

Engineering and Scientific Subroutine Library for AIX,  
Version 4 Release 2, and  
Engineering and Scientific Subroutine Library for Linux  
on POWER,  
Version 4 Release 2.2



# Guide and Reference



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on POWER,  
Version 4 Release 2.2



# Guide and Reference

**Note:**

Before using this information and the product it supports, read the information in "Notices" on page 1045.

| **Fourth Edition (November 2005)**

This edition applies to:

- | • Version 4 Release 2 of the IBM Engineering and Scientific Subroutine Library (ESSL) for Advanced Interactive Executive (AIX) licensed program, program number 5765-F82
- | • Version 4 Release 2.2 of the IBM Engineering and Scientific Subroutine Library (ESSL) for Linux on POWER licensed program, program number 5765-G17

and to all subsequent releases and modifications until otherwise indicated by new editions.

In this document, ESSL refers to both of the above products (unless a differentiation between ESSL for AIX and ESSL for Linux is explicitly specified).

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# Contents

## About This Book. . . . . xi

How to Use This Book . . . . .	xi
How to Find a Subroutine Description . . . . .	xii
Where to Find Related Publications . . . . .	xiii
How to Look Up a Bibliography Reference . . . . .	xiii
Special Terms . . . . .	xiii
Short and Long Precision . . . . .	xiii
Subroutines and Subprograms . . . . .	xiii
How to Interpret the Subroutine Names with a Prefix Underscore . . . . .	xiii
Abbreviated Names . . . . .	xiv
Conventions and terminology used in this book . . . . .	xiv
Fonts . . . . .	xv
Special Notations and Conventions . . . . .	xv
Special Characters, Symbols, Expressions, and Abbreviations . . . . .	xviii
How to Interpret the Subroutine Descriptions. . . . .	xix
Description . . . . .	xix
Syntax . . . . .	xx
On Entry . . . . .	xx
On Return. . . . .	xx
Notes . . . . .	xx
Function . . . . .	xx
Special Usage . . . . .	xxi
Error Conditions . . . . .	xxi
Examples . . . . .	xxi

## Summary of changes. . . . . xxiii

What's New for ESSL Version 4 Release 2.2 . . . . .	xxiii
What's New for ESSL Version 4 Release 2.1 . . . . .	xxiii
What's New for ESSL Version 4 Release 2 . . . . .	xxiii
What's New for ESSL Version 4 Release 1 . . . . .	xxiii
Future Migration . . . . .	xxiv

## Part 1. Guide Information . . . . . 1

### Chapter 1. Introduction and Requirements . . . . . 3

Overview of ESSL . . . . .	3
Performance and Functional Capability . . . . .	3
Usability. . . . .	3
The Variety of Mathematical Functions . . . . .	4
Accuracy of the Computations . . . . .	5
High Performance of ESSL. . . . .	6
The Fortran Language Interface to the Subroutines . . . . .	7
Software and Hardware Products That Can Be Used with ESSL . . . . .	7
Hardware Products Supported by ESSL . . . . .	8
Operating Systems Supported by ESSL . . . . .	8
Software Products Required by ESSL . . . . .	8
Software Products for Installing and Customizing ESSL . . . . .	10
Software Products for Displaying ESSL Documentation . . . . .	11

ESSL Internet Resources . . . . .	11
Blue Gene documentation . . . . .	11
Getting on the ESSL Mailing List . . . . .	12
List of ESSL Subroutines . . . . .	12
Linear Algebra Subprograms . . . . .	12
Matrix Operations . . . . .	16
Linear Algebraic Equations . . . . .	16
Eigensystem Analysis . . . . .	20
Fourier Transforms, Convolutions and Correlations, and Related Computations. . . . .	21
Sorting and Searching . . . . .	22
Interpolation . . . . .	22
Numerical Quadrature. . . . .	23
Random Number Generation . . . . .	23
Utilities. . . . .	23

### Chapter 2. Planning Your Program . . . . . 25

Selecting an ESSL Subroutine . . . . .	25
Which ESSL Library Do You Want to Use? . . . . .	25
What Type of Data Are You Processing in Your Program? . . . . .	31
How Is Your Data Structured? And What Storage Technique Are You Using? . . . . .	32
What about Performance and Accuracy?. . . . .	32
Avoiding Conflicts with Internal ESSL Routine   Names That are Exported. . . . .	32
Setting Up Your Data . . . . .	33
How Do You Set Up Your Scalar Data? . . . . .	33
How Do You Set Up Your Arrays?. . . . .	33
How Should Your Array Data Be Aligned?. . . . .	33
What Storage Mode Should You Use for Your Data? . . . . .	34
How Do You Convert from One Storage Mode to Another? . . . . .	34
Setting Up Your ESSL Calling Sequences . . . . .	34
What Is an Input-Output Argument? . . . . .	35
What Are the General Rules to Follow when Specifying Data for the Arguments? . . . . .	35
What Happens When a Value of 0 Is Specified for N? . . . . .	35
How Do You Specify the Beginning of the Data Structure in the ESSL Calling Sequence?. . . . .	35
Using Auxiliary Storage in ESSL . . . . .	36
Dynamic Allocation of Auxiliary Storage . . . . .	37
Setting Up Auxiliary Storage When Dynamic Allocation Is Not Used . . . . .	37
Who Do You Want to Calculate the Size? You or ESSL? . . . . .	37
How Do You Calculate the Size Using the Formulas?. . . . .	37
How Do You Get ESSL to Calculate the Size Using ESSL Error Handling?. . . . .	38
Providing a Correct Transform Length to ESSL . . . . .	42
What ESSL Subroutines Require Transform Lengths? . . . . .	42

Who Do You Want to Calculate the Length? You or ESSL? . . . . .	42
How Do You Calculate the Length Using the Table or Formula? . . . . .	43
How Do You Get ESSL to Calculate the Length Using ESSL Error Handling?. . . . .	43
Getting the Best Accuracy . . . . .	47
What Precisions Do ESSL Subroutines Operate On? . . . . .	47
How does the Nature of the ESSL Computation Affect Accuracy?. . . . .	48
What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About? . . . . .	48
How is Underflow Handled? . . . . .	48
Where Can You Find More Information on Accuracy? . . . . .	48
Getting the Best Performance . . . . .	49
What General Coding Techniques Can You Use to Improve Performance?. . . . .	49
Where Can You Find More Information on Performance?. . . . .	50
Dealing with Errors when Using ESSL . . . . .	50
What Can You Do about Program Exceptions?. . . . .	50
What Can You Do about ESSL Input-Argument Errors? . . . . .	50
What Can You Do about ESSL Computational Errors? . . . . .	51
What Can You Do about ESSL Resource Errors? . . . . .	53
What Can You Do about ESSL Attention Messages? . . . . .	54
How Do You Control Error Handling by Setting Values in the ESSL Error Option Table? . . . . .	54
How does Error Handling Work in a Threaded Environment? . . . . .	56
Where Can You Find More Information on Errors? . . . . .	57

<b>Chapter 3. Setting Up Your Data Structures . . . . .</b>	<b>59</b>
Concepts . . . . .	59
Vectors . . . . .	59
Transpose of a Vector . . . . .	60
Conjugate Transpose of a Vector . . . . .	60
In Storage . . . . .	61
How Stride Is Used for Vectors . . . . .	62
Sparse Vector . . . . .	64
Matrices . . . . .	65
Transpose of a Matrix . . . . .	66
Conjugate Transpose of a Matrix . . . . .	66
In Storage . . . . .	66
How Leading Dimension Is Used for Matrices . . . . .	67
Symmetric Matrix . . . . .	69
Positive Definite or Negative Definite Symmetric Matrix . . . . .	73
Symmetric Indefinite Matrix . . . . .	73
Complex Hermitian Matrix . . . . .	73
Positive Definite or Negative Definite Complex Hermitian Matrix . . . . .	75
Positive Definite or Negative Definite Symmetric Toeplitz Matrix . . . . .	75

Positive Definite or Negative Definite Complex Hermitian Toeplitz Matrix . . . . .	76
Triangular Matrix . . . . .	77
General Band Matrix . . . . .	80
Symmetric Band Matrix . . . . .	85
Positive Definite Symmetric Band Matrix . . . . .	87
Complex Hermitian Band Matrix . . . . .	88
Triangular Band Matrix . . . . .	88
General Tridiagonal Matrix . . . . .	92
Symmetric Tridiagonal Matrix . . . . .	93
Positive Definite Symmetric Tridiagonal Matrix . . . . .	94
Sparse Matrix. . . . .	94
Sequences . . . . .	106
Real and Complex Elements in Storage . . . . .	106
One-Dimensional Sequences . . . . .	106
Two-Dimensional Sequences . . . . .	106
Three-Dimensional Sequences . . . . .	106
How Stride Is Used for Three-Dimensional Sequences . . . . .	108

## **Chapter 4. Coding Your Program . . . 111**

Fortran Programs . . . . .	111
Calling ESSL Subroutines and Functions in Fortran . . . . .	111
Setting Up a User-Supplied Subroutine for ESSL in Fortran. . . . .	111
Setting Up Scalar Data in Fortran. . . . .	112
Setting Up Arrays in Fortran . . . . .	112
Creating Multiple Threads and Calling ESSL from Your Fortran Program. . . . .	117
Handling Errors in Your Fortran Program . . . . .	118
Example of Handling Errors in a Multithreaded Application Program . . . . .	127
C Programs . . . . .	129
Calling ESSL Subroutines and Functions in C . . . . .	129
Passing Arguments in C. . . . .	130
Setting Up a User-Supplied Subroutine for ESSL in C . . . . .	131
Setting Up Scalar Data in C . . . . .	131
Setting Up Complex Data Types in C . . . . .	132
Using Logical Data in C. . . . .	133
Setting Up Arrays in C . . . . .	133
Creating Multiple Threads and Calling ESSL from Your C Program . . . . .	134
Handling Errors in Your C Program . . . . .	136
C++ Programs . . . . .	145
Calling ESSL Subroutines and Functions in C++ . . . . .	145
Passing Arguments in C++. . . . .	145
Setting Up a User-Supplied Subroutine for ESSL in C++ . . . . .	147
Setting Up Scalar Data in C++. . . . .	147
Using Complex Data in C++ . . . . .	148
Using Logical Data in C++ . . . . .	150
Setting Up Arrays in C++ . . . . .	150
Creating Multiple Threads and Calling ESSL from Your C++ Program. . . . .	150
Handling Errors in Your C++ Program . . . . .	152

## **Chapter 5. Processing Your Program 163**

Processing Your Program on AIX. . . . .	163
---	-----

Dynamic Linking Versus Static Linking on AIX	163
Fortran Program Procedures on AIX	163
C Program Procedures on AIX	164
C++ Program Procedures on AIX	165
Processing Your Program on Linux	166
Dynamic Linking Versus Static Linking on Linux	167
Fortran Program Procedures on Linux	167
C Program Procedures on Linux	168
C++ Program Procedures on Linux	168

## Chapter 6. Migrating Your Programs . . . . . 171

Migrating ESSL Version 4 Release 2.1 Programs to Version 4 Release 2.2	171
Migrating ESSL Version 4 Release 2 Programs to Version 4 Release 2.1	171
Migrating ESSL Version 4 Release 1 Programs to Version 4 Release 2	171
Migrating ESSL Version 3 Release 3 Programs to Version 4 Release 1	172
ESSL Subroutines	172
Planning for Future Migration	172
Migrating From One Hardware Platform to Another	172
Auxiliary Storage	172
Bitwise-Identical Results	173
Migrating from Other Libraries to ESSL	173
Migrating from ESSL/370	173
Migrating from Another IBM Subroutine Library	173
Migrating from LAPACK	173
Migrating from a Non-IBM Subroutine Library	173

## Chapter 7. Handling Problems . . . . . 175

Where to Find More Information About Errors	175
Getting Help from IBM Support	175
National Language Support	176
Dealing with Errors	177
Program Exceptions	177
ESSL Input-Argument Error Messages	177
ESSL Computational Error Messages	178
ESSL Resource Error Messages	178
ESSL Informational and Attention Messages	179
Miscellaneous Error Messages	179
Messages	179
Message Conventions	179
Input-Argument Error Messages(2001-2099)	180
Computational Error Messages(2100-2199)	186
Input-Argument Error Messages(2200-2299)	187
Resource Error Messages(2400-2499)	188
Informational and Attention Error Messages(2600-2699)	188
Miscellaneous Error Messages(2700-2799)	188

## Part 2. Reference Information . . . . . 191

### Chapter 8. Linear Algebra Subprograms . . . . . 193

Overview of the Linear Algebra Subprograms	193
Vector-Scalar Linear Algebra Subprograms	193

Sparse Vector-Scalar Linear Algebra Subprograms	194
Matrix-Vector Linear Algebra Subprograms	195
Sparse Matrix-Vector Linear Algebra Subprograms	196
Use Considerations	196
Performance and Accuracy Considerations	196
<b>Vector-Scalar Subprograms</b>	198
ISAMAX, IDAMAX, ICAMAX, and IZAMAX — Position of the First or Last Occurrence of the Vector Element Having the Largest Magnitude	199
ISAMIN and IDAMIN — Position of the First or Last Occurrence of the Vector Element Having Minimum Absolute Value	202
ISMAY and IDMAX — Position of the First or Last Occurrence of the Vector Element Having the Maximum Value	205
ISMIN and IDMIN — Position of the First or Last Occurrence of the Vector Element Having Minimum Value	208
SASUM, DASUM, SCASUM, and DZASUM — Sum of the Magnitudes of the Elements in a Vector	211
SAXPY, DAXPY, CAXPY, and ZAXPY — Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y	214
SCOPY, DCOPY, CCOPY, and ZCOPY — Copy a Vector	217
SDOT, DDOT, CDOTU, ZDOTU, CDOTC, and ZDOTC — Dot Product of Two Vectors	220
SNAXPY and DNAXPY — Compute SAXPY or DAXPY N Times	224
SNDOT and DNDOT — Compute Special Dot Products N Times	229
SNRM2, DNRM2, SCNRM2, and DZNRM2 — Euclidean Length of a Vector with Scaling of Input to Avoid Destructive Underflow and Overflow	234
SNORM2, DNORM2, CNORM2, and ZNORM2 — Euclidean Length of a Vector with No Scaling of Input	237
SROTG, DROTG, CROTG, and ZROTG — Construct a Givens Plane Rotation	240
SROT, DROT, CROT, ZROT, CSROT, and ZDROT — Apply a Plane Rotation	247
SSCAL, DSCAL, CSCAL, ZSCAL, CSSCAL, and ZDSCAL — Multiply a Vector X by a Scalar and Store in the Vector X	251
SSWAP, DSWAP, CSWAP, and ZSWAP — Interchange the Elements of Two Vectors	254
SVEA, DVEA, CVEA, and ZVEA — Add a Vector X to a Vector Y and Store in a Vector Z	257
SVES, DVES, CVES, and ZVES — Subtract a Vector Y from a Vector X and Store in a Vector Z	261
SVEM, DVEM, CVEM, and ZVEM — Multiply a Vector X by a Vector Y and Store in a Vector Z	265
SYAX, DYAX, CYAX, ZYAX, CSYAX, and ZDYAX — Multiply a Vector X by a Scalar and Store in a Vector Y	269
SZAXPY, DZAXPY, CZAXPY, and ZZAXPY — Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in a Vector Z	272
<b>Sparse Vector-Scalar Subprograms</b>	276

SSCTR, DSCTR, CSCTR, ZSCTR — Scatter the Elements of a Sparse Vector X in Compressed-Vector Storage Mode into Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode . . . . .	277
SGTHR, DGTHR, CGTHR, and ZGTHR — Gather Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode into a Sparse Vector X in Compressed-Vector Storage Mode . . . . .	280
SGTHRZ, DGTHRZ, CGTHRZ, and ZGTHRZ — Gather Specified Elements of a Sparse Vector Y in Full-Vector Mode into a Sparse Vector X in Compressed-Vector Mode, and Zero the Same Specified Elements of Y . . . . .	283
SAXPYI, DAXPYI, CAXPYI, and ZAXPYI — Multiply a Sparse Vector X in Compressed-Vector Storage Mode by a Scalar, Add to a Sparse Vector Y in Full-Vector Storage Mode, and Store in the Vector Y . . . . .	286
SDOTI, DDOTI, CDOTUI, ZDOTUI, CDOTCI, and ZDOTCI — Dot Product of a Sparse Vector X in Compressed-Vector Storage Mode and a Sparse Vector Y in Full-Vector Storage Mode . . . . .	289
<b>Matrix-Vector Subprograms</b> . . . . .	293
SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX — Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose . . . . .	294
SGER, DGER, CGERU, ZGERU, CGERC, and ZGERC — Rank-One Update of a General Matrix . . . . .	305
SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, ZHEMV, SSLMX, and DSLMX — Matrix-Vector Product for a Real Symmetric or Complex Hermitian Matrix . . . . .	312
SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, ZHER, SSLR1, and DSLR1 — Rank-One Update of a Real Symmetric or Complex Hermitian Matrix. . . . .	320
SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, ZHER2, SSLR2, and DSLR2 — Rank-Two Update of a Real Symmetric or Complex Hermitian Matrix. . . . .	327
SGBMV, DGBMV, CGBMV, and ZGBMV — Matrix-Vector Product for a General Band Matrix, Its Transpose, or Its Conjugate Transpose . . . . .	336
SSBMV, DSBMV, CHBMV, and ZHBMV — Matrix-Vector Product for a Real Symmetric or Complex Hermitian Band Matrix . . . . .	343
STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, and ZTPMV — Matrix-Vector Product for a Triangular Matrix, Its Transpose, or Its Conjugate Transpose . . . . .	348
STBMV, DTBMV, CTBMV, and ZTBMV — Matrix-Vector Product for a Triangular Band Matrix, Its Transpose, or Its Conjugate Transpose . . . . .	354
<b>Sparse Matrix-Vector Subprograms</b> . . . . .	359
DSMMX — Matrix-Vector Product for a Sparse Matrix in Compressed-Matrix Storage Mode . . . . .	360
DSMTM — Transpose a Sparse Matrix in Compressed-Matrix Storage Mode . . . . .	363

DSDMX — Matrix-Vector Product for a Sparse Matrix or Its Transpose in Compressed-Diagonal Storage Mode . . . . .	367
--	-----

## Chapter 9. Matrix Operations. . . . . 373

Overview of the Matrix Operation Subroutines . . . . .	373
Use Considerations . . . . .	374
Specifying Normal, Transposed, or Conjugate Transposed Input Matrices . . . . .	374
Transposing or Conjugate Transposing: . . . . .	374
Performance and Accuracy Considerations . . . . .	375
In General . . . . .	375
For Large Matrices . . . . .	375
For Combined Operations . . . . .	375
<b>Matrix Operation Subroutines</b> . . . . .	376
SGEADD, DGEADD, CGEADD, and ZGEADD — Matrix Addition for General Matrices or Their Transposes . . . . .	377
SGESUB, DGESUB, CGESUB, and ZGESUB — Matrix Subtraction for General Matrices or Their Transposes . . . . .	383
SGEMUL, DGEMUL, CGEMUL, and ZGEMUL — Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes . . . . .	389
SGEMMS, DGEMMS, CGEMMS, and ZGEMMS — Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes Using Winograd's Variation of Strassen's Algorithm. . . . .	398
SGEMM, DGEMM, CGEMM, and ZGEMM — Combined Matrix Multiplication and Addition for General Matrices, Their Transposes, or Conjugate Transposes . . . . .	404
SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, and ZHEMM — Matrix-Matrix Product Where One Matrix is Real or Complex Symmetric or Complex Hermitian . . . . .	412
STRMM, DTRMM, CTRMM, and ZTRMM — Triangular Matrix-Matrix Product . . . . .	419
SSYRK, DSYRK, CSYRK, ZSYRK, CHERK, and ZHERK — Rank-K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix . . . . .	426
SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, and ZHER2K — Rank-2K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix. . . . .	432
SGETMI, DGETMI, CGETMI, and ZGETMI — General Matrix Transpose (In-Place) . . . . .	439
SGETMO, DGETMO, CGETMO, and ZGETMO — General Matrix Transpose (Out-of-Place) . . . . .	442

## Chapter 10. Linear Algebraic Equations . . . . . 445

Overview of the Linear Algebraic Equation Subroutines . . . . .	445
Dense Linear Algebraic Equation Subroutines . . . . .	445
Banded Linear Algebraic Equation Subroutines . . . . .	447
Sparse Linear Algebraic Equation Subroutines . . . . .	447
Linear Least Squares Subroutines. . . . .	448
Dense and Banded Linear Algebraic Equation Considerations . . . . .	448



Use Considerations . . . . .	448	SGETRI, DGETRI, CGETRI, ZGETRI, SGEICD, and	
Performance and Accuracy Considerations . . . . .	449	DGEICD — General Matrix Inverse, Condition	
Sparse Matrix Direct Solver Considerations . . . . .	449	Number Reciprocal, and Determinant . . . . .	539
Use Considerations . . . . .	449	SPOTRI, DPOTRI, CPOTRI, ZPOTRI, SPOICD,	
Performance and Accuracy Considerations . . . . .	449	DPOICD, SPPTRI, DPPTRI, SPPICD, and DPPICD	
Sparse Matrix Skyline Solver Considerations . . . . .	450	— Positive Definite Real Symmetric or Complex	
Use Considerations . . . . .	450	Hermitian Matrix Inverse, Condition Number	
Performance and Accuracy Considerations . . . . .	450	Reciprocal, and Determinant . . . . .	547
Sparse Matrix Iterative Solver Considerations . . . . .	451	STRSV, DTRSV, CTRSV, ZTRSV, STPSV, DTSPV,	
Use Considerations . . . . .	451	CTPSV, and ZTPSV — Solution of a Triangular	
Performance and Accuracy Considerations . . . . .	451	System of Equations with a Single Right-Hand Side	557
Linear Least Squares Considerations . . . . .	452	STRSM, DTRSM, CTRSM, and ZTRSM — Solution	
Use Considerations . . . . .	452	of Triangular Systems of Equations with Multiple	
Performance and Accuracy Considerations . . . . .	452	Right-Hand Sides . . . . .	563
<b>Dense Linear Algebraic Equation Subroutines</b>	453	STRTRI, DTRTRI, CTRTRI, ZTRTRI, STPTRI,	
SGESV, DGESV, CGESV, ZGESV — General Matrix		DTPTRI, CTPTRI, and ZTPTRI — Triangular	
Factorization and Multiple Right-Hand Side Solve . . . . .	454	Matrix Inverse . . . . .	570
SGETRF, DGETRF, CGETRF and ZGETRF —		<b>Banded Linear Algebraic Equation Subroutines</b>	578
General Matrix Factorization . . . . .	458	SGBF and DGBF — General Band Matrix	
SGETRS, DGETRS, CGETRS, and ZGETRS —		Factorization . . . . .	579
General Matrix Multiple Right-Hand Side Solve . . . . .	462	SGBS and DGBS — General Band Matrix Solve . . . . .	583
SGEF, DGEF, CGEF, and ZGEF — General Matrix		SPBF, DPBF, SPBCHF, and DPBCHF — Positive	
Factorization . . . . .	467	Definite Symmetric Band Matrix Factorization . . . . .	586
SGES, DGES, CGES, and ZGES — General Matrix,		SPBS, DPBS, SPBCHS, and DPBCHS — Positive	
Its Transpose, or Its Conjugate Transpose Solve . . . . .	470	Definite Symmetric Band Matrix Solve . . . . .	590
SGESM, DGESM, CGESM, and ZGESM — General		SGTF and DGTF — General Tridiagonal Matrix	
Matrix, Its Transpose, or Its Conjugate Transpose		Factorization . . . . .	593
Multiple Right-Hand Side Solve . . . . .	474	SGTS and DGTS — General Tridiagonal Matrix	
SGEFCD and DGEFCD — General Matrix		Solve . . . . .	596
Factorization, Condition Number Reciprocal, and		SGTNP, DGTNP, CGTNP, and ZGTNP — General	
Determinant . . . . .	479	Tridiagonal Matrix Combined Factorization and	
SPPSV, DPPSV, CPPSV, and ZPPSV — Positive		Solve with No Pivoting . . . . .	598
Definite Real Symmetric and Complex Hermitian		SGTNPF, DGTNPF, CGTNPF, and ZGTNPF —	
Matrix Factorization and Multiple Right-Hand Side		General Tridiagonal Matrix Factorization with No	
Solve . . . . .	483	Pivoting . . . . .	601
SPOSV, DPOSV, CPOSV, and ZPOSV — Positive		SGTNPS, DGTNPS, CGTNPS, and ZGTNPS —	
Definite Real Symmetric or Complex Hermitian		General Tridiagonal Matrix Solve with No Pivoting	604
Matrix Factorization and Multiple Right-Hand Side		SPTF and DPTF — Positive Definite Symmetric	
Solve . . . . .	489	Tridiagonal Matrix Factorization . . . . .	607
SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF,		SPTS and DPTS — Positive Definite Symmetric	
DPOF, CPOF, ZPOF, SPPTRF, DPPTRF, CPPTRF,		Tridiagonal Matrix Solve . . . . .	609
ZPPTRF, SPPF, and DPPF — Positive Definite Real		STBSV, DTBSV, CTBSV, and ZTBSV — Triangular	
Symmetric or Complex Hermitian Matrix		Band Equation Solve . . . . .	611
Factorization . . . . .	495	<b>Sparse Linear Algebraic Equation Subroutines</b>	616
SPOTRS, DPOTRS, CPOTRS, ZPOTRS, SPOSM,		DGSF — General Sparse Matrix Factorization	
DPOSM, CPOSM, ZPOSM, SPPTRS, DPPTRS,		Using Storage by Indices, Rows, or Columns . . . . .	617
CPPTRS, and ZPPTRS — Positive Definite Real		DGSS — General Sparse Matrix or Its Transpose	
Symmetric or Complex Hermitian Matrix Multiple		Solve Using Storage by Indices, Rows, or Columns . . . . .	623
Right-Hand Side Solve . . . . .	507	DGKFS — General Sparse Matrix or Its Transpose	
SPPS and DPPS — Positive Definite Real		Factorization, Determinant, and Solve Using	
Symmetric Matrix Solve . . . . .	515	Skyline Storage Mode . . . . .	627
SPPFCD, DPPFCD, SPOFCD, and DPOFCD —		DSKFS — Symmetric Sparse Matrix Factorization,	
Positive Definite Real Symmetric Matrix		Determinant, and Solve Using Skyline Storage	
Factorization, Condition Number Reciprocal, and		Mode . . . . .	644
Determinant . . . . .	518	DSRIS — Iterative Linear System Solver for a	
DBSSV — Symmetric Indefinite Matrix		General or Symmetric Sparse Matrix Stored by	
Factorization and Multiple Right-Hand Side Solve . . . . .	524	Rows . . . . .	662
DBSTRF — Symmetric Indefinite Matrix		DSMCG — Sparse Positive Definite or Negative	
Factorization . . . . .	530	Definite Symmetric Matrix Iterative Solve Using	
DBSTRS — Symmetric Indefinite Matrix Multiple		Compressed-Matrix Storage Mode . . . . .	673
Right-Hand Side Solve . . . . .	535		

DSDCG — Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Diagonal Storage Mode . . . . .	681
DSMGCG — General Sparse Matrix Iterative Solve Using Compressed-Matrix Storage Mode . . . . .	689
DSDGCG — General Sparse Matrix Iterative Solve Using Compressed-Diagonal Storage Mode . . . . .	696
<b>Linear Least Squares Subroutines</b> . . . . .	703
SGESVF and DGESVF — Singular Value Decomposition for a General Matrix. . . . .	704
SGESVS and DGESVS — Linear Least Squares Solution for a General Matrix Using the Singular Value Decomposition. . . . .	712
DGEQRF — General Matrix QR Factorization . . . . .	717
DGELS — Linear Least Squares Solution for a General Matrix . . . . .	721
SGELLS and DGELLS — Linear Least Squares Solution for a General Matrix with Column Pivoting . . . . .	728

**Chapter 11. Eigensystem Analysis 735**

Overview of the Eigensystem Analysis Subroutines	735
Performance and Accuracy Considerations . . . . .	735
<b>Eigensystem Analysis Subroutines</b> . . . . .	736
SGEEV, DGEEV, CGEEV, and ZGEEV — Eigenvalues and, Optionally, All or Selected Eigenvectors of a General Matrix . . . . .	737
SSPEV, DSPEV, CHPEV, and ZHPEV — Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix. . . . .	748
SSPSV, DSPSV, CHPSV, and ZHPSV — Extreme Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix. . . . .	757
SGEGV and DGEV — Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Eigensystem, $Az=wBz$ , where A and B Are Real General Matrices . . . . .	764
SSYGV and DSYGV — Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Symmetric Eigensystem, $Az=wBz$ , where A Is Real Symmetric and B Is Real Symmetric Positive Definite . . . . .	770

**Chapter 12. Fourier Transforms, Convolutions and Correlations, and Related Computations . . . . . 777**

Overview of the Signal Processing Subroutines . . . . .	777
Fourier Transforms Subroutines . . . . .	777
Convolution and Correlation Subroutines . . . . .	777
Related-Computation Subroutines . . . . .	778
Fourier Transforms, Convolutions, and Correlations Considerations . . . . .	778
Use Considerations . . . . .	778
Initializing Auxiliary Working Storage . . . . .	781
Determining the Amount of Auxiliary Working Storage That You Need . . . . .	781
Performance and Accuracy Considerations . . . . .	781
When Running on the Workstation Processors . . . . .	781

Defining Arrays . . . . .	782
Fourier Transform Considerations . . . . .	782
How the Fourier Transform Subroutines Achieve High Performance. . . . .	783
Convolution and Correlation Considerations . . . . .	783
Related Computation Considerations . . . . .	785
Accuracy Considerations . . . . .	785
<b>Fourier Transform Subroutines</b> . . . . .	786
SCFT and DCFT — Complex Fourier Transform	787
SRCFT and DRCFT — Real-to-Complex Fourier Transform . . . . .	796
SCRFT and DCRFT — Complex-to-Real Fourier Transform . . . . .	804
SCOSF and DCOSF — Cosine Transform . . . . .	812
SSINF and DSINF — Sine Transform . . . . .	820
SCFT2 and DCFT2 — Complex Fourier Transform in Two Dimensions . . . . .	828
SRCFT2 and DRCFT2 — Real-to-Complex Fourier Transform in Two Dimensions. . . . .	835
SCRFT2 and DCRFT2 — Complex-to-Real Fourier Transform in Two Dimensions. . . . .	842
SCFT3 and DCFT3 — Complex Fourier Transform in Three Dimensions . . . . .	850
SRCFT3 and DRCFT3 — Real-to-Complex Fourier Transform in Three Dimensions . . . . .	856
SCRFT3 and DCRFT3 — Complex-to-Real Fourier Transform in Three Dimensions . . . . .	862
<b>Convolution and Correlation Subroutines</b> . . . . .	868
SCON and SCOR — Convolution or Correlation of One Sequence with One or More Sequences . . . . .	869
SCOND and SCORD — Convolution or Correlation of One Sequence with Another Sequence Using a Direct Method . . . . .	875
SCONF and SCORF — Convolution or Correlation of One Sequence with One or More Sequences Using the Mixed-Radix Fourier Method . . . . .	881
SDCON, DDCON, SDCOR, and DDCOR — Convolution or Correlation with Decimated Output Using a Direct Method . . . . .	891
SACOR — Autocorrelation of One or More Sequences . . . . .	896
SACORF — Autocorrelation of One or More Sequences Using the Mixed-Radix Fourier Method . . . . .	900
<b>Related-Computation Subroutines</b> . . . . .	906
SPOLY and DPOLY — Polynomial Evaluation . . . . .	907
SIZC and DIZC — I-th Zero Crossing . . . . .	910
STREC and DTREC — Time-Varying Recursive Filter . . . . .	913
SQINT and DQINT — Quadratic Interpolation . . . . .	916
SWLEV, DWLEV, CWLEV, and ZWLEV — Wiener-Levinson Filter Coefficients . . . . .	920

**Chapter 13. Sorting and Searching 925**

Overview of the Sorting and Searching Subroutines	925
Use Considerations . . . . .	925
Performance and Accuracy Considerations . . . . .	925
<b>Sorting and Searching Subroutines</b> . . . . .	926
ISORT, SSORT, and DSORT — Sort the Elements of a Sequence . . . . .	927

ISORTX, SSORTX, and DSORTX — Sort the Elements of a Sequence and Note the Original Element Positions . . . . .	929
ISORTS, SSORTS, and DSORTS — Sort the Elements of a Sequence Using a Stable Sort and Note the Original Element Positions. . . . .	932
IBSRCH, SBSRCH, and DBSRCH — Binary Search for Elements of a Sequence X in a Sorted Sequence Y . . . . .	936
ISSRCH, SSSRCH, and DSSRCH — Sequential Search for Elements of a Sequence X in the Sequence Y . . . . .	940

**Chapter 14. Interpolation . . . . . 945**

Overview of the Interpolation Subroutines . . . . .	945
Use Considerations . . . . .	945
Performance and Accuracy Considerations . . . . .	945
<b>Interpolation Subroutines . . . . . 946</b>	
SPINT and DPINT — Polynomial Interpolation . . . . .	947
STPINT and DTPINT — Local Polynomial Interpolation . . . . .	952
SCSINT and DCSINT — Cubic Spline Interpolation . . . . .	955
SCSIN2 and DCSIN2 — Two-Dimensional Cubic Spline Interpolation . . . . .	961

**Chapter 15. Numerical Quadrature . . . . . 965**

Overview of the Numerical Quadrature Subroutines . . . . .	965
Use Considerations . . . . .	965
Choosing the Method . . . . .	965
Performance and Accuracy Considerations . . . . .	965
Programming Considerations for the SUBF Subroutine . . . . .	966
Designing SUBF . . . . .	966
Coding and Setting Up SUBF in Your Program . . . . .	966
<b>Numerical Quadrature Subroutines. . . . . 968</b>	
SPTNQ and DPTNQ — Numerical Quadrature Performed on a Set of Points . . . . .	969
SGLNQ and DGLNQ — Numerical Quadrature Performed on a Function Using Gauss-Legendre Quadrature . . . . .	972
SGLNQ2 and DGLNQ2 — Numerical Quadrature Performed on a Function Over a Rectangle Using Two-Dimensional Gauss-Legendre Quadrature . . . . .	975
SGLGQ and DGLGQ — Numerical Quadrature Performed on a Function Using Gauss-Laguerre Quadrature . . . . .	981
SGRAQ and DGRAQ — Numerical Quadrature Performed on a Function Using Gauss-Rational Quadrature . . . . .	984
SGHMQ and DGHMQ — Numerical Quadrature Performed on a Function Using Gauss-Hermite Quadrature . . . . .	988

**Chapter 16. Random Number . . . . . 991**

<b>Generation . . . . . 991</b>	
Overview of the Random Number Generation Subroutines . . . . .	991
Use Considerations . . . . .	991
<b>Random Number Generation Subroutines . . . . . 992</b>	

SURAND and DURAND — Generate a Vector of Uniformly Distributed Random Numbers . . . . .	993
SNRAND and DNRAND — Generate a Vector of Normally Distributed Random Numbers . . . . .	996
SURXOR and DURXOR — Generate a Vector of Long Period Uniformly Distributed Random Numbers . . . . .	1000

**Chapter 17. Utilities . . . . . 1005**

Overview of the Utility Subroutines . . . . .	1005
Use Considerations . . . . .	1005
Determining the Level of ESSL Installed . . . . .	1005
Finding the Optimal Stride(s) for Your Fourier Transforms . . . . .	1005
Converting Sparse Matrix Storage . . . . .	1006
<b>Utility Subroutines . . . . . 1007</b>	
EINFO — ESSL Error Information-Handler Subroutine . . . . .	1008
ERRSAV — ESSL ERRSAV Subroutine . . . . .	1011
ERRSET — ESSL ERRSET Subroutine . . . . .	1012
ERRSTR — ESSL ERRSTR Subroutine . . . . .	1014
IESSL — Determine the Level of ESSL Installed . . . . .	1015
STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines . . . . .	1017
DSRSM — Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode. . . . .	1026
DGKTRN — For a General Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode . . . . .	1030
DSKTRN — For a Symmetric Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode . . . . .	1035

**Part 3. Appendixes . . . . . 1039**

**Appendix A. Basic Linear Algebra Subprograms (BLAS) . . . . . 1041**

Level 1 BLAS . . . . .	1041
Level 2 BLAS . . . . .	1041
Level 3 BLAS . . . . .	1042

**Appendix B. LAPACK . . . . . 1043**

LAPACK Subroutines . . . . .	1043
Non-LAPACK-Conforming Subroutines . . . . .	1043

**Notices . . . . . 1045**

Trademarks . . . . .	1046
Software Update Protocol . . . . .	1047
Programming Interfaces . . . . .	1047

**Glossary . . . . . 1049**

**Bibliography . . . . . 1055**

References . . . . .	1055
ESSL Publications . . . . .	1060
Related Publications. . . . .	1060

**Index . . . . . 1061**

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## About This Book

The Engineering and Scientific Subroutine Library (ESSL) is a set of high-performance mathematical subroutines. ESSL is provided as run-time libraries, running on the following:

<b>Servers</b>	IBM® @server Cluster 1600, IBM @server POWER™ servers, SP™ systems, BladeCenter® JS20, or IBM @server Blue Gene® Solution
<b>Processors</b>	POWER3™, POWER3-II, POWER4™, POWER4+™, POWER5™, POWER5+™, PowerPC® 970, PowerPC 440, and PowerPC 440D processors

ESSL can be used with Fortran, C, and C++ programs operating under the AIX® and Linux® operating systems.

This book is a guide and reference manual for using ESSL in doing application programming. It includes:

- An overview of ESSL and guidance information for designing, coding, and processing your program, as well as migrating existing programs, and diagnosing problems
- Reference information for coding each ESSL calling sequence

This book is written for a wide class of ESSL users: scientists, mathematicians, engineers, statisticians, computer scientists, and system programmers. It assumes a basic knowledge of mathematics in the areas of ESSL computation. It also assumes that users are familiar with Fortran, C, and C++ programming.

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## How to Use This Book

**Front Matter** consists of the Table of Contents and the Preface. Use these to find or interpret information in the book.

**Part 1, “Guide Information,” on page 1** provides guidance information for using ESSL. It covers the user-oriented tasks of learning, designing, coding, migrating, processing, and diagnosing. Use the following chapters when performing any of these tasks:

- **Chapter 1, “Introduction and Requirements,” on page 3** gives an introduction to ESSL, providing highlights and general information. Read this chapter first to determine the aspects of ESSL you want to use.
- **Chapter 2, “Planning Your Program,” on page 25** provides ESSL-specific information that helps you design your program. Read this chapter before designing your program.
- **Chapter 3, “Setting Up Your Data Structures,” on page 59** describes all types of data structures, such as vectors, matrices, and sequences. Use this information when designing and coding your program.
- **Chapter 4, “Coding Your Program,” on page 111** tells you how to code your scalar and array data, how to code calls to ESSL in Fortran, C, and C++ programs, and how to do the coding necessary to handle errors. Use this information when coding your program.

- **Chapter 5, “Processing Your Program,” on page 163** describes how to process your program under your particular operating system on your hardware. Use this information after you have coded your program and are ready to run it.
- **Chapter 6, “Migrating Your Programs,” on page 171** explains all aspects of migration to ESSL, to this version of ESSL, to different processors, and to future releases and future processors. Read this chapter before starting to design your program.
- **Chapter 7, “Handling Problems,” on page 175** provides diagnostic procedures for analyzing all ESSL problems. When you encounter a problem, use the symptom indexes at the beginning of this chapter to guide you to the appropriate diagnostic procedure.

**Part 2, “Reference Information,” on page 191** provides reference information you need to code the ESSL calling sequences. It covers each of the mathematical areas of ESSL, and the utility subroutines. Each chapter begins with an introduction, followed by the subroutine descriptions. Each introduction applies to all the subroutines in that chapter and is especially important in planning your use of the subroutines and avoiding problems. To understand the information in the subroutine descriptions, see “How to Interpret the Subroutine Descriptions” on page xix. Use the appropriate chapter when coding your program:

- **Chapter 8, “Linear Algebra Subprograms,” on page 193**
- **Chapter 9, “Matrix Operations,” on page 373**
- **Chapter 10, “Linear Algebraic Equations,” on page 445**
- **Chapter 11, “Eigensystem Analysis,” on page 735**
- **Chapter 12, “Fourier Transforms, Convolutions and Correlations, and Related Computations,” on page 777**
- **Chapter 13, “Sorting and Searching,” on page 925**
- **Chapter 14, “Interpolation,” on page 945**
- **Chapter 15, “Numerical Quadrature,” on page 965**
- **Chapter 16, “Random Number Generation,” on page 991**
- **Chapter 17, “Utilities,” on page 1005**

**Appendix A, “Basic Linear Algebra Subprograms (BLAS),” on page 1041** provides a list of the Level 1, 2, and 3 Basic Linear Algebra Subprograms (BLAS) included in ESSL.

**Appendix B, “LAPACK,” on page 1043** provides a list of the LAPACK subroutines included in ESSL.

**“Glossary” on page 1049** contains definitions of terms used in this book.

**“Bibliography” on page 1055** provides information about publications related to ESSL. Use it when you need more information than this book provides.

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## How to Find a Subroutine Description

If you want to locate a subroutine description and you know the subroutine name, you can find it listed individually or under the entry “subroutines, ESSL” in the Index.

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## Where to Find Related Publications

If you have a question about IBM clustered servers, PSSP, or a related product, the online resources listed in Table 7 on page 11 make it easy to find the information for which you are looking.

A list of all ESSL publications, as well as related programming and hardware publications, are listed in the bibliography of this book. Also included is a list of math background publications you may find helpful, along with the necessary information for ordering them from independent sources. See “Bibliography” on page 1055.

---

## How to Look Up a Bibliography Reference

Special references are made throughout this book to mathematical background publications and software libraries, available through IBM, publishers, or other companies. All of these are described in detail in the bibliography. A reference to one of these is made by using a bracketed number. The number refers to the item listed under that number in the bibliography. For example, reference [1] cites the first item listed in the bibliography.

---

## Special Terms

Standard data processing and mathematical terms are used in this book. Terminology is generally consistent with that used for Fortran. See the Glossary for definitions of terms used in this book.

### Short and Long Precision

Because ESSL can be used with more than one programming language, the terms **short precision** and **long precision** are used in place of the Fortran terms **single precision** and **double precision**.

### Subroutines and Subprograms

An ESSL **subroutine** is a named sequence of instructions within the ESSL product library whose execution is invoked by a call. A subroutine can be called in one or more user programs and at one or more times within each program. The ESSL subroutines are referred to as **subprograms** in the area of linear algebra subprograms. The term subprograms is used because it is consistent with the BLAS. Many of the linear algebra subprograms correspond to the BLAS; these are listed in Appendix A, “Basic Linear Algebra Subprograms (BLAS),” on page 1041.

---

## How to Interpret the Subroutine Names with a Prefix Underscore

A name specified in this book with an underscore (`_`) prefix, such as `_GEMUL`, refers to all the versions of the subroutine with that name. To get the entire list of subroutines that name refers to, substitute the first letter for each version of the subroutine. For example, `_GEMUL`, refers to all versions of the matrix multiplication subroutine: `SGEMUL`, `DGEMUL`, `CGEMUL`, and `ZGEMUL`. You do **not** use the underscore in coding the names of the ESSL subroutines in your program. You code a complete name, such as `SGEMUL`. For details about these names, see “The Variety of Mathematical Functions” on page 4.

---

## Abbreviated Names

The abbreviated names used in this book are defined below.

Short Name	Full Name
AIX	Advanced Interactive Executive
BLAS	Basic Linear Algebra Subprograms
ESSL	IBM Engineering and Scientific Subroutine Library
HTML	Hypertext Markup Language
IBM @server Cluster 1600	Highly scalable cluster solution comprised of POWER architecture-based symmetric multiprocessing (SMP) AIX 5L™ or Linux servers
LAPACK	Linear Algebra Package
SL MATH	Subroutine Library—Mathematics
SMP	Symmetric Multi-Processing
SSP	Scientific Subroutine Package

---

## Conventions and terminology used in this book

Table 1 describes the typographic conventions used in this book.

*Table 1. Summary of typographic conventions*

Typographic	Usage
<b>Bold</b>	<b>Bold</b> words or characters represent system elements that you must use literally, such as commands, flags, and path names.
<i>Italic</i>	<ul style="list-style-type: none"><li>• <i>Italic</i> words or characters represent variable values that you must supply.</li><li>• <i>Italics</i> are also used for book titles and for general emphasis in text.</li></ul>
Constant width	Examples and information that the system displays appear in constant width typeface.
[ ]	Brackets enclose optional items in format and syntax descriptions.
{ }	Braces enclose a list from which you must choose an item in format and syntax descriptions.
	A vertical bar separates items in a list of choices. (In other words, it means “or.”)
< >	Angle brackets (less-than and greater-than) enclose the name of a key on the keyboard. For example, <Enter> refers to the key on your terminal or workstation that is labeled with the word Enter.
...	An ellipsis indicates that you can repeat the preceding item one or more times.
<Ctrl-x>	The notation <Ctrl-x> indicates a control character sequence. For example, <Ctrl-c> means that you hold down the control key while pressing <c>.
\	The continuation character is used in coding examples in this book for formatting purposes.

The following sections list additional conventions used in this book that are consistent with traditional mathematical usage.



## Fonts

This book uses a variety of special fonts to distinguish between many mathematical and programming items. These are defined below.

Special Font	Example	Description
Italic with no subscripts	<i>m, inc1x, aux, iopt</i>	Calling sequence argument or mathematical variable
Italic with subscripts	<i>x<sub>1</sub>, a<sub>mnr</sub>, x<sub>j1,j2</sub></i>	Element of a vector, matrix, or sequence
Bold italic lowercase	<b><i>x, y, z</i></b>	Vector or sequence
Bold italic uppercase	<b><i>A, B, C</i></b>	Matrix
Gothic uppercase	A, B, C, AGB IM=ISMAX(4,X,2)	Array Fortran statement

## Special Notations and Conventions

This section explains the special notations and conventions used in this book to describe various types of data.

### Scalar Data

Following are the special notations used in the examples in this book for scalar data items. These notations are used to simplify the examples, and they do not imply usage of any precision. For a definition of scalar data in Fortran, C, and C++, see Chapter 4, “Coding Your Program,” on page 111.

Data Item	Example	Description
Character item	'T'	Character(s) in single quotation marks
Hexadecimal string	X'97FA00C1'	String of 4-bit hexadecimal characters
Logical item	.TRUE. .FALSE.	True or false logical value, as indicated
Integer data	1	Number with no decimal point
Real data	1.6	Number with a decimal point
Complex data	(1.0,-2.9)	Real part followed by the imaginary part
Continuation	- 1.6666	Continue the last digit (1.6666666... and so forth)

### Vectors

A vector is represented as a single row or column of subscripted elements enclosed in square brackets. The subscripts refer to the element positions within the vector:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \quad [x_1 \ x_2 \ x_3 \ \dots \ x_n]$$

For a definition of vector, see “Vectors” on page 59.

### Matrices

A matrix is represented as a block of elements enclosed in square brackets. Subscripts refer to the row and column positions, respectively:

$$\begin{bmatrix} a_{11} & \cdot & \cdot & \cdot & a_{1n} \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ a_{m1} & \cdot & \cdot & \cdot & a_{mn} \end{bmatrix}$$

For a definition of matrix, see “Matrices” on page 65.

### Sequences

Sequences are used in the areas of sorting, searching, Fourier transforms, convolutions, and correlations. For a definition of sequences, see “Sequences” on page 106.

**One-Dimensional Sequences:** A one-dimensional sequence is represented as a series of elements enclosed in parentheses. Subscripts refer to the element position within the sequence:

$$(x_1, x_2, x_3, \dots, x_n)$$

**Two-Dimensional Sequences:** A two-dimensional sequence is represented as a series of columns of elements. (They are represented in the same way as a matrix without the square brackets.) Subscripts refer to the element positions within the first and second dimensions, respectively:

$$\begin{array}{cccc} a_{11} & a_{12} & \cdot & \cdot & a_{1n} \\ a_{21} & a_{22} & & & a_{2n} \\ \cdot & \cdot & & & \cdot \\ \cdot & \cdot & & & \cdot \\ \cdot & \cdot & & & \cdot \\ a_{m1} & a_{m2} & \cdot & \cdot & a_{mn} \end{array}$$

**Three-Dimensional Sequences:** A three-dimensional sequence is represented as a series of blocks of elements. Subscripts refer to the elements positions within the first, second, and third dimensions, respectively:

$$\begin{array}{ccc}
 a_{111} & a_{121} \cdot \cdot \cdot a_{1n1} & a_{112} & a_{122} \cdot \cdot \cdot a_{1n2} & a_{11p} & a_{12p} \cdot \cdot \cdot a_{1np} \\
 a_{211} & a_{221} & a_{2n1} & a_{212} & a_{222} & a_{2n2} & a_{21p} & a_{22p} & a_{2np} \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\
 a_{m11} & a_{m21} \cdot \cdot \cdot a_{mn1} & a_{m12} & a_{m22} \cdot \cdot \cdot a_{mn2} & a_{m1p} & a_{m2p} \cdot \cdot \cdot a_{mnp}
 \end{array}$$

## Arrays

Arrays contain vectors, matrices, or sequences. For a definition of array, see “How Do You Set Up Your Arrays?” on page 33.

**One-Dimensional Arrays:** A one-dimensional array is represented as a single row of numeric elements enclosed in parentheses:

$$(1.0, 2.0, 3.0, 4.0, 5.0)$$

Elements not significant to the computation are usually not shown in the array. One dot appears for each element not shown. In the following array, five elements are significant to the computation, and two elements not used in the computation exist between each of the elements shown:

$$(1.0, \cdot, \cdot, \cdot, 2.0, \cdot, \cdot, \cdot, 3.0, \cdot, \cdot, \cdot, 4.0, \cdot, \cdot, \cdot, 5.0)$$

This notation is used to show vector elements inside an array.

**Two-Dimensional Arrays:** A two-dimensional array is represented as a block of numeric elements enclosed in square brackets:

$$\left[ \begin{array}{cccc}
 1.0 & 11.0 & 5.0 & 25.0 \\
 2.0 & 12.0 & 6.0 & 26.0 \\
 3.0 & 13.0 & 7.0 & 27.0 \\
 4.0 & 14.0 & 8.0 & 28.0
 \end{array} \right]$$

Elements not significant to the computation are usually not shown in the array. One dot appears for each element not shown. The following array contains three rows and two columns not used in the computation:

$$\left[ \begin{array}{cccccc}
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1.0 & 2.0 & 5.0 & 4.0 & \cdot \\
 \cdot & 2.0 & 3.0 & 6.0 & 3.0 & \cdot \\
 \cdot & 3.0 & 4.0 & 7.0 & 2.0 & \cdot \\
 \cdot & 4.0 & 5.0 & 8.0 & 1.0 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{array} \right]$$

This notation is used to show matrix elements inside an array.

**Three-Dimensional Arrays:** A three-dimensional array is represented as a series of blocks of elements separated by ellipses. Each block appears like a two-dimensional array:

$$\begin{bmatrix} 1.0 & 11.0 & 5.0 & 25.0 \\ 2.0 & 12.0 & 6.0 & 26.0 \\ 3.0 & 13.0 & 7.0 & 27.0 \\ 4.0 & 14.0 & 8.0 & 28.0 \end{bmatrix} \quad \begin{bmatrix} 10.0 & 111.0 & 15.0 & 125.0 \\ 20.0 & 112.0 & 16.0 & 126.0 \\ 30.0 & 113.0 & 17.0 & 127.0 \\ 40.0 & 114.0 & 18.0 & 128.0 \end{bmatrix} \quad \dots \quad \begin{bmatrix} 100.0 & 11.0 & 15.0 & 25.0 \\ 200.0 & 12.0 & 16.0 & 26.0 \\ 300.0 & 13.0 & 17.0 & 27.0 \\ 400.0 & 14.0 & 18.0 & 28.0 \end{bmatrix}$$

Elements not significant to the computation are usually not shown in the array. One dot appears for each element not shown, just as for two-dimensional arrays.

## Special Characters, Symbols, Expressions, and Abbreviations

The mathematical and programming notations used in this book are consistent with traditional mathematical and programming usage. These conventions are explained below, along with special abbreviations that are associated with specific values.

Item	Description
Greek letters: $\alpha, \sigma, \omega, \Omega$	Symbolic scalar values
$ a $	The absolute value of $a$
$a \cdot b$	The dot product of $a$ and $b$
$x_i$	The $i$ -th element of vector $x$
$c_{ij}$	The element in matrix $C$ at row $i$ and column $j$
$x_1 \dots x_n$	Elements from $x_1$ to $x_n$
$i = 1, n$	$i$ is assigned the values 1 to $n$
$y \leftarrow x$	Vector $y$ is replaced by vector $x$
$xy$	Vector $x$ times vector $y$
$AX \cong B$	$AX$ is congruent to $B$
$a^k$	$a$ raised to the $k$ power
$e^x$	Exponential function of $x$
$A^T; x^T$	The transpose of matrix $A$ ; the transpose of vector $x$
$\bar{x}; \bar{A}$	The complex conjugate of vector $x$ ; the complex conjugate of matrix $A$
$\bar{x}_i; \bar{c}_{jk}$	The complex conjugate of the complex vector element $x_i$ , where: if $x_i = (a_i, b_i)$ , then $\bar{x}_i = (a_i, -b_i)$  The complex conjugate of the complex matrix element $c_{jk}$
$x^H; A^H$	The complex conjugate transpose of vector $x$ ; the complex conjugate transpose of matrix $A$
$\sum_{i=1}^n x_i$	The sum of elements $x_1$ to $x_n$
$\sqrt{a+b}$	The square root of $a+b$

Item	Description
$\int_a^b f(x) dx$	The integral from $a$ to $b$ of $f(x) dx$
$\ x\ _2$	The Euclidean norm of vector $x$ , defined as: $\sqrt{\sum_{j=1}^n  x_j ^2}$
$\ A\ _1$	The one norm of matrix $A$ , defined as: $\max \left\{ \sum_{i=1}^m  a_{ij} , 1 \leq j \leq n \right\}$
$\ A\ _2$	The spectral norm of matrix $A$ , defined as: $\max\{\ Ax\ _2 : \ x\ _2 = 1\}$
$\ A\ _F$	The Frobenius norm of matrix $A$ , defined as: $\sqrt{\sum_{i=1}^m \sum_{j=1}^n  a_{ij} ^2}$
$A^{-1}$	The inverse of matrix $A$
$A^{-T}$	The transpose of $A$ inverse
$ A $	The determinant of matrix $A$
$m$ by $n$ matrix $A$	Matrix $A$ has $m$ rows and $n$ columns
$\sin a$	The sine of $a$
$\cos b$	The cosine of $b$
$\text{SIGN}(a)$	The sign of $a$ ; the result is either + or -
address $\{a\}$	The storage address of $a$
$\max(x)$	The maximum element in vector $x$
$\min(x)$	The minimum element in vector $x$
$\text{ceiling}(x)$	The smallest integer that is greater than or equal to $x$
$\text{floor}(x)$	The largest integer that is not greater than $x$
$\text{int}(x)$	The largest integer that is less than or equal to $x$
$x \bmod(m)$	$x$ modulo $m$ ; the remainder when $x$ is divided by $m$
$\infty$	Infinity
$\pi$	Pi, 3.14159265...

---

## How to Interpret the Subroutine Descriptions

This section explains how to interpret the information in the subroutine descriptions in Part 2 of this book.

### Description

Each subroutine description begins with a brief explanation of what the subroutine does. When we combine the description of multiple versions of a subroutine, we

give enough information to enable you to easily tell the differences among the subroutines. Differences usually occur in either the function performed or the data types required for each subroutine.

## Syntax

This shows the syntax for the Fortran, C, and C++ calling statements:

Fortran	CALL NAME-1   NAME-2   ...   NAME-n ( <i>arg-1, arg-2, ... ,arg-m, ...</i> )
C and C++	name-1   name-2   ...   name-n ( <i>arg-1, ... ,arg-m</i> );

The syntax indicates:

- The programming language (Fortran, C, or C++)
- Each possible subroutine name that you can code in the calling sequence. Each name is separated by the | (or) symbol. You specify only one of these names in your calling sequence. (You do not code the | in the calling sequence.)
- The arguments, listed in the order in which you code them in the calling sequence. You must code them all in your calling sequence.

You can distinguish between input arguments and output arguments by looking at the “On Entry” and “On Return” sections, respectively. An argument used for both input and output is described in both the “On Entry” and “On Return” sections. In this case, the input value for the argument is overlaid with the output value.

The names of the arguments give an indication of the type of data that you should specify for the argument; for example:

- Names beginning with the letters *i* through *n*, such as *m*, *incx*, *iopt*, and *isign*, indicate that you specify integer data.
- Names beginning with the letters *a* through *h* and *o* through *z*, such as *b*, *t*, *alpha*, *sigma*, and *omega*, indicate that you specify real or complex data.

## On Entry

This lists the input arguments, which are the arguments you pass to the ESSL subroutine. Each argument description first gives the meaning of the argument, and then gives the form of data required for the argument. (To help you avoid errors, output arguments are also listed, along with a reference to the On Return section.)

## On Return

This lists the output arguments, which are the arguments passed back to your program from the ESSL subroutine. Each argument description first gives the meaning of the argument, and then gives the form of data passed back to your program for the argument.

## Notes

The notes describe any programming considerations and restrictions that apply to the arguments or the data for the arguments. There may be references to other parts of the book for further information.

## Function

This is a functional, or mathematical, description of the function performed by this subroutine. **It explains what computation is performed, not the implementation.** It explains the variations in the computation depending on the input arguments.

References are made, where appropriate, to mathematical background books listed in the bibliography. References appear as a number enclosed in square brackets, where the number refers to the item listed under that number in the bibliography. For example, reference [1] cites the first item listed.

## Special Usage

These are unique ways you can use the subroutine in your application. In most cases, this book does not address applications of the ESSL subroutines; however, in special situations where the functional capability of the subroutine can be extended by following certain rules for its use, these rules are described in this section.

## Error Conditions

These are all the ESSL run-time errors that can occur in the subroutine. They are organized under three headings; Computational Errors, Input-Argument Errors, and Resource Errors. The return code values resulting from these errors are also explained.

## Examples

**The examples show how you would call the subroutine from a Fortran program.** They show a variety of uses of the subroutine. Except where it is important to show differences in use between the various versions of the subroutine, the simplest version of the subroutine is used in the examples. In most cases, this is the short-precision real version of the subroutine. Each example provides a description of the important features of the example, followed by the Fortran calling sequence, the input data, and the resulting output data.





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## Summary of changes

This section summarizes the changes that were introduced in each release of ESSL Version 4.

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### What's New for ESSL Version 4 Release 2.2

- This release of ESSL for Linux on POWER provides the following new library:
  - ESSL Blue Gene Library, which provides 32-bit versions of the ESSL subroutines for use on Blue Gene

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### What's New for ESSL Version 4 Release 2.1

- This release of ESSL for Linux on POWER is supported on the following new distribution:
  - Red Hat Linux Enterprise Server 4 (RHEL4)

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### What's New for ESSL Version 4 Release 2

- This release of ESSL is supported on the following operating system versions or distributions:
  - AIX 5L Version 5.2
  - AIX 5L Version 5.3
  - SuSE Linux Enterprise Server 9 for POWER (SLES9)
  - Red Hat Enterprise Linux 3 (RHEL3) (Update 3)
- The ESSL Libraries are now tuned for the POWER5 and the PowerPC 970.
- The Dense Linear Algebraic Equation Subroutines now include these new LAPACK subroutines:
  - CPPSV and ZPPSV; see the subroutine description for Positive Definite Complex Hermitian Matrix Factorization and Multiple Right-Hand Side Solve on page 483.
  - CPPTRF and ZPPTRF; see the subroutine description for Positive Definite Complex Hermitian Matrix Factorization on page 495.
  - CPPTRS and ZPPTRS; see the subroutine description for Positive Definite Complex Hermitian Matrix Multiple Right-Hand Side Solve on page 507.
  - SPPTRI and DPPTRI; see the subroutine description for Positive Definite Real Symmetric Matrix Inverse on page 547.

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### What's New for ESSL Version 4 Release 1

- ESSL now runs on the SuSE Linux Enterprise Server 8 for pSeries® (SLES8) operating system (in addition to AIX 5L for POWER Version 5.2B or later).
- The ESSL Libraries are tuned for the POWER4+.
- The Dense Linear Algebraic Equation Subroutines now include these new LAPACK subroutines:
  - SGESV, DGESV, CGESV, and ZGESV; see the subroutine description for General Matrix Factorization and Multiple Right-Hand Side Solve on page 454.

- SPPSV and DPPSV; see the subroutine description for Positive Definite Real Symmetric Matrix Factorization and Multiple Right-Hand Side Solve on page 483.
- SPOSV, DPOSV, CPOSV, and ZPOSV; see the subroutine description for Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization and Multiple Right-Hand Side Solve on page 489.
- SPTRF and DPPTRF; see the subroutine description for Positive Definite Real Symmetric Matrix Factorization on page 495.)
- SPTRS and DPPTRS; see the subroutine description for Positive Definite Real Symmetric Matrix Multiple Right-Hand Side Solve on page 507.
- CGETRI and ZGETRI; see the subroutine description for General Matrix Inverse on page 539.
- CPOTRI and ZPOTRI; see the subroutine description for Positive Definite Complex Hermitian Matrix Inverse on page 547.
- CTRTRI, ZTRTRI, CTPTRI, and ZTPTRI; see the subroutine description for Triangular Matrix Inverse on page 570.
- SMP support has been added to the SCFT and DCFT subroutines when computing a single large transform.
- Manpages of the subroutine descriptions are now available.
- Documentation is no longer being shipped with the product. It can be viewed or downloaded from the URLs listed in Table 7 on page 11.
- The ESSL software license agreement is now shipped, viewed, and accepted electronically. (See the *ESSL for AIX Installation Guide* for details.)

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## Future Migration

If you are concerned with migration to possible future releases of ESSL or possible future hardware, you should read “Planning for Future Migration” on page 172. **That section explains what you can do now to prevent future migration problems.**

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## Part 1. Guide Information

This part of the book is organized into the following chapters, which provide guidance information on how to use ESSL. It is organized as follows:

- Learning about ESSL
- Designing your program
- Setting up your data structures
- Coding your program
- Processing your program
- Migrating your programs
- Handling problems



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# Chapter 1. Introduction and Requirements

This chapter introduces you to the Engineering and Scientific Subroutine Library (ESSL).

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## Overview of ESSL

This section gives an overview of the ESSL capabilities and requirements.

ESSL is a state-of-the-art collection of subroutines providing a wide range of mathematical functions for many different scientific and engineering applications. Its primary characteristics are performance, functional capability, and usability.

To order ESSL, specify one of the program numbers below:

**ESSL for AIX**  
5765-F82

**ESSL for Linux**  
5765-G17

## Performance and Functional Capability

The mathematical subroutines, in nine computational areas, are tuned for performance. The computational areas are:

- Linear Algebra Subprograms
- Matrix Operations
- Linear Algebraic Equations
- Eigensystem Analysis
- Fourier Transforms, Convolutions and Correlations, and Related Computations
- Sorting and Searching
- Interpolation
- Numerical Quadrature
- Random Number Generation

ESSL runs under the AIX and Linux operating systems.

ESSL provides the following run-time libraries (described in detail in “Which ESSL Library Do You Want to Use?” on page 25):

- ESSL Symmetric Multi-Processing (SMP) Library
- ESSL Serial Library
- ESSL Blue Gene Library

All libraries are designed to provide high levels of performance for numerically intensive computing jobs. All versions provide mathematically equivalent results.

The ESSL subroutines can be called from application programs written in Fortran, C, and C++.

## Usability

ESSL is designed for usability:

- It has an easy-to-use call interface.

- If your existing application programs use the ESSL Serial library, you only need to re-link your program to take advantage of the increased performance of the ESSL SMP Library.
- It supports a 64-bit environment.  
The data model used for the 64-bit environment is referred to as LP64. This data model supports 32-bit integers and 64-bit pointers. In accordance with the LP64 data model, all ESSL integer arguments remain 32-bit except for the **iusadr** argument for ERRSET. See “ERRSET — ESSL ERRSET Subroutine” on page 1012.
- It has informative error-handling capabilities, enabling you to calculate auxiliary storage sizes and transform lengths.
- An online book that can be displayed using an Hypertext Markup Language (HTML) document browser, is available for use with ESSL.

## The Variety of Mathematical Functions

This section describes the mathematical functions included in ESSL.

### Areas of Application

ESSL provides a variety of mathematical functions for many different types of scientific and engineering applications. Some of the industries using these applications are: Aerospace, Automotive, Electronics, Petroleum, Finance, Utilities, and Research. Examples of applications in these industries are:

Structural Analysis	Time Series Analysis
Computational Chemistry	Computational Techniques
Fluid Dynamics Analysis	Mathematical Analysis
Seismic Analysis	Dynamic Systems Simulation
Reservoir Modeling	Nuclear Engineering
Quantitative Analysis	Electronic Circuit Design

### What ESSL Provides

ESSL provides run-time libraries that are designed to provide high levels of performance for numerically intensive computing jobs.

The subroutines provided in ESSL, summarized in Table 2, fall into the following groups:

- Nine major areas of mathematical computation, providing the computations commonly used by the industry applications listed above
- Utilities, performing general-purpose functions

Most of the subroutine calls are compatible with those in the ESSL/370 product.

**To help you select the ESSL subroutines that fulfill your needs for performance, accuracy, storage, and so forth, see “Selecting an ESSL Subroutine” on page 25.**

Table 2. Summary of ESSL Subroutines

ESSL Area of Computation	Integer Subroutines	Short-Precision Subroutines	Long-Precision Subroutines
<b>Linear Algebra Subprograms:</b>			
Vector-scalar	0	41	41
Sparse vector-scalar	0	11	11
Matrix-vector	0	32	32
Sparse matrix-vector	0	0	3
<b>Matrix Operations:</b>			
Addition, subtraction, multiplications, rank-k updates, rank-2k updates, and matrix transposes	0	25	26
<b>Linear Algebraic Equations:</b>			
Dense linear algebraic equations	0	53	58
Banded linear algebraic equations	0	18	18
Sparse linear algebraic equations	0	0	11
Linear least squares	0	3	5
<b>Eigensystem Analysis:</b>			
Solutions to the algebraic eigensystem analysis problem and the generalized eigensystem analysis problem	0	8	8
<b>Signal Processing Computations:</b>			
Fourier transforms	0	15	11
Convolutions and correlations	0	10	2
Related computations	0	6	6
<b>Sorting and Searching:</b>			
Sorting, sorting with index, and binary and sequential searching	5	5	5
<b>Interpolation:</b>			
Polynomial and cubic spline interpolation	0	4	4
<b>Numerical Quadrature:</b>			
Numerical quadrature on a set of points or on a function	0	6	6
<b>Random Number Generation:</b>			
Generating vectors of uniformly distributed and normally distributed random numbers	0	3	3
<b>Utilities:</b>			
General service operations	8	0	3
<b>Total ESSL Subroutines</b>	<b>13</b>	<b>240</b>	<b>253</b>

## Accuracy of the Computations

ESSL provides accuracy comparable to libraries using equivalent algorithms with identical precision formats. Both short- and long-precision real versions of the subroutines are provided in most areas of ESSL. In some areas, short- and long-precision complex versions are also provided, and, occasionally, an integer version is provided. The data types operated on by the short-precision, long-precision, and integer versions of the subroutines are ANSI/IEEE 32-bit and

64-bit binary floating-point format, and 32-bit integer. See the *ANSI/IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Standard 754–1985*, for more detail. (There are ESSL-specific rules that apply to the results of computations on workstation processors using the ANSI/IEEE standards. For details, see “What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?” on page 48.)

For more information on accuracy, see “Getting the Best Accuracy” on page 47.

## High Performance of ESSL

The ESSL subroutines have been designed to provide high performance, as described in the following sections. (See references [32], [43], and [44].)

### Algorithms

To achieve high performance, the subroutines use state-of-the-art algorithms tailored to specific operational characteristics of the hardware, such as cache size, Translation Lookaside Buffer (TLB) size, and page size.

Most subroutines use the following techniques to optimize performance:

- Managing the cache and TLB efficiently so the hit ratios are maximized; that is, data is blocked so it stays in the cache or TLB for its computation.
- Accessing data stored contiguously—that is, using stride-1 computations.
- Exploiting the large number of available floating-point registers.
- Using algorithms that minimize paging.
- Structuring the ESSL subroutines so, where applicable, the compiled code fully utilizes the dual floating-point execution units. Because two Multiply-Add instructions can be executed each cycle, neglecting overhead, this allows four floating-point operations per cycle to be performed.
- Structuring the ESSL subroutines so, where applicable, the compiled code takes full advantage of the hardware data prefetching.

### Obtaining High Performance

The following sections explain how to obtain high performance depending on the type of processor you are using:

1. “Obtaining High Performance on SMP Processors”
2. “Obtaining High Performance on SIMD Processors” on page 7

**Obtaining High Performance on SMP Processors:** The ESSL SMP Library is designed to exploit the processing power and shared memory of the SMP processor. In addition, a subset of the ESSL SMP subroutines have been coded to take advantage of increased performance from multithreaded (parallel) programming techniques. For a list of the multithreaded subroutines in the ESSL SMP Library, see Table 26 on page 26.

Choosing the number of threads depends on the problem size, the specific subroutine being called, and the number of physical processors you are running on. To achieve optimal performance, experimentation is necessary; however, picking the number of threads equal to the number of online processors generally provides good performance in most cases. In some cases, performance may increase if you choose the number of threads to be less than the number of online processors.

You should use either the XL Fortran XLSMPOPTS or the OMP\_NUM\_THREADS environment variable to specify the number of threads you want to create.



**Obtaining High Performance on SIMD Processors:** The ESSL Blue Gene Library is designed to exploit the processing power of the PowerPC 440D SIMD processor. For details about how to use it to achieve optimal performance, see “ESSL Blue Gene Library” on page 28.

### **POWER5 SMT Mode**

The following operating systems support simultaneous multithreading (SMT) on servers with POWER5 and POWER5+ processors:

- AIX 5L Version 5.3
- SuSE Linux Enterprise Server 9 for POWER (SLES9)
- Red Hat Enterprise Linux 3 (RHEL3) (Update 3)
- Red Hat Enterprise Linux 4 (RHEL4)

SMT is a processor technology that allows two separate instruction streams (threads) to run concurrently on the same physical processor, improving overall throughput. To the operating system, each hardware thread is treated as an independent logical processor.

Not all applications benefit from SMT. Having two threads executing on the same processor will not increase the performance of applications with execution-unit-limited performance or applications that consume all the chip’s memory bandwidth. For this reason, these processors support single-threaded (ST) execution mode. In this mode, these processors give all the physical resources to the active thread.

In most cases, ESSL subroutines will not benefit from SMT. However, this can vary depending on the nature of the application; therefore, you may wish to verify this by testing your own applications in this mode.

Any partition can be booted in either in ST mode or SMT mode (which is the default).

### **Mathematical Techniques**

All areas of ESSL use state-of-the-art mathematical techniques to achieve high performance. For example, the matrix-vector linear algebra subprograms operate on a higher-level data structure, matrix-vector rather than vector-scalar. As a result, they optimize performance directly for your program and indirectly through those ESSL subroutines using them.

## **The Fortran Language Interface to the Subroutines**

The ESSL subroutines follow standard Fortran calling conventions and must run in the Fortran run-time environment. When ESSL subroutines are called from a program in a language other than Fortran, such as C or C++, the Fortran conventions must be used. This applies to all aspects of the interface, such as the linkage conventions and the data conventions. For example, array ordering must be consistent with Fortran array ordering techniques. Data and linkage conventions for each language are given in Chapter 4, “Coding Your Program,” on page 111.

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## **Software and Hardware Products That Can Be Used with ESSL**

This section describes the hardware and software products you can use with ESSL, as well as those products for installing ESSL and displaying the online documentation. It is divided into the following sections:

- “Hardware Products Supported by ESSL” on page 8

- “Operating Systems Supported by ESSL”
- “Software Products Required by ESSL”
- “Software Products for Installing and Customizing ESSL” on page 10
- “Software Products for Displaying ESSL Documentation” on page 11

## Hardware Products Supported by ESSL

ESSL runs on the following hardware platforms:

<b>Servers</b>	IBM @server Cluster 1600, IBM @server POWER servers, SP systems, BladeCenter JS20, or IBM @server Blue Gene Solution
<b>Processors</b>	POWER3, POWER3-II, POWER4, POWER4+, POWER5, POWER5+, PowerPC 970, PowerPC 440, and PowerPC 440D processors

64-bit applications require 64-bit hardware.

## Operating Systems Supported by ESSL

ESSL is supported in the following operating system environments:

*Table 3. Operating systems supported by ESSL*

Product	Supported Environment
Engineering and Scientific Subroutine Library for AIX, Version 4 Release 2 (program number 5765-G82)	<p>Either of the following operating systems:</p> <ul style="list-style-type: none"> <li>• AIX 5L Version 5.2 with the appropriate Recommended Maintenance Package, or later.</li> <li>• AIX 5L Version 5.3, or later.</li> </ul>
Engineering and Scientific Subroutine Library (ESSL) for Linux on POWER, Version 4 Release 2.2 (program number 5765-G17)	<p>For users of the ESSL Serial and ESSL SMP libraries, any of the following Linux distributions:</p> <ul style="list-style-type: none"> <li>• SUSE Linux Enterprise Server 9 (SLES9) Service Pack 1 (SP1)</li> <li>• Red Hat Linux Enterprise Server 3 (Update 3) (RHEL3)</li> <li>• Red Hat Linux Enterprise Server 4 (Update 1) (RHEL4)</li> </ul> <p><b>Note:</b> Verify that you have the minimum required service level for your hardware.</p> <p>For users of the ESSL Blue Gene library:</p> <ul style="list-style-type: none"> <li>• Blue Gene compute node kernel (CNK), also known as the Blue Gene Runtime System (BLRTS)</li> </ul>

## Software Products Required by ESSL

This section describes the software products that are required by ESSL. It is divided into the following sections:

- “Software Products Required by ESSL for AIX”
- “Software Products Required by ESSL for Linux” on page 9

### Software Products Required by ESSL for AIX

ESSL for AIX requires the software products shown in Table 4 on page 9 for compiling and running.

To assist C and C++ users, an ESSL header file is provided. Use of this file is described in “C Programs” on page 129 and “C++ Programs” on page 145.

**Required Software Products:** The following table lists the required software products for ESSL for AIX.

Table 4. Required Software Products for ESSL for AIX

Purpose	Required Software Product
For Compiling	IBM XL Fortran Enterprise Edition Version 9.1 for AIX or later (program number 5724-I08)
	<i>or</i>
	IBM XL C/C++ Enterprise Edition Version 7.0 for AIX or later (program number 5724-I11)
	<i>or</i>
	IBM XL C Enterprise Edition for AIX, Version 7.0 or later (program number 5724-I10)
For Linking, Loading, or Running	IBM XL Fortran Enterprise Edition Run-Time Environment Version 9.1 for AIX or later. (See Note 1.)
	<b>and</b>
	C libraries. (See Note 2.)
<b>Notes:</b> 1. IBM XL Fortran Enterprise Edition Run-Time Environment Version 9.1 for AIX is automatically shipped with the compiler. It is also available for downloading from the following Web site: <a href="http://www.ibm.com/software/awdtools/fortran">http://www.ibm.com/software/awdtools/fortran</a> 2. The AIX product includes the C and math libraries in the Application Development Toolkit.	

### Software Products Required by ESSL for Linux

ESSL for Linux requires the software products shown in Table 5 for compiling and running.

To assist C and C++ users, an ESSL header file is provided. Use of this file is described in “C Programs” on page 129 and “C++ Programs” on page 145.

**Required Software Products:** The following table lists the required software products for ESSL for Linux on POWER:

Table 5. Required Software Products for ESSL for Linux on POWER

Purpose	Required Software Product
For Compiling	IBM XL Fortran Advanced Edition Version 9.1.1 for Linux or later
	IBM XL C/C++ Advanced Edition Version 7.0.1 for Linux or later

Table 5. Required Software Products for ESSL for Linux on POWER (continued)

Purpose	Required Software Product
For Linking, Loading, or Running	<p><b>On RHEL3 and SLES9</b></p> <p>IBM XL Fortran Advanced Edition Run-Time Environment Version 9.1.1 for Linux or later<sup>1</sup></p> <p>—and—</p> <p>GCC 3.3.3 32-bit libraries on SLES9</p> <p>gcc-64bit-9 libraries on SLES9</p> <p>GCC 3.2.3 32-bit and 64-bit libraries on RHEL3 (Update 3)</p> <p><b>On RHEL4</b></p> <p>IBM XL Fortran Advanced Edition Run-Time Environment Version 9.1.1 for Linux or later<sup>1</sup></p> <p>—and—</p> <p>GCC 3.4.3 32-bit and 64-bit libraries</p>
<p><b>Notes:</b></p> <ol style="list-style-type: none"> <li>1. IBM XL Fortran Advanced Edition Run-Time Environment for Linux is automatically shipped with the compiler. It is also available for downloading from the following Web site: <a href="http://www.ibm.com/software/awdtools/fortran">http://www.ibm.com/software/awdtools/fortran</a></li> <li>2. <b>Blue Gene users only</b> should also download the IBM XLF Compiler Runtime Add-on for Blue Gene from the Blue Gene Software Delivery Web site (IBM ID sign-in required).</li> <li>3. Optional RPMs are required for building applications. For details, consult the Linux and compiler documentation.</li> </ol>	

## Software Products for Installing and Customizing ESSL

The ESSL licensed program is distributed on a CD. The following sections provide information about software products that are used for installing and customizing ESSL:

- “Software Products for Installing and Customizing ESSL for AIX”
- “Software Products for Installing and Customizing ESSL for Linux”

### Software Products for Installing and Customizing ESSL for AIX

The *ESSL for AIX Installation Guide* provides the detailed information you need to install ESSL for AIX.

ESSL for AIX is packaged according to the AIX guidelines, as described in the *AIX General Programming Concepts: Writing and Debugging Programs* manual. The product can be installed using the `smi t` command, as described in the *AIX System Management Guide: Operating System and Devices* manual.

### Software Products for Installing and Customizing ESSL for Linux

The *ESSL for Linux Installation Guide* provides the detailed information you need to install ESSL for Linux.

ESSL for Linux is packaged as RPM packages. The product can be installed using the `rpm` command, as described at the following URL:

<http://www.rpm.org/>

## Software Products for Displaying ESSL Documentation

The software products needed to display ESSL online information are listed in Table 6.

Table 6. Software needed to display various formats of ESSL online information

Format of online information	Software needed
HTML	HTML document browser (such as Microsoft® Internet Explorer)
PDF	Adobe Acrobat Reader, which is freely available for downloading from the Adobe Web site at: <a href="http://www.adobe.com">http://www.adobe.com</a>
Manpages	No additional software needed. To display a specific manpage, use the <b>man</b> command as follows:  <b>man</b> <i>subroutine-name</i> <b>Note:</b> These manpages will be installed in the following directory: /usr/share/man/man3 The manpages provided by LAPACK are installed in the /usr/share/man/man1 directory. By default, ESSL manpages will be displayed rather than BLAS or LAPACK manpages with the same names. If you want to access the BLAS or LAPACK manpages, you must set the MANPATH environment variable. See the documentation for the <b>man</b> command.

## ESSL Internet Resources

ESSL documentation, as well as other related information, can be displayed or downloaded from the Internet at the URLs listed in Table 7.

Table 7. Online resources for ESSL documentation

Web Site	Type of Information Provided	File Formats Available	
		PDF	HTML
IBM @server Cluster Information Center: <a href="http://publib.boulder.ibm.com/infocenter/clresctr/index.jsp">http://publib.boulder.ibm.com/infocenter/clresctr/index.jsp</a>	Documentation for IBM clustered-server and pSeries software products	Yes	Yes
IBM Publications Center: <a href="http://www.ibm.com/shop/publications/order">http://www.ibm.com/shop/publications/order</a>	Documentation for any IBM product	Yes	No

## Blue Gene documentation

For Blue Gene documentation, see the URLs listed in “Related Publications” on page 1060.

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## Getting on the ESSL Mailing List

Late breaking information about ESSL can be obtained by being placed on the ESSL mailing list. In addition, users on the mailing list will receive information about new ESSL function and may receive customer satisfaction surveys and requirements surveys, to provide feedback to ESSL Development on the product and user requirements.

You can be placed on the mailing list by sending a request to either of the following, asking to be placed on the ESSL mailing list:

International Business Machines Corporation  
ESSL Development  
Department 85BAMail Station P963  
2455 South Rd.  
Poughkeepsie, N.Y. 12601-5400

e-mail: [essl@us.ibm.com](mailto:essl@us.ibm.com)

**Note:** You should send us e-mail if you would like to be withdrawn from the ESSL mailing list.

When requesting to be placed on the mailing list or asking any questions, please provide the following information:

- Your name
- The name of your company
- Your mailing address
- Your Internet address
- Your phone number

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## List of ESSL Subroutines

This section provides an overview of the subroutines in each of the areas of ESSL.

Appendix A, “Basic Linear Algebra Subprograms (BLAS),” on page 1041 contains a list of Level 1, 2, and 3 Basic Linear Algebra Subprograms (BLAS) included in ESSL.

Appendix B, “LAPACK,” on page 1043 contains a list of Linear Algebra Package (LAPACK) subroutines included in ESSL.

### Linear Algebra Subprograms

The linear algebra subprograms consist of:

- Vector-scalar linear algebra subprograms (Table 8)
- Sparse vector-scalar linear algebra subprograms (Table 9)
- Matrix-vector linear algebra subprograms (Table 10)
- Sparse matrix-vector linear algebra subprograms (Table 11)

**Notes:**

1. The term **subprograms** is used to be consistent with the Basic Linear Algebra Subprograms (BLAS), because many of these subprograms correspond to the BLAS.
2. Some of the linear algebra subprograms were designed in accordance with the Level 1 and Level 2 BLAS de facto standard. If these subprograms do not

comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subprograms, the updates could require modifications of the calling application program.

### Vector-Scalar Linear Algebra Subprograms

The vector-scalar linear algebra subprograms include a subset of the standard set of Level 1 BLAS. For details on the BLAS, see reference [82]. The remainder of the vector-scalar linear algebra subprograms are commonly used computations provided for your applications. Both real and complex versions of the subprograms are provided.

Table 8. List of Vector-Scalar Linear Algebra Subprograms

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Position of the First or Last Occurrence of the Vector Element Having the Largest Magnitude	ISAMAX <sup>+</sup> ICAMAX <sup>+</sup>	IDAMAX <sup>+</sup> IZAMAX <sup>+</sup>	199
Position of the First or Last Occurrence of the Vector Element Having Minimum Absolute Value	ISAMIN <sup>+</sup>	IDAMIN <sup>+</sup>	202
Position of the First or Last Occurrence of the Vector Element Having Maximum Value	ISMAX <sup>+</sup>	IDMAX <sup>+</sup>	205
Position of the First or Last Occurrence of the Vector Element Having Minimum Value	ISMIN <sup>+</sup>	IDMIN <sup>+</sup>	208
Sum of the Magnitudes of the Elements in a Vector	SASUM <sup>+</sup> SCASUM <sup>+</sup>	DASUM <sup>+</sup> DZASUM <sup>+</sup>	211
Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y	SAXPY <sup>*</sup> CAXPY <sup>*</sup>	DAXPY <sup>*</sup> ZAXPY <sup>*</sup>	214
Copy a Vector	SCOPY <sup>*</sup> CCOPY <sup>*</sup>	DCOPY <sup>*</sup> ZCOPY <sup>*</sup>	217
Dot Product of Two Vectors	SDOT <sup>+</sup> CDOTU <sup>+</sup> CDOTC <sup>+</sup>	DDOT <sup>+</sup> ZDOTU <sup>+</sup> ZDOTC <sup>+</sup>	220
Compute SAXPY or DAXPY N Times	SNAXPY	DNAXPY	224
Compute Special Dot Products N Times	SNDOT	DNDOT	229
Euclidean Length of a Vector with Scaling of Input to Avoid Destructive Underflow and Overflow	SNRM2 <sup>+</sup> SCNRM2 <sup>+</sup>	DNRM2 <sup>+</sup> DZNRM2 <sup>+</sup>	234
Euclidean Length of a Vector with No Scaling of Input	SNORM2 <sup>+</sup> CNORM2 <sup>+</sup>	DNORM2 <sup>+</sup> ZNORM2 <sup>+</sup>	237
Construct a Givens Plane Rotation	SROTG <sup>*</sup> CROTG <sup>*</sup>	DROTG <sup>*</sup> ZROTG <sup>*</sup>	240
Apply a Plane Rotation	SROT <sup>*</sup> CROT <sup>*</sup> CSROT <sup>*</sup>	DROT <sup>*</sup> ZROT <sup>*</sup> ZDROT <sup>*</sup>	247
Multiply a Vector X by a Scalar and Store in the Vector X	SSCAL <sup>*</sup> CSCAL <sup>*</sup> CSSCAL <sup>*</sup>	DSCAL <sup>*</sup> ZSCAL <sup>*</sup> ZDSCAL <sup>*</sup>	251
Interchange the Elements of Two Vectors	SSWAP <sup>*</sup> CSWAP <sup>*</sup>	DSWAP <sup>*</sup> ZSWAP <sup>*</sup>	254
Add a Vector X to a Vector Y and Store in a Vector Z	SVEA CVEA	DVEA ZVEA	257
Subtract a Vector Y from a Vector X and Store in a Vector Z	SVES CVES	DVES ZVES	261

Table 8. List of Vector-Scalar Linear Algebra Subprograms (continued)

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Multiply a Vector X by a Vector Y and Store in a Vector Z	SVEM CVEM	DVEM ZVEM	265
Multiply a Vector X by a Scalar and Store in a Vector Y	SYAX CYAX CSYAX	DYAX ZYAX ZDYAX	269
Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in a Vector Z	SZAXPY CZAXPY	DZAXPY ZZAXPY	272
† This subprogram is invoked as a function in a Fortran program. * Level 1 BLAS			

### Sparse Vector-Scalar Linear Algebra Subprograms

The sparse vector-scalar linear algebra subprograms operate on sparse vectors; that is, only the nonzero elements of the vector are stored. These subprograms provide similar functions to the vector-scalar subprograms. These subprograms represent a subset of the sparse extensions to the Level 1 BLAS described in reference [31]. Both real and complex versions of the subprograms are provided.

Table 9. List of Sparse Vector-Scalar Linear Algebra Subprograms

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Scatter the Elements of a Sparse Vector X in Compressed-Vector Storage Mode into Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode	SSCTR CSCTR	DSCTR ZSCTR	277
Gather Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode into a Sparse Vector X in Compressed-Vector Storage Mode	SGTHR CGTHR	DGTHR ZGTHR	280
Gather Specified Elements of a Sparse Vector Y in Full-Vector Mode into a Sparse Vector X in Compressed-Vector Mode, and Zero the Same Specified Elements of Y	SGTHRZ CGTHRZ	DGTHRZ ZGTHRZ	283
Multiply a Sparse Vector X in Compressed-Vector Storage Mode by a Scalar, Add to a Sparse Vector Y in Full-Vector Storage Mode, and Store in the Vector Y	SAXPYI CAXPYI	DAXPYI ZAXPYI	286
Dot Product of a Sparse Vector X in Compressed-Vector Storage Mode and a Sparse Vector Y in Full-Vector Storage Mode	SDOTI <sup>†</sup> CDOTCI <sup>†</sup> CDOTUI <sup>†</sup>	DDOTI <sup>†</sup> ZDOTCI <sup>†</sup> ZDOTUI <sup>†</sup>	289
† This subprogram is invoked as a function in a Fortran program.			

### Matrix-Vector Linear Algebra Subprograms

The matrix-vector linear algebra subprograms operate on a higher-level data structure—matrix-vector rather than vector-scalar—using optimized algorithms to improve performance. These subprograms include a subset of the standard set of Level 2 BLAS. For details on the Level 2 BLAS, see [36] and [37]. Both real and complex versions of the subprograms are provided.



Table 10. List of Matrix-Vector Linear Algebra Subprograms

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose	SGEMV <sup>†</sup> CGEMV <sup>†</sup> SGEMX <sup>§</sup> SGEMTX <sup>§</sup>	DGEMV <sup>†</sup> ZGEMV <sup>†</sup> DGEMX <sup>§</sup> DGEMTX <sup>§</sup>	294
Rank-One Update of a General Matrix	SGER <sup>†</sup> CGERU <sup>†</sup> CGERC <sup>†</sup>	DGER <sup>†</sup> ZGERU <sup>†</sup> ZGERC <sup>†</sup>	305
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Matrix	SSPMV <sup>†</sup> CHPMV <sup>†</sup> SSYMV <sup>†</sup> CHEMV <sup>†</sup> SSLMX <sup>§</sup>	DSPMV <sup>†</sup> ZHPMV <sup>†</sup> DSYMV <sup>†</sup> ZHEMV <sup>†</sup> DSLMX <sup>§</sup>	312
Rank-One Update of a Real Symmetric or Complex Hermitian Matrix	SSPR <sup>†</sup> CHPR <sup>†</sup> SSYR <sup>†</sup> CHER <sup>†</sup> SSLR1 <sup>§</sup>	DSPR <sup>†</sup> ZHPR <sup>†</sup> DSYR <sup>†</sup> ZHER <sup>†</sup> DSL1 <sup>§</sup>	320
Rank-Two Update of a Real Symmetric or Complex Hermitian Matrix	SSPR2 <sup>†</sup> CHPR2 <sup>†</sup> SSYR2 <sup>†</sup> CHER2 <sup>†</sup> SSLR2 <sup>§</sup>	DSPR2 <sup>†</sup> ZHPR2 <sup>†</sup> DSYR2 <sup>†</sup> ZHER2 <sup>†</sup> DSL2 <sup>§</sup>	327
Matrix-Vector Product for a General Band Matrix, Its Transpose, or Its Conjugate Transpose	SGBMV <sup>†</sup> CGBMV <sup>†</sup>	DGBMV <sup>†</sup> ZGBMV <sup>†</sup>	336
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Band Matrix	SSBMV <sup>†</sup> CHBMV <sup>†</sup>	DSBMV <sup>†</sup> ZHBMV <sup>†</sup>	343
Matrix-Vector Product for a Triangular Matrix, Its Transpose, or Its Conjugate Transpose	STRMV <sup>†</sup> CTRMV <sup>†</sup> STPMV <sup>†</sup> CTPMV <sup>†</sup>	DTRMV <sup>†</sup> ZTRMV <sup>†</sup> DTPMV <sup>†</sup> ZTPMV <sup>†</sup>	348
Matrix-Vector Product for a Triangular Band Matrix, Its Transpose, or Its Conjugate Transpose	STBMV <sup>†</sup> CTBMV <sup>†</sup>	DTBMV <sup>†</sup> ZTBMV <sup>†</sup>	354
<sup>†</sup> Level 2 BLAS			
<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs.			

## Sparse Matrix-Vector Linear Algebra Subprograms

The sparse matrix-vector linear algebra subprograms operate on sparse matrices; that is, only the nonzero elements of the matrix are stored. These subprograms provide similar functions to the matrix-vector subprograms.

Table 11. List of Sparse Matrix-Vector Linear Algebra Subprograms

Descriptive Name	Long- Precision Subprogram	Page
Matrix-Vector Product for a Sparse Matrix in Compressed-Matrix Storage Mode	DSMMX	360
Transpose a Sparse Matrix in Compressed-Matrix Storage Mode	DSMTM	363
Matrix-Vector Product for a Sparse Matrix or Its Transpose in Compressed-Diagonal Storage Mode	DSDMX	367

## Matrix Operations

Some of the matrix operation subroutines were designed in accordance with the Level 3 BLAS de facto standard. If these subroutines do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subroutines, the updates could require modifications of the calling application program. For details on the Level 3 BLAS, see reference [34]. The matrix operation subroutines also include the commonly used matrix operations: addition, subtraction, multiplication, and transposition.

Table 12. List of Matrix Operation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Matrix Addition for General Matrices or Their Transposes	SGEADD CGEADD	DGEADD ZGEADD	377
Matrix Subtraction for General Matrices or Their Transposes	SGESUB CGESUB	DGESUB ZGESUB	383
Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes	SGEMUL CGEMUL	DGEMUL ZGEMUL DGEMPLP <sup>§</sup>	389
Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes Using Winograd's Variation of Strassen's Algorithm	SGEMMS CGEMMS	DGEMMS ZGEMMS	398
Combined Matrix Multiplication and Addition for General Matrices, Their Transposes, or Conjugate Transposes	SGEMM* CGEMM*	DGEMM* ZGEMM*	404
Matrix-Matrix Product Where One Matrix is Real or Complex Symmetric or Complex Hermitian	SSYMM* CSYMM* CHEMM*	DSYMM* ZSYMM* ZHEMM*	412
Triangular Matrix-Matrix Product	STRMM* CTRMM*	DTRMM* ZTRMM*	419
Rank-K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYRK* CSYRK* CHERK*	DSYRK* ZSYRK* ZHERK*	426
Rank-2K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYR2K* CSYR2K* CHER2K*	DSYR2K* ZSYR2K* ZHER2K*	432
General Matrix Transpose (In-Place)	SGETMI CGETMI	DGETMI ZGETMI	439
General Matrix Transpose (Out-of-Place)	SGETMO CGETMO	DGETMO ZGETMO	442
* Level 3 BLAS			
§ This subroutine is provided only for migration from earlier release of ESSL and is not intended for use in new programs.			

## Linear Algebraic Equations

The linear algebraic equations consist of:

- "Dense Linear Algebraic Equations" on page 17
- "Banded Linear Algebraic Equations" on page 18
- "Sparse Linear Algebraic Equations" on page 19
- "Linear Least Squares" on page 20

**Note:** Some of the linear algebraic equations were designed in accordance with the Level 2 BLAS, Level 3 BLAS, and LAPACK de facto standard. If these subprograms do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subprograms, the updates could require modifications of the calling application program. For details on the Level 2 and 3 BLAS, see [34] and [36]. For details on LAPACK, see [8].

## Dense Linear Algebraic Equations

The dense linear algebraic equation subroutines provide solutions to linear systems of equations for both real and complex general matrices and their transposes, positive definite real symmetric and complex Hermitian matrices, real symmetric indefinite matrices and triangular matrices. Some of these subroutines correspond to the Level 2 BLAS, Level 3 BLAS, and LAPACK routines described in references [34], [36] and [8].

Table 13. List of Dense Linear Algebraic Equation Subroutines

Descriptive Name	Short-Precision Subroutine	Long-Precision Subroutine	Page
General Matrix Factorization and Multiple Right-Hand Side Solve	SGESV <sup>△</sup> CGESV <sup>△</sup>	DGESV <sup>△</sup> ZGESV <sup>△</sup>	454
General Matrix Factorization	SGETRF <sup>△</sup> CGETRF <sup>△</sup>	DGETRF <sup>△</sup> ZGETRF <sup>△</sup>	458
	SGEF CGEF	DGEF ZGEF DGEFP <sup>§</sup>	467
General Matrix, Its Transpose, or Its Conjugate Transpose Multiple Right-Hand Side Solve	SGETRS <sup>△</sup> CGETRS <sup>△</sup>	DGETRS <sup>△</sup> ZGETRS <sup>△</sup>	462
	SGESM CGESM	DGESM ZGESM	474
General Matrix, Its Transpose, or Its Conjugate Transpose Solve	SGES CGES	DGES ZGES	470
General Matrix Factorization, Condition Number Reciprocal, and Determinant	SGEFCD	DGEFCD	479
Positive Definite Real Symmetric Matrix Factorization and Multiple Right-Hand Side Solve	SPPSV <sup>△</sup> CPPSV <sup>△</sup>	DPPSV <sup>△</sup> ZPPSV <sup>△</sup>	483
Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization and Multiple Right-Hand Side Solve	SPOSV <sup>△</sup> CPOSV <sup>△</sup>	DPOSV <sup>△</sup> ZPOSV <sup>△</sup>	489
Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization	SPOTRF <sup>△</sup> CPOTRF <sup>△</sup> SPOF CPOF SPPTRF <sup>△</sup> CPPTRF <sup>△</sup> SPPF	DPOTRF <sup>△</sup> ZPOTRF <sup>△</sup> DPOF ZPOF DPPTRF <sup>△</sup> ZPPTRF <sup>△</sup> DPPF DPPFP <sup>§</sup>	495
Positive Definite Real Symmetric or Complex Hermitian Matrix Multiple Right-Hand Side Solve	SPOTRS <sup>△</sup> CPOTRS <sup>△</sup> SPOSM CPOSM SPPTRS <sup>△</sup> CPPTRS <sup>△</sup>	DPOTRS <sup>△</sup> ZPOTRS <sup>△</sup> DPOSM ZPOSM DPPTRS <sup>△</sup> ZPPTRS <sup>△</sup>	507
Positive Definite Real Symmetric Matrix Solve	SPPS	DPPS	515

Table 13. List of Dense Linear Algebraic Equation Subroutines (continued)

Descriptive Name	Short-Precision Subroutine	Long-Precision Subroutine	Page
Positive Definite Real Symmetric Matrix Factorization, Condition Number Reciprocal, and Determinant	SPPFCD SPOFCD	DPPFCD DPOFCD	518
Symmetric Indefinite Matrix Factorization and Multiple Right-Hand Side Solve		DBSSV	524
Symmetric Indefinite Matrix Factorization		DBSTRF	530
Symmetric Indefinite Matrix Multiple Right-Hand Side Solve		DBSTRS	535
General Matrix Inverse, Condition Number Reciprocal, and Determinant	SGETRI <sup>△</sup> CGETRI <sup>△</sup> SGEICD	DGETRI <sup>△</sup> ZGETRI <sup>△</sup> DGEICD	539
Positive Definite Real Symmetric or Complex Hermitian Matrix Inverse, Condition Number Reciprocal, and Determinant	SPOTRI <sup>△</sup> CPOTRI <sup>△</sup> SPPTRI <sup>△</sup> SPPICD SPOICD	DPOTRI <sup>△</sup> ZPOTRI <sup>△</sup> DPPTRI <sup>△</sup> DPPICD DPOICD	547
Solution of a Triangular System of Equations with a Single Right-Hand Side	STRSV <sup>♣</sup> CTRSV <sup>♣</sup> STPSV <sup>♣</sup> CTPSV <sup>♣</sup>	DTRSV <sup>♣</sup> ZTRSV <sup>♣</sup> DTPSV <sup>♣</sup> ZTPSV <sup>♣</sup>	557
Solution of Triangular Systems of Equations with Multiple Right-Hand Sides	STRSM <sup>♣</sup> CTRSM <sup>♣</sup>	DTRSM <sup>♣</sup> ZTRSM <sup>♣</sup>	563
Triangular Matrix Inverse	STRTRI <sup>△</sup> CTRTRI <sup>△</sup> STPTRI <sup>△</sup> CTPTRI <sup>△</sup> STRI <sup>§</sup> STPI <sup>§</sup>	DTRTRI <sup>△</sup> ZTRTRI <sup>△</sup> DTPTRI <sup>△</sup> ZTPTRI <sup>△</sup> DTRI <sup>§</sup> DTPI <sup>§</sup>	570
<sup>♣</sup> Level 2 BLAS <sup>♣</sup> Level 3 BLAS <sup>△</sup> LAPACK <sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.			

## Banded Linear Algebraic Equations

The banded linear algebraic equation subroutines provide solutions to linear systems of equations for real general band matrices, real positive definite symmetric band matrices, real or complex general tridiagonal matrices, real positive definite symmetric tridiagonal matrices, and real or complex triangular band matrices.

Table 14. List of Banded Linear Algebraic Equation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
General Band Matrix Factorization	SGBF	DGBF	579
General Band Matrix Solve	SGBS	DGBS	583
Positive Definite Symmetric Band Matrix Factorization	SPBF SPBCHF	DPBF DPBCHF	586

Table 14. List of Banded Linear Algebraic Equation Subroutines (continued)

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Positive Definite Symmetric Band Matrix Solve	SPBS SPBCHS	DPBS DPBCHS	590
General Tridiagonal Matrix Factorization	SGTF	DGTF	593
General Tridiagonal Matrix Solve	SGTS	DGTS	596
General Tridiagonal Matrix Combined Factorization and Solve with No Pivoting	SGTNP CGTNP	DGTNP ZGTNP	598
General Tridiagonal Matrix Factorization with No Pivoting	SGTNPF CGTNPF	DGTNPF ZGTNPF	601
General Tridiagonal Matrix Solve with No Pivoting	SGTNPS CGTNPS	DGTNPS ZGTNPS	604
Positive Definite Symmetric Tridiagonal Matrix Factorization	SPTF	DPTF	607
Positive Definite Symmetric Tridiagonal Matrix Solve	SPTS	DPTS	609
Triangular Band Equation Solve	STBSV <sup>†</sup> CTBSV <sup>†</sup>	DTBSV <sup>†</sup> ZTBSV <sup>†</sup>	611
<sup>†</sup> Level 2 BLAS			

## Sparse Linear Algebraic Equations

The sparse linear algebraic equation subroutines provide direct and iterative solutions to linear systems of equations both for general sparse matrices and their transposes and for sparse symmetric matrices.

Table 15. List of Sparse Linear Algebraic Equation Subroutines

Descriptive Name	Long- Precision Subroutine	Page
General Sparse Matrix Factorization Using Storage by Indices, Rows, or Columns	DGSF	617
General Sparse Matrix or Its Transpose Solve Using Storage by Indices, Rows, or Columns	DGSS	623
General Sparse Matrix or Its Transpose Factorization, Determinant, and Solve Using Skyline Storage Mode	DGKFS DGKFSP <sup>§</sup>	627
Symmetric Sparse Matrix Factorization, Determinant, and Solve Using Skyline Storage Mode	DSKFS DSKFSP <sup>§</sup>	644
Iterative Linear System Solver for a General or Symmetric Sparse Matrix Stored by Rows	DSRIS	662
Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Matrix Storage Mode	DSMCG <sup>‡</sup>	673
Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Diagonal Storage Mode	DSDCG	681
General Sparse Matrix Iterative Solve Using Compressed-Matrix Storage Mode	DSMGCG <sup>‡</sup>	689
General Sparse Matrix Iterative Solve Using Compressed-Diagonal Storage Mode	DSDGCG	696
<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.		
<sup>‡</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Use DSRIS instead.		

## Linear Least Squares

The linear least squares subroutines provide least squares solutions to linear systems of equations for real general matrices. Three methods are provided: one that uses the singular value decomposition; one that uses a QR decomposition with column pivoting; and another that uses a QR decomposition without column pivoting. Some of these subroutines correspond to the LAPACK routines described in reference [8].

Table 16. List of Linear Least Squares Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Singular Value Decomposition for a General Matrix	SGESVF	DGESVF	704
Linear Least Squares Solution for a General Matrix Using the Singular Value Decomposition	SGESVS	DGESVS	712
General Matrix QR Factorization		DGEQRF <sup>△</sup>	717
Linear Least Squares Solution for a General Matrix		DGELS <sup>△</sup>	721
Linear Least Squares Solution for a General Matrix with Column Pivoting	SGELLS	DGELLS	728
<sup>△</sup> LAPACK			

## Eigensystem Analysis

The eigensystem analysis subroutines provide solutions to the algebraic eigensystem analysis problem  $Az = wz$  and the generalized eigensystem analysis problem  $Az = wBz$  (Table 17). Many of the eigensystem analysis subroutines use the algorithms presented in *Linear Algebra* by Wilkinson and Reinsch [103] or use adaptations of EISPACK routines, as described in the *EISPACK Guide Lecture Notes in Computer Science* in reference [91] or in the *EISPACK Guide Extension Lecture Notes in Computer Science* in reference [60]. (EISPACK is available from the sources listed in reference [51].)

Table 17. List of Eigensystem Analysis Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Eigenvalues and, Optionally, All or Selected Eigenvectors of a General Matrix	SGEEV <sup>‡</sup> CGEEV <sup>‡</sup>	DGEEV <sup>‡</sup> ZGEEV <sup>‡</sup>	737
Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix	SSPEV <sup>‡</sup> CHPEV <sup>‡</sup>	DSPEV <sup>‡</sup> ZHPEV <sup>‡</sup>	748
Extreme Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix	SSPSV <sup>‡</sup> CHPSV <sup>‡</sup>	DSPSV <sup>‡</sup> ZHPSV <sup>‡</sup>	757
Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Eigensystem, $Az=wBz$ , where A and B Are Real General Matrices	SGEGV <sup>‡</sup>	DGEGV <sup>‡</sup>	764
Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Symmetric Eigensystem, $Az=wBz$ , where A Is Real Symmetric and B Is Real Symmetric Positive Definite	SSYGV <sup>‡</sup>	DSYGV <sup>‡</sup>	770
<sup>‡</sup> Not LAPACK. Although this subroutine has the same name as an existing LAPACK subroutine, its calling-sequence arguments and functionality are different from that LAPACK subroutine.			

## Fourier Transforms, Convolutions and Correlations, and Related Computations

This signal processing area provides:

- Fourier transform subroutines (Table 18)
- Convolution and correlation subroutines (Table 19)
- Related-computation subroutines (Table 20)

### Fourier Transforms

The Fourier transform subroutines perform mixed-radix transforms in one, two, and three dimensions.

Table 18. List of Fourier Transform Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Complex Fourier Transform	SCFT SCFTP <sup>§</sup>	DCFT	787
Real-to-Complex Fourier Transform	SRCFT	DRCFT	796
Complex-to-Real Fourier Transform	SCRFT	DCRFT	804
Cosine Transform	SCOSF SCOSFT <sup>§</sup>	DCOSF	812
Sine Transform	SSINF	DSINF	820
Complex Fourier Transform in Two Dimensions	SCFT2 SCFT2P <sup>§</sup>	DCFT2	828
Real-to-Complex Fourier Transform in Two Dimensions	SRCFT2	DRCFT2	835
Complex-to-Real Fourier Transform in Two Dimensions	SCRFT2	DCRFT2	842
Complex Fourier Transform in Three Dimensions	SCFT3 SCFT3P <sup>§</sup>	DCFT3	850
Real-to-Complex Fourier Transform in Three Dimensions	SRCFT3	DRCFT3	856
Complex-to-Real Fourier Transform in Three Dimensions	SCRFT3	DCRFT3	862

<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.

### Convolutions and Correlations

The convolution and correlation subroutines provide the choice of using Fourier methods or direct methods. The Fourier-method subroutines contain a high-performance mixed-radix capability. There are also several direct-method subroutines that provide decimated output.

Table 19. List of Convolution and Correlation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Convolution or Correlation of One Sequence with One or More Sequences	SCON <sup>§</sup> SCOR <sup>§</sup>		869
Convolution or Correlation of One Sequence with Another Sequence Using a Direct Method	SCOND SCORD		875
Convolution or Correlation of One Sequence with One or More Sequences Using the Mixed-Radix Fourier Method	SCONF SCORF		881
Convolution or Correlation with Decimated Output Using a Direct Method	SDCON SDCOR	DDCON DDCOR	891

Table 19. List of Convolution and Correlation Subroutines (continued)

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Autocorrelation of One or More Sequences	SACOR <sup>§</sup>		896
Autocorrelation of One or More Sequences Using the Mixed-Radix Fourier Method	SACORF		900

<sup>§</sup> These subroutines are provided only for migration from earlier releases of ESSL and are not intended for use in new programs.

## Related Computations

The related-computation subroutines consist of a group of computations that can be used in general signal processing applications. They are similar to those provided on the IBM 3838 Array Processor; however, the ESSL subroutines generally solve a wider range of problems.

Table 20. List of Related-Computation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Polynomial Evaluation	SPOLY	DPOLY	907
I-th Zero Crossing	SIZC	DIZC	910
Time-Varying Recursive Filter	STREC	DTREC	913
Quadratic Interpolation	SQINT	DQINT	916
Wiener-Levinson Filter Coefficients	SWLEV CWLEV	DWLEV ZWLEV	920

## Sorting and Searching

The sorting and searching subroutines operate on three types of data: integer, short-precision real, and long-precision real (Table 21). The sorting subroutines perform sorts with or without index designations. The searching subroutines perform either a binary or sequential search.

Table 21. List of Sorting and Searching Subroutines

Descriptive Name	Integer Subroutine	Short- Precision Subroutine	Long- Precision Subroutine	Page
Sort the Elements of a Sequence	ISORT	SSORT	DSORT	927
Sort the Elements of a Sequence and Note the Original Element Positions	ISORTX	SSORTX	DSORTX	929
Sort the Elements of a Sequence Using a Stable Sort and Note the Original Element Positions	ISORTS	SSORTS	DSORTS	932
Binary Search for Elements of a Sequence X in a Sorted Sequence Y	IBSRCH	SBSRCH	DBSRCH	936
Sequential Search for Elements of a Sequence X in the Sequence Y	ISSRCH	SSSRCH	DSSRCH	940

## Interpolation

The interpolation subroutines provide the capabilities of doing polynomial interpolation, local polynomial interpolation, and both one- and two-dimensional cubic spline interpolation (Table 22).



Table 22. List of Interpolation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Polynomial Interpolation	SPINT	DPINT	947
Local Polynomial Interpolation	STPINT	DTPINT	952
Cubic Spline Interpolation	SCSINT	DCSINT	955
Two-Dimensional Cubic Spline Interpolation	SCSIN2	DCSIN2	961

## Numerical Quadrature

The numerical quadrature subroutines provide Gaussian quadrature methods for integrating a tabulated function and a user-supplied function over a finite, semi-infinite, or infinite region of integration (Table 23).

Table 23. List of Numerical Quadrature Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Numerical Quadrature Performed on a Set of Points	SPTNQ	DPTNQ	969
Numerical Quadrature Performed on a Function Using Gauss-Legendre Quadrature	SGLNQ <sup>†</sup>	DGLNQ <sup>†</sup>	972
Numerical Quadrature Performed on a Function Over a Rectangle Using Two-Dimensional Gauss-Legendre Quadrature	SGLNQ2 <sup>†</sup>	DGLNQ2 <sup>†</sup>	975
Numerical Quadrature Performed on a Function Using Gauss-Laguerre Quadrature	SGLGQ <sup>†</sup>	DGLGQ <sup>†</sup>	981
Numerical Quadrature Performed on a Function Using Gauss-Rational Quadrature	SGRAQ <sup>†</sup>	DGRAQ <sup>†</sup>	984
Numerical Quadrature Performed on a Function Using Gauss-Hermite Quadrature	SGHMQ <sup>†</sup>	DGHMQ <sup>†</sup>	988

<sup>†</sup> This subprogram is invoked as a function in a Fortran program.

## Random Number Generation

Random number generation subroutines generate uniformly distributed random numbers or normally distributed random numbers (Table 24).

Table 24. List of Random Number Generation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Generate a Vector of Uniformly Distributed Random Numbers	SURAND	DURAND	993
Generate a Vector of Normally Distributed Random Numbers	SNRAND	DNRAND	996
Generate a Vector of Long Period Uniformly Distributed Random Numbers	SURXOR	DURXOR	1000

## Utilities

The utility subroutines perform general service functions that support ESSL, rather than mathematical computations (Table 25).

Table 25. List of Utility Subroutines

Descriptive Name	Subroutine	Page
ESSL Error Information-Handler Subroutine	EINFO	1008
ESSL ERRSAV Subroutine	ERRSAV	1011
ESSL ERRSET Subroutine	ERRSET	1012
ESSL ERRSTR Subroutine	ERRSTR	1014
Set the Vector Section Size (VSS) for the ESSL/370 Scalar Library	IVSSET <sup>§</sup>	
Set the Extended Vector Operations Indicator for the ESSL/370 Scalar Library	IEVOPS <sup>§</sup>	
Determine the Level of ESSL Installed	IESSL	1015
Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines	STRIDE	1017
Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode	DSRSM	1026
For a General Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode	DGKTRN	1030
For a Symmetric Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode	DSKTRN	1035
<sup>§</sup> This subroutine is provided for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.		

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## Chapter 2. Planning Your Program

This chapter provides information about ESSL that you need when planning your program. Its purpose is to help you in performing the following tasks:

- “Selecting an ESSL Subroutine”
- “Avoiding Conflicts with Internal ESSL Routine Names That are Exported” on page 32
- “Setting Up Your Data” on page 33
- “Setting Up Your ESSL Calling Sequences” on page 34
- “Using Auxiliary Storage in ESSL” on page 36
- “Providing a Correct Transform Length to ESSL” on page 42
- “Getting the Best Accuracy” on page 47
- “Getting the Best Performance” on page 49
- “Dealing with Errors when Using ESSL” on page 50

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### Selecting an ESSL Subroutine

Your choice of which ESSL subroutine to use is based mainly on the functional needs of your program. However, you have a choice of several variations of many of the subroutines. In addition, there are instances where certain subroutines cannot be used. This section describes these variations and limitations. See the answers to each question below that applies to you.

#### Which ESSL Library Do You Want to Use?

ESSL provides the run-time libraries described in the following sections:

- “ESSL SMP Library”
- “ESSL Serial Library” on page 28
- “ESSL Blue Gene Library” on page 28

For additional details about using these libraries, see Chapter 4, “Coding Your Program,” on page 111 and Chapter 5, “Processing Your Program,” on page 163.

#### ESSL SMP Library

This library provides thread-safe versions of the ESSL subroutines for use on all SMP processors. In addition, a subset of these subroutines are also multithreaded versions; that is, they support the shared memory parallel processing programming model.

The number of threads you choose to use depends on the problem size, the specific subroutine being called, and the number of physical processors you are running on. To achieve optimal performance, experimentation is necessary; however, picking the number of threads equal to the number of online processors generally provides good performance in most cases. In a few cases, performance may increase if you choose the number of threads to be less than the number of online processors. For more information about thread concepts, see *AIX General Programming Concepts: Writing and Debugging Programs* and reference [87].

You do not have to change your existing application programs that call ESSL to take advantage of the increased performance of using the SMP processors; you can simply re-link your existing application programs.

The multithreaded subroutines in the ESSL SMP Library are listed in Table 26.

**Note:** The ESSL SMP Library supports both 32-bit environment and 64-bit environment applications.

*Table 26. Multithreaded ESSL SMP Subroutines*

Subroutine Names
Vector-Scalar Linear Algebra Subprograms:  SASUM, DASUM, SCASUM, DZASUM SAXPY, DAXPY, CAXPY, ZAXPY SCOPY, DCOPY, CCOPY, ZCOPY SDOT, DDOT, CDOTU, ZDOTU, CDOTC, ZDOTC SNDOT, DNDOT SNORM2, DNORM2, CNORM2, ZNORM2 SROT, DROT, CROT, ZROT, CSROT, ZDROT SSCAL, DSCAL, CSCAL, ZSCAL, CSSCAL, ZDSCAL SSWAP, DSWAP, CSWAP, ZSWAP SVEA, DVEA, CVEA, ZVEA SVES, DVES, CVES, ZVES SVEM, DVEM, CVEM, ZVEM SYAX, DYAX, CYAX, ZYAX, CSYAX, ZDYAX SZAXPY, DZAXPY, CZAXPY, ZZAXPY
Matrix-Vector Linear Algebra Subprograms:  SGEMV, DGEMV, CGEMV, ZGEMV SGER, DGER, CGERU, ZGERU, CGERC, ZGERC SSPMV, DSPMV, CHPMV, ZHPMV SSYMV, DSYMV, CHEMV, ZHEMV SSPR, DSPR, CHPR, ZHPR SSYR, DSYR, CHER, ZHER SSPR2, DSPR2, CHPR2, ZHPR2 SSYR2, DSYR2, CHER2, ZHER2 SGBMV*, DGBMV* CGBMV*, ZGBMV* SSBMV*, DSBMV* CHBMV*, ZHBMV* STRMV, DTRMV, CTRMV, ZTRMV STPMV, DTPMV, CTPMV, ZTPMV STBMV*, DTBMV* CTBMV*, ZTBMV*
Matrix Operations:  SGEADD, DGEADD, CGEADD, ZGEADD SGESUB, DGESUB, CGESUB, ZGESUB SGEMUL, DGEMUL, CGEMUL, ZGEMUL SGEMM, DGEMM, CGEMM, ZGEMM SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, ZHEMM STRMM, DTRMM, CTRMM, ZTRMM SSYRK, DSYRK, CSYRK, ZSYRK, CHERK, ZHERK SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, ZHER2K SGETMI, DGETMI, CGETMI, ZGETMI SGETMO, DGETMO, CGETMO, ZGETMO

Table 26. Multithreaded ESSL SMP Subroutines (continued)

Subroutine Names
<p>Dense Linear Algebraic Equations:</p> <p>SGESV, DGESV, CGESV, ZGESV            SGEF, DGEF, CGEF, ZGEF            SGES, DGES, CGES, ZGES            SGETRF, DGETRF, CGETRF, ZGETRF            SGETRS, DGETRS, CGETRS, ZGETRS            SPPSV, DPPSV, CPPSV, ZPPSV            SPPE, DPPE, SPPTRE, DPPTRE, CPPTRE, ZPPTRE, DPOE, DPOTRF            SPPTRS, DPPTRS, CPPTRS, ZPPTRS            SPOSV, DPOSV, CPOSV, ZPOSV            SPOSM, DPOSM, CPOSM, ZPOSM            SPPFCD*, DPPFCD*, DPOFCD*            SPPTRI, DPPTRI, SPPICD*, DPPICD*, DPOICD*            STRSV, DTRSV, CTRSV, ZTRSV            STPSV, DTPSV, CTPSV, ZTPSV            STRSM, DTRSM, CTRSM, ZTRSM            STRI, DTRI, STRTRI, DTRTRI, CTRTRI, ZTRTRI</p>
<p>Sparse Linear Algebraic Equations:</p> <p>DSRIS<sup>†</sup></p>
<p>Linear Least Squares:</p> <p>DGEQRF</p>
<p>Fourier Transforms:</p> <p>SCFT, DCFT            SRCFT, DRCFT            SCRFT, DCRFT            SCFT2, DCFT2            SRCFT2, DRCFT2            SCRFT2, DCRFT2            SCFT3, DCFT3            SRCFT3, DRCFT3            SCRFT3, DCRFT3</p>
<p>Convolution and Correlation:</p> <p>SCOND, SCORD            SDCON, SDCOR, DDCON, DDCOR</p>

1

Table 26. Multithreaded ESSL SMP Subroutines (continued)

Subroutine Names	
<p>Many of the dense linear algebraic equations and eigensystem analysis subroutines make one or more calls to the multithreaded versions of the matrix-vector linear algebra and matrix operation subroutines shown in this table. These subroutines benefit from the increased performance of the multithreaded versions of the ESSL SMP subroutines.</p> <p>Your performance may be improved by setting the Environment variables:</p>	
<b>ESSL for AIX</b>	export MALLOCMULTIHEAP=true
	—and—
	export XLSMPOPTS="spins=0:yields=0"
<b>ESSL for Linux</b>	export XLSMPOPTS="spins=0:yields=0"
<p>For additional information, see the <i>AIX Performance Management Guide</i> and the XLF Manuals.</p> <p>† DSRIS only uses multiple threads when <math>IPARM(4) = 1</math> or <math>2</math>.</p> <p>• The Level 2 Banded BLAS use multiple threads only when the bandwidth is sufficiently large.</p> <p>* Multiple threads are used for the factor or inverse computation.</p>	

### ESSL Serial Library

This library provides thread-safe versions of the ESSL subroutines for use on all processors. You may choose to use this library if you decide to develop your own multithreaded programs that call the thread-safe ESSL subroutines.

**Note:** The ESSL Serial Library supports both 32-bit environment and 64-bit environment applications.

### ESSL Blue Gene Library

This library provides 32-bit versions of the ESSL subroutines for use on Blue Gene.

The Blue Gene custom chip contains two standard 32-bit embedded PowerPC 440 cores. Each core has a double floating-point unit (FPU) that can perform four double-precision floating-point operations per cycle. This custom FPU consists of two conventional FPUs joined together, each of which has a 64-bit register file with 32 registers. The PowerPC instruction set has been extended to perform SIMD floating-point operations on the two FPUs and allows for two double-precision values to be loaded or stored in parallel in a single cycle, provided that the address is aligned such that it does not cross a cache-line boundary (which is 32 bytes).

A subset of the ESSL Blue Gene Library subroutines use SIMD algorithms that utilize the PowerPC 440 dual FPUs. These SIMD algorithms need to use the load and store quadword instructions to effectively utilize the dual FPUs. Alignment requirements for the SIMD algorithms are described in Table 27 on page 29 and Table 28 on page 29.

Table 27. Alignment Requirements for SIMD Algorithms in Linear Algebra Subroutines

Data Type	Vector and Matrix Alignment	Vector Stride	Leading Dimensions
Long-precision real	Quadword and doubleword	Varies depending on the type of subroutine: <b>1</b> For vector-scalar linear algebra subroutines <b>Any</b> For matrix-vector linear algebra subprograms	Any
Short-precision real	Doubleword and singleword	Varies depending on the type of subroutine: <b>1</b> For vector-scalar linear algebra subroutines <b>Any</b> For matrix-vector linear algebra subprograms	Any
Long-precision complex	Quadword	Any	Any
Short-precision complex	Doubleword	Any	Any

**Notes:**

- As long as the alignment requirements described in this table are met, you do not have to change your existing application programs that call ESSL to take advantage of the increased performance produced by the SIMD subroutines. However, you will obtain optimal performance for these subroutines when the following additional conditions are met:
  - Long-precision real vectors and matrices are quadword aligned.
  - Short-precision real vectors and matrices are doubleword aligned.
  - LDAs are even for real matrices.
  - Stride is 1 for real vectors.
- If the alignment restrictions in this table are not met, in some cases attention message 2610 will be issued. The default behavior for message 2610 is for the message to be suppressed. To change the default behavior, see “ERRSET — ESSL ERRSET Subroutine” on page 1012.

Table 28. Alignment Requirements for SIMD Algorithms in Fourier Transform Subroutines and Convolution and Correlation Subroutines

Data Type	Vector and Matrix Alignment	Stride Between Elements Within Sequence	Stride Between Sequences
Long-precision real (see Note 1)	Quadword	1 (see Note 2)	Even (see Note 2)
Short-precision real	Doubleword	1 (see Note 2)	Even (see Note 2)
Long-precision complex	Quadword	Any	Any
Short-precision complex	Doubleword	Any	Any

Table 28. Alignment Requirements for SIMD Algorithms in Fourier Transform Subroutines and Convolution and Correlation Subroutines (continued)

Data Type	Vector and Matrix Alignment	Stride Between Elements Within Sequence	Stride Between Sequences
<p><b>Notes:</b></p> <ol style="list-style-type: none"> <li>In addition, AUX and AUX2 must either be aligned on a quadword boundary or dynamically allocated.</li> <li>For <code>_COSF</code> and <code>_SINE</code>, the stride between elements within a sequence and the stride between sequences can have any value.</li> <li>As long as the alignment requirements described in this table are met, you do not have to change your existing application programs that call ESSL to take advantage of the increased performance produced by the SIMD subroutines. However, some subroutines require separate calls for initialization and computation, and it can occur that the alignment of an array meets the requirements during initialization but does not meet the requirements during computation. When this happens, in some cases error 2152 will be issued and your program will terminate. If you want your program to continue processing, use <code>ERRSET</code> with an ESSL error exit routine, <code>ENOTRM</code>, to make error 2152 recoverable.</li> <li>If the alignment restrictions in this table are not met, in some cases one or both of the following attention messages will be issued: <ul style="list-style-type: none"> <li>2610</li> <li>2611</li> </ul>                     The default behavior for these messages is for the message to be suppressed. To change the default behavior, see “<code>ERRSET — ESSL ERRSET Subroutine</code>” on page 1012.                 </li> </ol>			

See Table 29 for a list of the ESSL Blue Gene Library subroutines that automatically use SIMD algorithms when the appropriate alignment requirements (as described in Table 27 on page 29 and Table 28 on page 29) are met.

**Note:** The ESSL Blue Gene Library supports only 32-bit environment applications.

Table 29. Blue Gene ESSL SIMD Subroutines

Subroutine Names
Vector-Scalar Linear Algebra Subprograms:  ISAMAX, IDAMAX, ICAMAX, IZAMAX ISAMIN, IDAMIN ISMAX, IDMAX ISMIN, IDMIN SASUM, DASUM, SCASUM, DZASUM SAXPY, DAXPY, CAXPY, ZAXPY SCOPY, DCOPY, CCOPY, ZCOPY SDOT, DDOT, CDOTU, ZDOTU, CDOTC, ZDOTC SNRM2, DNRM2, SCNRM2, DZNRM2 SNORM2, DNORM2, CNORM2, ZNORM2 SROT, DROT, CROT, ZROT, CSROT, ZDROT SSCAL, DSCAL, CSCAL, ZSCAL, CSSCAL, ZDSCAL SSWAP, DSWAP, CSWAP, ZSWAP SVEA, DVEA, CVEA, ZVEA SVES, DVES, CVES, ZVES SVEM, DVEM, CVEM, ZVEM SYAX, DYAX, CYAX, ZYAX, CSYAX, ZDYAX SZAXPY, DZAXPY, CZAXPY, ZZAXPY



Table 29. Blue Gene ESSL SIMD Subroutines (continued)

Subroutine Names
<p>Matrix-Vector Linear Algebra Subprograms:</p> <p>SGEMV, DGEMV, CGEMV, ZGEMV            SGER, DGER, CGERU, ZGERU, CGERC, ZGERC            SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, ZHEMV            SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, ZHER            SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, ZHER2            STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, ZTPMV</p>
<p>Matrix Operations:</p> <p>SGEADD, DGEADD, CGEADD, ZGEADD            SGESUB, DGESUB, CGESUB, ZGESUB            SGEMUL, DGEMUL, CGEMUL, ZGEMUL            SGEMM, DGEMM, CGEMM, ZGEMM            SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, ZHEMM            STRMM, DTRMM, CTRMM, ZTRMM            SSYRK, DSYRK, CSYRK, ZSYRK, CHERK, ZHERK            SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, ZHER2K            SGETMI, DGETMI, CGETMI, ZGETMI            SGETMO, DGETMO, CGETMO, ZGETMO</p>
<p>Dense Linear Algebraic Equations:</p> <p>STRSV, DTRSV, CTRSV, ZTRSV, STPSV, DTPSV, CTPSV, ZTPSV            STRSM, DTRSM, CTRSM, ZTRSM</p>
<p>Fourier Transforms:</p> <p>SCFT, DCFT            SRCFT, DRCFT            SCRFT, DCRFT            SCOSF, DCOSF            SSINF, DSINF            SCFT2, DCFT2            SRCFT2, DRCFT2            SCRFT2, DCRFT2            SCFT3, DCFT3            SRCFT3, DRCFT3            SCRFT3, DCRFT3</p>
<p>Convolutions and Correlations:</p> <p>SCOND, SCORD            SCONE, SCORF            SDCON, SDCOR, DDCON, DDCOR            SACORF</p>
<p><b>Note:</b> Many of the dense linear algebraic equations and eigensystem analysis subroutines make one or more calls to the SIMD versions of the matrix-vector linear algebra and matrix operation subroutines shown in this table. These subroutines benefit from the increased performance of the SIMD versions of the ESSL Blue Gene Library subroutines.</p>

## What Type of Data Are You Processing in Your Program?

The version of the ESSL subroutine you select should agree with the data you are using. ESSL provides a short- and long-precision version of most of its subroutines processing short- and long-precision data, respectively. In a few cases, it also

provides an integer version processing integer data or returning just integer data. The subroutine names are distinguished by a one- or two-letter prefix based on the following letters:

S for short-precision real  
D for long-precision real  
C for short-precision complex  
Z for long-precision complex  
I for integer

The precision of your data affects the accuracy of your results. This is discussed in “Getting the Best Accuracy” on page 47. For a description of these data types, see “How Do You Set Up Your Scalar Data?” on page 33.

## How Is Your Data Structured? And What Storage Technique Are You Using?

Some subroutines process specific data structures, such as sparse vectors and matrices or dense and banded matrices. In addition, these data structures can be stored using various storage techniques. You should select the proper subroutine on the basis of the type of data structure you have and the storage technique you want to use. If possible, you should use a storage technique that conserves storage and potentially improves performance. For more about storage techniques, see “Setting Up Your Data” on page 33.

## What about Performance and Accuracy?

ESSL provides variations among some of its subroutines. You should consider performance and accuracy when deciding which subroutine is the best to use. Study the “Function” section in each subroutine description. It helps you understand exactly what each subroutine does, and helps you determine which subroutine is best for you. For example, some subroutines perform multiple computations of a certain type. This might give you better performance than a subroutine that does each computation individually. In other cases, one subroutine may do scaling while another does not. If scaling is not necessary for your data, you get better performance by using the subroutine without scaling.

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## Avoiding Conflicts with Internal ESSL Routine Names That are Exported

Do not use names for your own subroutines, functions, and global variables that are the same as the ESSL exported names. The following list explains how to avoid using these names, depending on the type of ESSL library you are using:

### ESSL shared libraries

For the ESSL shared libraries, all internal ESSL routine names that are exported begin with the **ESV** prefix, so you should avoid using this prefix for your own names.

### ESSL Blue Gene static library

For the ESSL Blue Gene static library, the internal ESSL routine names can begin with any prefix, not just the **ESV** prefix. Therefore, it is not sufficient for you to avoid using only this prefix for your own names; you must check each of your names individually to make sure that it is not the same as an ESSL Blue Gene routine name.

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## Setting Up Your Data

This section explains how to set up your scalar and array data and points you to where you can find more detail.

### How Do You Set Up Your Scalar Data?

A scalar item is a single item of data, whether it is a constant, a variable, or an element of an array. ESSL assumes that your scalar data conforms to the appropriate standards, as described below. The scalar data types and how you should code them for each programming language are listed under “Coding Your Scalar Data” in each language section in Chapter 4, “Coding Your Program,” on page 111.

#### Internal Representation

Scalar data passed to ESSL from all types of programs, including Fortran, C, and C++, should conform to the ANSI/IEEE 32-bit and 64-bit binary floating-point format, as described in the *ANSI/IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Standard 754–1985*.

### How Do You Set Up Your Arrays?

An array represents an area of storage in your program, containing data stored in a series of locations. An array has a single name. It is made up of one or more pieces of scalar data, all the same type. These are the elements of the array. It can be passed to the ESSL subroutine as input, returned to your program as output, or used for both input and output, in which case the original contents are overwritten.

Arrays can contain conceptual (mathematical) data structures, such as vectors, matrices, or sequences. There are many different types of data structures. Each type of data structure requires a unique arrangement of data in an array and does not necessarily have to include all the elements of the array. In addition, the elements of these data structures are not always contiguous in storage within an array. Stride and leading dimension arguments passed to ESSL subroutines define the separations in array storage for the elements of the vector, matrix, and sequence. All these aspects of data structures are described in Chapter 3, “Setting Up Your Data Structures,” on page 59. You must first understand array storage techniques to fully understand the concepts of data structures, stride, and leading dimension, especially if you are using them in unconventional ways.

ESSL subroutines assume that all arrays passed to them are stored using the Fortran array storage techniques (in column-major order), and they process your data accordingly. For details, see “Setting Up Arrays in Fortran” on page 112. On the other hand, C, and C++ programs store arrays in row-major order. For details on what you can do, see:

- For C, see page “Setting Up Arrays in C” on page 133.
- For C++, see page “Setting Up Arrays in C++” on page 150.

### How Should Your Array Data Be Aligned?

The following list explains how to align your array data for optimal performance, depending on the type of ESSL library you are using:

#### ESSL Serial and SMP libraries

All arrays, regardless of the type of data, should be aligned on a doubleword boundary to ensure optimal performance. For

information about how your programming language aligns data, see your programming language manuals.

#### **ESSL Blue Gene library**

See Table 27 on page 29.

## **What Storage Mode Should You Use for Your Data?**

The amount of storage used by arrays and the storage arrangement of data in the arrays can affect overall program performance. As a result, ESSL provides subroutines that operate on different types of data structures, stored using various storage modes. You should choose a storage mode that conserves storage and potentially improves performance. For definitions of the various data structures and their corresponding storage modes, see Chapter 3, “Setting Up Your Data Structures,” on page 59. You can also find special storage considerations, where applicable, in the “Notes” section of each subroutine description.

## **How Do You Convert from One Storage Mode to Another?**

This section describes how you can convert from one storage mode to another.

### **Conversion Subroutines**

ESSL provides several subroutines that help you convert from one storage mode to another:

- DSRSM is used to migrate your existing program from sparse matrices stored by rows to sparse matrices stored in compressed-matrix storage mode. This converts the matrices into a storage format that is compatible with the input requirements for some ESSL sparse matrix subroutines, such as DSMMX.
- DGKTRN and DSKTRN are used to convert your sparse matrix from one skyline storage mode to another, if necessary, before calling the subroutines DGKFS/DGKFSP or DSKFS/DSKFSP, respectively.

### **Sample Programs**

In addition, sample programs are provided with many of the storage mode descriptions in Chapter 3, “Setting Up Your Data Structures,” on page 59. You can use these sample programs to convert your data to the desired storage mode by adapting them to your application program.

---

## **Setting Up Your ESSL Calling Sequences**

This section gives the general rules for setting up the ESSL calling sequences. The information given here applies to all types of programs, running in all environments. For a description and examples of how to code the ESSL calling sequences in your particular programming language, see the following sections:

- “Fortran Programs” on page 111
- “C Programs” on page 129
- “C++ Programs” on page 145

For details on the conventions used in this book to describe the calling sequence syntax, see “How to Interpret the Subroutine Descriptions” on page xix. It describes how required and optional arguments are indicated in the calling sequence and the naming conventions used for different data types.

## What Is an Input-Output Argument?

Some arguments are used for both input and output. The contents of the input argument are overlaid with the output value(s) on return to your program. Be careful that you save any data you need to preserve before calling the ESSL subroutine.

## What Are the General Rules to Follow when Specifying Data for the Arguments?

You should follow the syntax rules given for each argument in “On Entry” in the subroutine description. Input-argument error messages may be issued, and your program may terminate when you make an error specifying the input arguments. For example:

- Data passed to ESSL must be of the correct type: integer, character, real, complex, short-precision, or long-precision. There is no conversion of data. Assuming you are using the ESSL header file with your C and C++ programs, you first need to define the following:
  - Complex and logical data in C programs, using the guidelines given on page 132.
  - Short-precision complex and logical data in C++ programs, using the guidelines given on page 148.
- Character values must be one of the specified values. For example, it may have to be 'N', 'T', or 'C'.
- Numeric values must fall within the correct range for that argument. For example, a numeric value may need to be greater than or equal to 0, or it may have to be a nonzero value.
- Arrays must be defined correctly; that is, they must have the correct dimensions, or the dimensions must fall within the correct range. For example, input and output matrices may need to be conformable, or the number of rows in the matrix must be less than or equal to the leading dimension specified. (ESSL assumes all arrays are stored in column-major order.)

## What Happens When a Value of 0 Is Specified for N?

For most ESSL subroutines, if you specify 0 for the number of elements to be processed in a vector or the order of a matrix (usually argument  $n$ ), no computation is performed. After checking for input-argument errors, the subroutine returns immediately and no result is returned. In the other subroutines, an error message may be issued.

## How Do You Specify the Beginning of the Data Structure in the ESSL Calling Sequence?

When you specify a vector, matrix, or sequence in your calling sequence, it does not necessarily have to start at the beginning of the array. It can begin at any point in the array. For example, if you want vector  $x$  to start at element 3 in array  $A$ , which is declared  $A(1:12)$ , specify  $A(3)$  in your calling sequence for argument  $x$ , such as in the following SASUM calling sequence in your Fortran program:

```
      N   X   INCX
      |   |   |
X = SASUM( 4 , A(3) , 2 )
```

Also, for example, if you want matrix *A* to start at the second row and third column of array *A*, which is declared `A(0:10,2:8)`, specify `A(1,4)` in your calling sequence for argument *a*, such as in the following SGEADD calling sequence in your Fortran program:

```

      A      LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
      |      |      |      |      |      |      |      |
CALL  SGEADD( A(1,4) , 11 , 'N' , B , 4 , 'N' , C , 4 , 4 , 3 )

```

For more examples of specifying vectors and matrices, see Chapter 3, “Setting Up Your Data Structures,” on page 59.

## Using Auxiliary Storage in ESSL

For the ESSL subroutines listed in Table 30, you need to provide extra working storage to perform the computation. This section describes the use of dynamic allocation for providing auxiliary storage in ESSL and how to calculate the amount of auxiliary storage you need by use of formulas or error-handling capabilities provided in ESSL, if dynamic allocation is not an option.

Auxiliary storage, or working storage, is supplied through one or more arguments, such as *aux*, in the calling sequence for the ESSL subroutine. **If the working storage does not need to persist after the subroutine call, it is suggested you use dynamic allocation.** For example, in the Fourier Transforms subroutines, you may allocate *aux2* dynamically, but not *aux1*. See the subroutine descriptions in Part 2 of this book for details and variations.

Table 30. ESSL Subroutines Requiring Auxiliary Working Storage

Subroutine Names
Linear Algebra Subprograms: DSMTM
Matrix Operations: _GEMMS
Dense Linear Algebraic Equations: _GEFCD _PPFCD _GEICD _PPICD _POFCD _POICD DGEFP <sup>A</sup> DPPFP <sup>A</sup>
Sparse Linear Algebraic Equations: DGSF DGSS DGKFS DGKFSP <sup>A</sup> DSKFS DSKFSP <sup>A</sup> DSRIS DSMCG DSDCG DSMGCG DSDGCG
Linear Least Squares: _GESVF _GELLS
Eigensystem Analysis: _GEEV _SPEV _HPEV _SPSV _HPSV _GEGV _SYGV
Fourier Transforms: _CFT _RCFT _CRFT _COSF _SINF SCOSFT <sup>A</sup> _CFT2 _RCFT2 _CRFT2 _CFT3 _RCFT3 _CRFT3 SCFTP <sup>A</sup> SCFT2P <sup>A</sup> SCFT3P <sup>A</sup>
Convolutions and Correlations: SCONF SCORF SACORF
Related Computations: _WLEV
Interpolation: _TPINT _CSIN2

Table 30. ESSL Subroutines Requiring Auxiliary Working Storage (continued)

<b>Subroutine Names</b>
Random Number Generation: _NRAND
Utilities: DGKTRN DSKTRN
<sup>^</sup> Documentation for this subroutine is no longer provided. The <i>aux</i> and <i>naux</i> arguments for the subroutine are specified the same as for the corresponding serial ESSL subroutine.

## Dynamic Allocation of Auxiliary Storage

Dynamic allocation for the auxiliary storage is performed when error 2015 is unrecoverable and *naux*=0. For details on which *aux* arguments allow dynamic allocation, see the subroutine descriptions in Part 2 of this book.

## Setting Up Auxiliary Storage When Dynamic Allocation Is Not Used

You set up the storage area in your program and pass it to ESSL through arguments, specifying the size of the *aux* work area in the *naux* argument.

## Who Do You Want to Calculate the Size? You or ESSL?

You have a choice of two methods for determining how much auxiliary storage you should specify:

- Use the formulas provided in the subroutine description to derive **sufficient values** for your current and future needs. Use them if **ease of migration** to future machines and future releases of ESSL is your primary concern. For details, see “How Do You Calculate the Size Using the Formulas?”
- Use the ESSL error-handling facilities to return to you a **minimum value** for the particular processor you are currently running on. (Values vary by platform.) Use this approach if **conserving storage** is your primary concern. For details, see “How Do You Get ESSL to Calculate the Size Using ESSL Error Handling?” on page 38.

## How Do You Calculate the Size Using the Formulas?

The formulas provided for calculating *naux* indicate a **sufficient** amount of auxiliary storage required, which, in most cases, is larger than the minimum amount, returned by ESSL error handling. There are two types of formulas:

- **Simple formulas**  
These are given in the *naux* argument syntax descriptions. In general, these formulas result in the minimum required value, but, in a few cases, they provide overestimates.
- **Processor-independent formulas**  
These are given in separate sections in the subroutine description. In general, these provide overestimates.

Both types of formulas provide values that are sufficient for all processors. As a result, you can migrate to any other processor and to future releases of ESSL without being concerned about having to increase the amount of storage for *aux*. You do, of course, need to weigh your storage requirements against the convenience of using this larger value.

To calculate the amount of storage using the formulas, you must substitute values for specific variables, such as  $n$ ,  $m$ ,  $n1$ , or  $n2$ . These variables are arguments specified in the ESSL calling sequence or derived from the arguments in the calling sequence.

## How Do You Get ESSL to Calculate the Size Using ESSL Error Handling?

This section describes how you can get ESSL to calculate auxiliary storage.

### Here Are the Two Ways You Can Do It

Ask yourself which of the following ways you prefer to obtain the information from ESSL:

- **By leaving error 2015 unrecoverable**, you can obtain the minimum required value of  $naux$  from the input-argument error message, but your program terminates.
- **By making error 2015 recoverable**, you can obtain the minimum required value of  $naux$  from the input-argument error message and have the updated  $naux$  argument returned to your program.

For both techniques, the amount returned by the ESSL error-handling facility is the **minimum** amount of auxiliary storage required to run your program successfully **on the particular processor you are currently running on**. The ESSL error-handling capability usually returns a smaller value than you derive by using the formulas listed for the subroutine. This is because the formulas provide a good estimate, but ESSL can calculate exactly what is needed on the basis of your data.

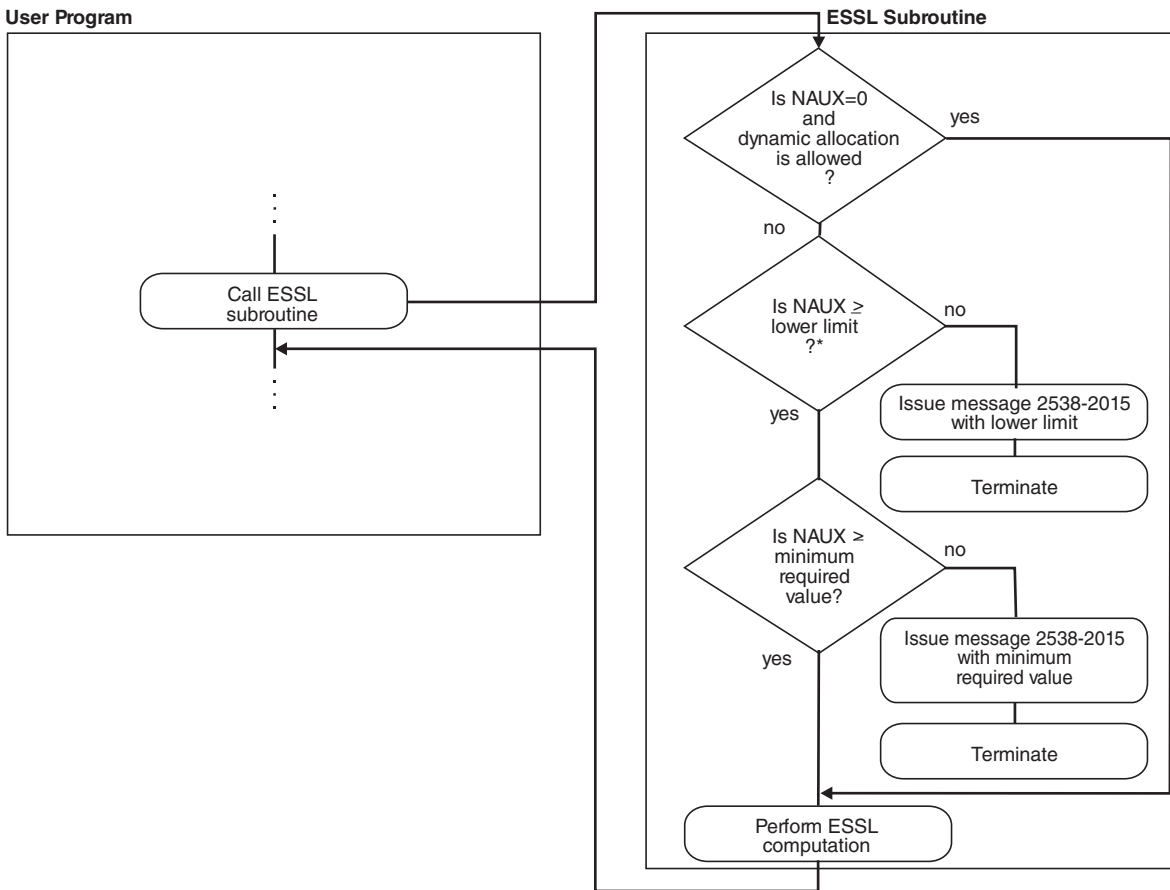
The values returned by ESSL error handling **may not apply to future processors**. You should not use them if you plan to run your program on a future processor. You should use them only if you are concerned with minimizing the amount of auxiliary storage used by your program.

### The First Way

In this case, you obtain the minimum required value of  $naux$  from the error message, but your program terminates. The following description assumes that dynamic allocation is not selected as an option.

Leave error 2015 as unrecoverable, without calls to EINFO and ERRSET. Run your program with the  $naux$  values smaller than required by the subroutine for the particular processor you are running on. As a general guideline, specify values smaller than those listed in the formulas. However, if a lower limit is specified in the syntax (only for several  $naux1$  arguments in the Fourier transform, convolution, and correlation subroutines), you should not go below that limit. The ESSL error monitor returns the necessary sizes of the  $aux$  storage areas in the input-argument error message. This does, however, terminate your program when the error is encountered. (If you accidentally specify a sufficient amount of storage for the ESSL subroutine to perform the computation, error handling does not issue an error message and processing continues normally.) Figure 1 on page 39 illustrates what happens when error 2015 is unrecoverable.





\* This check applies only to several NAUX1 arguments in the Fourier transform, convolution, and correlation subroutines.

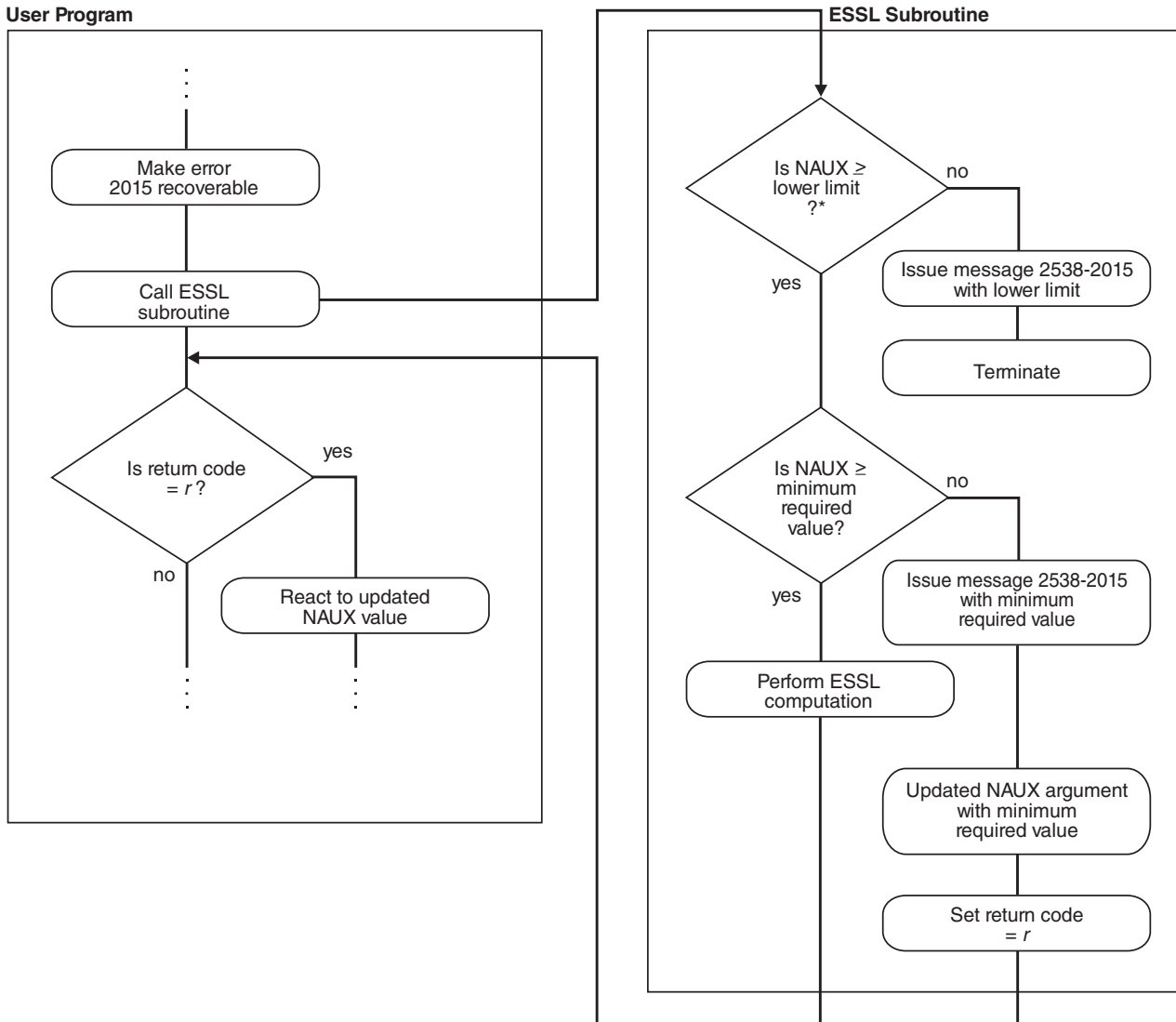
Figure 1. How to Obtain an NAUX Value from an Error Message, but Terminate

## The Second Way

In this case, you obtain the minimum required value of *naux* from the error message and from the updated *naux* argument returned to your program.

Use EINFO and ERRSET with an ESSL error exit routine, ENOTRM, to make error 2015 recoverable. This allows you to dynamically determine in your program the minimum sizes required for the auxiliary working storage areas, specified in the *naux* arguments. Run your program with the *naux* values smaller than required by the subroutine for the particular processor you are running on. As a general guideline, specify values smaller than those listed in the formulas. However, if a lower limit is specified in the syntax (only for several *naux1* arguments in the Fourier transform, convolution, and correlation subroutines), you should not go below that limit. The ESSL error monitor returns the necessary sizes of the *aux* storage areas in the input-argument error message and a return code is passed

back to your program, indicating that updated values are also returned in the *naux* arguments. You can then react to these updated values during run time in your program. ESSL does not perform any computation when this error occurs. For details on how to do this, see Chapter 4, “Coding Your Program,” on page 111. (If you accidentally specify a sufficient amount of storage for the ESSL subroutine to perform the computation, error handling does not issue an error message and processing continues normally.) Figure 2 illustrates what happens when error 2015 is recoverable.



\* This check applies only to several NAUX1 arguments in the Fourier transform, convolution, and correlation subroutines.

Figure 2. How to Obtain an NAUX Value from an Error Message and in Your Program

### Here Is an Example of What Happens When You Use These Two Techniques

The following example illustrates all the actions taken by the ESSL error-handling facility for each possible value of a recoverable input argument, *naux*. A key point here is that if you want to have the updated argument value returned to your

program, you must make error 2015 recoverable and then specify an *naux* value greater than or equal to 20 and less than 300. For values out of that range, the error recovery facility is not in effect. (These values of *naux*, 20 and 300, are used only for the purposes of this example and do not relate to any of the ESSL subroutines.)

### NAUX Meaning of the NAUX Value

- 20 Lower limit of *naux* required for using recoverable input-argument error-handling facilities in ESSL. (This applies only to several *naux1* arguments in the Fourier transform, convolution, and correlation subroutines. You can find the lower limit in the syntax description for the *naux1* argument. For a list of subroutines, see Table 30 on page 36.)
- 300 Minimum value of *naux*, required for successful running (on the processor the program is being run on).

Table 31 describes the actions taken by ESSL in every possible situation for the values given in this example.

Table 31. Example of Input-Argument Error Recovery for Auxiliary Storage Sizes

NAUX Value	Action When 2015 Is an Unrecoverable Input-Argument Error	Action When 2015 Is a Recoverable Input-Argument Error
$naux < 20$	An input-argument error message is issued. The value in the error message is the lower limit, 20. The application program stops.	An input-argument error message is issued. The value in the error message is the lower limit, 20. The application program stops.
$20 \leq naux < 300$	An input-argument error message is issued. The value in the error message is the minimum required value, 300. The application program stops.	ESSL returns the value of <i>naux</i> as 300 to the application program, and an input-argument error message is issued. The value in the error message is the minimum required value, 300. ESSL does no computation, and control is returned to the application program.
$naux \geq 300$	Your application program runs successfully.	Your application program runs successfully.

### Here Is How You Code It in Your Program

If you leave error 2015 unrecoverable, you **do not code anything** in your program. You just look at the error messages to get the sizes of auxiliary storage. On the other hand, if you want to make error 2015 recoverable to obtain the auxiliary storage sizes dynamically in your program, you need to **add some coding statements** to your program. For details on coding these statements in each programming language, see the following examples:

- For Fortran, see page 121
- For C, see page 139
- For C++, see page 155

You may want to provide a separate subroutine to calculate the auxiliary storage size whenever you need it. Figure 3 on page 42 shows how you might code a separate Fortran subroutine. Before calling SCFT in your program, call this subroutine, SCFT which calculates the minimum size and stores it in the *naux* arguments. Upon return, your program checks the return code. If it is nonzero, the *naux* arguments were updated, as planned. You should then make sure adequate storage is available and call SCFT. On the other hand, if the return code is zero, error handling was not invoked, the *naux* arguments were not updated, and the initialization step was performed for SCFT.

```

SUBROUTINE SCFT
* N, M, ISIGN, SCALE, AUX1, NAUX1,AUX2,NAUX2)
REAL*4 X(0:*),Y(0:*),SCALE
REAL*8 AUX1(7),AUX2(0:*)
INTEGER*4 INIT,INC1X,INC2X,INC1Y,INC2Y,N,M,ISIGN,NAUX1,NAUX2
EXTERNAL ENOTRM
CHARACTER*8 S2015
CALL EINFO(0)
CALL ERRSAV(2015,S2015)
CALL ERRSET(2015,0,-1,1,ENOTRM,0)
C SETS NAUX1 AND NAUX2 TO THE MINIMUM VALUES REQUIRED TO USE
C THE RECOVERABLE INPUT-ARGUMENT ERROR-HANDLING FACILITY
NAUX1 = 7
NAUX2 = 0
CALL SCFT(INIT,X,INC1X,INC2X,Y,INC1Y,INC2Y,
* N,M,ISIGN,SCALE,AUX1,NAUX1,AUX2,NAUX2,*10)
CALL ERRSTR(2015,S2015)
RETURN
10 CONTINUE
CALL ERRSTR(2015,S2015)
RETURN 1
END

```

Figure 3. Fortran Subroutine to Calculate Auxiliary Storage Sizes

## Providing a Correct Transform Length to ESSL

This section describes how to calculate the length of your transform by use of formulas or error-handling capabilities provided in ESSL.

### What ESSL Subroutines Require Transform Lengths?

For the ESSL subroutines listed in Table 32, you need to provide one or more transform lengths for the computation of a Fourier transform. These transform lengths are supplied through one or more arguments, such as  $n$ ,  $n1$ ,  $n2$ , and  $n3$ , in the calling sequence for the ESSL subroutine. Only certain lengths of transforms are permitted in the computation.

Table 32. ESSL Subroutines Requiring Transform Lengths

Subroutine Names
Fourier Transforms: _CFT _RCFT _CRFT _COSF _SINF SCOSFT _CFT2 _RCFT2 _CRFT2 _CFT3 _RCFT3 _CRFT3 SCFTP SCFT2P SCFT3P

### Who Do You Want to Calculate the Length? You or ESSL?

You have a choice of two methods for determining an acceptable length for your transform to be processed by ESSL:

- Use the formula or large table in “Acceptable Lengths for the Transforms” on page 779 to determine an acceptable length. For details, see “How Do You Calculate the Length Using the Table or Formula?” on page 43.
- Use the ESSL error-handling facilities to return to you an acceptable length. For details, see “How Do You Get ESSL to Calculate the Length Using ESSL Error Handling?” on page 43.

## How Do You Calculate the Length Using the Table or Formula?

The lengths ESSL accepts for transforms in the Fourier transform subroutines are listed in “Acceptable Lengths for the Transforms” on page 779. You should use the table in that section to find the two values your length falls between. You then specify the **larger** length for your transform. If you find a perfect match, you can use that value without having to change it. The formula provided in that section expresses how to calculate the acceptable values listed in the table. If necessary, you can use the formula to dynamically check lengths in your program.

## How Do You Get ESSL to Calculate the Length Using ESSL Error Handling?

This section describes how to get ESSL to calculate transform lengths.

### Here Are the Two Ways You Can Do It

Ask yourself which of the following ways you prefer to obtain the information from ESSL:

- **By leaving error 2030 unrecoverable**, you can obtain an acceptable value for  $n$  from the input-argument error message, but your program terminates.
- **By making error 2030 recoverable**, you obtain an acceptable value for  $n$  from the input-argument error message and have the updated  $n$  argument returned to your program.

Because the Fourier transform subroutines allow only certain lengths for transforms, ESSL provides this error-handling capability to return acceptable lengths to your program. It returns them in the transform length arguments. The value ESSL returns is the **next larger acceptable length** for a transform, based on the length you specify in the  $n$  argument.

### The First Way

In this case, you obtain an acceptable value of  $n$  from the error message, but your program terminates.

Leave error 2030 as unrecoverable, without calls to EINFO and ERRSET. Run your program with a close approximation of the transform length you want to use. If this happens not to be an acceptable length, the ESSL error monitor returns an acceptable length of the transform in input-argument error message. This does, however, terminate your program when the error is encountered. (If you do happen to specify an acceptable length for the transform, error handling does not issue an error message and processing continues normally.) Figure 4 on page 44 illustrates what happens when error 2030 is unrecoverable.

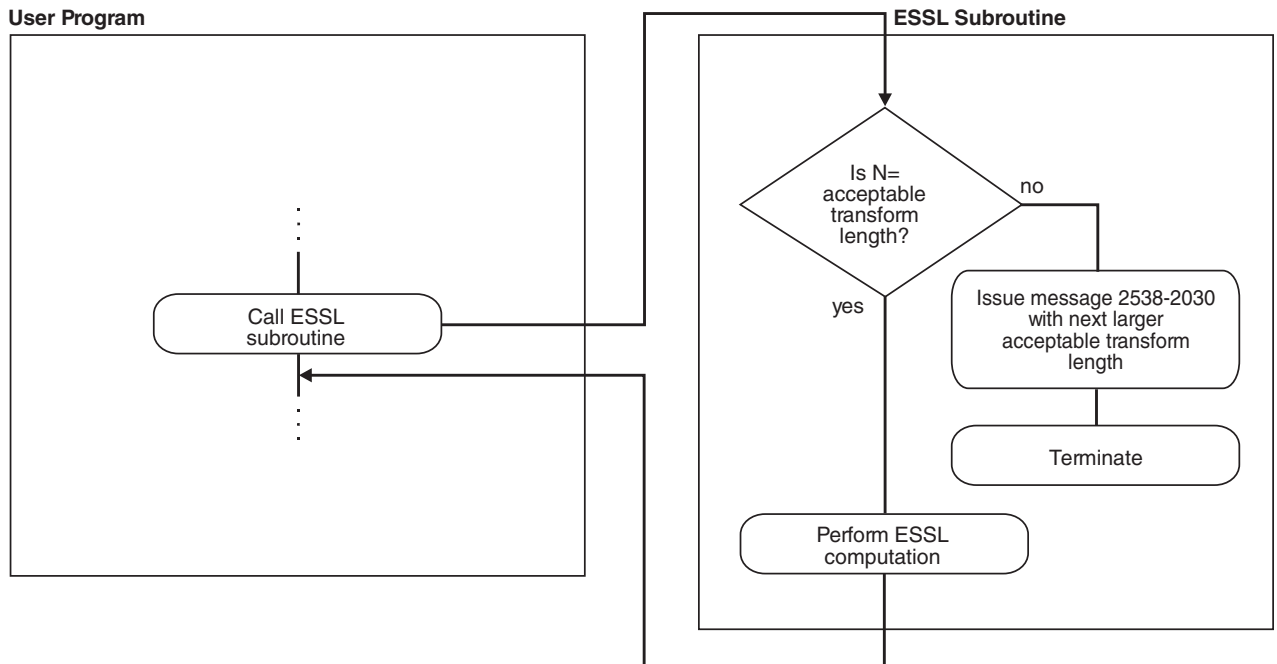


Figure 4. How to Obtain an  $N$  Value from an Error Message, but Terminate

### The Second Way

In this case, you obtain an acceptable value of  $n$  from the error message and from the updated  $n$  argument returned to your program.

Use EINFO and ERRSET with an ESSL error exit routine, ENOTRM, to make error 2030 recoverable. This allows you to dynamically determine in your program an acceptable length for your transform, specified in the  $n$  argument(s). Run your program with a close approximation of the transform length you want to use. If this happens not to be an acceptable length, the ESSL error monitor returns an acceptable length of the transform in the input-argument error message and a return code is passed back to your program, indicating that updated values are also returned in the  $n$  argument(s). You can then react to these updated values during run time in your program. ESSL does not perform any computation when this error occurs. For details on how to do this, see Chapter 4, “Coding Your Program,” on page 111. (If you do happen to specify an acceptable length for the transform, error handling does not issue an error message and processing continues normally.) Figure 5 on page 45 illustrates what happens when error 2030 is recoverable.

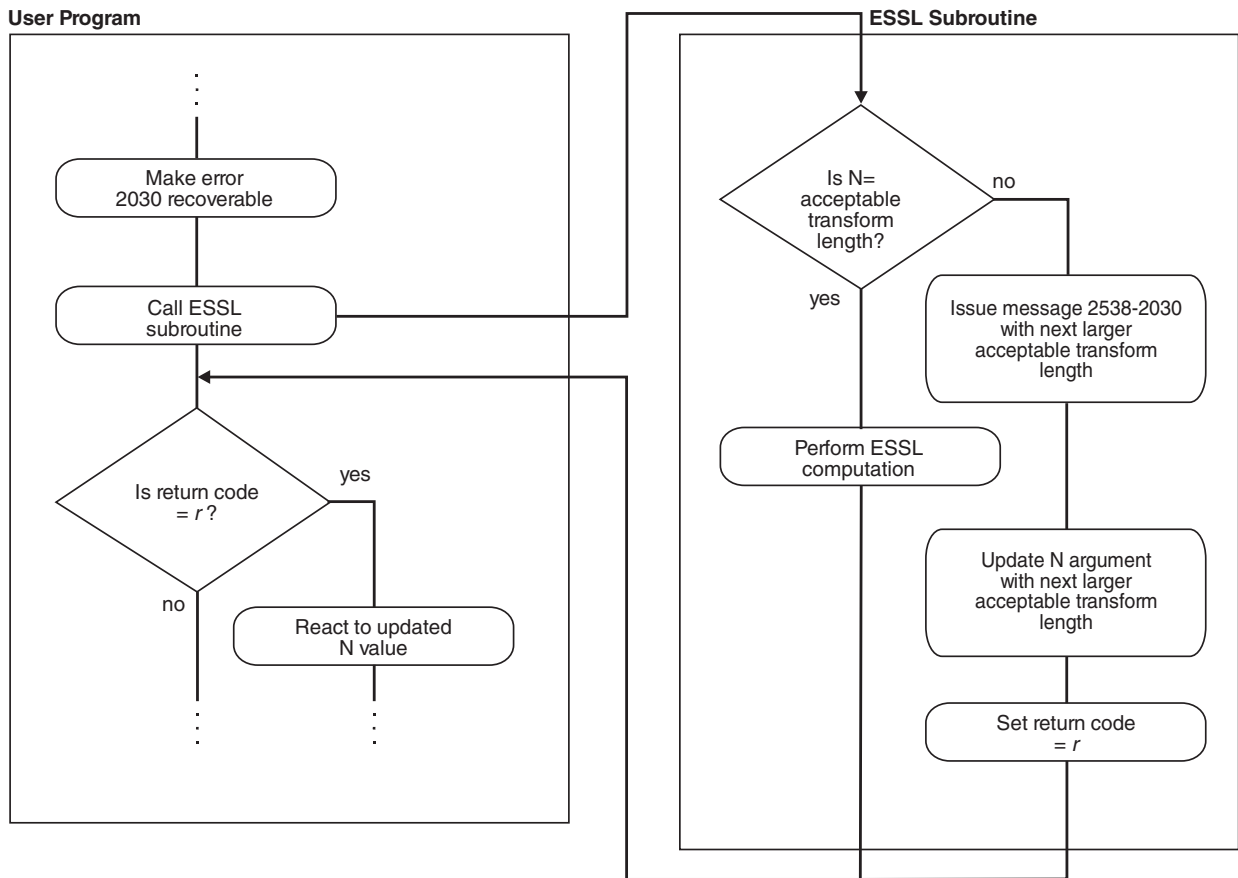


Figure 5. How to Obtain an N Value from an Error Message and in Your Program

### Here Is an Example of What Happens When You Use These Two Techniques

The following example illustrates all the actions taken by the ESSL error-handling facility for each possible value of a recoverable input argument,  $n$ . The values of  $n$  used in the example are as follows:

N	Meaning of the N Value
7208960	An acceptable transform length, required for successful computing of a Fourier transform
7340032	The next larger acceptable transform length, required for successful computing of a Fourier transform

Table 33 on page 46 describes the actions taken by ESSL in every possible situation for the values given in this example.

Table 33. Example of Input-Argument Error Recovery for Transform Lengths

N Value	Action When 2030 Is an Unrecoverable Input-Argument Error	Action When 2030 Is a Recoverable Input-Argument Error
$n = 7208960$ -or- $n = 7340032$	Your application program runs successfully.	Your application program runs successfully.
$7208960 < n < 7340032$	An input-argument error message is issued. The value in the error message is 7340032. The application program stops.	ESSL returns the value of $n$ as 7340032 to the application program, and an input-argument error message is issued. The value in the error message is 7340032. ESSL does no computation, and control is returned to the application program.

### Here Is How You Code It in Your Program

If you leave error 2030 unrecoverable, you **do not code anything** in your program. You just look at the error messages to get the transform lengths. On the other hand, if you want to make error 2030 recoverable to obtain the transform lengths dynamically in your program, you need to **add some coding statements** to your program. For details on coding these statements in each programming language, see the following examples:

- For Fortran, see page 121
- For C, see page 139
- For C++, see page 155

You may want to provide a separate subroutine to calculate the transform length whenever you need it. Figure 6 shows how you might code a separate Fortran subroutine. Before calling SCFT in your program, you call this subroutine, SCFT which calculates the correct length and stores it in  $n$ . Upon return, your program checks the return code. If it is nonzero, the  $n$  argument was updated, as planned. You then do any necessary data setup and call SCFT. On the other hand, if the return code is zero, error handling was not invoked, the  $n$  argument was not updated, and the initialization step was performed for SCFT.

```

SUBROUTINE SCFT
* N, M, ISIGN, SCALE, AUX1, NAUX1,AUX2,NAUX2)
REAL*4 X(0:*),Y(0:*),SCALE
REAL*8 AUX1(7),AUX2(0:*)
INTEGER*4 INIT,INC1X,INC2X,INC1Y,INC2Y,N,M,ISIGN,NAUX1,NAUX2
EXTERNAL ENOTRM
CHARACTER*8 S2030
CALL EINFO(0)
CALL ERRSAV(2030,S2030)
CALL ERRSET(2030,0,-1,1,ENOTRM,0)
CALL SCFT(INIT,X,INC1X,INC2X,Y,INC1Y,INC2Y,
*          N,M,ISIGN,SCALE,AUX1,NAUX1,AUX2,NAUX2,*10)
CALL ERRSTR(2030,S2030)
RETURN
10 CONTINUE
CALL ERRSTR(2030,S2030)
RETURN 1
END

```

Figure 6. Fortran Subroutine to Calculate Transform Length

You might want to combine the request for auxiliary storage sizes along with your request for transform lengths. Figure 7 on page 47 shows how you might code a



separate Fortran subroutine combining both requests. It combines the functions performed by the subroutines in Figure 3 on page 42 and Figure 6 on page 46.

```

SUBROUTINE SCFT
* N, M, ISIGN, SCALE, AUX1, NAUX1,AUX2,NAUX2)
REAL*4 X(0:*),Y(0:*),SCALE
REAL*8 AUX1(7),AUX2(0:*)
INTEGER*4 INIT,INC1X,INC2X,INC1Y,INC2Y,N,M,ISIGN,NAUX1,NAUX2
EXTERNAL ENOTRM
CHARACTER*8 S2015,S2030
CALL EINFO(0)
CALL ERRSAV(2015,S2015)
CALL ERRSAV(2030,S2030)
CALL ERRSET(2015,0,-1,1,ENOTRM,0)
CALL ERRSET(2030,0,-1,1,ENOTRM,0)
C SETS NAUX1 AND NAUX2 TO THE MINIMUM VALUES REQUIRED TO USE
C THE RECOVERABLE INPUT-ARGUMENT ERROR-HANDLING FACILITY
NAUX1 = 7
NAUX2 = 0
CALL SCFT(INIT,X,INC1X,INC2X,Y,INC1Y,INC2Y,
* N,M,ISIGN,SCALE,AUX1,NAUX1,AUX2,NAUX2,*10)
CALL ERRSTR(2015,S2015)
CALL ERRSTR(2030,S2030)
RETURN
10 CONTINUE
CALL ERRSTR(2015,S2015)
CALL ERRSTR(2030,S2030)
RETURN 1
END

```

Figure 7. Fortran Subroutine to Calculate Auxiliary Storage Sizes and Transform Length

## Getting the Best Accuracy

This section explains how accuracy of your results can be affected in various situations and what you can do to achieve the best possible accuracy.

### What Precisions Do ESSL Subroutines Operate On?

Both short- and long-precision real versions of the subroutines are provided in most areas of ESSL. In some areas, short- and long-precision complex versions are also provided, and, occasionally, an integer version is provided. The subroutine names are distinguished by a one- or two-letter prefix based on the following letters:

S for short-precision real  
D for long-precision real  
C for short-precision complex  
Z for long-precision complex  
I for integer

For a description of these data types, see “How Do You Set Up Your Scalar Data?” on page 33. The scalar data types and how you should code them for each programming language are listed under “Coding Your Scalar Data” in each language section in Chapter 4, “Coding Your Program,” on page 111.

## How does the Nature of the ESSL Computation Affect Accuracy?

In subroutines performing operations such as copy and swap, the accuracy of data is not affected. In subroutines performing computations involving mathematical operations on array data, the accuracy of the result may be affected by the following:

- The algorithm, which can vary depending on values or array sizes within the computation or the number of threads used.
- The matrix and vector sizes

For this reason, the ESSL subroutines do **not** have a closed formula for the error of computation. In other words, there is no formula with which you can calculate the error of computation in each subroutine.

Short-precision subroutines sometimes provide increased accuracy of results by accumulating intermediate results in long precision. This is also noted in the functional description for each subroutine.

Where applicable, the ESSL subroutines use the Multiply-Add instructions, which combine a Multiply and Add operation without an intermediate rounding operation.

For the **ESSL Serial Library** and the **ESSL SMP Library**, results obtained by 32-bit environment and 64-bit environment applications using the same ESSL library are mathematically equivalent but may not be bit identical.

## What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?

The data types operated on by the short-precision, long-precision, and integer versions of the subroutines are ANSI/IEEE 32-bit and 64-bit binary floating-point format, and 32-bit integer. See the *ANSI/IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Standard 754–1985* for more detail.

There are ESSL-specific rules that apply to the results of computations using the ANSI/IEEE standards. When running your program, the result of a multiplication of NaN (“Not-a-Number”) by a scalar zero, under certain circumstances, may differ in the ESSL subroutines from the result you expect.

Usually, when NaN is multiplied by a scalar zero, the result is NaN; however, in some ESSL subroutines where scaling is performed, the result may be zero. For example, in computing  $\alpha A$ , where  $\alpha$  is a scalar and  $A$  is a matrix, if  $\alpha$  is zero and one (or more) of the elements of  $A$  is NaN, the scaled result, using that element, may be a zero, rather than NaN. To avoid problems, you should consider this when designing your program.

## How is Underflow Handled?

ESSL does not mask underflow. If your program incurs a number of unmasked underflows, its overall performance decreases. Floating-point exception trapping is disabled by default. Therefore, you do not have to mask underflow unless you have changed the default.

## Where Can You Find More Information on Accuracy?

Information about accuracy can be found in the following places:

- Migration considerations concerning accuracy of results between releases, platforms, and so forth are described in Chapter 6, “Migrating Your Programs,” on page 171.
- Specific information on accuracy for each area of ESSL is given in “Performance and Accuracy Considerations” in each chapter introduction in Part 2.
- The functional description under “Function” for each subroutine explains what you need to know about the accuracy of the computation. Varying implementation techniques are sometimes used to improve performance. To let you know how accuracy is affected, the functional description may explain in general terms the different techniques used in the computation.

---

## Getting the Best Performance

This section describes how you can achieve the best possible performance from the ESSL subroutines.

### What General Coding Techniques Can You Use to Improve Performance?

There are many ways in which you can improve the performance of your program. Here are some of them:

- Use the basic linear algebra subprograms and matrix operations in the order of optimum performance: matrix-matrix computations, matrix-vector computations, and vector-scalar computations. When data is presented in matrices or vectors, rather than vectors or scalars, multiple operations can be performed by a single ESSL subroutine.
- Where possible, use subroutines that do multiple computations, such as SNDOT and SNAXPY, rather than individual computations, such as SDOT and SAXPY.
- Use a stride of 1 for the data in your computations. Not having vector elements consecutively accessed in storage can degrade your performance. The closer the vector elements are to each other in storage, the better your performance. For an explanation of stride, see “How Stride Is Used for Vectors” on page 62.
- Do **not** specify the size of the leading dimension of an array (*lda*) or stride of a vector (*inc*) equal to or near a multiple of:
  - 128 for a long-precision array
  - 256 for a short-precision array
- **For ESSL Blue Gene Library users:** Specify the size of the leading dimension of a real array to be even.
- Do **not** specify the individual sizes of your one-dimensional arrays as multiples of 128. This is especially important when you are passing several one-dimensional arrays to an ESSL subroutine. (The multiplicity can cause a performance problem that otherwise might not occur.)
- For small problems, avoid using a large leading dimension (*lda*) for your matrix.
- The following list explains how to align your data arrays for optimal performance, depending on the type of ESSL library you are using:

#### ESSL serial and SMP libraries

In general, align your arrays on doubleword boundaries, regardless of the type of data. For information on how your programming language aligns data, see your programming language manuals.

#### ESSL Blue Gene library

See Table 27 on page 29.

- One subroutine may do scaling while another does not. If scaling is not necessary for your data, you get better performance by using the subroutine without scaling. SNORM2 and DNORM2 are examples of subroutines that do not do scaling, versus SNRM2 and DNRM2, which do scaling.
- Use the STRIDE subroutine to calculate the optimal stride values for your input or output data when using any of the Fourier transform subroutines, except \_RCFT and \_CRFT. Using these stride values for your data allows the Fourier transform subroutines to achieve maximum performance. You first obtain the optimal stride values from STRIDE, calling it once for each stride value desired. You then arrange your data using these stride values. After the data is set up, you call the Fourier transform subroutine. For details on the STRIDE subroutine and how to use it for each Fourier transform subroutine, see “STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines” on page 1017. For additional information, see “Setting Up Your Data” on page 782.

## Where Can You Find More Information on Performance?

Information about performance can be found in the following places:

- Many of the techniques ESSL uses to achieve the best possible performance are described in the “High Performance of ESSL” on page 6.
- Migration considerations concerning performance are described in Chapter 6, “Migrating Your Programs,” on page 171.
- Specific information on performance for each area of ESSL is given in “Performance and Accuracy Considerations” in each chapter introduction in Part 2.
- Detailed performance information for selected subroutines can be found in reference [32], [43], [44].

---

## Dealing with Errors when Using ESSL

At run time, you can encounter different types of errors or messages that are related to the use of the ESSL subroutines:

- Program exceptions
- ESSL input-argument errors
- ESSL computational errors
- ESSL resource errors
- ESSL attention messages

This section explains how to handle all these situations.

### What Can You Do about Program Exceptions?

The program exceptions you can encounter in ESSL are described in the *ANSI/IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Standard 754–1985*.

### What Can You Do about ESSL Input-Argument Errors?

This section gives an overview on how you can handle input-argument errors.

#### All Input-Argument Errors

ESSL checks the validity of most input arguments. If it finds that any are invalid, it issues the appropriate error messages. Also, except for the three recoverable errors described below, it terminates your program. You should use standard programming techniques to diagnose and fix unrecoverable input-argument errors, as described in Chapter 7, “Handling Problems,” on page 175.

You can determine the input-argument errors that can occur in a subroutine by looking under “Error Conditions” in the subroutine description in Part 2 of this book. Error messages for all input-argument errors are listed in “Input-Argument Error Messages(2001-2099)” on page 180.

### **Recoverable Errors 2015, 2030 and 2200 Can Return Updated Values in the NAUX, N and NSINFO Arguments**

For three input-argument errors, 2015, 2030, and 2200 in Fortran, C, and C++ programs, you have the option to continue running and have an updated value of the input argument returned to your program for subsequent use. These are called recoverable errors. This recoverable error-handling capability gives you flexibility in determining the correct values for the arguments. You can:

- Determine the correct size of an auxiliary work area by using error 2015. For help in deciding whether you want to use this capability and details on how to use it, see “Using Auxiliary Storage in ESSL” on page 36.
- Determine the correct length of a transform by using error 2030. For help in deciding whether you want to use this capability and details on how to use it, see “Providing a Correct Transform Length to ESSL” on page 42.
- Determine the minimal size of the array AP for DBSTRF and DBSSV by using error 2200. For help deciding whether you want to use this capability, see “DBSTRF — Symmetric Indefinite Matrix Factorization” on page 530 and “DBSSV — Symmetric Indefinite Matrix Factorization and Multiple Right-Hand Side Solve” on page 524

If you chose to leave errors 2015, 2030 and 2200 unrecoverable, you do not need to make any coding changes to your program. The input-argument error message is issued upon termination, containing the updated values you could have specified for the program to run successfully. You then make the necessary corrections in your program and rerun it.

If you choose to make errors 2015, 2030 and 2200 recoverable, you call the ERRSET subroutine to set up the ESSL error exit routine, ENOTRM, and then call the ESSL subroutine. When one or more of these errors occurs, the input-argument error message is issued with the updated values. In addition, the updated values are returned to your program in the input arguments named in the error message, along with a nonzero return code and processing continues. Return code values associated with these recoverable errors are described under “Error Conditions” for each ESSL subroutine in Part 2.

For details on how to code the necessary statements in your program to make 2015, 2030 and 2200 recoverable, see the following sections:

- “Input-Argument Errors in Fortran” on page 119
- “Input-Argument Errors in C” on page 136
- “Input-Argument Errors in C++” on page 152

## **What Can You Do about ESSL Computational Errors?**

This section gives an overview on how you can handle computational errors.

### **All Computational Errors**

ESSL computational errors are errors occurring in the computational data, such as in your vectors and matrices. You can determine the computational errors that can occur in a subroutine by looking under “Error Conditions” in the subroutine description in Part 2 of this book. These errors cause your program to terminate abnormally unless you take preventive action. A message is also provided in your

output, containing information about the error. Messages are listed in “Computational Error Messages(2100-2199)” on page 186.

When a computational error occurs, you should assume that the results are unpredictable. The result of the computation is valid only if no errors have occurred. In this case, a zero return code is returned.

Figure 8 shows what happens when a computational error occurs.

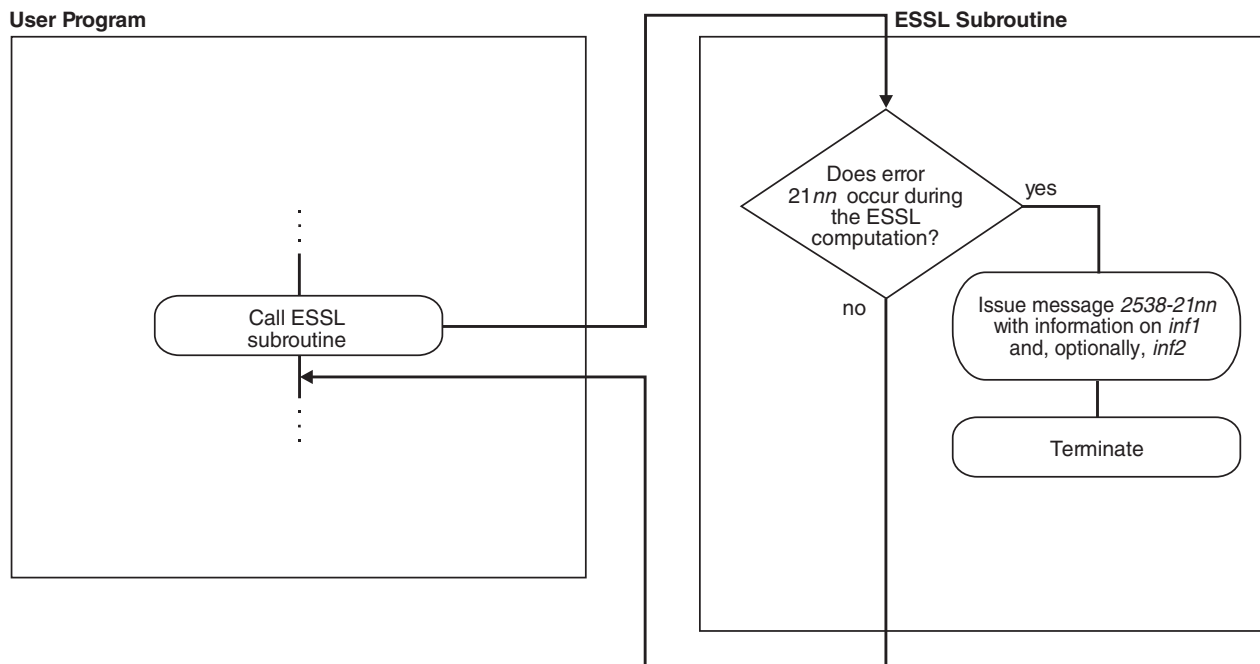


Figure 8. How to Obtain Computational Error Information from an Error Message, but Terminate

### Recoverable Computational Errors Can Return Values Through EINFO

In Fortran, C, and C++ programs, you have the capability to make certain computational errors recoverable and have information returned to your program about the errors. Recoverable computational errors are listed in Table 182 on page 1008. First, you call EINFO in the beginning of your program to initialize the ESSL error option table. You then call ERRSET to reset the number of allowable errors for the computational error codes in which you are interested. When a computational error occurs, a nonzero return code is returned for each computational error. Return code values associated with these errors are described under “Error Conditions” in each subroutine description. Based on the return code, your program can branch to an appropriate statement to call the ESSL error information-handler subroutine, EINFO, to obtain specific information about the data involved in the error. This information is returned in the EINFO output arguments, *inf1* and, optionally, *inf2*. You can then check the information returned and continue processing, if you choose. The syntax for EINFO is described under “EINFO — ESSL Error Information-Handler Subroutine” on page 1008. You also get a message in your output for each computational error encountered, containing information about the error. The EINFO subroutine provides the same information in the messages as it provides to your program.

For details on how to code the necessary statements in your program to obtain specific information on computational errors, see the following sections:

- “Computational Errors in Fortran” on page 122
- “Computational Errors in C” on page 141
- “Computational Errors in C++” on page 157

Figure 9 shows what happens if you make a computational error recoverable.

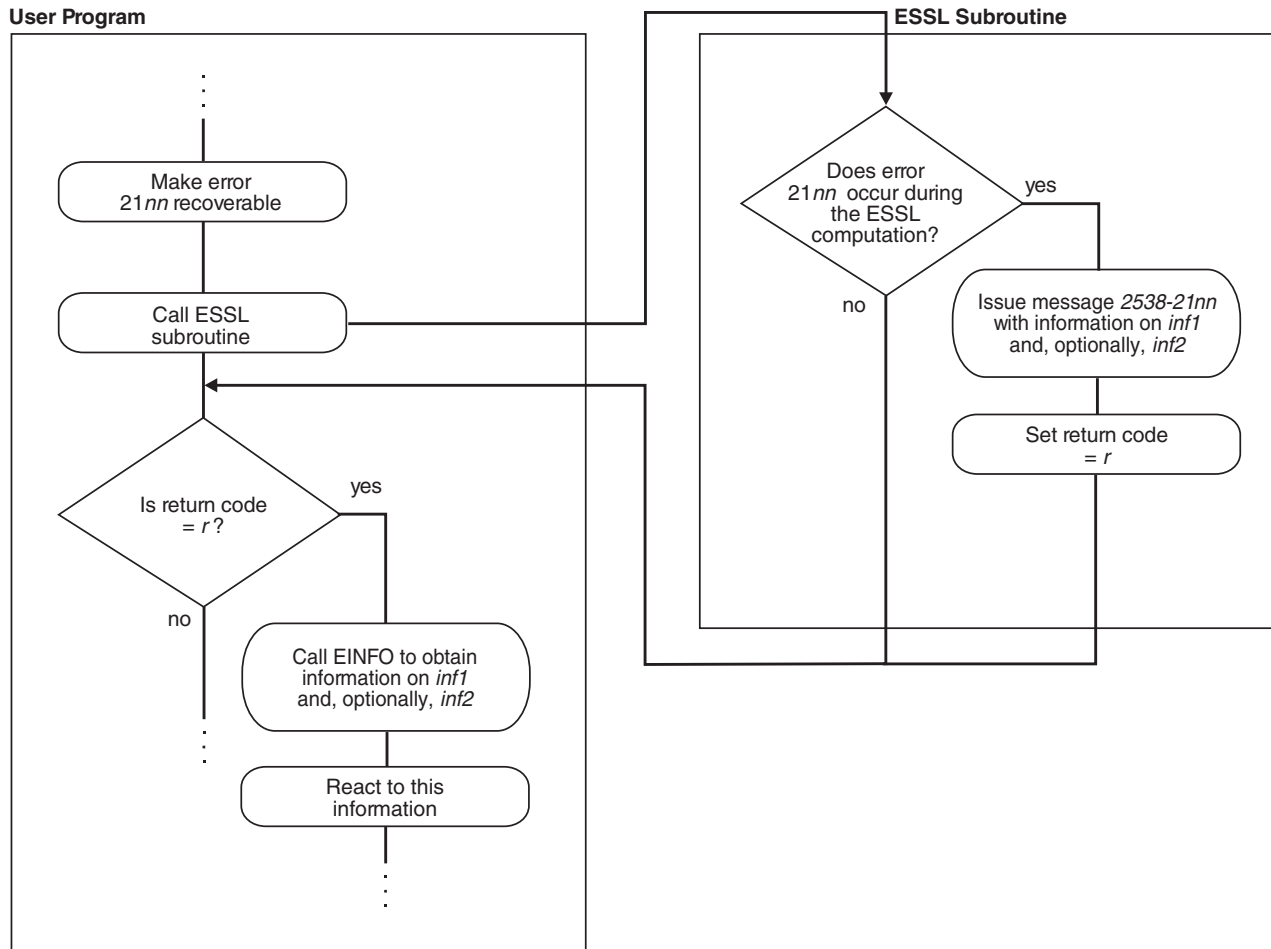


Figure 9. How to Obtain Computational Error Information in an Error Message and in Your Program

## What Can You Do about ESSL Resource Errors?

This section gives an overview on how you can handle resource errors.

### All Resource Errors

ESSL returns a resource error and terminates your program when an attempt to allocate work area fails. Some ESSL subroutines attempt to allocate work area for their internal use. Other ESSL subroutines attempt to dynamically allocate auxiliary storage when a user requests it through calling sequence arguments, such as *aux* and *naux*. For information on how you could reduce memory constraints on the system or increase the amount of memory available before rerunning the application program, see “ESSL Resource Error Messages” on page 178.

You can determine the resource errors that can occur in a subroutine by looking under “Error Conditions” in the subroutine description in Part 2 of this book. Error messages for all resource errors are listed in “Resource Error Messages(2400-2499)” on page 188.

## What Can You Do about ESSL Attention Messages?

This section gives an overview on how you can handle attention messages.

### All Attention Messages

ESSL returns an attention message to describe a condition that occurred, however, ESSL is able to continue processing. For information on how you could reduce memory constraints on the system or increase the amount of memory available, see “ESSL Resource Error Messages” on page 178.

For example, an attention message may be issued when enough work area was available to continue processing, but was not the amount initially requested. An attention message would be issued to indicate that performance may be degraded.

For a list of attention messages, see “Informational and Attention Error Messages(2600-2699)” on page 188.

## How Do You Control Error Handling by Setting Values in the ESSL Error Option Table?

This section explains all aspects of using the ESSL error option table.

### What Values Are Set in the ESSL Error Option Table?

The ESSL error option table contains information that tells ESSL what to do every time it encounters an ESSL-generated error. Table 34 shows the default values established in the table when ESSL is installed.

Table 34. ESSL Error Option Table Default Values

Range of Error Messages (From-To)	Number of Allowable Errors (ALLOW)	Number of Messages Printed (PRINT)	Modifiable Table Entry (MODENT)
2538-2000	Unlimited	255	NO
2538-2001 through 2538-2073	Unlimited	255	YES
2538-2074	Unlimited	5	YES
2538-2075 through 2538-2098	Unlimited	255	YES
2538-2099	1	255	YES
2538-2100 through 2538-2101	1	255	YES
2538-2102	Unlimited	255	YES
2538-2103 through 2538-2113	1	255	YES
2538-2114	Unlimited	255	YES
2538-2115 through 2538-2122	1	255	YES
2538-2123 through 2538-2124	Unlimited	255	YES
2538-2125 through 2538-2126	1	255	YES
2538-2127	Unlimited	255	YES
2538-2128 through 2538-2137	1	255	YES
2538-2138 through 2538-2143	Unlimited	255	YES
2538-2144 through 2538-2145	1	255	YES
2538-2146 through 2538-2149	Unlimited	255	YES
2538-2150	1	255	YES
2538-2151 through 2538-2152	Unlimited	255	YES



Table 34. ESSL Error Option Table Default Values (continued)

Range of Error Messages (From-To)	Number of Allowable Errors (ALLOW)	Number of Messages Printed (PRINT)	Modifiable Table Entry (MODENT)
2538–2153 through 2538–2198	1	255	YES
2538–2199	1	255	YES
2538–2200 through 2538–2299	Unlimited	255	YES
2538–2400 through 2538–2499	1	255	NO
2538–2600 through 2538–2609	Unlimited	255	NO
2538–2610 through 2538–2611	Unlimited	-1	YES
2538–2612 through 2538–2699	Unlimited	255	NO
2538–2700 through 2538–2799	1	255	NO

### How Can You Change the Values in the Error Option Table?

You can change any of the values in the ESSL error option table by calling the ERRSET subroutine in your program. This dynamically changes values at run time. You can also save and restore entries in the table by using the ERRSAV and ERRSTR subroutines, respectively. For a description of the ERRSET, ERRSAV, and ERRSTR subroutines see Chapter 17, “Utilities,” on page 1005.

### When Do You Change the Values in the Error Option Table?

Because you can change the information in the error option table, you can control what happens when any of the ESSL errors occur. There are a number of instances when you may want to do this:

**To Customize Your Error-Handling Environment:** You may simply want to adjust the number of times an error is allowed to occur before your program terminates. You can use any of the capabilities available in ERRSET.

**To Obtain Auxiliary Storage Sizes and Transform Lengths:** You may want to make ESSL input-argument error 2015 or 2030 recoverable, so ESSL returns updated auxiliary storage sizes or transform lengths, respectively, to your program. For a more detailed discussion, see “What Can You Do about ESSL Input-Argument Errors?” on page 50. For how to use ERRSET to do this, see the section for your programming language in Chapter 4, “Coding Your Program,” on page 111.

**To Obtain the Minimal Size of the Array AP for DBSTRF and DBSSV:** You may want to make ESSL input-argument error 2200 recoverable, so ESSL returns an updated size to your program. For a more detailed discussion, see “What Can You Do about ESSL Input-Argument Errors?” on page 50. For how to use ERRSET to do this, see the section for your programming language in Chapter 4, “Coding Your Program,” on page 111.

**To Get More Information About a Computational Error:** You may want ESSL to return information about a computational error to your program. For a more detailed discussion, see “What Can You Do about ESSL Computational Errors?” on page 51. For how to do use ERRSET to do this, see the section for your programming language in Chapter 4, “Coding Your Program,” on page 111.

**To Allow Parts of Your Application to Have Unique Error-Handling Environments:** If your program is part of a large application, you may want to dynamically save and restore entries in the error option table that have been

altered by ERRSET. This ensures the integrity of the error option table when it is used by multiple programs within an application. For a more detailed discussion, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” For how to use ERRSAV and ERRSTR, see the section for your programming language in Chapter 4, “Coding Your Program,” on page 111.

### **How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?**

When your program is part of a larger application, you should consider that one of the following can occur:

- If you use ERRSET in your program to reset any of the values in the error option table for any of the ESSL input-argument errors or computational errors, some other program in the application may be adversely affected. It may be expecting its original values.
- If some other program in the application uses ERRSET to reset any of the values in the error option table for any of the ESSL input-argument errors or computational errors, your program may be adversely affected. You may need a certain value in the error option table, and the application may have reset that value.

These situations can be avoided if every program that uses ERRSET, in the large application, also uses the ERRSAV and ERRSTR facilities. For a particular error number, ERRSAV saves an entry from the error option table in an area accessible to your program. ERRSTR then stores the entry back into the error option table from the storage area. You code an ERRSAV and ERRSTR for each input-argument error number and computational error number for which you do an ERRSET to reset the values in the error option table. Call ERRSAV at the beginning of your program after you call EINFO, and then call ERRSTR at the end of your program after all ESSL computations are completed. This saves the original contents of the error option table while your program is running with different values, and then restores it to its original contents when your program is done. For details on how to code these statements in your program, see Chapter 4, “Coding Your Program,” on page 111.

### **How does Error Handling Work in a Threaded Environment?**

When your application program or Fortran first creates a thread, ESSL initializes the error option table information to the default settings shown in Table 34 on page 54. You can change the default settings for each thread you created by calling the appropriate error handling subroutines (ERRSET, ERRSAV, or ERRSTR) from each thread. An example of how to initialize the error option table and change the default settings on multiple threads is shown in “Example of Handling Errors in a Multithreaded Application Program” on page 127.

ESSL issues error messages as they occur in a threaded environment. Error messages issued from any of the existing threads are written to standard output in the order in which they occur.

When a terminating condition occurs on any of the existing threads (for example, the number of allowable errors was exceeded), ESSL terminates your application program. One set of summary information corresponding to the terminating thread is always printed. Summary information corresponding to other threads may also be printed.

## Where Can You Find More Information on Errors?

Information about errors and how to handle them can be found in the following places:

- How to code your program to use the ESSL error-handling facilities is described in Chapter 4, “Coding Your Program,” on page 111.
- All ESSL error messages are listed under “Messages” on page 179.
- The errors and return codes associated with each ESSL subroutine are listed under “Error Conditions” in each subroutine description in Part 2.
- Complete diagnostic procedures for all types of ESSL programming and documentation problems, along with how to collect information and report a problem, are provided in Chapter 7, “Handling Problems,” on page 175.



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## Chapter 3. Setting Up Your Data Structures

This chapter provides you with information that you need to set up your data structures, consisting of vectors, matrices, and sequences. These techniques apply to programs in all programming languages.

---

### Concepts

Vectors, matrices, and sequences are conceptual data structures contained in arrays. In many cases, ESSL uses stride or leading dimension to select the elements of the vector, matrix, or sequence from an array. In other cases, ESSL uses a specific mapping, or storage layout, that identifies the elements of the vector, matrix, or sequence in an array, sometimes requiring several arrays to help define the mapping. These elements selected from the array(s) make up the conceptual data structure.

When you call an ESSL subroutine, it assumes that the data structure is set up properly in the array(s) you pass to it. If it is not, your results are unpredictable. ESSL also uses these same storage layouts for data structures passed back to your program.

The use of the terms vector, matrix, and sequence in this book is consistent with standard mathematical definitions, and their representations are consistent with conventions used in mathematical texts. Special notations and conventions used in this book for describing vectors, matrices, and sequences are explained in “Special Notations and Conventions” on page xv.

**Overlapping Data Structures:** Most of the subroutines do not allow vectors, matrices, or sequences to overlap. If this occurs, results are unpredictable. Where this applies, it is explained in Notes in each subroutine description. This means the elements of the data structure cannot reside in the same storage locations as any of the other data structures. It is possible, however, to have elements of different data structures in the same array, as long as the elements are interleaved through storage using strides greater than 1. For example, using vectors  $x$  and  $y$  with strides of 2, where  $x$  starts at  $A(1)$  and  $y$  starts at  $A(2)$ , the elements reside in array  $A$  in the order  $x_1, y_1, x_2, y_2, x_3, y_3, \dots$  and so forth.

When you use this technique, you should be careful that you specify different starting locations for each data structure contained in the array.

---

### Vectors

A vector is a one-dimensional, ordered collection of numbers. It can be a column vector, which represents an  $n$  by 1 ordered collection, or a row vector, which represents a 1 by  $n$  ordered collection.

The column vector appears symbolically as follows:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

A row vector appears symbolically as follows:

$$\mathbf{x} = [x_1 \ x_2 \ x_3 \ \dots \ x_n]$$

Vectors can contain either real or complex numbers. When they contain real numbers, they are sometimes called real vectors. When they contain complex numbers, they are called complex vectors.

## Transpose of a Vector

The transpose of a vector changes a column vector to a row vector, or vice versa:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \quad \mathbf{x}^T = [x_1 \ x_2 \ x_3 \ \dots \ x_n] \quad (\mathbf{x}^T)^T = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

The ESSL subroutines use the vector as it is intended in the computation, as either a column vector or a row vector; therefore, no movement of data is necessary.

In the examples provided with the subroutine descriptions in Part 2, "Reference Information" of this book, both types of vectors are represented in the same way, showing the elements of the array that make up the vector  $\mathbf{x}$ , as follows:

$$(1.0, 2.0, 3.0, 4.0, 5.0, 6.0)$$

## Conjugate Transpose of a Vector

The conjugate transpose of a vector  $\mathbf{x}$ , containing complex numbers, is denoted by  $\mathbf{x}^H$  and is expressed as follows:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \quad \mathbf{x}^H = [\bar{x}_1 \ \bar{x}_2 \ \bar{x}_3 \ \dots \ \bar{x}_n]$$

Just as for the transpose of a vector, no movement of data is necessary for the conjugate transpose of a vector.

## In Storage

A vector is usually stored within a one- or two-dimensional array. Its elements are stored sequentially in the array, but not necessarily contiguously.

The **location** of the vector in the array is specified by the argument for the vector in the ESSL calling sequence. It can be specified in a number of ways. For example, if  $A$  is an array of length 12, and you want to specify vector  $x$  as starting at the first element of array  $A$ , specify  $A$  as the argument, such as in:

```
X = SASUM (4,A,2)
```

where the number of elements to be summed in the vector is 4, the location of the vector is  $A$ , and the stride is 2.

If you want to specify vector  $x$  as starting at element 3 in array  $A$ , which is declared as  $A(1:12)$ , specify:

```
X = SASUM (4,A(3),2)
```

If  $A$  is declared as  $A(-1:8)$ , specify the following for element 3:

```
X = SASUM (4,A(1),2)
```

If  $A$  is a two-dimensional array and declared as  $A(1:4,1:10)$ , and you want vector  $x$  to start at the second row and third column of  $A$ , specify the following:

```
X = SASUM (4,A(2,3),2)
```

The **stride** specified in the ESSL calling sequence is used to step through the array to select the vector elements. The direction in which the vector elements are selected from the array—that is, front to back or back to front—is indicated by the sign (+ or -) of the stride. The absolute value of the stride gives the spacing between each element selected from the array.

To calculate the total number of elements needed in an array for a vector, you can use the following formula, which takes into account the number of elements,  $n$ , in the array and the stride,  $inc$ , specified for the vector:

$$1+(n-1)|inc|$$

**An array can be much larger than the vector that it contains; that is, there can be many elements following the vector in the array, as well as elements preceding the vector.**

For a complete description of how vectors are stored within arrays, see “How Stride Is Used for Vectors” on page 62.

For a complex vector, a special storage arrangement is used to accommodate the two parts,  $a$  and  $b$ , of each complex number ( $a+bi$ ) in the array. For each complex number, two sequential storage locations are required in the array. Therefore, exactly twice as much storage is required for complex vectors and matrices as for real vectors and matrices of the same precision. See “How Do You Set Up Your Scalar Data?” on page 33 for a description of real and complex numbers, and “How Do You Set Up Your Arrays?” on page 33 for a description of how real and complex data is stored in arrays.

## How Stride Is Used for Vectors

The stride for a vector is an increment that is used to step through array storage to select the vector elements from an array. To define exactly which elements become the conceptual vector in the array, the following items are used together:

- The location of the vector within the array
- The stride for the vector
- The number of elements,  $n$ , to be processed

The stride can be positive, negative, or 0. For positive and negative strides, if you specify vector elements beyond the range of the array, your results are be unpredictable, and you may get program errors.

This section explains how each of the three types of stride is used to select the vector elements from the array.

### Positive Stride

When a positive stride is specified for a vector, the location specified by the argument for the vector is the location of the first element in the vector, element  $x_1$ . The vector is in forward order in the array:  $(x_1, x_2, \dots, x_n)$ . For example, if you specify  $X(1)$  for vector  $x$ , where  $X$  is declared as  $X(0:12)$  and defined as:

```
X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0, 12.0, 13.0)
```

then processing begins at the second element in  $X$ , which is 2.0.

To find each successive element, the stride is added cumulatively to the starting point of vector  $x$  in the array. In this case, the starting point is  $X(1)$ . If the stride specified for vector  $x$  is 3 and the number of elements to be processed is 4, then the resulting elements selected from  $X$  for vector  $x$  are:  $X(1), X(4), X(7)$ , and  $X(10)$ .

Vector  $x$  is then:

```
(2.0, 5.0, 8.0, 11.0)
```

As shown in this example, a vector does not have to extend to the end of the array. Elements are selected from the second to the eleventh element of the array, and the array elements after that are not used.

This element selection can be expressed in general terms. Using  $BEGIN$  as the starting point in an array  $X$  and  $inc$  as the stride, this results in the following elements being selected from the array:

```
X(BEGIN)
X(BEGIN+inc)
X(BEGIN+(2)inc)
X(BEGIN+(3)inc)
.
.
.
X(BEGIN+(n-1)inc)
```

The following general formula can be used to calculate each vector element position in a one-dimensional array:

$$x_i = X(BEGIN + (i-1)(inc)) \text{ for } i = 1, n$$



When using an array with more than one dimension, you should understand how the array elements are stored to ensure that elements are selected properly. For a description of array storage, see “Setting Up Arrays in Fortran” on page 112. You should remember that the elements of an array are selected as they are arranged in storage, regardless of the number of dimensions defined in the array. Stride is used to step through array storage until  $n$  elements are selected. ESSL processing stops at that point. For example, given the following two-dimensional array, declared as  $A(1:7,1:4)$ .

Matrix A is:

$$\begin{bmatrix} 1.0 & 8.0 & 15.0 & 22.0 \\ 2.0 & 9.0 & 16.0 & 23.0 \\ 3.0 & 10.0 & 17.0 & 24.0 \\ 4.0 & 11.0 & 18.0 & 25.0 \\ 5.0 & 12.0 & 19.0 & 26.0 \\ 6.0 & 13.0 & 20.0 & 27.0 \\ 7.0 & 14.0 & 21.0 & 28.0 \end{bmatrix}$$

with  $A(3,1)$  specified for vector  $x$ , a stride of 2, and the number of elements to be processed as 12, the resulting vector  $x$  is:

$$(3.0, 5.0, 7.0, 9.0, 11.0, 13.0, 15.0, 17.0, 19.0, 21.0, 23.0, 25.0)$$

This is not a conventional use of arrays, and you should be very careful when using this technique.

### Zero Stride

When a zero stride is specified for a vector, the starting point for the vector is the only element used in the computation. The starting point for the vector is at the location specified by the argument for the vector, just as though you had specified a positive stride. For example, if you specify  $\chi$  for vector  $x$ , where  $\chi$  is defined as:

$$\chi = (5.0, 4.0, 3.0, 2.0, 1.0)$$

and you specify the number of elements,  $n$ , to be processed as 6, then processing begins at the first element, which is 5.0. This element is used for each of the six elements in vector  $x$ .

This makes the conceptual vector  $x$  appear as:

$$(5.0, 5.0, 5.0, 5.0, 5.0, 5.0)$$

The following general formula shows how to calculate each vector position in a one-dimensional array:

$$x_i = \chi(\text{BEGIN}) \text{ for } i = 1, n$$

### Negative Stride

When a negative stride is specified for a vector, the location specified for the vector is actually the location of the last element in the vector. In other words, the vector is in reverse order in the array:  $(x_n, x_{n-1}, \dots, x_1)$ . You specify the end of the vector,  $(x_n)$ . ESSL then calculates where the starting point  $(x_1)$  is by using the following arguments:

- The location of the vector in the array
- The stride for the vector,  $inc$
- The number of elements,  $n$ , to be processed

If you specify vector  $x$  at location  $X(\text{BEGIN})$  in array  $X$  with a negative stride of  $inc$  and  $n$  elements to be processed, then the following formula gives the starting point of vector  $x$  in the array:

$$X(\text{BEGIN} + (-n+1)(inc))$$

For example, if you specify  $X(2)$  for vector  $x$ , where  $X$  is declared as  $X(1:9)$  and defined as:

$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0)$$

and if you specify a stride of  $-2$ , and four elements to be processed, processing begins at the following element in  $X$ :

$$X(2+(-4+1)(-2)) = X(8)$$

where element  $X(8)$  is 8.0.

To find each of the  $n$  successive element positions in the array, you successively add the stride to the starting point  $n-1$  times. Suppose the formula calculated a starting point of  $X(\text{SP})$ ; the elements selected are:

$$\begin{aligned} &X(\text{SP}) \\ &X(\text{SP}+inc) \\ &X(\text{SP}+(2)inc) \\ &X(\text{SP}+(3)inc) \\ &\cdot \\ &\cdot \\ &\cdot \\ &X(\text{SP}+(n-1)inc) \end{aligned}$$

In the above example, the resulting elements selected from  $X$  for vector  $x$  are  $X(8)$ ,  $X(6)$ ,  $X(4)$ , and  $X(2)$ . This makes the resulting vector  $x$  appear as follows:

$$(8.0, 6.0, 4.0, 2.0)$$

The following general formula can be used to calculate each vector element position in a one-dimensional array:

$$x_i = X(\text{BEGIN} + (-n+i)(inc)) \text{ for } i = 1, n$$

## Sparse Vector

A sparse vector is a vector having a relatively small number of nonzero elements.

Consider the following as an example of a sparse vector  $x$  with  $n$  elements, where  $n$  is 11, and vector  $x$  is:

$$(0.0, 0.0, 1.0, 0.0, 2.0, 3.0, 0.0, 4.0, 0.0, 5.0, 0.0)$$

### In Storage

There are two storage modes that apply to sparse vectors: full-vector storage mode and compressed-vector storage mode. When a sparse vector is stored in **full-vector storage mode**, all its elements, including its zero elements, are stored in an array.

For example, sparse vector  $x$  is stored in full-vector storage mode in a one-dimensional array  $X$ , as follows:

$$X = (0.0, 0.0, 1.0, 0.0, 2.0, 3.0, 0.0, 4.0, 0.0, 5.0, 0.0)$$

When a sparse vector is stored in **compressed-vector storage mode**, it is stored without its zero elements. It consists of two one-dimensional arrays, each with a length of  $nz$ , where  $nz$  is the number of nonzero elements in vector  $x$ :

- The first array contains the nonzero elements of the sparse vector  $x$ , stored contiguously within the array.

**Note:** The ESSL subroutines do not check that all elements are nonzero. You do not get an error if any elements are zero.

- The second array contains a sequence of integers indicating the element positions (indices) of the nonzero elements of the sparse vector  $x$  stored in full-vector storage mode. This is referred to as the indices array.

For example, the sparse vector  $x$  shown above might have its five nonzero elements stored in ascending order in array  $X$  of length 5, as follows:

$$X = (1.0, 2.0, 3.0, 4.0, 5.0)$$

in which case, the array of indices,  $INDX$ , also of length 5, contains:

$$INDX = (3, 5, 6, 8, 10)$$

If the sparse vector  $x$  has its elements stored in random order in the array  $X$  as:

$$X = (5.0, 3.0, 4.0, 1.0, 2.0)$$

then the array  $INDX$  contains:

$$INDX = (10, 6, 8, 3, 5)$$

In general terms, this storage technique can be expressed as follows:

For each  $x_j \neq 0$ , for  $j = 1, n$   
there exists  $i$ , where  $1 \leq i \leq nz$ ,  
such that  $X(i) = x_j$  and  $INDX(i) = j$ .

where:

$x_1, \dots, x_n$  are the  $n$  elements of sparse vector  $x$ , stored in full-vector storage mode.

$X$  is the array containing the  $nz$  nonzero elements of sparse vector  $x$ ; that is, vector  $x$  is stored in compressed-vector storage mode.

$INDX$  is the array containing the  $nz$  indices indicating the element positions.

To avoid an error when using the  $INDX$  array to access the elements in any other target vector, the length of the target vector must be greater than or equal to  $\max(INDX(i))$  for  $i = 1, nz$ .

---

## Matrices

A matrix, also referred to as a general matrix, is an  $m$  by  $n$  ordered collection of numbers. It is represented symbolically as:

$$A = \begin{bmatrix} a_{11} & \cdot & \cdot & \cdot & a_{1n} \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ a_{m1} & \cdot & \cdot & \cdot & a_{mn} \end{bmatrix}$$

where the matrix is named  $A$  and has  $m$  rows and  $n$  columns. The elements of the matrix are  $a_{ij}$ , where  $i = 1, m$  and  $j = 1, n$ .

Matrices can contain either real or complex numbers. Those containing real numbers are called real matrices; those containing complex numbers are called complex matrices.

## Transpose of a Matrix

The transpose of a matrix  $A$  is a matrix formed from  $A$  by interchanging the rows and columns such that row  $i$  of matrix  $A$  becomes column  $i$  of the transposed matrix. The transpose of  $A$  is denoted by  $A^T$ . Each element  $a_{ij}$  in  $A$  becomes element  $a_{ji}$  in  $A^T$ . If  $A$  is an  $m$  by  $n$  matrix, then  $A^T$  is an  $n$  by  $m$  matrix. The following represents a matrix and its transpose:

$$A = \begin{bmatrix} a_{11} & \cdot & \cdot & \cdot & a_{1n} \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ a_{m1} & \cdot & \cdot & \cdot & a_{mn} \end{bmatrix} \quad A^T = \begin{bmatrix} a_{11} & \cdot & \cdot & \cdot & a_{m1} \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ a_{1n} & \cdot & \cdot & \cdot & a_{mn} \end{bmatrix}$$

ESSL assumes that all matrices are stored in untransformed format, such as matrix  $A$  shown above. No movement of data is necessary in your application program when you are processing transposed matrices. The ESSL subroutines adjust their selection of elements from the matrix when an argument in the calling sequence indicates that the transposed matrix is to be used in the computation. Examples of this are the *transa* and *transb* arguments specified for SGEADD, matrix addition.

## Conjugate Transpose of a Matrix

The conjugate transpose of a matrix  $A$ , containing complex numbers, is denoted by  $A^H$  and is expressed as follows:

$$A = \begin{bmatrix} a_{11} & \cdot & \cdot & \cdot & a_{1n} \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ a_{m1} & \cdot & \cdot & \cdot & a_{mn} \end{bmatrix} \quad A^H = \begin{bmatrix} \bar{a}_{11} & \cdot & \cdot & \cdot & \bar{a}_{m1} \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \bar{a}_{1n} & \cdot & \cdot & \cdot & \bar{a}_{mn} \end{bmatrix}$$

Just as for the transpose of a matrix, the conjugate transpose of a matrix is stored in untransformed format. No movement of data is necessary in your program.

## In Storage

A matrix is usually stored in a two-dimensional array. Its elements are stored successively within the array. Each column of the matrix is stored successively in

the array. The leading dimension argument is used to select the matrix elements from each successive column of the array. The starting point of the matrix in the array is specified as the argument for the matrix in the ESSL calling sequence. For example, if matrix  $A$  is contained in array  $A$  and starts at the first element in the first row and first column of  $A$ , you should specify  $A$  as the argument for matrix  $A$ , such as in:

```
CALL SGEMX (5,2,1.0,A,6,X,1,Y,1)
```

where, in the matrix-vector product, the number of rows in matrix  $A$  is 5, the number of columns in matrix  $A$  is 2, the scaling constant is 1.0, the location of the matrix is  $A$ , the leading dimension is 6, the vectors used in the matrix-vector product are  $X$  and  $Y$ , and their strides are 1.

If matrix  $A$  is contained in the array  $BIG$ , declared as  $BIG(1:20,1:30)$ , and starts at the second row and third column of  $BIG$ , you should specify  $BIG(2,3)$  as the argument for matrix  $A$ , such as in:

```
CALL SGEMX (5,2,1.0,BIG(2,3),6,X,1,Y,1)
```

See “How Leading Dimension Is Used for Matrices” for a complete description of how matrices are stored within arrays.

For a complex matrix, a special storage arrangement is used to accommodate the two parts,  $a$  and  $b$ , of each complex number ( $a+bi$ ) in the array. For each complex number, two sequential storage locations are required in the array. Therefore, exactly twice as much storage is required for complex matrices as for real matrices of the same precision. See “How Do You Set Up Your Scalar Data?” on page 33 for a description of real and complex numbers, and “How Do You Set Up Your Arrays?” on page 33 for a description of how real and complex data is stored in arrays.

## How Leading Dimension Is Used for Matrices

The leading dimension for a two-dimensional array is an increment that is used to find the starting point for the matrix elements in each successive column of the array. To define exactly which elements become the conceptual matrix in the array, the following items are used together:

- The location of the matrix within the array
- The leading dimension
- The number of rows,  $m$ , to be processed in the array
- The number of columns,  $n$ , to be processed in the array

The leading dimension must always be positive. It must always be greater than or equal to  $m$ , the number of rows in the matrix to be processed. For an array,  $A$ , declared as  $A(E1:E2,F1:F2)$ , the leading dimension is equal to:

$$(E2-E1+1)$$

The starting point for selecting the matrix elements from the array is at the location specified by the argument for the matrix in the ESSL calling sequence. For example, if you specify  $A(3,0)$  for a 4 by 4 matrix  $A$ , where  $A$  is declared as  $A(1:7,0:4)$ :

$$\begin{bmatrix} 1.0 & 8.0 & 15.0 & 22.0 & 29.0 \\ 2.0 & 9.0 & 16.0 & 23.0 & 30.0 \\ 3.0 & 10.0 & 17.0 & 24.0 & 31.0 \\ 4.0 & 11.0 & 18.0 & 25.0 & 32.0 \\ 5.0 & 12.0 & 19.0 & 26.0 & 33.0 \end{bmatrix}$$

$$\begin{bmatrix} 6.0 & 13.0 & 20.0 & 27.0 & 34.0 \\ 7.0 & 14.0 & 21.0 & 28.0 & 35.0 \end{bmatrix}$$

then processing begins at the element at row 3 and column 0 in array A, which is 3.0.

The leading dimension is used to find the starting point for the matrix elements in each of the  $n$  successive columns in the array. ESSL subroutines assume that the arrays are stored in column-major order, as described under "How Do You Set Up Your Arrays?" on page 33, and they add the leading dimension (times the size of the element in bytes) to the starting point. They do this  $n-1$  times. This finds the starting point in each of the  $n$  columns of the array.

In the above example, the leading dimension is:

$$E2-E1+1 = 7-1+1 = 7$$

If the number of columns,  $n$ , to be processed is 4, the starting points are:  $A(3,0)$ ,  $A(3,1)$ ,  $A(3,2)$ , and  $A(3,3)$ . These are elements 3.0, 10.0, 17.0, and 24.0 for  $a_{11}$ ,  $a_{12}$ ,  $a_{13}$ , and  $a_{14}$ , respectively.

In general terms, this results in the following starting positions of each column in the matrix being calculated as follows:

```
A(BEGINI, BEGINJ)
A(BEGINI, BEGINJ+1)
A(BEGINI, BEGINJ+2)
.
.
.
A(BEGINI, BEGINJ+n-1)
```

To find the elements in each column of the array, 1 is added successively to the starting point in the column until  $m$  elements are selected. This is why the leading dimension must be greater than or equal to  $m$ ; otherwise, you go past the end of each dimension of the array. In the above example, if the number of elements,  $m$ , to be processed in each column is 4, the following elements are selected from array A for the first column of the matrix:  $A(3,0)$ ,  $A(4,0)$ ,  $A(5,0)$ , and  $A(6,0)$ . These are elements 3.0, 4.0, 5.0, and 6.0, corresponding to the matrix elements  $a_{11}$ ,  $a_{21}$ ,  $a_{31}$ , and  $a_{41}$ , respectively.

Column element selection can also be expressed in general terms. Using  $A(\text{BEGINI}, \text{BEGINJ})$  as the starting point in the array, this results in the following elements being selected from each column in the array:

```
A(BEGINI, BEGINJ)
A(BEGINI+1, BEGINJ)
A(BEGINI+2, BEGINJ)
.
.
.
A(BEGINI+m-1, BEGINJ)
```

Combining this with the technique already described for finding the starting point in each column of the array, the resulting matrix in the example is:

$$A = \begin{bmatrix} a_{11} & \cdot & \cdot & \cdot & a_{14} \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ a_{41} & \cdot & \cdot & \cdot & a_{44} \end{bmatrix} = \begin{bmatrix} 3.0 & 10.0 & 17.0 & 24.0 \\ 4.0 & 11.0 & 18.0 & 25.0 \\ 5.0 & 12.0 & 19.0 & 26.0 \\ 6.0 & 13.0 & 20.0 & 27.0 \end{bmatrix}$$

As shown in this example, a matrix does not have to include all columns and rows of an array. The elements of matrix  $A$  are selected from rows 3 through 6 and columns 0 through 3 of the array. Rows 1, 2, and 7 and column 4 of the array are not used.

## Symmetric Matrix

The matrix  $A$  is symmetric if it has the property  $A = A^T$ , which means:

- It has the same number of rows as it has columns; that is, it has  $n$  rows and  $n$  columns.
- The value of every element  $a_{ij}$  on one side of the main diagonal equals its mirror image  $a_{ji}$  on the other side:  $a_{ij} = a_{ji}$  for  $1 \leq i \leq n$  and  $1 \leq j \leq n$ .

The following matrix illustrates a symmetric matrix of order  $n$ ; that is, it has  $n$  rows and  $n$  columns. The subscripts on each side of the diagonal appear the same to show which elements are equal:

$$A = \begin{bmatrix} a_{11} & a_{21} & a_{31} & \cdot & \cdot & \cdot & a_{n1} \\ a_{21} & a_{22} & a_{32} & & & & \cdot \\ a_{31} & a_{32} & a_{33} & & & & \cdot \\ \cdot & & & \cdot & & & \cdot \\ \cdot & & & & \cdot & & \cdot \\ \cdot & & & & & \cdot & \cdot \\ a_{n1} & \cdot & \cdot & \cdot & \cdot & \cdot & a_{nn} \end{bmatrix}$$

## In Storage

The four storage modes used for storing symmetric matrices are described in the following sections:

- “Lower-Packed Storage Mode”
- “Upper-Packed Storage Mode” on page 71
- “Lower Storage Mode” on page 72
- “Upper Storage Mode” on page 72

The storage technique you should use depends on the ESSL subroutine you are using and is given under Notes in each subroutine description.

**Lower-Packed Storage Mode:** When a symmetric matrix is stored in lower-packed storage mode, the lower triangular part of the symmetric matrix is stored, including the diagonal, in a one-dimensional array. The lower triangle is packed by columns. (This is equivalent to packing the upper triangle by rows.) The matrix is packed sequentially column by column in  $n(n+1)/2$  elements of a

one-dimensional array. To calculate the location of each element  $a_{ij}$  of matrix  $A$  in an array, AP, using the lower triangular packed technique, use the following formula:

$$AP(i + ((2n-j)(j-1)/2)) = a_{ij} \quad \text{where } i \geq j$$

This results in the following storage arrangement for the elements of a symmetric matrix  $A$  in an array AP:

<b>AP(1)</b>	= $a_{11}$ (start the first column)
<b>AP(2)</b>	= $a_{21}$
<b>AP(3)</b>	= $a_{31}$
.	.
.	.
.	.
<b>AP(n)</b>	= $a_{n1}$
<b>AP(n+1)</b>	= $a_{22}$ (start the second column)
<b>AP(n+2)</b>	= $a_{32}$
.	.
.	.
.	.
<b>AP(2n-1)</b>	= $a_{n2}$
<b>AP(2n)</b>	= $a_{33}$ (start the third column and so forth)
<b>AP(2n+1)</b>	= $a_{43}$
.	.
.	.
.	.
<b>AP(n(n+1)/2)</b>	= $a_{nn}$

Following is an example of a symmetric matrix that uses the element values to show the order in which the matrix elements are stored in the array.

Given the following matrix  $A$ :

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 6 & 7 & 8 & 9 \\ 3 & 7 & 10 & 11 & 12 \\ 4 & 8 & 11 & 13 & 14 \\ 5 & 9 & 12 & 14 & 15 \end{bmatrix}$$

the array is:

$$AP = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15)$$

**Note:** Additional work storage is required in the array for some ESSL subroutines; for example, in the simultaneous linear algebraic equation subroutines SPPF, DPPF, SPPS, and DPPS. See the description of those subroutines in Part 2, "Reference Information" for details.



Following is an example of how to transform your symmetric matrix to lower-packed storage mode:

```

      K = 0
      DO 1 J=1,N
        DO 2 I=J,N
          K = K+1
          AP(K)=A(I,J)
        2   CONTINUE
      1   CONTINUE

```

**Upper-Packed Storage Mode:** When a symmetric matrix is stored in upper-packed storage mode, the upper triangular part of the symmetric matrix is stored, including the diagonal, in a one-dimensional array. The upper triangle is packed by columns. (This is equivalent to packing the lower triangle by rows.) The matrix is packed sequentially column by column in  $n(n+1)/2$  elements of a one-dimensional array. To calculate the location of each element  $a_{ij}$  of matrix  $A$  in an array  $AP$  using the upper triangular packed technique, use the following formula:

$$AP(i+(j(j-1)/2)) = a_{ij} \quad \text{where } j \geq i$$

This results in the following storage arrangement for the elements of a symmetric matrix  $A$  in an array  $AP$ :

<b>AP(1)</b>	= $a_{11}$ (start the first column)
<b>AP(2)</b>	= $a_{12}$ (start the second column)
<b>AP(3)</b>	= $a_{22}$
<b>AP(4)</b>	= $a_{13}$ (start the third column)
<b>AP(5)</b>	= $a_{23}$
<b>AP(6)</b>	= $a_{33}$
<b>AP(7)</b>	= $a_{14}$ (start the fourth column)
.	.
.	.
.	.
<b>AP(<math>j(j-1)/2+1</math>)</b>	= $a_{1j}$ (start the $j$ -th column)
<b>AP(<math>j(j-1)/2+2</math>)</b>	= $a_{2j}$
<b>AP(<math>j(j-1)/2+3</math>)</b>	= $a_{3j}$
.	.
.	.
.	.
<b>AP(<math>j(j-1)/2+j</math>)</b>	= $a_{jj}$ (end of the $j$ -th column)
.	.
.	.
.	.
<b>AP(<math>n(n+1)/2</math>)</b>	= $a_{nn}$

Following is an example of a symmetric matrix that uses the element values to show the order in which the matrix elements are stored in the array. Given the following matrix *A*:

$$\begin{bmatrix} 1 & 2 & 4 & 7 & 11 \\ 2 & 3 & 5 & 8 & 12 \\ 4 & 5 & 6 & 9 & 13 \\ 7 & 8 & 9 & 10 & 14 \\ 11 & 12 & 13 & 14 & 15 \end{bmatrix}$$

the array is:

$$AP = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15)$$

Following is an example of how to transform your symmetric matrix to upper-packed storage mode:

```

      K = 0
      DO 1 J=1,N
        DO 2 I=1,J
          K = K+1
          AP(K)=A(I,J)
2        CONTINUE
1      CONTINUE

```

**Lower Storage Mode:** When a symmetric matrix is stored in lower storage mode, the lower triangular part of the symmetric matrix is stored, including the diagonal, in a two-dimensional array. These elements are stored in the array in the same way they appear in the matrix. The upper part of the matrix is not required to be stored in the array.

Following is an example of a symmetric matrix *A* of order 5 and how it is stored in an array *AL*.

Given the following matrix *A*:

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 6 & 7 & 8 & 9 \\ 3 & 7 & 10 & 11 & 12 \\ 4 & 8 & 11 & 13 & 14 \\ 5 & 9 & 12 & 14 & 15 \end{bmatrix}$$

the array is:

$$AL = \begin{bmatrix} 1 & * & * & * & * \\ 2 & 6 & * & * & * \\ 3 & 7 & 10 & * & * \\ 4 & 8 & 11 & 13 & * \\ 5 & 9 & 12 & 14 & 15 \end{bmatrix}$$

where “\*” means you do not have to store a value in that position in the array. However, these storage positions are required.

**Upper Storage Mode:** When a symmetric matrix is stored in upper storage mode, the upper triangular part of the symmetric matrix is stored, including the diagonal, in a two-dimensional array. These elements are stored in the array in the same way they appear in the matrix. The lower part of the matrix is not required to be stored in the array.

Following is an example of a symmetric matrix  $A$  of order 5 and how it is stored in an array  $AU$ .

Given the following matrix  $A$ :

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 6 & 7 & 8 & 9 \\ 3 & 7 & 10 & 11 & 12 \\ 4 & 8 & 11 & 13 & 14 \\ 5 & 9 & 12 & 14 & 15 \end{bmatrix}$$

the array is:

$$AU = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ * & 6 & 7 & 8 & 9 \\ * & * & 10 & 11 & 12 \\ * & * & * & 13 & 14 \\ * & * & * & * & 15 \end{bmatrix}$$

where “\*” means you do not have to store a value in that position in the array. However, these storage positions are required.

## Positive Definite or Negative Definite Symmetric Matrix

A real symmetric matrix  $A$  is positive definite if and only if  $x^T Ax$  is positive for all nonzero vectors  $x$ .

A real symmetric matrix  $A$  is negative definite if and only if  $x^T Ax$  is negative for all nonzero vectors  $x$ .

### In Storage

The positive definite or negative definite symmetric matrix is stored in the same way the symmetric matrix is stored. For a description of this storage technique, see “Symmetric Matrix” on page 69.

## Symmetric Indefinite Matrix

A real symmetric matrix  $A$  is indefinite if and only if  $(x^T Ax) (y^T Ay) < 0$  for some non-zero vectors  $x$  and  $y$ .

### In Storage

The symmetric indefinite matrix is stored in the same way the symmetric matrix is stored. For a description of this storage technique, see “Symmetric Matrix” on page 69.

## Complex Hermitian Matrix

A complex matrix is Hermitian if it is equal to its conjugate transpose:

$$H = H^H$$

### In Storage

The complex Hermitian matrix is stored using the same four techniques used for symmetric matrices:

- Lower-packed storage mode, as described in “Lower-Packed Storage Mode” on page 69. (The complex Hermitian matrix is not symmetric; therefore, lower-packed storage mode is not equivalent to packing the upper triangle by rows, as it is for a symmetric matrix.)
- Upper-packed storage mode, as described in “Upper-Packed Storage Mode” on page 71. (The complex Hermitian matrix is not symmetric; therefore, upper-packed storage mode is not equivalent to packing the lower triangle by rows, as it is for a symmetric matrix.)
- Lower storage mode, as described in “Lower Storage Mode” on page 72.
- Upper storage mode, as described in “Upper Storage Mode” on page 72.

Following is an example of a complex Hermitian matrix  $H$  of order 5.

Given the following matrix  $H$ :

$$\begin{bmatrix} (11, 0) & (21, -1) & (31, 1) & (41, -1) & (51, -1) \\ (21, 1) & (22, 0) & (32, -1) & (42, -1) & (52, 1) \\ (31, -1) & (32, 1) & (33, 0) & (43, -1) & (53, -1) \\ (41, 1) & (42, 1) & (43, 1) & (44, 0) & (54, -1) \\ (51, 1) & (52, -1) & (53, 1) & (54, 1) & (55, 0) \end{bmatrix}$$

it is stored in a one-dimensional array, HP, in  $n(n+1)/2 = 15$  elements as follows:

- In lower-packed storage mode:

$$\text{HP} = ((11, *), (21, 1), (31, -1), (41, 1), (51, 1), (22, *), (32, 1), (42, 1), (52, -1), (33, *), (43, 1), (53, 1), (44, *), (54, 1), (55, *))$$

- In upper-packed storage mode:

$$\text{HP} = ((11, *), (21, -1), (22, *), (31, 1), (32, -1), (33, *), (41, -1), (42, -1), (43, -1), (44, *), (51, -1), (52, 1), (53, -1), (54, -1), (55, *))$$

or it is stored in a two-dimensional array, HP, as follows:

- In lower storage mode:

$$\text{HP} = \begin{bmatrix} (11, *) & * & * & * & * \\ (21, 1) & (22, *) & * & * & * \\ (31, -1) & (32, 1) & (33, *) & * & * \\ (41, 1) & (42, 1) & (43, 1) & (44, *) & * \\ (51, 1) & (52, -1) & (53, 1) & (54, 1) & (55, *) \end{bmatrix}$$

- In upper storage mode

$$\text{HP} = \begin{bmatrix} (11, *) & (21, -1) & (31, 1) & (41, -1) & (51, -1) \\ * & (22, *) & (32, -1) & (42, -1) & (52, 1) \\ * & * & (33, *) & (43, -1) & (53, -1) \\ * & * & * & (44, *) & (54, -1) \\ * & * & * & * & (55, *) \end{bmatrix}$$

where “\*” means you do not have to store a value in that position in the array. The imaginary parts of the diagonal elements of a complex Hermitian matrix are always 0, so you do not need to set these values. The ESSL subroutines always assume that the values in these positions are 0.

## Positive Definite or Negative Definite Complex Hermitian Matrix

A complex Hermitian matrix  $A$  is positive definite if and only if  $x^H A x$  is positive for all nonzero vectors  $x$ .

A complex Hermitian matrix  $A$  is negative definite if and only if  $x^H A x$  is negative for all nonzero vectors  $x$ .

### In Storage

The positive definite or negative definite complex Hermitian matrix is stored in the same way the complex Hermitian matrix is stored. For a description of this storage technique, see “Complex Hermitian Matrix” on page 73.

## Positive Definite or Negative Definite Symmetric Toeplitz Matrix

A positive definite or negative definite symmetric matrix  $A$  of order  $n$  is also a Toeplitz matrix if and only if:

$$a_{ij} = a_{i-1,j-1} \quad \text{for } i = 2, n \text{ and } j = 2, n$$

The elements on each diagonal of the Toeplitz matrix have a constant value. For the definition of a positive definite or negative definite symmetric matrix, see “Positive Definite or Negative Definite Symmetric Matrix” on page 73.

The following matrix illustrates a symmetric Toeplitz matrix of order  $n$ ; that is, it has  $n$  rows and  $n$  columns:

$$A = \begin{bmatrix} a_{11} & a_{21} & a_{31} & \cdot & \cdot & \cdot & a_{n1} \\ a_{21} & a_{11} & a_{21} & \cdot & \cdot & \cdot & \cdot \\ a_{31} & a_{21} & a_{11} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & a_{31} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & a_{21} & \cdot \\ a_{n1} & \cdot & \cdot & \cdot & a_{31} & a_{21} & a_{11} \end{bmatrix}$$

A symmetric Toeplitz matrix of order  $n$  is represented by a vector  $x$  of length  $n$  containing the elements of the first column of the matrix (or the elements of the first row), such that  $x_i = a_{i1}$  for  $i = 1, n$ .

The following vector represents the matrix  $A$  shown above:

$$x = \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ \cdot \\ \cdot \\ a_{n1} \end{bmatrix}$$

## In Storage

The elements of the vector  $x$ , which represent a positive definite symmetric Toeplitz matrix, are stored sequentially in an array. This is called packed-symmetric-Toeplitz storage mode. Following is an example of a positive definite symmetric Toeplitz matrix  $A$  and how it is stored in an array  $x$ .

Given the following matrix  $A$ :

$$\begin{bmatrix} 99 & 12 & 13 & 14 & 15 & 16 \\ 12 & 99 & 12 & 13 & 14 & 15 \\ 13 & 12 & 99 & 12 & 13 & 14 \\ 14 & 13 & 12 & 99 & 12 & 13 \\ 15 & 14 & 13 & 12 & 99 & 12 \\ 16 & 15 & 14 & 13 & 12 & 99 \end{bmatrix}$$

the array is:

$$x = (99, 12, 13, 14, 15, 16)$$

## Positive Definite or Negative Definite Complex Hermitian Toeplitz Matrix

A positive definite or negative definite complex Hermitian matrix  $A$  of order  $n$  is also a Toeplitz matrix if and only if:

$$a_{ij} = a_{i-1,j-1} \quad \text{for } i = 2, n \text{ and } j = 2, n$$

The real part of the diagonal elements of the Toeplitz matrix must have a constant value. The imaginary part of the diagonal elements must be zero.

For the definition of a positive definite or negative definite complex Hermitian matrix, see "Positive Definite or Negative Definite Complex Hermitian Matrix" on page 75.

The following matrix illustrates a complex Hermitian Toeplitz matrix of order  $n$ ; that is, it has  $n$  rows and  $n$  columns:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdot & \cdot & \cdot & a_{1n} \\ \bar{a}_{12} & a_{11} & a_{12} & \cdot & & & \cdot \\ \bar{a}_{13} & \bar{a}_{12} & a_{11} & \cdot & & & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & a_{13} & & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & a_{12} & \cdot \\ \bar{a}_{1n} & \cdot & \cdot & \cdot & \bar{a}_{13} & \bar{a}_{12} & a_{11} \end{bmatrix}$$

A complex Hermitian Toeplitz matrix of order  $n$  is represented by a vector  $x$  of length  $n$  containing the elements of the first row of the matrix.

The following vector represents the matrix  $A$  shown above.

$$\mathbf{x} = \begin{bmatrix} a_{11} \\ a_{12} \\ a_{13} \\ \vdots \\ a_{1n} \end{bmatrix}$$

## In Storage

The elements of the vector  $\mathbf{x}$ , which represent a positive definite complex Hermitian Toeplitz matrix, are stored sequentially in an array. This is called packed-Hermitian-Toeplitz storage mode. Following is an example of a positive definite complex Hermitian Toeplitz matrix  $A$  and how it is stored in an array  $\mathbf{x}$ .

Given the following matrix  $A$ :

$$\begin{bmatrix} (10.0, 0.0) & (2.0, -3.0) & (-3.0, 1.0) & (1.0, 1.0) \\ (2.0, 3.0) & (10.0, 0.0) & (2.0, -3.0) & (-3.0, 1.0) \\ (-3.0, -1.0) & (2.0, 3.0) & (10.0, 0.0) & (2.0, -3.0) \\ (1.0, -1.0) & (-3.0, -1.0) & (2.0, 3.0) & (10.0, 0.0) \end{bmatrix}$$

the array is:

$$\mathbf{x} = ((10.0, 0.0), (2.0, -3.0), (-3.0, 1.0), (1.0, 1.0))$$

## Triangular Matrix

There are two types of triangular matrices: upper triangular matrix and lower triangular matrix. Triangular matrices have the same number of rows as they have columns; that is, they have  $n$  rows and  $n$  columns.

A matrix  $\mathbf{U}$  is an upper triangular matrix if its nonzero elements are found only in the upper triangle of the matrix, including the main diagonal; that is:

$$u_{ij} = 0 \quad \text{if } i > j$$

A matrix  $\mathbf{L}$  is a lower triangular matrix if its nonzero elements are found only in the lower triangle of the matrix, including the main diagonal; that is:

$$l_{ij} = 0 \quad \text{if } i < j$$

The following matrices,  $\mathbf{U}$  and  $\mathbf{L}$ , illustrate upper and lower triangular matrices of order  $n$ , respectively:

$$\mathbf{U} = \begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & & \cdot \\ 0 & 0 & u_{33} & & \cdot \\ \cdot & & & \cdot & \cdot \\ \cdot & & & & \cdot \\ 0 & \cdot & \cdot & \cdot & u_{nn} \end{bmatrix} \quad \mathbf{L} = \begin{bmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ l_{21} & l_{22} & 0 & & \cdot \\ l_{31} & l_{32} & l_{33} & & \cdot \\ \cdot & & & \cdot & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & 0 \\ l_{n1} & \cdot & \cdot & \cdot & l_{nn} \end{bmatrix}$$

A unit triangular matrix is a triangular matrix in which all the diagonal elements have a value of one; that is:

- For an upper triangular matrix,  $u_{ij} = 1$  if  $i = j$ .
- For a lower triangular matrix,  $l_{ij} = 1$  if  $i = j$ .

The following matrices,  $\mathbf{U}$  and  $\mathbf{L}$ , illustrate upper and lower unit real triangular matrices of order  $n$ , respectively:

$$\mathbf{U} = \begin{bmatrix} 1 & u_{12} & u_{13} & \dots & u_{1n} \\ 0 & 1 & u_{23} & & \cdot \\ 0 & 0 & 1 & & \cdot \\ \cdot & & & \cdot & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ 0 & \cdot & \cdot & \cdot & 1 \end{bmatrix} \quad \mathbf{L} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ l_{21} & 1 & 0 & & \cdot \\ l_{31} & l_{32} & 1 & & \cdot \\ \cdot & & \cdot & \cdot & \cdot \\ \cdot & & & \cdot & \cdot \\ \cdot & & & & 0 \\ l_{n1} & \cdot & \cdot & \cdot & 1 \end{bmatrix}$$

### In Storage

The four storage modes used for storing triangular matrices are described in the following sections:

- “Upper-Triangular-Packed Storage Mode”
- “Lower-Triangular-Packed Storage Mode”
- “Upper-Triangular Storage Mode” on page 79
- “Lower-Triangular Storage Mode” on page 79

**It is important to note that because the diagonal elements of a unit triangular matrix are always one, you do not need to set these values in the array for these four storage modes. ESSL always assumes that the values in these positions are one.**

**Upper-Triangular-Packed Storage Mode:** When an upper-triangular matrix is stored in upper-triangular-packed storage mode, the upper triangle of the matrix is stored, including the diagonal, in a one-dimensional array. The upper triangle is packed by columns. The elements are packed sequentially, column by column, in  $n(n+1)/2$  elements of a one-dimensional array. To calculate the location of each element of the triangular matrix in the array, use the technique described in “Upper-Packed Storage Mode” on page 71.

Following is an example of an upper triangular matrix  $\mathbf{U}$  of order 5 and how it is stored in array UP. It uses the element values to show the order in which the elements are stored in the one-dimensional array.

Given the following matrix  $\mathbf{U}$ :

$$\begin{bmatrix} 1 & 2 & 4 & 7 & 11 \\ 0 & 3 & 5 & 8 & 12 \\ 0 & 0 & 6 & 9 & 13 \\ 0 & 0 & 0 & 10 & 14 \\ 0 & 0 & 0 & 0 & 15 \end{bmatrix}$$

the array is:

$$\text{UP} = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15)$$

**Lower-Triangular-Packed Storage Mode:** When a lower-triangular matrix is stored in lower-triangular-packed storage mode, the lower triangle of the matrix is



stored, including the diagonal, in a one-dimensional array. The lower triangle is packed by columns. The elements are packed sequentially, column by column, in  $n(n+1)/2$  elements of a one-dimensional array. To calculate the location of each element of the triangular matrix in the array, use the technique described in “Lower-Packed Storage Mode” on page 69.

Following is an example of a lower triangular matrix  $L$  of order 5 and how it is stored in array LP. It uses the element values to show the order in which the elements are stored in the one-dimensional array.

Given the following matrix  $L$ :

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 2 & 6 & 0 & 0 & 0 \\ 3 & 7 & 10 & 0 & 0 \\ 4 & 8 & 11 & 13 & 0 \\ 5 & 9 & 12 & 14 & 15 \end{bmatrix}$$

the array is:

$$LP = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15)$$

**Upper-Triangular Storage Mode:** A triangular matrix is stored in upper-triangular storage mode in a two-dimensional array. Only the elements in the upper triangle of the matrix, including the diagonal, are stored in the upper triangle of the array.

Following is an example of an upper triangular matrix  $U$  of order 5 and how it is stored in array UTA.

Given the following matrix  $U$ :

$$\begin{bmatrix} 11 & 12 & 13 & 14 & 15 \\ 0 & 22 & 23 & 24 & 25 \\ 0 & 0 & 33 & 34 & 35 \\ 0 & 0 & 0 & 44 & 45 \\ 0 & 0 & 0 & 0 & 55 \end{bmatrix}$$

the array is:

$$UTA = \begin{bmatrix} 11 & 12 & 13 & 14 & 15 \\ * & 22 & 23 & 24 & 25 \\ * & * & 33 & 34 & 35 \\ * & * & * & 44 & 45 \\ * & * & * & * & 55 \end{bmatrix}$$

where “\*” means you do not have to store a value in that position in the array.

**Lower-Triangular Storage Mode:** A triangular matrix is stored in lower-triangular storage mode in a two-dimensional array. Only the elements in the lower triangle of the matrix, including the diagonal, are stored in the lower triangle of the array.

Following is an example of a lower triangular matrix  $L$  of order 5 and how it is stored in array LTA.

Given the following matrix  $L$ :

$$\begin{bmatrix} 11 & 0 & 0 & 0 & 0 \\ 21 & 22 & 0 & 0 & 0 \\ 31 & 32 & 33 & 0 & 0 \\ 41 & 42 & 43 & 44 & 0 \\ 51 & 52 & 53 & 54 & 55 \end{bmatrix}$$

the array is:

$$\text{LTA} = \begin{bmatrix} 11 & * & * & * & * \\ 21 & 22 & * & * & * \\ 31 & 32 & 33 & * & * \\ 41 & 42 & 43 & 44 & * \\ 51 & 52 & 53 & 54 & 55 \end{bmatrix}$$

where “\*” means you do not have to store a value in that position in the array.

## General Band Matrix

A general band matrix has its nonzero elements arranged uniformly near the diagonal, such that:

$$a_{ij} = 0 \quad \text{if } (i-j) > ml \text{ or } (j-i) > mu$$

where  $ml$  and  $mu$  are the lower and upper band widths, respectively, and  $ml+mu+1$  is the total band width.

The following matrix illustrates a **square** general band matrix of order  $n$ , where the band widths are  $ml = q-1$  and  $mu = p-1$ :

$$A = \begin{array}{c} \begin{array}{c} | \leftarrow mu \rightarrow | \\ \uparrow \\ ml \\ \downarrow \\ - \end{array} \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdot & \cdot & a_{1p} & 0 & \cdot & \cdot & 0 \\ a_{21} & a_{22} & a_{23} & & & & \cdot & 0 & & \cdot \\ a_{31} & a_{32} & a_{33} & & & & & \cdot & 0 & \cdot \\ \cdot & & & & & & & & \cdot & 0 \\ \cdot & & & & & & & & & \cdot \\ a_{q1} & & & & & & & & & \cdot \\ 0 & & & & & & & & & \cdot \\ \cdot & 0 & & & & & & & & \cdot \\ \cdot & & 0 & & & & & & & \cdot \\ 0 & & \cdot & 0 & & & & & & \cdot \\ & & & & & & & & & a_{nn} \end{bmatrix} \end{array}$$

Some special types of band matrices are:

- Tridiagonal matrix:  $ml = mu = 1$
- 9-diagonal matrix:  $ml = mu = 4$

The following two matrices illustrate  $m$  by  $n$  **rectangular** general band matrices, where the band widths are  $ml = q-1$  and  $mu = p-1$ . For both matrices, the leading diagonal is  $a_{11}, a_{22}, a_{33}, \dots, a_{nn}$ . Following is a general band matrix with  $m > n$ :

$$\begin{array}{c}
 \begin{array}{c}
 \left| \leftarrow mu \rightarrow \right| \\
 \left[ \begin{array}{cccccccc}
 a_{11} & a_{12} & a_{13} & \cdot & \cdot & a_{1p} & 0 & \cdot & \cdot & 0 \\
 a_{21} & a_{22} & a_{23} & & & & \cdot & 0 & & \cdot \\
 a_{31} & a_{32} & a_{33} & & & & & \cdot & 0 & \cdot \\
 \cdot & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & \cdot \\
 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & \cdot & \cdot & a_{mn}
 \end{array} \right] \\
 \begin{array}{c}
 - \\
 \uparrow \\
 ml \\
 \downarrow \\
 -
 \end{array}
 \end{array}
 \end{array}
 A =$$

Following is a general band matrix with  $m < n$ :

$$\begin{array}{c}
 \begin{array}{c}
 \left| \leftarrow mu \rightarrow \right| \\
 \left[ \begin{array}{cccccccccccc}
 a_{11} & a_{12} & a_{13} & \cdot & \cdot & a_{1p} & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\
 a_{21} & a_{22} & a_{23} & & & & \cdot & 0 & & & & \cdot \\
 a_{31} & a_{32} & a_{33} & & & & & \cdot & 0 & & & \cdot \\
 \cdot & & & & & & & & \cdot & 0 & & \cdot \\
 \cdot & & & & & & & & & \cdot & 0 & \cdot \\
 \cdot & & & & & & & & & & \cdot & 0 \\
 \cdot & & & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & & & \cdot \\
 0 & \cdot & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a_{nm} & \cdot & \cdot & a_{mn}
 \end{array} \right] \\
 \begin{array}{c}
 - \\
 \uparrow \\
 ml \\
 \downarrow \\
 -
 \end{array}
 \end{array}
 \end{array}
 A =$$

### In Storage

The two storage modes used for storing general band matrices are described in the following sections:

- "General-Band Storage Mode"
- "BLAS-General-Band Storage Mode" on page 83

**General-Band Storage Mode:** (This storage mode is used only for square matrices.) Only the band elements of a general band matrix are stored for general-band storage mode. Additional storage must also be provided for fill-in. General-band storage mode packs the matrix elements by columns into a two-dimensional array, such that each diagonal of the matrix appears as a row in the packed array.

For a matrix  $A$  of order  $n$  with band widths  $ml$  and  $mu$ , the array must have a leading dimension,  $lda$ , greater than or equal to  $2ml+mu+16$ . The size of the second dimension must be (at least)  $n$ , the number of columns in the matrix.

Using array AGB, which is declared as  $AGB(2ml+mu+16, n)$ , the columns of elements in matrix  $A$  are stored in each column in array AGB as follows, where  $a_{11}$  is stored at  $AGB(ml+mu+1, 1)$ :

$$\begin{array}{c}
 \leftarrow \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \rightarrow \\
 \begin{array}{c}
 \uparrow \\
 ml \\
 \downarrow \\
 \uparrow \\
 \\
 mu \\
 \downarrow \\
 \uparrow \\
 ml \\
 \downarrow \\
 \uparrow \\
 15 \\
 \downarrow \\
 \downarrow
 \end{array}
 \left[ \begin{array}{cccccccc}
 * & \cdot & \cdot & \cdot & & & & * \\
 \cdot & & & & & & & \cdot \\
 \cdot & & & & & & & * \\
 \cdot & & & & & a_{1p} & a_{2,p+1} & \cdot & \cdot & \cdot & \cdot & \cdot & a_{n-mu,n} \\
 \cdot & & & & & \cdot & \cdot & \cdot & & & & & \cdot \\
 \cdot & & & & & \cdot & \cdot & \cdot & & & & & \cdot \\
 \cdot & & & a_{13} & & \cdot & \cdot & \cdot & & & & & \cdot \\
 * & a_{12} & \cdot & & & & & & & & & & \cdot \\
 a_{11} & \cdot & \cdot & & & & & & & & & & a_{m} \\
 \cdot & \cdot & \cdot & & & & & & & & & & \cdot \\
 \cdot & \cdot & & & & & & & & & & & * \\
 \cdot & & & & & & & & & & & & \cdot \\
 a_{q1} & a_{q+1,2} & \cdot & & & a_{q+mu,p} & \cdot & \cdot & & & a_{n,n-ml} & & \cdot \\
 * & & & & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & & & & \cdot \\
 \cdot & & & & & & & & & & & & \cdot \\
 * & \cdot & \cdot & \cdot & & & & & & & & & *
 \end{array} \right]
 \end{array}$$

where “\*” means you do not store an element in that position in the array.

In the ESSL subroutine computation, some of the positions in the array indicated by an “\*” are used for fill-in. Other positions may not be accessed at all.

Following is an example of a band matrix  $A$  of order 9 and band widths of  $ml = 2$  and  $mu = 3$ .

Given the following matrix  $A$ :

$$\begin{bmatrix}
 11 & 12 & 13 & 14 & 0 & 0 & 0 & 0 & 0 \\
 21 & 22 & 23 & 24 & 25 & 0 & 0 & 0 & 0 \\
 31 & 32 & 33 & 34 & 35 & 36 & 0 & 0 & 0 \\
 0 & 42 & 43 & 44 & 45 & 46 & 47 & 0 & 0 \\
 0 & 0 & 53 & 54 & 55 & 56 & 57 & 58 & 0 \\
 0 & 0 & 0 & 64 & 65 & 66 & 67 & 68 & 69 \\
 0 & 0 & 0 & 0 & 75 & 76 & 77 & 78 & 79 \\
 0 & 0 & 0 & 0 & 0 & 86 & 87 & 88 & 89 \\
 0 & 0 & 0 & 0 & 0 & 0 & 97 & 98 & 99
 \end{bmatrix}$$

you store it in general-band storage mode in a 23 by 9 array AGB as follows, where  $a_{11}$  is stored in  $AGB(6,1)$ :

$$\begin{bmatrix}
 * & * & * & * & * & * & * & * & * \\
 * & * & * & * & * & * & * & * & *
 \end{bmatrix}$$

	*	*	*	14	25	36	47	58	69
	*	*	13	24	35	46	57	68	79
	*	12	23	34	45	56	67	78	89
11	22	33	44	55	66	77	88	99	
21	32	43	54	65	76	87	98	*	*
31	42	53	64	75	86	97	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
AGB =	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*
	*	*	*	*	*	*	*	*	*

Following is an example of how to transform your general band matrix, of order  $n$ , to general-band storage mode:

```

MD=ML+MU+1
DO 1 J=1,N
    DO 1 I=MAX(J-MU,1),MIN(J+ML,N)
        AGB(I-J+MD,J)=A(I,J)
1    CONTINUE

```

**BLAS-General-Band Storage Mode:** (This storage mode is used for both square and rectangular matrices.) Only the band elements of a general band matrix are stored for BLAS-general-band storage mode. The storage mode packs the matrix elements by columns into a two-dimensional array, such that each diagonal of the matrix appears as a row in the packed array.

For an  $m$  by  $n$  matrix  $A$  with band widths  $ml$  and  $mu$ , the array AGB must have a leading dimension,  $lda$ , greater than or equal to  $ml+mu+1$ . The size of the second dimension must be (at least)  $n$ , the number of columns in the matrix.

Using the array AGB, which is declared as  $AGB(ml+mu+1, n)$ , the columns of elements in matrix  $A$  are stored in each column in array AGB as follows, where  $a_{11}$  is stored at  $AGB(mu+1, 1)$ :

$$\text{AGB} = \begin{array}{c} \overline{\uparrow} \\ \text{mu} \\ \downarrow \overline{1} \\ \uparrow \\ \text{ml} \\ \downarrow \overline{2} \end{array} \left[ \begin{array}{cccccccc} \leftarrow & & & & & n & & \rightarrow \\ * & \cdot & \cdot & \cdot & * & a_{1p} & a_{2,p+1} & \cdot & \cdot & \cdot \\ \cdot & & & & \cdot & \cdot & \cdot & & & \\ \cdot & & a_{13} & & & \cdot & \cdot & & & \\ * & a_{12} & \cdot & & & \cdot & \cdot & & & \\ \overline{1} & a_{11} & \cdot & & & & & & & \\ \cdot & \cdot & \cdot & & & & & & & \\ \cdot & \cdot & & & & & & & & \\ \cdot & & & & & & & & & \\ \downarrow \overline{2} & a_{q1} & a_{q+1,2} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{array} \right]$$

where “\*” means you do not store an element in that position in the array. These positions are not accessed by ESSL. **Unused positions in the array always occur in the upper left triangle of the array, but may not occur in the lower right triangle of the array, as you can see from the examples given here.**

Following is an example where  $m > n$ , and general band matrix  $A$  is 9 by 8 with band widths of  $ml = 2$  and  $mu = 3$ .

Given the following matrix  $A$ :

$$\begin{bmatrix} 11 & 12 & 13 & 14 & 0 & 0 & 0 & 0 \\ 21 & 22 & 23 & 24 & 25 & 0 & 0 & 0 \\ 31 & 32 & 33 & 34 & 35 & 36 & 0 & 0 \\ 0 & 42 & 43 & 44 & 45 & 46 & 47 & 0 \\ 0 & 0 & 53 & 54 & 55 & 56 & 57 & 58 \\ 0 & 0 & 0 & 64 & 65 & 66 & 67 & 68 \\ 0 & 0 & 0 & 0 & 75 & 76 & 77 & 78 \\ 0 & 0 & 0 & 0 & 0 & 86 & 87 & 88 \\ 0 & 0 & 0 & 0 & 0 & 0 & 97 & 98 \end{bmatrix}$$

you store it in array  $\text{AGB}$ , declared as  $\text{AGB}(6,8)$ , as follows, where  $a_{11}$  is stored in  $\text{AGB}(4,1)$ :

$$\text{AGB} = \begin{bmatrix} * & * & * & 14 & 25 & 36 & 47 & 58 \\ * & * & 13 & 24 & 35 & 46 & 57 & 68 \\ * & 12 & 23 & 34 & 45 & 56 & 67 & 78 \\ 11 & 22 & 33 & 44 & 55 & 66 & 77 & 88 \\ 21 & 32 & 43 & 54 & 65 & 76 & 87 & 98 \\ 31 & 42 & 53 & 64 & 75 & 86 & 97 & * \end{bmatrix}$$

Following is an example where  $m < n$ , and general band matrix  $A$  is 7 by 9 with band widths of  $ml = 2$  and  $mu = 3$ .

Given the following matrix  $A$ :

$$\begin{bmatrix} 11 & 12 & 13 & 14 & 0 & 0 & 0 & 0 & 0 \\ 21 & 22 & 23 & 24 & 25 & 0 & 0 & 0 & 0 \\ 31 & 32 & 33 & 34 & 35 & 36 & 0 & 0 & 0 \\ 0 & 42 & 43 & 44 & 45 & 46 & 47 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 53 & 54 & 55 & 56 & 57 & 58 & 0 \\ 0 & 0 & 0 & 64 & 65 & 66 & 67 & 68 & 69 \\ 0 & 0 & 0 & 0 & 75 & 76 & 77 & 78 & 79 \end{bmatrix}$$

you store it in array AGB, declared as AGB(6,9), as follows, where  $a_{11}$  is stored in AGB(4,1) and the leading diagonal does not fill up the whole row:

$$\text{AGB} = \begin{bmatrix} * & * & * & 14 & 25 & 36 & 47 & 58 & 69 \\ * & * & 13 & 24 & 35 & 46 & 57 & 68 & 79 \\ * & 12 & 23 & 34 & 45 & 56 & 67 & 78 & * \\ 11 & 22 & 33 & 44 & 55 & 66 & 77 & * & * \\ 21 & 32 & 43 & 54 & 65 & 76 & * & * & * \\ 31 & 42 & 53 & 64 & 75 & * & * & * & * \end{bmatrix}$$

and where “\*” means you do not store an element in that position in the array.

Following is an example of how to transform your general band matrix, for all values of  $m$  and  $n$ , to BLAS-general-band storage mode:

```

DO 20 J=1,N
  K=MU+1-J
  DO 10 I=MAX(1,J-MU),MIN(M,J+ML)
    AGB(K+I,J)=A(I,J)
10  CONTINUE
20  CONTINUE

```

## Symmetric Band Matrix

A symmetric band matrix is a symmetric matrix whose nonzero elements are arranged uniformly near the diagonal, such that:

$$a_{ij} = 0 \quad \text{if } |i-j| > k$$

where  $k$  is the half band width.

The following matrix illustrates a symmetric band matrix of order  $n$ , where the half band width  $k = q-1$ :

$$A = \begin{array}{c} | \leftarrow k \rightarrow | \\ \begin{bmatrix} a_{11} & a_{21} & a_{31} & \cdot & \cdot & a_{q1} & 0 & \cdot & \cdot & 0 \\ a_{21} & a_{22} & a_{32} & & & & 0 & \cdot & & \\ a_{31} & a_{32} & a_{33} & & & & & 0 & \cdot & \\ \cdot & & & \cdot & & & & & 0 & \\ \cdot & & & & \cdot & & & & & \cdot \\ a_{q1} & & & & & \cdot & & & & \cdot \\ 0 & & & & & & \cdot & & & \cdot \\ \cdot & 0 & & & & & & \cdot & & \cdot \\ \cdot & & 0 & & & & & & \cdot & \\ 0 & \cdot & \cdot & 0 & \cdot & \cdot & \cdot & & & a_{nn} \end{bmatrix} \end{array}$$

## In Storage

The two storage modes used for storing symmetric band matrices are described in the following sections:

- “Upper-Band-Packed Storage Mode” on page 86

- “Lower-Band-Packed Storage Mode” on page 87

**Upper-Band-Packed Storage Mode:** Only the band elements of the upper triangular part of a symmetric band matrix, including the main diagonal, are stored for upper-band-packed storage mode.

For a matrix  $A$  of order  $n$  and a half band width of  $k$ , the array must have a leading dimension,  $lda$ , greater than or equal to  $k+1$ , and the size of the second dimension must be (at least)  $n$ .

Using array  $ASB$ , which is declared as  $ASB(lda,n)$ , where  $p = lda = k+1$ , the elements of a symmetric band matrix are stored as follows:

$$ASB = \begin{bmatrix} * & \cdot & \cdot & \cdot & * & a_{1p} & a_{2,p+1} & \cdot & \cdot & \cdot & a_{n-k,n} \\ \cdot & & & & \cdot & & & & & & \\ \cdot & & & & \cdot & & & & & & \\ \cdot & & & & \cdot & & & & & & \\ & & * & a_{13} & a_{24} & \cdot & \cdot & \cdot & & & \\ * & a_{12} & a_{23} & \cdot & \cdot & \cdot & & & & & \\ a_{11} & a_{22} & \cdot & \cdot & \cdot & & & & & & a_{nn} \end{bmatrix}$$

where “\*” means you do not store an element in that position in the array.

Following is an example of a symmetric band matrix  $A$  of order 6 and a half band width of 3.

Given the following matrix  $A$ :

$$\begin{bmatrix} 11 & 12 & 13 & 14 & 0 & 0 \\ 12 & 22 & 23 & 24 & 25 & 0 \\ 13 & 23 & 33 & 34 & 35 & 36 \\ 14 & 24 & 34 & 44 & 45 & 46 \\ 0 & 25 & 35 & 45 & 55 & 56 \\ 0 & 0 & 36 & 46 & 56 & 66 \end{bmatrix}$$

you store it in upper-band-packed storage mode in array  $ASB$ , declared as  $ASB(4,6)$ , as follows.

$$ASB = \begin{bmatrix} * & * & * & 14 & 25 & 36 \\ * & * & 13 & 24 & 35 & 46 \\ * & 12 & 23 & 34 & 45 & 56 \\ 11 & 22 & 33 & 44 & 55 & 66 \end{bmatrix}$$

Following is an example of how to transform your symmetric band matrix to upper-band-packed storage mode:

```

DO 20 J=1,N
  M=K+1-J
  DO 10 I=MAX(1,J-K),J
    ASB(M+I,J)=A(I,J)
  10 CONTINUE
20 CONTINUE

```



**Lower-Band-Packed Storage Mode:** Only the band elements of the lower triangular part of a symmetric band matrix, including the main diagonal, are stored for lower-band-packed storage mode.

For a matrix  $A$  of order  $n$  and a half band width of  $k$ , the array must have a leading dimension,  $lda$ , greater than or equal to  $k+1$ , and the size of the second dimension must be (at least)  $n$ .

Using array  $ASB$ , which is declared as  $ASB(lda,n)$ , where  $q = lda = k+1$ , the elements of a symmetric band matrix are stored as follows:

$$ASB = \begin{bmatrix} a_{11} & a_{22} & \dots & & a_{nn} \\ a_{21} & a_{32} & & & * \\ a_{31} & a_{42} & & & \cdot \\ \cdot & \cdot & & & \cdot \\ \cdot & \cdot & & & \cdot \\ \cdot & \cdot & & & \cdot \\ a_{q1} & a_{q+1,2} & \dots & a_{n,n-k} & * & \dots & * \end{bmatrix}$$

where “\*” means you do not store an element in that position in the array.

Following is an example of a symmetric band matrix  $A$  of order 6 and a half band width of 2.

Given the following matrix  $A$ :

$$\begin{bmatrix} 11 & 21 & 31 & 0 & 0 & 0 \\ 21 & 22 & 32 & 42 & 0 & 0 \\ 31 & 32 & 33 & 43 & 53 & 0 \\ 0 & 42 & 43 & 44 & 54 & 64 \\ 0 & 0 & 53 & 54 & 55 & 65 \\ 0 & 0 & 0 & 64 & 65 & 66 \end{bmatrix}$$

you store it in lower-band-packed storage mode in array  $ASB$ , declared as  $ASB(3,6)$ , as follows:

$$ASB = \begin{bmatrix} 11 & 22 & 33 & 44 & 55 & 66 \\ 21 & 32 & 43 & 54 & 65 & * \\ 31 & 42 & 53 & 64 & * & * \end{bmatrix}$$

Following is an example of how to transform your symmetric band matrix to lower-band-packed storage mode:

```
DO 20 J=1,N
  DO 10 I=J,MIN(J+K,N)
    ASB(I-J+1,J)=A(I,J)
  10 CONTINUE
20 CONTINUE
```

## Positive Definite Symmetric Band Matrix

A real symmetric band matrix  $A$  is positive definite if and only if  $x^T A x$  is positive for all nonzero vectors  $x$ .

## In Storage

The positive definite symmetric band matrix is stored in the same way a symmetric band matrix is stored. For a description of this storage technique, see “Symmetric Band Matrix” on page 85.

## Complex Hermitian Band Matrix

A complex band matrix is Hermitian if it is equal to its conjugate transpose:

$$H = H^H$$

### In Storage

The complex Hermitian band matrix is stored using the same two techniques used for symmetric band matrices:

- Lower-band-packed storage mode, as described in “Lower-Band-Packed Storage Mode” on page 87
- Upper-band-packed storage mode, as described in “Upper-Band-Packed Storage Mode” on page 86

Following is an example of a complex Hermitian band matrix  $H$  of order 5, having a half band width of 2.

Given the following matrix  $H$ :

$$\begin{bmatrix} (11, 0) & (21, -1) & (31, 1) & (0, 0) & (0, 0) \\ (21, 1) & (22, 0) & (32, -1) & (42, -1) & (0, 0) \\ (31, -1) & (32, 1) & (33, 0) & (43, -1) & (53, -1) \\ (0, 0) & (42, 1) & (43, 1) & (44, 0) & (54, -1) \\ (0, 0) & (0, 0) & (53, 1) & (54, 1) & (55, 0) \end{bmatrix}$$

you store it in a two-dimensional array HP, as follows:

- In lower-band-packed storage mode:

$$HP = \begin{bmatrix} (11, *) & (22, *) & (33, *) & (44, *) & (55, *) \\ (21, 1) & (32, 1) & (43, 1) & (54, 1) & * \\ (31, -1) & (42, 1) & (53, 1) & * & * \end{bmatrix}$$

- In upper-band-packed storage mode:

$$HP = \begin{bmatrix} * & * & (31, 1) & (42, -1) & (53, -1) \\ * & (21, -1) & (32, -1) & (43, -1) & (54, -1) \\ (11, *) & (22, *) & (33, *) & (44, *) & (55, *) \end{bmatrix}$$

where “\*” means you do not have to store a value in that position in the array.

The imaginary parts of the diagonal elements of a complex Hermitian band matrix are always 0, so you do not need to set these values. The ESSL subroutines always assume that the values in these positions are 0.

## Triangular Band Matrix

There are two types of triangular band matrices: upper triangular band matrix and lower triangular band matrix. Triangular band matrices have the same number of rows as they have columns; that is, they have  $n$  rows and  $n$  columns. They have an upper or lower band width of  $k$ .

A band matrix  $\mathbf{U}$  is an upper triangular band matrix if its nonzero elements are found only in the upper triangle of the matrix, including the main diagonal; that is:

$$u_{ij} = 0 \quad \text{if } i > j$$

Its band elements are arranged uniformly near the diagonal in the upper triangle of the matrix, such that:

$$u_{ij} = 0 \quad \text{if } j-i > k$$

The following matrix  $\mathbf{U}$  illustrates an upper triangular band matrix of order  $n$  with an upper band width  $k = q-1$ :

$$\mathbf{U} = \begin{array}{c} | \leftarrow k \rightarrow | \\ \left[ \begin{array}{cccccccc} u_{11} & u_{21} & u_{31} & \cdot & \cdot & u_{q1} & 0 & \cdot & \cdot & 0 \\ 0 & u_{22} & u_{32} & & & & 0 & & \cdot & \\ \cdot & 0 & u_{33} & & & & & & 0 & \cdot \\ \cdot & & & \cdot & & & & & & 0 \\ \cdot & & & & \cdot & & & & & \cdot \\ \cdot & & & & & \cdot & & & & \cdot \\ \cdot & & & & & & \cdot & & & \cdot \\ 0 & \cdot & \cdot & \cdot & & & & \cdot & & 0 \\ & & & & & & & & & u_{nn} \end{array} \right] \end{array}$$

A band matrix  $\mathbf{L}$  is a lower triangular band matrix if its nonzero elements are found only in the lower triangle of the matrix, including the main diagonal; that is:

$$l_{ij} = 0 \quad \text{if } i < j$$

Its band elements are arranged uniformly near the diagonal in the lower triangle of the matrix such that:

$$l_{ij} = 0 \quad \text{if } i-j > k$$

The following matrix  $\mathbf{L}$  illustrates an upper triangular band matrix of order  $n$  with a lower band width  $k = q-1$ :

$$\mathbf{L} = \begin{array}{c} - \\ \uparrow \\ k \\ \downarrow \\ - \end{array} \left[ \begin{array}{cccccccc} l_{11} & 0 & \cdot & \cdot & \cdot & & & 0 \\ l_{21} & l_{22} & 0 & & & & & \cdot \\ l_{31} & l_{32} & l_{33} & & & & & \cdot \\ \cdot & & & \cdot & & & & \cdot \\ \cdot & & & & \cdot & & & \cdot \\ l_{q1} & & & & & \cdot & & \cdot \\ 0 & & & & & & \cdot & \\ \cdot & 0 & & & & & & \cdot \\ \cdot & & 0 & & & & & \cdot \\ 0 & \cdot & \cdot & 0 & \cdot & \cdot & \cdot & 0 \\ & & & & & & & l_{nn} \end{array} \right]$$

A triangular band matrix can also be a unit triangular band matrix if all the diagonal elements have a value of 1. For an illustration of a unit triangular matrix, see "Triangular Matrix" on page 77.

## In Storage

The two storage modes used for storing triangular band matrices are described in the following sections:

- "Upper-Triangular-Band-Packed Storage Mode"
- "Lower-Triangular-Band-Packed Storage Mode" on page 91

**It is important to note that because the diagonal elements of a unit triangular band matrix are always one, you do not need to set these values in the array for these two storage modes. ESSL always assumes that the values in these positions are one.**

**Upper-Triangular-Band-Packed Storage Mode:** Only the band elements of the upper triangular part of an upper triangular band matrix, including the main diagonal, are stored for upper-triangular-band-packed storage mode.

For a matrix  $U$  of order  $n$  and an upper band width of  $k$ , the array must have a leading dimension,  $lda$ , greater than or equal to  $k+1$ , and the size of the second dimension must be (at least)  $n$ .

Using array  $UTB$ , which is declared as  $UTB(lda,n)$ , where  $p = lda = k+1$ , the elements of an upper triangular band matrix are stored as follows:

$$UTB = \begin{bmatrix} * & \cdot & \cdot & \cdot & * & u_{1p} & u_{2,p+1} & \cdot & \cdot & \cdot & u_{n-k,n} \\ \cdot & & & & \cdot & & & & & & \\ \cdot & & & & \cdot & & & & & & \\ \cdot & & & & \cdot & & & & & & \\ & & * & u_{13} & u_{24} & \cdot & \cdot & \cdot & & & \cdot \\ * & u_{12} & u_{23} & \cdot & \cdot & \cdot & & & & & \cdot \\ u_{11} & u_{22} & \cdot & \cdot & \cdot & & & & & & u_{nn} \end{bmatrix}$$

where "\*" means you do not store an element in that position in the array.

Following is an example of an upper triangular band matrix  $U$  of order 6 and an upper band width of 3.

Given the following matrix  $U$ :

$$\begin{bmatrix} 11 & 12 & 13 & 14 & 0 & 0 \\ 0 & 22 & 23 & 24 & 25 & 0 \\ 0 & 0 & 33 & 34 & 35 & 36 \\ 0 & 0 & 0 & 44 & 45 & 46 \\ 0 & 0 & 0 & 0 & 55 & 56 \\ 0 & 0 & 0 & 0 & 0 & 66 \end{bmatrix}$$

you store it in upper-triangular-band-packed storage mode in array  $UTB$ , declared as  $UTB(4,6)$ , as follows:

$$UTB = \begin{bmatrix} * & * & * & 14 & 25 & 36 \\ * & * & 13 & 24 & 35 & 46 \\ * & 12 & 23 & 34 & 45 & 56 \\ 11 & 22 & 33 & 44 & 55 & 66 \end{bmatrix}$$

Following is an example of how to transform your upper triangular band matrix to upper-triangular-band-packed storage mode:

```

DO 20 J=1,N
  M=K+1-J
  DO 10 I=MAX(1,J-K),J
    UTB(M+I,J)=U(I,J)
  10 CONTINUE
20 CONTINUE

```

**Lower-Triangular-Band-Packed Storage Mode:** Only the band elements of the lower triangular part of a lower triangular band matrix, including the main diagonal, are stored for lower-triangular-band-packed storage mode.

**Note:** As an alternative to this storage mode, you can specify your arguments in your subroutine in a special way so that ESSL selects the matrix elements properly, and you can leave your matrix stored in full-matrix storage mode. For details, see the Notes in the subroutine description in Part 2 of this book.

For a matrix  $L$  of order  $n$  and a lower band width of  $k$ , the array must have a leading dimension,  $lda$ , greater than or equal to  $k+1$ , and the size of the second dimension must be (at least)  $n$ .

Using array LTB, which is declared as  $LTB(lda,n)$ , where  $q = lda = k+1$ , the elements of a lower triangular band matrix are stored as follows:

$$LTB = \begin{bmatrix} l_{11} & l_{22} & \dots & & & l_{nn} \\ l_{21} & l_{32} & & & & * \\ l_{31} & l_{42} & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ l_{q1} & l_{q+1,2} & \dots & l_{n,n-k} & * & \dots & * \end{bmatrix}$$

where “\*” means you do not store an element in that position in the array.

Following is an example of a lower triangular band matrix  $L$  of order 6 and a lower band width of 2.

Given the following matrix  $L$ :

$$\begin{bmatrix} 11 & 0 & 0 & 0 & 0 & 0 \\ 21 & 22 & 0 & 0 & 0 & 0 \\ 31 & 32 & 33 & 0 & 0 & 0 \\ 0 & 42 & 43 & 44 & 0 & 0 \\ 0 & 0 & 53 & 54 & 55 & 0 \\ 0 & 0 & 0 & 64 & 65 & 66 \end{bmatrix}$$

you store it in lower-triangular-band-packed storage mode in array LTB, declared as LTB(3,6), as follows:

$$\text{LTB} = \begin{bmatrix} 11 & 22 & 33 & 44 & 55 & 66 \\ 21 & 32 & 43 & 54 & 65 & * \\ 31 & 42 & 53 & 64 & * & * \end{bmatrix}$$

Following is an example of how to transform your lower triangular band matrix to lower-triangular-band-packed storage mode:

```

DO 20 J=1,N
  M=1-J
  DO 10 I=J,MIN(N,J+K)
    LTB(M+I,J)=L(I,J)
  10 CONTINUE
20 CONTINUE

```

## General Tridiagonal Matrix

A general tridiagonal matrix is a matrix whose nonzero elements are found only on the diagonal, subdiagonal, and superdiagonal of the matrix; that is:

$$a_{ij} = 0 \quad \text{if } |i-j| > 1$$

The following matrix illustrates a general tridiagonal matrix of order  $n$ :

$$A = \begin{bmatrix} a_{11} & a_{12} & 0 & \cdot & \cdot & \cdot & 0 \\ a_{21} & a_{22} & a_{23} & 0 & & & \cdot \\ 0 & a_{32} & a_{33} & a_{34} & 0 & & \cdot \\ \cdot & 0 & a_{43} & a_{44} & \cdot & \cdot & \cdot \\ \cdot & & 0 & \cdot & \cdot & \cdot & \cdot \\ \cdot & & & \cdot & \cdot & \cdot & \cdot \\ \cdot & & & & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & a_{nn} \end{bmatrix}$$

### In Storage

Only the diagonal, subdiagonal, and superdiagonal elements of the general tridiagonal matrix are stored. This is called tridiagonal storage mode. The elements of a general tridiagonal matrix,  $A$ , of order  $n$  are stored in three one-dimensional arrays, C, D, and E, each of length  $n$ , where array C contains the subdiagonal elements, stored as follows:

$$C = (*, a_{21}, a_{32}, a_{43}, \dots, a_{n,n-1})$$

and array D contains the main diagonal elements, stored as follows:

$$D = (a_{11}, a_{22}, a_{33}, \dots, a_{nn})$$

and array E contains the superdiagonal elements, stored as follows:

$$E = (a_{12}, a_{23}, a_{34}, \dots, a_{n-1,n}, *)$$

where "\*" means you do not store an element in that position in the array.

Following is an example of a general tridiagonal matrix  $A$  of order 5:

$$\begin{bmatrix} 11 & 12 & 0 & 0 & 0 \\ 21 & 22 & 23 & 0 & 0 \\ 0 & 32 & 33 & 34 & 0 \\ 0 & 0 & 43 & 44 & 45 \\ 0 & 0 & 0 & 54 & 55 \end{bmatrix}$$

which you store in tridiagonal storage mode in arrays C, D, and E, each of length 5, as follows:

$$C = (*, 21, 32, 43, 54)$$

$$D = (11, 22, 33, 44, 55)$$

$$E = (12, 23, 34, 45, *)$$

**Note:** Some ESSL subroutines provide an option for specifying at least  $n$  additional locations at the end of each of the arrays C, D, and E. These additional locations are used for working storage by the ESSL subroutine. The reasons for choosing this option are explained in the subroutine descriptions.

## Symmetric Tridiagonal Matrix

A tridiagonal matrix  $A$  is also symmetric if and only if its nonzero elements are found only on the diagonal, subdiagonal, and superdiagonal of the matrix, and its subdiagonal elements and superdiagonal elements are equal; that is:

$$(a_{ij} = 0 \quad \text{if } |i-j| > 1) \quad \text{and} \quad (a_{ij} = a_{ji} \quad \text{if } |i-j| = 1)$$

The following matrix illustrates a symmetric tridiagonal matrix of order  $n$ :

$$A = \begin{bmatrix} a_{11} & a_{21} & 0 & \cdot & \cdot & \cdot & 0 \\ a_{21} & a_{22} & a_{32} & 0 & & & \cdot \\ 0 & a_{32} & a_{33} & a_{43} & 0 & & \cdot \\ \cdot & 0 & a_{43} & a_{44} & \cdot & \cdot & \cdot \\ \cdot & & 0 & \cdot & \cdot & \cdot & \cdot \\ \cdot & & & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & a_{nn} \end{bmatrix}$$

### In Storage

Only the diagonal and subdiagonal elements of the positive definite symmetric tridiagonal matrix are stored. This is called symmetric-tridiagonal storage mode. The elements of a symmetric tridiagonal matrix  $A$  of order  $n$  are stored in two one-dimensional arrays C and D, each of length  $n$ , where array C contains the subdiagonal elements, stored as follows:

$$C = (*, a_{21}, a_{32}, a_{43}, \dots, a_{n,n-1})$$

where “\*” means you do not store an element in that position in the array. Then array D contains the main diagonal elements, stored as follows:

$$D = (a_{11}, a_{22}, a_{33}, \dots, a_{nn})$$

Following is an example of a symmetric tridiagonal matrix  $A$  of order 5:

$$\begin{bmatrix} 10 & 1 & 0 & 0 & 0 \\ 1 & 20 & 2 & 0 & 0 \\ 0 & 2 & 30 & 3 & 0 \\ 0 & 0 & 3 & 40 & 4 \\ 0 & 0 & 0 & 4 & 50 \end{bmatrix}$$

which you store in symmetric-tridiagonal storage mode in arrays C and D, each of length 5, as follows:

$$C = (*, 1, 2, 3, 4)$$

$$D = (10, 20, 30, 40, 50)$$

**Note:** Some ESSL subroutines provide an option for specifying at least  $n$  additional locations at the end of each of the arrays C and D. These additional locations are used for working storage by the ESSL subroutine. The reasons for choosing this option are explained in the subroutine descriptions.

## Positive Definite Symmetric Tridiagonal Matrix

A real symmetric tridiagonal matrix  $A$  is positive definite if and only if  $x^T A x$  is positive for all nonzero vectors  $x$ .

### In Storage

The positive definite symmetric tridiagonal matrix is stored in the same way the symmetric tridiagonal matrix is stored. For a description of this storage technique, see “Symmetric Tridiagonal Matrix” on page 93.

## Sparse Matrix

A sparse matrix is a matrix having a relatively small number of nonzero elements.

Consider the following as an example of a sparse matrix  $A$ :

$$\begin{bmatrix} 11 & 0 & 13 & 0 & 0 & 0 \\ 21 & 22 & 0 & 24 & 0 & 0 \\ 0 & 32 & 33 & 0 & 35 & 0 \\ 0 & 0 & 43 & 44 & 0 & 46 \\ 51 & 0 & 0 & 54 & 55 & 0 \\ 61 & 62 & 0 & 0 & 65 & 66 \end{bmatrix}$$

### In Storage

A sparse matrix can be stored in full-matrix storage mode or a packed storage mode. When a sparse matrix is stored in **full-matrix storage mode**, all its elements, including its zero elements, are stored in an array.

The seven packed storage modes used for storing sparse matrices are described in the following sections:

- “Compressed-Matrix Storage Mode” on page 95
- “Compressed-Diagonal Storage Mode” on page 96
- “Storage-by-Indices” on page 98
- “Storage-by-Columns” on page 99
- “Storage-by-Rows” on page 100
- “Diagonal-Out Skyline Storage Mode” on page 102
- “Profile-In Skyline Storage Mode” on page 104



**Note:** When the elements of a sparse matrix are stored using any of these storage modes, the ESSL subroutines do not check that all elements are nonzero. You do not get an error if any elements are zero.

**Compressed-Matrix Storage Mode:** The sparse matrix  $A$ , stored in compressed-matrix storage mode, uses two two-dimensional arrays to define the sparse matrix storage, AC and KA. See reference [76]. Given the  $m$  by  $n$  sparse matrix  $A$ , having a maximum of  $nz$  nonzero elements in each row:

- AC is defined as  $AC(lda,nz)$ , where the leading dimension,  $lda$ , must be greater than or equal to  $m$ . Each row of array AC contains the nonzero elements of the corresponding row of matrix  $A$ . For each row in matrix  $A$  containing less than  $nz$  nonzero elements, the corresponding row in array AC is padded with zeros. The elements in each row can be stored in any order.
- KA is an integer array defined as  $KA(lda,nz)$ , where the leading dimension,  $lda$ , must be greater than or equal to  $m$ . It contains the column numbers of the matrix  $A$  elements that are stored in the corresponding positions in array AC. For each row in matrix  $A$  containing less than  $nz$  nonzero elements, the corresponding row in array KA is padded with any values from 1 to  $n$ . **Because this array is used by the ESSL subroutines to access other target vectors in the computation, you must adhere to these required values to avoid errors.**

Unless all the rows of sparse matrix  $A$  contain approximately the same number of nonzero elements, this storage mode requires a large amount of storage. This diminishes the performance you can obtain by using this storage mode.

Consider the following as an example of a 6 by 6 sparse matrix  $A$  with a maximum of four nonzero elements in each row. It shows how matrix  $A$  can be stored in arrays AC and KA.

Given the following matrix  $A$ :

$$\begin{bmatrix} 11 & 0 & 13 & 0 & 0 & 0 \\ 21 & 22 & 0 & 24 & 0 & 0 \\ 0 & 32 & 33 & 0 & 35 & 0 \\ 0 & 0 & 43 & 44 & 0 & 46 \\ 51 & 0 & 0 & 54 & 55 & 0 \\ 61 & 62 & 0 & 0 & 65 & 66 \end{bmatrix}$$

the arrays are:

$$AC = \begin{bmatrix} 11 & 13 & 0 & 0 \\ 22 & 21 & 24 & 0 \\ 33 & 32 & 35 & 0 \\ 44 & 43 & 46 & 0 \\ 55 & 51 & 54 & 0 \\ 66 & 61 & 62 & 65 \end{bmatrix}$$

$$KA = \begin{bmatrix} 1 & 3 & * & * \\ 2 & 1 & 4 & * \\ 3 & 2 & 5 & * \\ 4 & 3 & 6 & * \\ 5 & 1 & 4 & * \\ 6 & 1 & 2 & 5 \end{bmatrix}$$

where “\*” means you can store any value from 1 to 6 in that position in the array.

Symmetric sparse matrices use the same storage technique as nonsymmetric sparse matrices; that is, all nonzero elements of a symmetric matrix  $A$  must be stored in array AC, not just the elements of the upper triangle and diagonal of matrix  $A$ .

In general terms, this storage technique can be expressed as follows:

For each  $a_{ij} \neq 0$ , for  $i = 1, m$  and  $j = 1, n$   
 there exists  $k$ , where  $1 \leq k \leq nz$ ,  
 such that  $AC(i,k) = a_{ij}$  and  $KA(i,k) = j$ .

For all other elements of AC and KA,  
 $AC(i,k) = 0$  and  $1 \leq KA(i,k) \leq n$

where:

- $a_{ij}$  are the elements of the  $m$  by  $n$  matrix  $A$  that has a maximum of  $nz$  nonzero elements in each row.
- Array AC is defined as  $AC(lda,nz)$ , where  $lda \geq m$ .
- Array KA is defined as  $KA(lda,nz)$ , where  $lda \geq m$ .

**Compressed-Diagonal Storage Mode:** The storage mode used for square sparse matrices stored in compressed-diagonal storage mode has two variations, depending on whether the matrix is a general sparse matrix or a symmetric sparse matrix. This section explains both of these variations. This section begins, however, by explaining the conventions used for numbering the diagonals in the matrix, which apply to the storage descriptions.

Matrix  $A$  of order  $n$  has  $2n-1$  diagonals. Because  $k = j-i$  is constant for the elements  $a_{ij}$  along each diagonal, each diagonal can be assigned a diagonal number,  $k$ , having a value from  $1-n$  to  $n-1$ . Then the diagonals can be referred to as  $d_k$ , where  $k = 1-n, n-1$ .

The following matrix shows the starting position of each diagonal,  $d_k$ :

$$\begin{array}{c}
 \mathbf{A} = \\
 \\
 \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{array}{r}
 \mathbf{d}_0 \quad \mathbf{d}_1 \quad \mathbf{d}_2 \quad \cdot \quad \cdot \quad \cdot \quad \mathbf{d}_{n-1} \\
 \left[ \begin{array}{cccccccc}
 a_{11} & a_{12} & a_{13} & \cdot & \cdot & \cdot & a_{1n} \\
 a_{21} & a_{22} & a_{23} & & & & \cdot \\
 a_{31} & a_{32} & a_{33} & & & & \cdot \\
 \cdot & \cdot & & \cdot & & & \cdot \\
 \cdot & & & & \cdot & & \cdot \\
 \cdot & & & & & \cdot & \cdot \\
 a_{n1} & \cdot & \cdot & \cdot & \cdot & \cdot & a_{nn}
 \end{array} \right]
 \end{array}$$

For a **general** (square) sparse matrix  $A$ , compressed-diagonal storage mode uses two arrays to define the sparse matrix storage, AD and LA. Using the above convention for numbering the diagonals, and given that sparse matrix  $A$  contains  $nd$  diagonals having nonzero elements, arrays AD and LA are set up as follows:

- AD is defined as  $AD(lda,nd)$ , where the leading dimension,  $lda$ , must be greater than or equal to  $n$ . Each diagonal of matrix  $A$  that has at least one nonzero element is stored in a column of array AD. All of the elements of the diagonal, including its zero elements, are stored in  $n$  contiguous locations in the array, in the same order as they appear in the diagonal. Padding with zeros is required as follows to fill the  $n$  locations in each column of array AD:

- Each superdiagonal ( $k > 0$ ), which has  $n-k$  elements, is padded with  $k$  trailing zeros.
- The main diagonal ( $k = 0$ ), which has  $n$  elements, does not require padding.
- Each subdiagonal ( $k < 0$ ), which has  $n-|k|$  elements, is padded with  $|k|$  leading zeros.

The diagonals can be stored in any columns in array AD.

- LA is a one-dimensional integer array of length  $nd$ , containing the diagonal numbers  $k$  for the diagonals stored in each corresponding column in array AD.

**Because this storage mode requires entire diagonals to be stored, if the nonzero elements in matrix A are not concentrated along a few diagonals, this storage mode requires a large amount of storage. This diminishes the performance you obtain by using this storage mode.**

Consider the following as an example of how a 6 by 6 general sparse matrix A with 5 nonzero diagonals is stored in arrays AD and LA.

Given the following matrix A:

$$\begin{bmatrix} 11 & 0 & 13 & 0 & 0 & 0 \\ 21 & 22 & 0 & 24 & 0 & 0 \\ 0 & 32 & 33 & 0 & 35 & 0 \\ 0 & 0 & 43 & 44 & 0 & 46 \\ 51 & 0 & 0 & 54 & 55 & 0 \\ 61 & 62 & 0 & 0 & 65 & 66 \end{bmatrix}$$

the arrays are:

$$\text{AD} = \begin{bmatrix} 11 & 13 & 0 & 0 & 0 \\ 22 & 24 & 21 & 0 & 0 \\ 33 & 35 & 32 & 0 & 0 \\ 44 & 46 & 43 & 0 & 0 \\ 55 & 0 & 54 & 51 & 0 \\ 66 & 0 & 65 & 62 & 61 \end{bmatrix}$$

$$\text{LA} = (0, 2, -1, -4, -5)$$

For a **symmetric** sparse matrix, where each superdiagonal  $k$  is equal to subdiagonal  $-k$ , compressed-diagonal storage mode uses the same storage technique as for the general sparse matrix, except that only the nonzero main diagonal and one diagonal of each couple of nonzero diagonals,  $k$  and  $-k$ , are used in setting up arrays AD and LA. You can store either the upper or the lower diagonal of each couple.

Consider the following as an example of a symmetric sparse matrix of order 6 and how it is stored in arrays AD and LA, using only three nonzero diagonals in the matrix.

Given the following matrix A:

$$\begin{bmatrix} 11 & 0 & 13 & 0 & 51 & 0 \\ 0 & 22 & 0 & 24 & 0 & 62 \\ 13 & 0 & 33 & 0 & 35 & 0 \\ 0 & 24 & 0 & 44 & 0 & 46 \end{bmatrix}$$

$$\begin{bmatrix} 51 & 0 & 35 & 0 & 55 & 0 \\ 0 & 62 & 0 & 46 & 0 & 66 \end{bmatrix}$$

the arrays are:

$$AD = \begin{bmatrix} 11 & 13 & 0 \\ 22 & 24 & 0 \\ 33 & 35 & 0 \\ 44 & 46 & 0 \\ 55 & 0 & 51 \\ 66 & 0 & 62 \end{bmatrix}$$

$$LA = (0, 2, -4)$$

In general terms, this storage technique can be expressed as follows:

For each  $d_k \neq (0, \dots, 0)$ , for  $k = 1-n, n-1$   
for **general** square sparse matrices, or

for each unique  $d_k \neq (0, \dots, 0)$ , for  $k = 1-n, n-1$   
for **symmetric** sparse matrices,

there exists  $l$ , where  $1 \leq l \leq nd$ ,

such that  $LA(l) = k$  and column  $l$  in array  $AD$  contains  $dp_k$ .

where:

- Array  $AD$  is defined as  $AD(lda, nd)$ , where  $lda \geq n$ , and where  $nd$  is the number of nonzero diagonals,  $d_k$  that are stored in array  $AD$ .
- Array  $LA$  has  $nd$  elements.
- $k$  is the diagonal number of each diagonal,  $d_k$ , where  $k = i-j$ .
- $dp_k$  are the diagonals,  $d_k$ , with padding, which are constructed from the sparse matrix  $A$  elements,  $a_{ij}$ , for  $i, j = 1, n$  as follows:  
For superdiagonals ( $k > 0$ ),  $dp_k$  has  $k$  trailing zeros:  $dp_k = (a_{1,k+1}, a_{2,k+2}, \dots, a_{n-k,n}, 0_1, \dots, 0_k)$   
For the main diagonal ( $k = 0$ ),  $dp_0$  has no padding:  $dp_0 = (a_{11}, a_{22}, \dots, a_{nn})$   
For subdiagonals ( $k < 0$ ),  $dp_k$  has  $|k|$  leading zeros:  $dp_k = (0_1, \dots, 0_{|k|}, a_{|k|+1,1}, a_{|k|+2,2}, \dots, a_{n, n-|k|})$

**Storage-by-Indices:** For a sparse matrix  $A$ , storage-by-indices uses three one-dimensional arrays to define the sparse matrix storage,  $AR$ ,  $IA$ , and  $JA$ . Given the  $m$  by  $n$  sparse matrix  $A$  having  $ne$  nonzero elements, the arrays are set up as follows:

- $AR$  of (at least) length  $ne$  contains the  $ne$  nonzero elements of the sparse matrix  $A$ , stored contiguously in **any** order.
- $IA$ , an integer array of (at least) length  $ne$  contains the corresponding row numbers of each nonzero element,  $a_{ij}$ , in matrix  $A$ .
- $JA$ , an integer array of (at least) length  $ne$  contains the corresponding column numbers of each nonzero element,  $a_{ij}$ , in matrix  $A$ .

Consider the following as an example of a 6 by 6 sparse matrix  $A$  and how it can be stored in arrays  $AR$ ,  $IA$ , and  $JA$ :

Given the following matrix  $A$ :

$$\begin{bmatrix} 11 & 0 & 13 & 0 & 0 & 0 \\ 21 & 22 & 0 & 24 & 0 & 0 \\ 0 & 32 & 33 & 0 & 35 & 0 \\ 0 & 0 & 43 & 44 & 0 & 46 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 61 & 62 & 0 & 0 & 65 & 66 \end{bmatrix}$$

the arrays are:

$$\text{AR} = (11, 22, 32, 33, 13, 21, 43, 24, 66, 46, 35, 62, 61, 65, 44)$$

$$\text{IA} = (1, 2, 3, 3, 1, 2, 4, 2, 6, 4, 3, 6, 6, 6, 4)$$

$$\text{JA} = (1, 2, 2, 3, 3, 1, 3, 4, 6, 6, 5, 2, 1, 5, 4)$$

In general terms, this storage technique can be expressed as follows:

For each  $a_{ij} \neq 0$ , for  $i = 1, m$  and  $j = 1, n$   
there exists  $k$ , where  $1 \leq k \leq ne$ , such that:

$$\text{AR}(k) = a_{ij}$$

$$\text{IA}(k) = i$$

$$\text{JA}(k) = j$$

where:

$a_{ij}$  are the elements of the  $m$  by  $n$  sparse matrix  $A$ .  
Arrays AR, IA, and JA each have  $ne$  elements.

**Storage-by-Columns:** For a sparse matrix,  $A$ , storage-by-columns uses three one-dimensional arrays to define the sparse matrix storage, AR, IA, and JA. Given the  $m$  by  $n$  sparse matrix  $A$  having  $ne$  nonzero elements, the arrays are set up as follows:

- AR of (at least) length  $ne$  contains the  $ne$  nonzero elements of the sparse matrix  $A$ , stored contiguously. The columns of matrix  $A$  are stored consecutively from 1 to  $n$  in AR. The elements in each column of  $A$  are stored in any order in AR.
- IA, an integer array of (at least) length  $ne$  contains the corresponding row numbers of each nonzero element,  $a_{ij}$ , in matrix  $A$ .
- JA, an integer array of (at least) length  $n+1$  contains the relative starting position of each column of matrix  $A$  in array AR; that is, each element  $\text{JA}(j)$  of the column pointer array indicates where column  $j$  begins in array AR. If all elements in column  $j$  are zero, then  $\text{JA}(j) = \text{JA}(j+1)$ . The last element,  $\text{JA}(n+1)$ , indicates the position after the last element in array AR, which is  $ne+1$ .

Consider the following as an example of a 6 by 6 sparse matrix  $A$  and how it can be stored in arrays AR, IA, and JA.

Given the following matrix  $A$ :

$$\begin{bmatrix} 11 & 0 & 13 & 0 & 0 & 0 \\ 21 & 22 & 0 & 24 & 0 & 0 \\ 0 & 32 & 33 & 0 & 0 & 0 \\ 0 & 0 & 43 & 44 & 0 & 46 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 61 & 62 & 0 & 0 & 0 & 66 \end{bmatrix}$$

the arrays are:

$$\text{AR} = (11, 61, 21, 62, 32, 22, 13, 33, 43, 44, 24, 46, 66)$$

$$\text{IA} = (1, 6, 2, 6, 3, 2, 1, 3, 4, 4, 2, 4, 6)$$

$$\text{JA} = (1, 4, 7, 10, 12, 12, 14)$$

In general terms, this storage technique can be expressed as follows:

For each  $a_{ij} \neq 0$ , for  $i = 1, m$  and  $j = 1, n$   
there exists  $k$ , where  $1 \leq k \leq ne$ , such that

$$\begin{aligned} \text{AR}(k) &= a_{ij} \\ \text{IA}(k) &= i \end{aligned}$$

And for  $j = 1, n$ ,

$\text{JA}(j) = k$ , where  $a_{ij}$ , in  $\text{AR}(k)$ , is the first element stored in AR for column  $j$

$\text{JA}(j) = \text{JA}(j+1)$ , where all  $a_{ij} = 0$  in column  $j$

$\text{JA}(n+1) = ne+1$

where:

$a_{ij}$  are the elements of the  $m$  by  $n$  sparse matrix  $A$ .

Arrays AR and IA each have  $ne$  elements.

Array JA has  $n+1$  elements.

**Storage-by-Rows:** The storage mode used for sparse matrices stored by rows has three variations, depending on whether the matrix is a general sparse matrix or a symmetric sparse matrix. This section explains these variations.

For a **general** sparse matrix  $A$ , storage-by-rows uses three one-dimensional arrays to define the sparse matrix storage, AR, IA, and JA. Given the  $m$  by  $n$  sparse matrix  $A$  having  $ne$  nonzero elements, the arrays are set up as follows:

- AR of (at least) length  $ne$  contains the  $ne$  nonzero elements of the sparse matrix  $A$ , stored contiguously. The rows of matrix  $A$  are stored consecutively from 1 to  $m$  in AR. The elements in each row of  $A$  are stored in any order in AR.
- IA, an integer array of (at least) length  $m+1$  contains the relative starting position of each row of matrix  $A$  in array AR; that is, each element  $\text{IA}(i)$  of the row pointer array indicates where row  $i$  begins in array AR. If all elements in row  $i$  are zero, then  $\text{IA}(i) = \text{IA}(i+1)$ . The last element,  $\text{IA}(m+1)$ , indicates the position after the last element in array AR, which is  $ne+1$ .
- JA, an integer array of (at least) length  $ne$  contains the corresponding column numbers of each nonzero element,  $a_{ij}$ , in matrix  $A$ .

Consider the following as an example of a 6 by 6 general sparse matrix  $A$  and how it can be stored in arrays AR, IA, and JA.

Given the following matrix  $A$ :

$$\begin{bmatrix} 11 & 0 & 13 & 0 & 0 & 0 \\ 21 & 22 & 0 & 24 & 0 & 0 \\ 0 & 32 & 33 & 0 & 0 & 0 \\ 0 & 0 & 43 & 44 & 0 & 46 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 61 & 62 & 0 & 0 & 0 & 66 \end{bmatrix}$$

the arrays are:

$$AR = (11, 13, 24, 22, 21, 32, 33, 44, 43, 46, 61, 62, 66)$$

$$IA = (1, 3, 6, 8, 11, 11, 14)$$

$$JA = (1, 3, 4, 2, 1, 2, 3, 4, 3, 6, 1, 2, 6)$$

For a **symmetric** sparse matrix of order  $m$ , storage-by-rows uses the same storage technique as for the general sparse matrix, except that only the upper or lower triangle and diagonal elements are used in setting up arrays AR, IA, and JA.

Consider the following as an example of a symmetric sparse matrix  $A$  of order 6 and how it can be stored in arrays AR, IA, and JA using upper-storage-by-rows, which stores only the upper triangle and diagonal elements.

Given the following matrix  $A$ :

$$\begin{bmatrix} 11 & 0 & 13 & 0 & 0 & 0 \\ 0 & 22 & 23 & 24 & 0 & 0 \\ 13 & 23 & 33 & 0 & 35 & 0 \\ 0 & 24 & 0 & 44 & 0 & 46 \\ 0 & 0 & 35 & 0 & 55 & 0 \\ 0 & 0 & 0 & 46 & 0 & 0 \end{bmatrix}$$

the arrays are:

$$AR = (11, 13, 22, 24, 23, 33, 35, 46, 44, 55)$$

$$IA = (1, 3, 6, 8, 10, 11, 11)$$

$$JA = (1, 3, 2, 3, 4, 3, 5, 4, 6, 5)$$

Using the same symmetric matrix  $A$ , consider the following as an example of how it can be stored in arrays AR, IA, and JA using lower-storage-by-rows, which stores only the lower triangle and diagonal elements:

$$AR = (11, 22, 23, 33, 13, 24, 44, 55, 35, 46)$$

$$IA = (1, 2, 3, 6, 8, 10, 11)$$

$$JA = (1, 2, 2, 3, 1, 2, 4, 5, 3, 4)$$

In general terms, this storage technique can be expressed as follows:

For each  $a_{ij} \neq 0$ ,

for  $i = 1, m$  and  $j = 1, n$  for general sparse matrices

or

for  $i = 1, m$  and  $j = i, m$  for symmetric sparse matrices using the lower triangle

or

for  $i = 1, m$  and  $j = 1, i$  for symmetric sparse matrices using the upper triangle

there exists  $k$ , where  $1 \leq k \leq ne$ , such that

$$AR(k) = a_{ij}$$

$$JA(k) = j$$

And for  $i = 1, m$ ,

$IA(i) = k$ , where  $a_{ij}$  in  $AR(k)$ , is the first element stored in AR for row  $i$

$IA(i) = IA(i+1)$ , where all  $a_{ij} = 0$  in row  $i$

$$IA(m+1) = ne+1$$

where:

- $a_{ij}$  are the elements of sparse matrix  $A$ , which is either an  $m$  by  $n$  general sparse matrix or a symmetric sparse matrix of order  $m$  containing  $ne$  nonzero elements.
- Arrays AR and JA each have  $ne$  elements.
- Array IA has  $m+1$  elements.

**Diagonal-Out Skyline Storage Mode:** The diagonal-out skyline storage mode used for sparse matrices has two variations, depending on whether the matrix is a general sparse matrix or a symmetric sparse matrix. Both of these variations are explained here.

For a **general** sparse matrix  $A$ , diagonal-out skyline storage mode uses four one-dimensional arrays to define the sparse matrix storage, AU, IDU, AL, and IDL. Given the sparse matrix  $A$  of order  $n$ , containing  $nu+nl-n$  elements under the top and left profiles, the arrays are set up as follows:

- AU of (at least) length  $nu$  contains the upper triangle of the sparse matrix  $A$ , where the columns are stored consecutively from 1 to  $n$  in AU in the following way. For each column, the elements starting at the diagonal element and ending at the topmost nonzero element in the column are stored contiguously in AU. The elements stored may include zero elements along with the nonzero elements. If all elements in the column to be stored are zero, the diagonal element,  $a_{ii}$  having a value of zero, is stored in AU for that column. A total of  $nu$  elements are stored for the upper triangle of  $A$ .
- IDU, an integer array of (at least) length  $n+1$  contains the relative position of each diagonal element of matrix  $A$  in array AU; that is, each element  $IDU(i)$  of the diagonal pointer array indicates where diagonal element  $a_{ii}$  is stored in array AU. One-origin is used, so the first element of IDU is always 1. The last element,  $IDU(n+1)$ , indicates the position after the last element in array AU, which is  $nu+1$ .
- AL of (at least) length  $nl$  contains the lower triangle of the sparse matrix  $A$ , where the rows are stored consecutively from 1 to  $n$  in AL in the following way. For each row, the elements starting at the diagonal element and ending at the leftmost nonzero element in the row are stored contiguously in AL. The elements stored may include zero elements along with the nonzero elements. If all elements in the row to be stored are zero, the diagonal element,  $a_{ii}$  having a value of zero, is stored in AL for that row. A total of  $nl$  elements are stored for the lower triangle of  $A$ . The values of the diagonal elements are meaningless, so you can store any values in those positions in AL.
- IDL, an integer array of (at least) length  $n+1$  contains the relative position of each diagonal element of matrix  $A$  in array AL; that is, each element  $IDL(i)$  of the diagonal pointer array indicates where diagonal element  $a_{ii}$  is stored in array AL. One-origin is used, so the first element of IDL is always 1. The last element,  $IDL(n+1)$ , indicates the position after the last element in array AL, which is  $nl+1$ .

Consider the following as an example of a 6 by 6 general sparse matrix  $A$  and how it is stored in arrays AU, IDU, AL, and IDL.

Given the following matrix  $A$ :

$$\begin{bmatrix} 0 & 12 & 13 & 0 & 0 & 0 \\ 21 & 22 & 0 & 24 & 0 & 0 \\ 31 & 0 & 33 & 34 & 0 & 36 \\ 41 & 42 & 43 & 44 & 45 & 0 \\ 0 & 0 & 0 & 54 & 55 & 56 \\ 0 & 0 & 63 & 0 & 65 & 66 \end{bmatrix}$$



the arrays are:

$$AU = (0, 22, 12, 33, 0, 13, 44, 34, 24, 55, 45, 66, 56, 0, 36)$$

$$IDU = (1, 2, 4, 7, 10, 12, 16) \text{ where } nu=15$$

$$AL = (*, *, 21, *, 0, 31, *, 43, 42, 41, *, 54, *, 65, 0, 63)$$

$$IDL = (1, 2, 4, 7, 11, 13, 17) \text{ where } nl=16$$

and where "\*" means you do not have to store a value in that position in the array. However, these storage positions are required.

For a **symmetric** sparse matrix of order  $n$ , diagonal-out skyline storage mode uses the same storage technique as for the upper triangle and diagonal elements of the general sparse matrix; therefore, only the AU and IDU arrays are needed.

Consider the following as an example of a symmetric sparse matrix  $A$  of order 6 and how it is stored in arrays AU and IDU.

Given the following matrix  $A$ :

$$\begin{bmatrix} 0 & 12 & 13 & 0 & 0 & 0 \\ 12 & 22 & 0 & 24 & 0 & 0 \\ 13 & 0 & 33 & 34 & 0 & 36 \\ 0 & 24 & 34 & 44 & 45 & 0 \\ 0 & 0 & 0 & 45 & 55 & 56 \\ 0 & 0 & 36 & 0 & 56 & 66 \end{bmatrix}$$

the arrays are:

$$AU = (0, 22, 12, 33, 0, 13, 44, 34, 24, 55, 45, 66, 56, 0, 36)$$

$$IDU = (1, 2, 4, 7, 10, 12, 16) \text{ where } nu=15$$

In general terms, this storage technique can be expressed as follows:

For general sparse matrices and symmetric sparse matrices:

For each  $a_{ij}$  for  $j = 1, n$  and  $i = j, k$ ,  
 where  $a_{kj}$  is the topmost  $a_{ij} \neq 0$  in each column  $j$ ,  
 there exists  $m$ , where  $1 \leq m \leq nu$ , such that  
 $AU(m+j-i) = a_{ij}$   
 $IDU(j) = m$  for each  $a_{jj}$   
 $IDU(n+1) = nu+1$

Also, for general sparse matrices:

For each  $a_{ij}$  for  $i = 1, n$  and  $i = j, k$ ,  
 where  $a_{ik}$  is the leftmost  $a_{ij} \neq 0$  in each row  $i$ ,  
 there exists  $m$ , where  $1 \leq m \leq nl$ , such that  
 $AL(m+i-j) = a_{ij}$   
 $IDL(i) = m$  for each  $a_{ii}$   
 $IDL(n+1) = nl+1$

where:

$a_{ij}$  are the elements of sparse matrix  $A$ , of order  $n$ .  
 Array AU has  $nu$  elements.

Array AL has  $nl$  elements.

Arrays IDU and IDL each have  $n+1$  elements.

**Profile-In Skyline Storage Mode:** The profile-in skyline storage mode used for sparse matrices has two variations, depending on whether the matrix is a general sparse matrix or a symmetric sparse matrix. Both of these variations are explained here.

For a **general** sparse matrix  $A$ , profile-in skyline storage mode uses four one-dimensional arrays to define the sparse matrix storage, AU, IDU, AL, and IDL. Given the sparse matrix  $A$  of order  $n$ , containing  $nu+nl-n$  elements under the top and left profiles, the arrays are set up as follows:

- AU of (at least) length  $nu$  contains the upper triangle of the sparse matrix  $A$ , where the columns are stored consecutively from 1 to  $n$  in AU in the following way. For each column, the elements starting at the topmost nonzero element in the column and ending at the diagonal element are stored contiguously in AU. The elements stored may include zero elements along with the nonzero elements. If all elements in the column to be stored are zero, the diagonal element,  $a_{ii}$ , having a value of zero, is stored in AU for that column. A total of  $nu$  elements are stored for the upper triangle of  $A$ .
- IDU, an integer array of (at least) length  $n+1$  contains the relative position of each diagonal element of matrix  $A$  in array AU; that is, each element  $IDU(i)$  of the diagonal pointer array indicates where diagonal element  $a_{ii}$  is stored in array AU. One-origin is used, so the first element of IDU is always 1. The last element,  $IDU(n+1)$ , indicates the position after the last element in array AU, which is  $nu+1$ .
- AL of (at least) length  $nl$  contains the lower triangle of the sparse matrix  $A$ , where the rows are stored consecutively from 1 to  $n$  in AL in the following way. For each row, the elements starting at the leftmost nonzero element in the row and ending at the diagonal element are stored contiguously in AL. The elements stored may include zero elements along with the nonzero elements. If all elements in the row to be stored are zero, the diagonal element,  $a_{ii}$ , having a value of zero, is stored in AL for that row. A total of  $nl$  elements are stored for the lower triangle of  $A$ . The values of the diagonal elements are meaningless, so you can store any values in those positions in AL.
- IDL, an integer array of (at least) length  $n+1$  contains the relative position of each diagonal element of matrix  $A$  in array AL; that is, each element  $IDL(i)$  of the diagonal pointer array indicates where diagonal element  $a_{ii}$  is stored in array AL. One-origin is used, so the first element of IDL is always 1. The last element,  $IDL(n+1)$ , indicates the position after the last element in array AL, which is  $nl+1$ .

Consider the following as an example of a 6 by 6 general sparse matrix  $A$  and how it is stored in arrays AU, IDU, AL, and IDL.

Given the following matrix  $A$ :

$$\begin{bmatrix} 0 & 12 & 13 & 0 & 0 & 0 \\ 21 & 22 & 0 & 24 & 0 & 0 \\ 31 & 0 & 33 & 34 & 0 & 36 \\ 41 & 42 & 43 & 44 & 45 & 0 \\ 0 & 0 & 0 & 54 & 55 & 56 \\ 0 & 0 & 63 & 0 & 65 & 66 \end{bmatrix}$$

the arrays are:

$$AU = (0, 12, 22, 13, 0, 33, 24, 34, 44, 45, 55, 36, 0, 56, 66)$$

$IDU = (1, 3, 6, 9, 11, 15, 16)$  where  $nu=15$   
 $AL = (*, 21, *, 31, 0, *, 41, 42, 43, *, 54, *, 63, 0, 65, *)$

$IDL = (1, 3, 6, 10, 12, 16, 17)$  where  $nl=16$

and where "\*" means you do not have to store a value in that position in the array. However, these storage positions are required.

For a **symmetric** sparse matrix of order  $n$ , profile-in skyline storage mode uses the same storage technique as for the upper triangle and diagonal elements of the general sparse matrix; therefore, only the AU and IDU arrays are needed.

Consider the following as an example of a symmetric sparse matrix  $A$  of order 6 and how it is stored in arrays AU and IDU.

Given the following matrix  $A$ :

$$\begin{bmatrix} 0 & 12 & 13 & 0 & 0 & 0 \\ 12 & 22 & 0 & 24 & 0 & 0 \\ 13 & 0 & 33 & 34 & 0 & 36 \\ 0 & 24 & 34 & 44 & 45 & 0 \\ 0 & 0 & 0 & 45 & 55 & 56 \\ 0 & 0 & 36 & 0 & 56 & 66 \end{bmatrix}$$

the arrays are:

$AU = (0, 12, 22, 13, 0, 33, 24, 34, 44, 45, 55, 36, 0, 56, 66)$

$IDU = (1, 3, 6, 9, 11, 15, 16)$  where  $nu=15$

In general terms, this storage technique can be expressed as follows:

For general sparse matrices and symmetric sparse matrices:

For each  $a_{ij}$  for  $j = 1, n$  and  $i = k, j$ ,  
 where  $a_{kj}$  is the topmost  $a_{ij} \neq 0$  in each column  $j$ ,  
 there exists  $m$ , where  $1 \leq m \leq nu$ , such that  
 $AU(m-j+i) = a_{ij}$   
 $IDU(j) = m$  for each  $a_{ij}$   
 $IDU(n+1) = nu+1$

Also, for general sparse matrices:

For each  $a_{ij}$  for  $i = 1, n$  and  $j = k, i$ ,  
 where  $a_{ik}$  is the leftmost  $a_{ij} \neq 0$  in each row  $i$ ,  
 there exists  $m$ , where  $1 \leq m \leq nl$ , such that  
 $AL(m-i+j) = a_{ij}$   
 $IDL(i) = m$  for each  $a_{ij}$   
 $IDL(n+1) = nl+1$

where:

$a_{ij}$  are the elements of sparse matrix  $A$ , of order  $n$ .  
 Array AU has  $nu$  elements.  
 Array AL has  $nl$  elements.  
 Arrays IDU and IDL each have  $n+1$  elements.

---

## Sequences

A sequence is an ordered collection of numbers. It can be a one-, two-, or three-dimensional sequence. Sequences are used in the areas of sorting, searching, Fourier transforms, convolutions, and correlations.

### Real and Complex Elements in Storage

Sequences can contain either real or complex data. For sequences containing complex data, a special storage arrangement is used to accommodate the two parts,  $a$  and  $b$ , of each complex number,  $a+bi$ , in the array. For each complex number, two sequential storage locations are required in the array. Therefore, exactly twice as much storage is required for complex sequences as for real sequences of the same precision. See “How Do You Set Up Your Scalar Data?” on page 33 for a description of real and complex numbers, and “How Do You Set Up Your Arrays?” on page 33 for a description of how real and complex data is stored in arrays.

### One-Dimensional Sequences

A one-dimensional sequence appears symbolically as follows, where the subscripts indicate the element positions within the sequence:

$$(x_1, x_2, x_3, \dots, x_n)$$

#### In Storage

A one-dimensional sequence is stored in an array using stride in the same way a vector uses stride. For details, see “How Stride Is Used for Vectors” on page 62.

### Two-Dimensional Sequences

A two-dimensional sequence appears symbolically as a series of columns of elements. (They are represented in the same way as a matrix without the square brackets.) The two subscripts indicate the element positions in the first and second dimensions, respectively:

$$\begin{array}{cccc} a_{0,0} & a_{0,1} & \cdot & \cdot & \cdot & a_{0,n-1} \\ a_{1,0} & a_{1,1} & \cdot & \cdot & \cdot & a_{1,n-1} \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ a_{m-1,0} & a_{m-1,1} & \cdot & \cdot & \cdot & a_{m-1,n-1} \end{array}$$

#### In Storage

A two-dimensional sequence is stored in an array using the stride for the second dimension in the same way that a matrix uses leading dimension. It uses a stride of 1 for the first dimension. For details, see “How Leading Dimension Is Used for Matrices” on page 67. (In the area of Fourier transforms, a two-dimensional sequence may be stored in transposed form in an array. In this case, the stride for the second dimension is 1, and the stride for the first dimension is the leading dimension of the array.)

### Three-Dimensional Sequences

A three-dimensional sequence is represented as a series of blocks of elements. Each block is equivalent to a two-dimensional sequence. The number of blocks indicates

the length of the third dimension. The three subscripts indicate the element positions in the first, second, and third dimensions, respectively:

**Plane 0:**

$$\begin{array}{ccc}
 a_{0,0,0} & \cdot \cdot \cdot & a_{0,n-1,0} \\
 a_{1,0,0} & \cdot \cdot \cdot & a_{1,n-1,0} \\
 \cdot & & \cdot \\
 \cdot & & \cdot \\
 \cdot & & \cdot \\
 a_{m-1,0,0} & \cdot \cdot \cdot & a_{m-1,n-1,0}
 \end{array}$$

**Plane 1:**

$$\begin{array}{ccc}
 a_{0,0,1} & \cdot \cdot \cdot & a_{0,n-1,1} \\
 a_{1,0,1} & \cdot \cdot \cdot & a_{1,n-1,1} \\
 \cdot & & \cdot \\
 \cdot & & \cdot \\
 \cdot & & \cdot \\
 a_{m-1,0,1} & \cdot \cdot \cdot & a_{m-1,n-1,1} \\
 \\
 \cdot \\
 \cdot \\
 \cdot
 \end{array}$$

**Plane (p-1):**

$$\begin{array}{ccc}
 a_{0,0,p-1} & \cdot \cdot \cdot & a_{0,n-1,p-1} \\
 a_{1,0,p-1} & \cdot \cdot \cdot & a_{1,n-1,p-1} \\
 \cdot & & \cdot \\
 \cdot & & \cdot \\
 \cdot & & \cdot \\
 a_{m-1,0,p-1} & \cdot \cdot \cdot & a_{m-1,n-1,p-1}
 \end{array}$$

**In Storage**

Each block of elements in a three-dimensional sequence is stored successively in an array. The stride for the third dimension is used to select the elements for each successive block of elements in the array. The starting point of the three-dimensional sequence is specified as the argument for the sequence in the ESSL calling statement. For example, if the three-dimensional sequence is contained in array BIG, declared as `BIG(1:20,1:30,1:10)`, and starts at the second element in the first dimension, the third element in the second dimension, and the first element in the third dimension of array BIG, you should specify `BIG(2,3,1)` as the argument for the sequence, such as in:

```
CALL SCFT3 (BIG(2,3,1),20,600,Y,32,2056,16,20,10,1,1.0,AUX,30000)
```

See “How Stride Is Used for Three-Dimensional Sequences” on page 108 for a detailed description of how three-dimensional sequences are stored within arrays using strides.

## How Stride Is Used for Three-Dimensional Sequences

The elements of the three-dimensional sequence can be defined as  $a_{ijk}$  for  $i = 1, m$ ,  $j = 1, n$ , and  $k = 1, p$ . The first two subscripts,  $i$  and  $j$ , define the elements in the first two dimensions of the sequence, and the third subscript,  $k$ , defines the elements in the third dimension. Using this definition of three-dimensional sequences, this section explains how these elements are mapped into an array using the concepts of stride. (Remember that the elements  $a_{ijk}$  are the elements of the conceptual data structure, the three-dimensional sequence to be processed by ESSL. The sequence does not have to include all the elements in the array. Strides are used by the ESSL subroutines to select the desired elements to be processed in the array.)

The sequence elements in the first two dimensions are mapped into an array in the same way a matrix or two-dimensional sequence is mapped into an array. It uses all the items listed in "How Leading Dimension Is Used for Matrices" on page 67, such as the starting point, the number of rows and columns, and the leading dimension. The stride for the first dimension,  $inc1$ , of a three-dimensional sequence is assumed to be 1, as for matrices. The stride for the second dimension,  $inc2$ , of a three-dimensional sequence is equivalent to the leading dimension for a matrix.

The stride for the third dimension,  $inc3$ , is used to define the array elements that make up the third dimension of the three-dimensional sequence. The stride for the third dimension is used as an increment to step through the array to find the starting point for each of the  $p$  successive blocks of elements in the array. The stride,  $inc3$ , must always be positive. It must always be greater than or equal to the number of elements to be processed in the first two dimensions; that is,  $inc3 \geq (inc2)(n)$ .

A three-dimensional sequence is usually stored in a one-, two-, or three-dimensional array; however, for the sake of this discussion, a three-dimensional array is used here. For an array,  $A$ , declared as  $A(E1:E2, F1:F2, G1:G2)$ , the strides in the first, second, and third dimensions are:

$$\begin{aligned} inc1 &= 1 \\ inc2 &= (E2-E1+1) \\ inc3 &= (E2-E1+1)(F2-F1+1) \end{aligned}$$

Given an array  $A$ , declared as  $A(1:7, 1:3, 0:3)$ , where the lengths of the first, second, and third dimensions are 7, 3, and 4, respectively, the resulting strides are  $inc1 = 1$ ,  $inc2 = 7$ , and  $inc3 = 21$ .

The starting point for a three-dimensional sequence in an array is at the location specified by the argument for the sequence in the ESSL calling statement. Using the array  $A$ , described above, if you specify  $A(2,2,1)$  for a three-dimensional sequence, where  $A$  is defined as follows, in four blocks, for planes 0 - 3, respectively:

1.0	8.0	15.0	22.0	29.0	36.0	43.0	50.0	57.0	64.0	71.0	78.0
2.0	9.0	16.0	23.0	30.0	37.0	44.0	51.0	58.0	65.0	72.0	79.0
3.0	10.0	17.0	24.0	31.0	38.0	45.0	52.0	59.0	66.0	73.0	80.0
4.0	11.0	18.0	25.0	32.0	39.0	46.0	53.0	60.0	67.0	74.0	81.0
5.0	12.0	19.0	26.0	33.0	40.0	47.0	54.0	61.0	68.0	75.0	82.0
6.0	13.0	20.0	27.0	34.0	41.0	48.0	55.0	62.0	69.0	76.0	83.0
7.0	14.0	21.0	28.0	35.0	42.0	49.0	56.0	63.0	70.0	77.0	84.0

then processing begins in the second block of elements at row 2 and column 2 in array A, which is 30.0. The stride in the third dimension is then used to find the starting point for each of the next  $p-1$  successive blocks of elements in the array. The stride, *inc3*, is added to the starting point  $p-1$  times. In this example, the stride for the third dimension is 21, and the number of blocks of elements,  $p$ , to be processed is 3, so the starting points in array A are A(2,2,1), A(2,2,2), and A(2,2,3). These are elements 30.0, 51.0, and 72.0. These array elements then correspond to the sequence elements  $a_{111}$ ,  $a_{112}$ , and  $a_{113}$ , respectively.

In general terms, this results in the following starting positions for the blocks of elements in the array:

```
A(BEGINI, BEGINJ, BEGINK)
A(BEGINI, BEGINJ, BEGINK+1)
A(BEGINI, BEGINJ, BEGINK+2)
.
.
A(BEGINI, BEGINJ, BEGINK+p-1)
```

Using  $m = 4$ ,  $n = 2$ , and  $p = 3$  to define the elements of the three-dimensional data structure in this example, the resulting three-dimensional sequence is defined as follows, in three blocks, for planes 0 - 2, respectively:

Plane 0:	Plane 1:	Plane 2:
$a_{000}$ $a_{010}$	$a_{001}$ $a_{011}$	$a_{002}$ $a_{012}$
$a_{100}$ $a_{110}$	$a_{101}$ $a_{111}$	$a_{102}$ $a_{112}$
$a_{200}$ $a_{210}$	$a_{201}$ $a_{211}$	$a_{202}$ $a_{212}$
$a_{300}$ $a_{310}$	$a_{301}$ $a_{311}$	$a_{302}$ $a_{312}$
Plane 0:	Plane 1:	Plane 2:
30.0 37.0	51.0 58.0	72.0 79.0
31.0 38.0	52.0 59.0	73.0 80.0
32.0 39.0	53.0 60.0	74.0 81.0
33.0 40.0	54.0 61.0	75.0 82.0

As shown in this example, the three-dimensional sequence does not have to include all the blocks of elements in the array. In this case, the three-dimensional sequence includes only the second through the fourth block of elements in the array. The first block is not used. Elements of an array are selected as they are arranged in storage, regardless of the number of dimensions defined in the array. Therefore, when using a one- or two-dimensional array to store your three-dimensional sequence, you should understand how your array elements are stored to ensure that elements are selected properly. See "Setting Up Arrays in Fortran" on page 112 for a description of array storage.

**Note:** Three-dimensional sequences are used by the three-dimensional Fourier transform subroutines. By specifying certain stride values for *inc2* and *inc3* and declaring your arrays to have certain number of dimensions, you achieve optimal performance in these subroutines. For details, see "Setting Up Your Data" on page 782 and the Notes section for each subroutine.





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## Chapter 4. Coding Your Program

This chapter provides you with information you need to code your Fortran, C, and C++ programs.

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### Fortran Programs

This section describes how to code your Fortran program using any of the ESSL run-time libraries.

#### Calling ESSL Subroutines and Functions in Fortran

In Fortran programs, most ESSL subroutines are invoked with the CALL statement:

```
CALL subroutine-name (argument-1, . . . , argument-n)
```

An example of a calling sequence for the SAXPY subroutine might be:

```
CALL SAXPY (5,A,X,J+INC,Y,1)
```

The remaining ESSL subroutines are invoked as functions by coding a function reference. You first declare the type of value returned by the function: short- or long-precision real, short- or long-precision complex, or integer. Then you code the function reference as part of an expression in a statement. An example of declaring and invoking the DASUM function might be:

```
DOUBLE PRECISION DASUM,SUM,X  
.  
.  
.  
SUM = DASUM (N,X,INCX)
```

Values are returned differently for ESSL subroutines and functions. For subroutines, the results of the computation are returned in an argument specified in the calling sequence. In the CALL statement above, the result is returned in argument Y. For functions, the result is returned as the value of the function. In the assignment statement above, the result is assigned to SUM.

See the Fortran publications for details on how to code the CALL statement and a function reference.

#### Setting Up a User-Supplied Subroutine for ESSL in Fortran

Some ESSL numerical quadrature subroutines call a user-supplied subroutine, *subf*, identified in the ESSL calling sequence. If your program that calls the numerical quadrature subroutines is coded in Fortran, there are some coding rules you must follow:

- You must declare *subf* as EXTERNAL in your program.
- You should code the *subf* subroutine to the specifications given in “Programming Considerations for the SUBF Subroutine” on page 966. For examples of coding a *subf* subroutine in Fortran, see the subroutine descriptions in that chapter.

## Setting Up Scalar Data in Fortran

Table 35 lists the scalar data types in Fortran that are used for ESSL. Only those types and lengths used by ESSL are listed.

Table 35. Scalar Data Types in Fortran Programs

Terminology Used by ESSL	Fortran Equivalent
Character item <sup>1</sup> 'N', 'T', 'C' or 'n', 't', 'c'	CHARACTER*1 'N', 'T', 'C'
Logical item .TRUE., .FALSE.	LOGICAL .TRUE., .FALSE.
32-bit environment integer 12345, -12345	INTEGER or INTEGER*4 12345, -12345
64-bit environment integer <sup>2</sup> 12345, -12345	INTEGER*8 12345_8, -12345_8
Short-precision real number <sup>3</sup> 12.345	REAL or REAL*4 0.12345E2
Long-precision real number <sup>3</sup> 12.345	DOUBLE PRECISION or REAL*8 0.12345D2
Short-precision complex number <sup>3</sup> (123.45, -54321.0)	COMPLEX or COMPLEX*8 (123.45E0, -543.21E2)
Long-precision complex number <sup>3</sup> (123.45, -54321.0)	COMPLEX*16 (123.45D0, -543.21D2)
<p><b>Note:</b> <sup>1</sup> ESSL accepts character data in either upper- or lowercase in its calling sequences.</p> <p><sup>2</sup> In accordance with the LP64 data model, all ESSL integer arguments remain 32 bits except for the <b>iusadr</b> argument for ERRSET.</p> <p><sup>3</sup> Short- and long-precision numbers look the same in this book.</p>	

## Setting Up Arrays in Fortran

Arrays are declared in Fortran by specifying the array name, the number of dimensions, and the range of each dimension in a DIMENSION statement or an explicit data type statement, such as REAL, DOUBLE PRECISION, and so forth.

### Real and Complex Array Elements

Each array element can be either a real or complex data item of short or long precision. The type of the array determines the size of the element storage locations. Short-precision data requires 4 bytes, and long-precision data requires 8 bytes. Complex data requires two storage locations of either 4 or 8 bytes each, for short or long precision, respectively, to accommodate the two parts of the complex number:  $c = a+bi$ . Therefore, exactly twice as much storage is required for complex data as for real data of the same precision. See "How Do You Set Up Your Scalar Data?" on page 33 for a description of real and complex numbers.

Even though complex data items require two storage locations, the same number of elements exist in the array as for real data. A reference to an element—for

example,  $C(3)$ —in an array containing complex data gives you the whole complex number; that is, it contains both  $a$  and  $b$ , where the complex number is expressed as follows:

$C(I) \leftarrow (a_i, b_i)$  for a one-dimensional array  
 $C(I,J) \leftarrow (a_{ij}, b_{ij})$  for a two-dimensional array  
 $C(I,J,K) \leftarrow (a_{ijk}, b_{ijk})$  for a three-dimensional array

## One-Dimensional Array

For a one-dimensional array in Fortran 77, you can code:

```
DIMENSION A(E1:E2)
```

where  $A$  is the name of the array,  $E1$  is the lower bound, and  $E2$  is the upper bound of the single dimension in the array. If the lower bound is not specified, such as in  $A(E2)$ , the value is assumed to be 1. The upper bound is required.

A one-dimensional array is stored in ascending storage locations (relative to some base storage address) in the following order:

Relative Location	Array Element
1	$A(E1)$
2	$A(E1+1)$
3	$A(E1+2)$
.	.
.	.
.	.
$E2-E1+1$	$A(E2)$

For example, the array  $A$  of length 4 specified in the DIMENSION statement as  $A(0:3)$  and containing the following elements:

$A = (1, 2, 3, 4)$

has its elements arranged in storage as follows:

Relative Location	Array Element Value
1	1
2	2
3	3
4	4

## Two-Dimensional Array

For a two-dimensional array in Fortran 77, you can code:

```
DIMENSION A(E1:E2,F1:F2)
```

where  $A$  is the name of the array.  $E1$  and  $F1$  are the lower bounds of the first and second dimensions, respectively, and  $E2$  and  $F2$  are the upper bounds of the first and second dimensions, respectively. If either of the lower bounds is not specified, such as in  $A(E2,F1:F2)$ , the value is assumed to be 1. The upper bounds are always required for each dimension. For examples of Fortran 77 usage, see “SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX — Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose” on page 294.

The elements of a two-dimensional array are stored in column-major order; that is, they are stored in the following ascending storage locations (relative to some base storage address) with the value of the first (row) subscript expression increasing

most rapidly and the value of the second (column) subscript expression increasing least rapidly. Following are the locations of the elements in the array:

Relative Location	Array Element
1	A(E1,F1) (starting column 1)
2	A(E1+1,F1)
.	.
.	.
.	.
E2-E1+1	A(E2,F1)
(E2-E1+1)+1	A(E1,F1+1) (starting column 2)
(E2-E1+1)+2	A(E1+1,F1+1)
.	.
.	.
.	.
(E2-E1+1)(2)	A(E2,F1+1)
(E2-E1+1)(2)+1	A(E1,F1+2) (starting column 3)
(E2-E1+1)(2)+2	A(E1+1,F1+2)
.	.
.	.
.	.
(E2-E1+1)(F2-F1)	A(E2,F2-1)
(E2-E1+1)(F2-F1)+1	A(E1,F2) (starting column F2-F1+1)
(E2-E1+1)(F2-F1)+2	A(E1+1,F2)
.	.
.	.
.	.
(E2-E1+1)(F2-F1+1)	A(E2,F2)

For example, the 3 by 4 array A specified in the DIMENSION statement as A(2:4,1:4) and containing the following elements:

$$A = \begin{bmatrix} 11 & 12 & 13 & 14 \\ 21 & 22 & 23 & 24 \\ 31 & 32 & 33 & 34 \end{bmatrix}$$

has its elements arranged in storage as follows:

Relative Location	Array Element Value
1	11 (starting column 1)
2	21
3	31
4	12 (starting column 2)
5	22
6	32
7	13 (starting column 3)
8	23
9	33
10	14 (starting column 4)
11	24
12	34

Each element A(I,J) of the array A, declared A(1:n, 1:m), containing real or complex data, occupies the storage location whose address is given by the following formula:

$$\text{address } \{A(I,J)\} = \text{address } \{A\} + (I-1 + n(J-1))f$$

for:

$$I = 1, n \text{ and}$$

$$J = 1, m$$

where:

$f = 4$  for short-precision real numbers

$f = 8$  for long-precision real numbers

$f = 8$  for short-precision complex numbers

$f = 16$  for long-precision complex numbers

### Three-Dimensional Array

For a three-dimensional array in Fortran 77, you can code:

```
DIMENSION A(E1:E2,F1:F2,G1:G2)
```

where A is the name of the array. E1, F1, and G1 are the lower bounds of the first, second, and third dimensions, respectively, and E2, F2, and G2 are the upper bounds of the first, second, and third dimensions, respectively. If any of the lower bounds are not specified, such as in A(E1:E2,F1:F2,G2), the value is assumed to be 1. The upper bounds are always required for each dimension. For examples of Fortran 77 usage, see “SCFT3 and DCFT3 — Complex Fourier Transform in Three Dimensions” on page 850.

The elements of a three-dimensional array can be thought of as a set of two-dimensional arrays, stored sequentially in ascending storage locations in the array. The elements in each two-dimensional array are stored as defined in the previous section. In the three-dimensional array, the value of the first (row) subscript expression increases most rapidly, the second (column) subscript expression increases less rapidly, and the third subscript expression (set of rows and columns) increases least rapidly. Following are the locations of the elements in the array:

Relative Location	Array Element
1	A(E1,F1,G1) (starting the first set)
2	A(E1+1,F1,G1)
.	.
.	.
.	.
(E2-E1+1)(F2-F1+1)	A(E2,F2,G1)
(E2-E1+1)(F2-F1+1)+1	A(E1,F1,G1+1) (starting the second set)
(E2-E1+1)(F2-F1+1)+2	A(E1+1,F1,G1+1)
.	.
.	.
.	.
(E2-E1+1)(F2-F1+1)(2)	A(E2,F2,G1+1)
(E2-E1+1)(F2-F1+1)(2)+1	A(E1,F1,G1+2) (starting the third set)
(E2-E1+1)(F2-F1+1)(2)+2	A(E1+1,F1+2)
.	.
.	.
.	.
(E2-E1+1)(F2-F1+1)(G2-G1)	A(E2,F2,G2-1)
(E2-E1+1)(F2-F1+1)(G2-G1)+1	A(E1,F1,G2) (starting the last set*)
(E2-E1+1)(F2-F1+1)(G2-G1)+2	A(E1+1,F1,G2)

.  
 .  
 .  
 (E2-E1+1)(F2-F1+1)(G2-G1+1) A(E2,F2,G2)

\* The last set is the G2-G1+1 set.

For example, the 3 by 2 by 4 array A specified in the DIMENSION statement as A(1:3,0:1,2:5) and containing the following sets of rows and columns of elements:

$$A = \begin{bmatrix} 111 & 121 \\ 211 & 221 \\ 311 & 321 \end{bmatrix} \begin{bmatrix} 112 & 122 \\ 212 & 222 \\ 312 & 322 \end{bmatrix} \begin{bmatrix} 113 & 123 \\ 213 & 223 \\ 313 & 323 \end{bmatrix} \begin{bmatrix} 114 & 124 \\ 214 & 224 \\ 314 & 324 \end{bmatrix}$$

has its elements arranged in storage as follows:

Relative Location	Array Element Value
1	111 (starting the first set)
2	211
3	311
4	121
5	221
6	321
7	112 (starting the second set)
8	212
9	312
10	122
11	222
12	322
13	113 (starting the third set)
14	213
15	313
16	123
17	223
18	323
19	114 (starting the fourth set)
20	214
21	314
22	124
23	224
24	324

Each element A(I,J,K) of the array A, declared A(1:n, 1:m, 1:p), containing real or complex data, occupies the storage location whose address is given by the following formula:

$$\text{address } \{A(I,J,K)\} = \text{address } \{A\} + (I-1 + n(J-1) + mn(K-1))f$$

for:

$$\begin{aligned} I &= 1, n \\ J &= 1, m \\ K &= 1, p \end{aligned}$$

where:

$f = 4$  for short-precision real numbers  
 $f = 8$  for long-precision real numbers  
 $f = 8$  for short-precision complex numbers  
 $f = 16$  for long-precision complex numbers

## Creating Multiple Threads and Calling ESSL from Your Fortran Program

The following example shows how to create up to a maximum of eight threads, where each thread calls the DURAND and DGEICD subroutines.

**Note:** Be sure to compile this program with the `xlf_r` command and the `-qnosave` option.

```

        program matinv_example
        implicit none
!
! program to invert m nxn random matrices
!
        real(8), allocatable :: A(:, :, :), det(:, :), rcond(:)
        real(8)                :: dummy_aux, seed=1998, sd
        integer                :: rc, i, m=8, n=500, iopt=3, naux=0
!
! allocate storage
!
        allocate(A(n,n,m),stat=rc)
        call error_exit(rc,"Allocation of matrix A")
        allocate(det(2,m),stat=rc)
        call error_exit(rc,"Allocation of det")
        allocate(rcond(m),stat=rc)
        call error_exit(rc,"Allocation of rcond")
!
! Calculate inverses in parallel
!
!SMP$ parallel do private(i,sd), schedule(static),
!SMP$&   share(n,a,iopt,rcond,det,dummy_aux,naux)
        do i=1,m

            sd = seed + 100*i
            call durand(sd,n*n,A(1,1,i))
            call dgeicd(A(1,1,i),n,n,iopt,rcond(i),det(1,i),
            &          dummy_aux,naux)
            enddo

            write(*,*)'Reciprocal condition numbers of the matrices are:'
            write(*,'(4E12.4)') rcond
!
            deallocate(A,stat=rc)

            call error_exit(rc,"Deallocation of matrix A")
            deallocate(det,stat=rc)
            call error_exit(rc,"Deallocation of det")
            deallocate(rcond,stat=rc)
            call error_exit(rc,"Deallocation of rcond")
            stop

            contains
            subroutine error_exit(error_code,string)
            character(*)      :: string
            integer          :: error_code
            if(error_code .eq. 0 ) return
            write(0,*)string,": failing return code was ",error_code
            stop 1
            end subroutine error_exit
        end
end

```

## Handling Errors in Your Fortran Program

ESSL provides you with flexibilities in handling both input-argument errors and computational errors:

- For input-argument errors 2015, 2030, and 2200 which are optionally-recoverable errors, ESSL allows you to obtain corrected input-argument values and react at run time.



**Note:** In the case where error 2015 is unrecoverable, you have the option of dynamic allocation for most of the *aux* arguments. For details see the subroutine descriptions in Part 2 of this book.

- For computational errors, ESSL provides a return code and additional information to help you analyze the problem in your program and react at run time.

“Input-Argument Errors in Fortran” and “Computational Errors in Fortran” on page 122 explain how to use these facilities by describing the additional statements you must code in your program.

For multithreaded application programs, if you want to initialize the error option table and change the default settings for input-argument and computational errors, you need to implement the steps shown in “Input-Argument Errors in Fortran” and “Computational Errors in Fortran” on page 122 on each thread that calls ESSL. An example is shown in “Example of Handling Errors in a Multithreaded Application Program” on page 127.

## Input-Argument Errors in Fortran

To obtain corrected input-argument values in a Fortran program and to avert program termination for the optionally-recoverable input-argument errors 2015, 2030, and 2200 add the statements in the following steps your program. Steps 3 and 7 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary.

### Step 1. Declare ENOTRM as External:

```
EXTERNAL ENOTRM
```

This declares the ESSL error exit routine ENOTRM as an external reference in your program. This should be coded in the beginning of your program before any of the following statements.

### Step 2. Call EINFO for Initialization:

```
CALL EINFO (0)
```

This calls the EINFO subroutine with one argument of value 0 to initialize the ESSL error option table. It is required only if you call ERRSET in your program. It is coded only once in the beginning of your program before any calls to ERRSET. For a description of EINFO, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008.

### Step 3. Call ERRSAV:

```
CALL ERRSAV (ierno, tabent)
```

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *tabent*, which is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 7, for ERRSTR. For information on whether

you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56. For an example, see “Example 3” on page 126, as the use is the same as for computational errors.

#### Step 4. Call ERRSET:

```
CALL ERRSET (ierno,inoal,inomes,itrace,iusadr,irange)
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For optionally-recoverable ESSL input-argument errors, you need to call ERRSET only if you want to avoid terminating your program and you want the input arguments associated with this error to be assigned correct values in your program when the error occurs. For one error (*ierno*) or a range of errors (*irange*), you can specify:

- How many times each error can occur before execution terminates (*inoal*)
- How many times each error message can be printed (*inomes*)
- The ESSL exit routine ENOTRM, to be invoked for the error indicated (*iusadr*)

ERRSET must be called for each error code you want to indicate as being recoverable. For ESSL, *ierno* should have a value of 2015, 2030 or 2200. If you want to eliminate error messages, you should indicate a negative number for *inomes*; otherwise, you should specify 0 for this argument. All the other ERRSET arguments should be specified as 0.

For a list of the default values set in the ESSL error option table, see Table 34 on page 54. For a description of the input-argument errors, see “Input-Argument Error Messages(2001-2099)” on page 180. For a description of ERRSET, see Chapter 17, “Utilities,” on page 1005.

#### Step 5. Call ESSL:

```
CALL name (arg-1,...,arg-n,*yyy,*zzz,...)
```

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- *name* specifies the ESSL subroutine.
- *arg-1*,..., *arg-n* are the input and output arguments.
- *yyy*, *zzz*, and any other statement numbers preceded by an “\*” are the Fortran statement numbers indicating where you want to branch when you get a nonzero return code. Each corresponds to a different ESSL value. Control goes to the corresponding statement number when a nonzero return code value is returned for the CALL statement. Return code values are described under “Error Conditions” in each ESSL subroutine description in Part 2 of this book.

**Step 6. Perform the Desired Action:** These are the statements at statement number *yyy* or *zzz*, shown in the CALL statement in Step 5, and preceded by an “\*”. The statement to which control is passed corresponds to the return code value for the error.

These statements perform whatever action is desired when the recoverable error occurs. These statements may check the new values set in the input arguments to

determine whether adequate program storage is available, and then decide whether to continue or terminate the program. Otherwise, these statements may check that the size of the working storage arrays or the length of the transform agrees with other data in the program. The program may also store this corrected input argument value for future reference.

**Step 7. Call ERRSTR:**

```
CALL ERRSTR (ierno,tabent)
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *tabent*, which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 3, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56. For an example, see “Example 3” on page 126, as the use is the same as for computational errors.

**Example**

This example shows an error code 2015, which resets the size of the work area *aux*, specified in *naux*, if the value specified is too small. It also indicates that no error messages should be issued.

```

      .
      .
      .
C      DECLARE ENOTRM AS EXTERNAL
      EXTERNAL ENOTRM
      .
      .
      .
C      INITIALIZE THE ESSL ERROR
C      OPTION TABLE
      CALL EINFO(0)
      .
      .
      .
C      MAKE ERROR CODE 2015 A RECOVERABLE
C      ERROR AND SUPPRESS PRINTING ALL
C      ERROR MESSAGES FOR IT
      CALL ERRSET(2015,0,-1,0,ENOTRM,2015)
      .
      .
      .
C      CALL ESSL ROUTINE SWLEV.
C      IF THE NAUX INPUT
C      ARGUMENT IS TOO SMALL, ERROR
C      2015 OCCURS. THE MINIMUM VALUE
C      REQUIRED IS STORED IN THE NAUX
C      INPUT ARGUMENT AND CONTROL GOES
C      TO LABEL 400.
      CALL SWLEV(X,INCX,U,INCY,Y,INCY,N,AUX,NAUX,*400)
      .
      .
      .
C      CHECK THE RESULTING INPUT ARGUMENT
C      VALUE IN NAUX AND TAKE THE
C      DESIRED ACTION
400  .
      .
      .

```

## Computational Errors in Fortran

To obtain information about an ESSL computational error in a Fortran program, add the statements in the following steps to your program. Steps 2 and 7 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary. For a list of those computational errors that return information and to which these steps apply, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008.

### Step 1. Call EINFO for Initialization:

```
CALL EINFO (0)
```

This calls the EINFO subroutine with one argument of value 0 to initialize the ESSL error option table. It is required only if you call ERRSET in your program. It

is coded only once in the beginning of your program before any calls to ERRSET. For a description of EINFO, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008.

### Step 2. Call ERRSAV:

```
CALL ERRSAV (ierno,tabent)
```

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *tabent*, which is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 7, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56.

### Step 3. Call ERRSET:

```
CALL ERRSET (ierno,inoal,inomes,itrace,iusadr,irange)
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For ESSL computational errors, you need to call ERRSET only if you want to change the default values in the ESSL error option table. For one error (*ierno*) or a range of errors (*irange*), you can specify:

- How many times each error can occur before execution terminates (*inoal*)
- How many times each error message can be printed (*inomes*)

ERRSET must be called for each error code for which you want to change the default values. For ESSL, *ierno* should be set to one of the eligible values listed in Table 182 on page 1008. To allow your program to continue after an error in the specified range occurs, *inoal* must be set to a value greater than 1. For ESSL, *iusadr* should be specified as either 0 or 1 in a 32-bit environment (0\_8 or 1\_8 in a 64-bit environment), so a user exit is not taken.

For a list of the default values set in the ESSL error option table, see Table 34 on page 54. For a description of the computational errors, see “Computational Error Messages(2100-2199)” on page 186. For a description of ERRSET, see Chapter 17, “Utilities,” on page 1005.

### Step 4. Call ESSL:

```
CALL name (arg-1,...,arg-n,*yyy,*zzz,...)
```

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- *name* specifies the ESSL subroutine.
- *arg-1*,..., *arg-n* are the input and output arguments.
- *yyy*, *zzz*, and any other statement numbers preceded by an “\*” are the Fortran statement numbers indicating where you want to branch when you get a nonzero return code. Each corresponds to a different ESSL value. Control goes to

the corresponding statement number when a nonzero return code value is returned for the CALL statement. Return code values are described under “Error Conditions” in each ESSL subroutine description in Part 2 of this book.

#### Step 5. Call EINFO for Information:

```
nbr CALL EINFO (icode, inf1)
-or-
nbr CALL EINFO (icode, inf1, inf2)
```

This calls the EINFO subroutine, which returns information about certain computational errors, where:

- *nbr* is the statement number *yyy*, *zzz*, or any of the other statement numbers preceded by an “\*” in the CALL statement in Step 4, corresponding to the return code value for this error code.
- *icode* is the error code of interest.
- *inf1* and *inf2* are the integer variables used to receive the information, where *inf1* is assigned a value for all errors, and *inf2* is assigned a value for some errors. For a description of EINFO, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008.

**Step 6. Check the Values in the Information Receivers:** These statements check the values returned in the output argument information receivers, *inf1* and *inf2*, which contain the information about the computational error.

#### Step 7. Call ERRSTR:

```
CALL ERRSTR (ierno, tabent)
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *tabent*, which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 2, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56.

#### Example 1

This 32-bit environment example shows an error code 2104, which returns one piece of information: the index of the last diagonal with nonpositive value (I1).

```

      .
      .
      .
C           INITIALIZE THE ESSL ERROR
C           OPTION TABLE
C     CALL EINFO(0)
      .
      .
      .
C           ALLOW 100 ERRORS FOR CODE 2104
C     CALL ERRSET(2104,100,0,0,0,2104)
      .
      .
      .
C           CALL ESSL ROUTINE DPPF.
C           IF THE INPUT MATRIX IS NOT
C           POSITIVE DEFINITE, CONTROL GOES TO
C           LABEL 400
C     IOPT=0
C     CALL DPPF(APP,N,IOPT,*400)
      .
      .
      .
C           CALL THE INFORMATION-HANDLER
C           ROUTINE FOR ERROR CODE 2104 TO
C           RETURN ONE PIECE OF INFORMATION
C           IN VARIABLE I1, THE INDEX OF THE
C           LAST NONPOSITIVE DIAGONAL FOUND
C           BY ROUTINE DPPF
400  CALL EINFO (2104,I1)
      .
      .
      .

```

## Example 2

This 32-bit environment example shows an error code 2103, which returns one piece of information: the index of the zero diagonal (I1) found by DGEF.

```

      .
      .
      .
C           INITIALIZE THE ESSL ERROR
C           OPTION TABLE
      CALL EINFO(0)
      .
      .
      .
C           ALLOW 100 ERRORS FOR CODE 2103
      CALL ERRSET(2103,100,0,0,0,2103)
      .
      .
      .
C           CALL ESSL SUBROUTINE DGEF.
C           IF THE INPUT MATRIX IS
C           SINGULAR, CONTROL GOES TO
C           LABEL 400
      CALL DGEF(A,LDA,N,IPVT,*400)
      .
      .
      .
C           CALL THE INFORMATION-HANDLER
C           ROUTINE FOR ERROR CODE 2103 TO
C           RETURN ONE PIECE OF INFORMATION
C           IN VARIABLE I1, THE INDEX OF THE
C           LAST ZERO DIAGONAL FOUND BY
C           SUBROUTINE DGEF
400      CALL EINFO (2103,I1)
      .
      .
      .

```

### Example 3

This 32-bit environment example shows an error code 2101, which returns two pieces of information: the eigenvalue (I1) that failed to converge after the indicated (I2) number of iterations. It uses ERRSAV and ERRSTR to insulate the effects of the error handling for error 2101 by this program.



```

      .
      .
C      DECLARE AN AREA TO SAVE THE
C      ERROR OPTION TABLE INFORMATION
C      FOR ERROR CODE 2101
      CHARACTER*8 SAV2101
      .
      .
C      INITIALIZE THE ESSL ERROR
C      OPTION TABLE
      CALL EINFO(0)
C      SAVE THE EXISTING ERROR OPTION
C      TABLE ENTRY FOR ERROR CODE 2101
      CALL ERRSAV(2101,SAV2101)
      .
      .
C      ALLOW 255 ERRORS FOR CODE 2101
      CALL ERRSET(2101,255,0,0,0,2101)
      .
      .
C      CALL ESSL SUBROUTINE DGEEV.
C      IF THE EIGENVALUE FAILED TO
C      CONVERGE, CONTROL GOES TO LABEL 400
      CALL DGEEV(IOPT,A,LDA,W,Z,LDZ,SELECT,N,AUX,NAUX,*400)
      .
      .
C      CALL THE INFORMATION-HANDLER
C      ROUTINE FOR ERROR CODE 2101 TO
C      RETURN TWO PIECES OF INFORMATION.
C      VARIABLE I1 CONTAINS THE EIGENVALUE
C      THAT FAILED TO CONVERGE.  VARIABLE
C      I2 CONTAINS THE NUMBER OF ITERATIONS.
400  CALL EINFO (2101,I1,I2)
      .
      .
C      RESTORE THE PREVIOUS ERROR OPTION
C      TABLE ENTRY FOR ERROR CODE 2101.
C      ERROR PROCESSING RETURNS TO HOW IT
C      WAS BEFORE IT WAS ALTERED BY THE ABOVE
C      ERRSET STATEMENT.
      CALL ERRSTR(2101,SAV2101)
      .
      .

```

## Example of Handling Errors in a Multithreaded Application Program

This 32-bit environment example shows how to modify the MATINV\_EXAMPLE program in “Creating Multiple Threads and Calling ESSL from Your Fortran Program” on page 117 with calls to the ESSL error handling subroutines. The ESSL error handling subroutines are called from each thread to: initialize the error option table, save the current error option table values for input-argument error 2015 and computational error 2105, change the default values for errors 2015 and 2105, and then restore the original default values for errors 2015 and 2105.

```

program matinv_example
    implicit none
!
!   program to invert m nxn random matrices
!
    real(8), allocatable :: A(:, :, :), det(:, :), rcond(:)
    real(8)                :: dummy_aux, seed=1998, sd
    integer                :: rc, i, m=8, n=500, iopt=3, naux=0
    integer                :: inf1(8)
    character(8)          :: sav2015(8)
    character(8)          :: sav2105(8)
    integer                :: ENOTRM
!
    external ENOTRM
!
! allocate storage
    allocate(A(n,n,m),stat=rc)
    call error_exit(rc,"Allocation of matrix A")
    allocate(det(2,m),stat=rc)
    call error_exit(rc,"Allocation of det")
    allocate(rcond(m),stat=rc)
!
    call error_exit(rc,"Allocation of rcond")
!
! Calculate inverses in parallel
!
!SMP$ parallel do private(i,sd), schedule(static),
!SMP$&   share(n,m,a,iopt,rcond,det,dummy_aux,naux,sav2015,sav2105,inf1)
do i=1,m
!
!   initialize error handling
    call einfo(0)
!
!   Save existing option table values for error 2015
    call errsav(2015,sav2015(i))
!
!   Set Error 2015 to be non-recoverable so dgeicd will dynamically
!   allocate the work area.
    call errset(2015,100,100,0,1,2015)
!
!   Save existing option table values for error 2105
    call errsav(2105,sav2105(i))
!
!   Set Error 2105 to be recoverable
    call errset(2105,100,100,0,ENOTRM,2105)
!
    sd = seed + 100*i
    call durand(sd,n*n,A(1,1,i))
    call dgeicd(A(1,1,i),n,n,iopt,rcond(i),det(1,i),
&             dummy_aux,naux,*10,*20)
10    goto 30
!
!   Catch singular matrix returned by dgeicd.
20    CALL EINFO(2105,inf1(i))
    WRITE(*,*) 'ERROR: Zero pivot found at location ',inf1(i)
!
!   Restore the error option table entries
30    continue
    call errstr(2015,SAV2015(i))
    call errstr(2105,SAV2105(i))

enddo

```

```
write(*,*)'Reciprocal condition numbers of the matrices are:'
write(*,'(4E12.4)') rcond
!
deallocate(A,stat=rc)
call error_exit(rc,"Deallocation of matrix A")
deallocate(det,stat=rc)
call error_exit(rc,"Deallocation of det")

deallocate(rcond,stat=rc)
call error_exit(rc,"Deallocation of rcond")
stop
contains
  subroutine error_exit(error_code,string)
    character(*)    :: string
    integer         :: error_code
    if(error_code .eq. 0 ) return
    write(0,*)string,": failing return code was ",error_code
    stop 1
  end subroutine error_exit
end
```

---

## C Programs

This section describes how to code your C program.

### Calling ESSL Subroutines and Functions in C

This section shows how to call ESSL subroutines and functions from your C program.

#### Before You Call ESSL

Before you can call the ESSL subroutines from your C program, you must have the appropriate ESSL header file installed on your system. The ESSL header file allows you to code your function calls as described in this section. It contains entries for all the ESSL subroutines. The ESSL header file is distributed with the ESSL package. The ESSL header file to be used with the C compiler is named `essl.h`. You should check with your system support group to verify that the appropriate ESSL header file is installed.

In the beginning of your program, before you call any of the ESSL subroutines, **you must code the following statement for the ESSL header file:**

```
#include <essl.h>
```

If you are planning to create your own threads for the ESSL Thread-Safety or SMP Library, you must include the `pthread.h` header file as the first include file in your C program. For an example, see “Creating Multiple Threads and Calling ESSL from Your C Program” on page 134.

#### Coding the Calling Sequences

In C programs, the ESSL subroutines, not returning a function value, are invoked with the following type of statement:

```
subroutine-name (argument-1, . . . , argument-n);
```

An example of a calling sequence for SAXPY might be:

```
saxpy (5,a,x,incx,y,1);
```

The ESSL subroutines returning a function value are invoked with the following type of statement:

```
function-value-name=subroutine-name (argument-1, . . . , argument-n);
```

An example of invoking DASUM might be:

```
sum = dasum (n,x,incx);
```

See the C publications for details about how to code the function calls.

## Passing Arguments in C

This section describes how to pass arguments in your C program.

### About the Syntax Shown in This Book

The argument syntax shown in this book assumes that you have installed and are using the ESSL header file. For further details, see “Calling ESSL Subroutines and Functions in C” on page 129.

### No Optional Arguments

In the ESSL calling sequences for C, there are no optional arguments, as for some programming languages. You must code all the arguments listed in the syntax.

### Arguments That Must Be Passed by Value

All scalar arguments that are not modified must be passed by value in the ESSL calling sequence. (This refers to input-only scalar arguments, such as *incx*, *m*, and *lda*.)

### Arguments That Must Be Passed by Reference

Following are the instances in which you pass your arguments by reference (as a pointer) in the ESSL calling sequence:

**Arrays:** Arguments that are arrays are passed by reference, as usual.

**Subroutine Names:** Some ESSL subroutines call a user-supplied subroutine. The name is part of the ESSL calling sequence. It must be passed by reference.

**Output Scalar Arguments:** When an output argument is a scalar data item, it must be passed by reference. This is true for all scalar data types: real, complex, and so forth. **When this occurs, it is listed in the notes of each subroutine description in Part 2 of this book.**

**Character Arguments:** Character arguments must be passed as strings, by reference. You specify the character, in upper- or lowercase, in the ESSL calling sequence with double quotation marks around it, as in "t". Following is an example of how you can call SGEADD, specifying the *transa* and *transb* arguments as strings *n* and *t*, respectively:

```
sgeadd (a,5,"n",b,3,"t",c,4,4,3);
```

**Altered Arguments When Using Error Handling:** If you use ESSL error handling in your C program, as described in “Handling Errors in Your C Program” on page 136, you must pass by reference all the arguments that can potentially be altered

by ESSL error handling. This applies to all your ESSL call statements after the point where you code the #define statement, shown in step 1 in “Input-Argument Errors in C” on page 136 and in step 1 in “Computational Errors in C” on page 141. The two types of ESSL arguments are:

- *naux* arguments for auxiliary storage
- *n* arguments for transform lengths

## Setting Up a User-Supplied Subroutine for ESSL in C

Some ESSL numerical quadrature subroutines call a user-supplied subroutine, *subf*, identified in the ESSL calling sequence. If your program that calls the numerical quadrature subroutines is coded in C, there are some coding rules you must follow for the *subf* subroutine:

- You can code the *subf* subroutine using only C or Fortran.
- You must declare *subf* as an external subroutine in your application program.
- You should code the *subf* subroutine to the specifications given in “Programming Considerations for the SUBF Subroutine” on page 966. For an example of coding a *subf* subroutine in C, see “Example 1” on page 978.

## Setting Up Scalar Data in C

Table 36 lists the scalar data types in C that are used for ESSL. Only those types and lengths used by ESSL are listed.

Table 36. Scalar Data Types in C Programs

Terminology Used by ESSL	C Equivalent
Character item <sup>1</sup> 'N', 'T', 'C' or 'n', 't', 'c'	char * "n", "t", "c"
Logical item .TRUE., .FALSE.	int For additional information, see “Using Logical Data in C” on page 133. <sup>2</sup>
32-bit environment integer 12345, -12345	int
64-bit environment integer <sup>3</sup> 12345l, -12345l	long
Short-precision real number <sup>4</sup> 12.345	float
Long-precision real number <sup>4</sup> 12.345	double
Short-precision complex number <sup>4</sup> (123.45, -54321.0)	Specify it as described in “Setting Up Complex Data Types in C” on page 132. <sup>2</sup>
Long-precision complex number <sup>4</sup> (123.45, -54321.0)	Specify it as described in “Setting Up Complex Data Types in C” on page 132. <sup>2</sup>

Table 36. Scalar Data Types in C Programs (continued)

Terminology Used by ESSL	C Equivalent
<b>Note:</b> <sup>1</sup> ESSL accepts character data in either upper- or lowercase in its calling sequences.	
<sup>2</sup> There are no equivalent data types for logical and complex data in C. These require special procedures. For details, see the referenced section.	
<sup>3</sup> In accordance with the LP64 data model, all ESSL integer arguments remain 32-bits except for the <b>iusadr</b> argument for ERRSET.	
<sup>4</sup> Short- and long-precision numbers look the same in this book.	

## Setting Up Complex Data Types in C

Complex data types are not part of the C language; however, some ESSL subroutines require arguments of these data types.

### Complex Data

ESSL provides identifiers, `cmplx` and `dcmplx`, for complex data types, defined in the ESSL header file, as well as two macro definitions, `RE` and `IM`, for handling the real and imaginary parts of complex numbers:

```
#ifndef _Cmplx
#define _Cmplx
#ifdef _REIM
#define _REIM 1
#endif
typedef union { struct { float _re, _im;
                        _data; double _align;} cmplx;
#ifdef _DCmplx
#ifdef _REIM
#define _REIM 1
#endif
typedef union { struct { double _re, _im;
                        _data; double _align;} dcplx;
#ifdef _REIM
#define RE(x) ((x)._data._re)
#define IM(x) ((x)._data._im)
#endif
#endif
```

You must, therefore, code an include statement for the ESSL header file in the beginning of your program to use these definitions. For details, see “Calling ESSL Subroutines and Functions in C” on page 129.

Assuming you are using the ESSL header file, if you declare data items to be of type `cmplx` or `dcmplx`, you can pass them as short- and long-precision complex data to ESSL, respectively. You may want to write a `CSET` macro to initialize complex variables, using the `RE` and `IM` macros provided in the ESSL header file. Following is an example of how to use the `CSET` macro to initialize the complex variable `alpha`:

```
#include <essl.h>
#define CSET(x,a,b) (RE(x)=a, IM(x)=b)
main()
{
  cmplx alpha,t[3],s[5];
  .
  .
  .
  CSET (alpha,2.0,3.0);
  caxpy (3,alpha,s,1,t,2);
```

```
.  
. .  
}
```

If you choose to use your own definitions for complex data, instead of those provided in the ESSL header file, you can define `_CMPLX` and `_DCMPLX` in your program for short- and long-precision complex data, respectively, using the following `#define` statements. These statements are coded with your global declares in the front of your program and must be coded before the `#include` statement for the ESSL header file.

```
#define _CMPLX  
#define _DCMPLX
```

If you prefer to define your complex data at compile time, you can use the job processing procedures described in Chapter 5, “Processing Your Program,” on page 163.

## Using Logical Data in C

Logical data types are not part of the C language; however, some ESSL subroutines require arguments of these data types.

By coding the following simple macro definitions in your program, you can then use `TRUE` or `FALSE` in assigning values to or specifying any logical arguments passed to ESSL:

```
#define FALSE 0  
#define TRUE 1
```

## Setting Up Arrays in C

C arrays are arranged in storage in row-major order. This means that the last subscript expression increases most rapidly, the next-to-the-last subscript expression increases less rapidly, and so forth, with the first subscript expression increasing least rapidly. ESSL subroutines require that arrays passed as arguments be in column-major order. This is the array storage convention used by Fortran, described in “Setting Up Arrays in Fortran” on page 112. To pass an array from your C program to ESSL, to have ESSL process the data correctly, and to get a result that is in the proper form for your C program, you can do any of the following:

- Build and process the matrix, logically transposed from the outset, and transpose the results as necessary.
- Before the ESSL call, transpose the input arrays. Then, following the ESSL call, transpose any arrays updated as output.
- If there are arguments in the ESSL calling sequence indicating whether the arrays are to be processed in normal or transposed form, such as the *transa* and *transb* arguments in the `_GEMM` subroutines, use these arguments in combination with the matrix equivalence rules to avoid having to transpose your data in separate operations. For further detail, see “SGEMMS, DGEMMS, CGEMMS, and ZGEMMS — Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes Using Winograd’s Variation of Strassen’s Algorithm” on page 398.

## Creating Multiple Threads and Calling ESSL from Your C Program

The example shown below shows how to create two threads, where each thread calls the ISAMAX subroutine. To use the AIX pthreads library, you must specify the pthread.h header file as the first include file in your program.

**Note:** Be sure to compile this program with the cc\_r command.



```

#include <pthread.h>
#include <stdio.h>
#include <unistd.h>
#include <essl.h>

/* Create structure for argument list */
typedef struct {
    int    n;
    float  *x;
    int    incx;
} arg_list;

/* Define prototype for thread routine */
void *Thread(void *v);

int main()
{
    float  sx1[9] = { 1., 2., 7., -8., -5., -10., -9., 10., 6. };
    float  sx2[8] = { 1.,12., 7., -8., -5., -10., -9., 19.};
    pthread_t first_th;
    pthread_t second_th;
    int rc;
    arg_list a_l,b_l;

    /* Creating argument list for the first thread */
    a_l.n = 9;
    a_l.incx = 1;
    a_l.x = sx1;

    /* Creating argument list for the second thread */
    b_l.n = 8;
    b_l.incx = 1;
    b_l.x = sx2;

    /* Creating first thread which calls the ESSL subroutine ISAMAX */
    rc = pthread_create(&first_th, NULL, Thread, (void *) &a_l);
    if (rc) exit(-1);

    /* Creating second thread which calls the ESSL subroutine ISAMAX */
    rc = pthread_create(&second_th, NULL, Thread, (void *) &b_l);
    if (rc) exit(-1);

    sleep(1);
    exit(0);
}

/* Thread routine which call ESSL routine ISAMAX */
void *Thread(void *v)
{
    arg_list *a_l;
    float *x;
    int n,incx;
    int i;

    a_l = (arg_list *) (v);
    x = a_l->x;
    n = a_l->n;
    incx = a_l->incx;

    /* Calling the ESSL subroutine ISAMAX */
    i = isamax(n,x,incx);
    if ( i == 8)
        printf("max for sx2 should be 8 = %d\n",i);
    else
        printf("max for sx1 should be 6 = %d\n",i);
}

```

## Handling Errors in Your C Program

ESSL provides you with flexibilities in handling both input-argument errors and computational errors:

- For input-argument errors 2015, 2030, and 2200, which are optionally-recoverable errors, ESSL allows you to obtain corrected input-argument values and react at run time.

**Note:** In the case where error 2015 is unrecoverable, you have the option of dynamic allocation for most of the *aux* arguments. For details see the subroutine descriptions in Part 2 of this book.

- For computational errors, ESSL provides a return code and additional information to help you analyze the problem in your program and react at run time.

“Input-Argument Errors in C” and “Computational Errors in C” on page 141 explain how to use these facilities by describing the additional statements you must code in your program.

For multithreaded application programs, if you want to initialize the error option table and change the default settings for input-argument and computational errors, you need to implement the steps shown in “Input-Argument Errors in C” and “Computational Errors in C” on page 141 on each thread that calls ESSL.

### Input-Argument Errors in C

To obtain corrected input-argument values in a C program and to avert program termination for the optionally-recoverable input-argument errors 2015, 2030, and 2200, add the statements in the following steps to your program. Steps 4 and 8 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary.

#### Step 1. Code the Global Statements for ESSL Error Handling:

```
/* Code two underscores */
/* before the letters ESVERR */
#define __ESVERR
#include <essl.h>
extern int enotrm();
```

These statements are coded with your global declares in the front of your program. The `#define` must be coded before the `#include` statement for the ESSL header file. The `extern` statement declares the ESSL error exit routine ENOTRM as an external reference in your program. **After the point where you code these statements in your program, you must pass by reference all ESSL calling sequence arguments that can potentially be altered by ESSL error handling.** This applies to all your ESSL call statements. The two types of arguments are:

- *n*<sub>aux</sub> arguments for auxiliary storage
- *n* arguments for transform lengths

## Step 2. Declare the Variables:

```
int (*iusadr) ();
int ierno, inoal, inomes, itrace, irange, irc, dummy;
char storarea[8];
```

This declares a pointer, *iusadr*, to be used for the ESSL error exit routine ENOTRM. Also included are declares for the variables used by the ESSL and Fortran error-handling subroutines. Note that *storarea* must be 8 characters long. These should be coded in the beginning of your program before any of the following statements.

## Step 3. Do Initialization for ESSL:

```
iusadr = enotrm;
einfo (0, &dummy, &dummy);
```

The first statement sets the function pointer, *iusadr*, to ENOTRM, the ESSL error exit routine. The last statement calls the EINFO subroutine to initialize the ESSL error option table, where *dummy* is a declared integer and is a placeholder. For a description of EINFO, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008. These statements should be coded only once in the beginning of your program before calls to ERRSET.

## Step 4. Call ERRSAV:

```
errsav (&ierno, storarea);
```

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *storarea*, which is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 8, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56. For an example, see “Example 1” on page 143, as the use is the same as for computational errors.

## Step 5. Call ERRSET:

```
errset (&ierno, &inoal, &inomes, &itrace, &iusadr, &irange);
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For optionally-recoverable ESSL input-argument errors, you need to call ERRSET only if you want to avoid terminating your program and you want the input arguments associated with this error to be assigned correct values in your program when the error occurs. For one error (*ierno*) or a range of errors (*irange*), you can specify:

- How many times each error can occur before execution terminates (*inoal*)
- How many times each error message can be printed (*inomes*)

- The ESSL exit routine ENOTRM, to be invoked for the error indicated (*iusadr*)

ERRSET must be called for each error code you want to indicate as being recoverable. For ESSL, *ierno* should have a value of 2015, 2030, or 2200. If you want to eliminate error messages, you should indicate a negative number for *inomes*; otherwise, you should specify 0 for this argument. All the other ERRSET arguments should be specified as 0.

For a list of the default values set in the ESSL error option table, see Table 34 on page 54. For a description of the input-argument errors, see “Input-Argument Error Messages(2001-2099)” on page 180. For a description of ERRSET, see Chapter 17, “Utilities,” on page 1005.

#### Step 6. Call ESSL:

```
irc = name (arg1,...,argn);
if irc == rc1
{
    .
    .
    .
}
```

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- *name* specifies the ESSL subroutine.
- *arg1,...,argn* are the input and output arguments. As explained in step 1, all arguments that can potentially be altered by error handling must be coded by reference.
- *irc* is the integer variable containing the return code resulting from the computation performed by the ESSL subroutine.
- *rc1, rc2*, and so forth are the possible return code values that can be passed back from the ESSL subroutine to C. The values can be 0, 1, 2, and so forth. Return code values are described under “Error Conditions” in each ESSL subroutine description in Part 2 of this book.

**Step 7. Perform the Desired Action:** These are the statements following the test for each value of the return code, returned in *irc* in step 6. These statements perform whatever action is desired when the recoverable error occurs. These statements may check the new values set in the input arguments to determine whether adequate program storage is available, and then decide whether to continue or terminate the program. Otherwise, these statements may check that the size of the working storage arrays or the length of the transform agrees with other data in the program. The program may also store this corrected input argument value for future reference.

#### Step 8. Call ERRSTR:

```
errstr (&ierno,storarea);
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *storarea*, which is accessible to your program. ERRSTR must be called for each

entry you want to store. This step is used, along with step 4, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56. For an example, see “Example 1” on page 143, as the use is the same as for computational errors.

### **Example 1**

This example shows an error code 2015, which resets the size of the work area *aux*, specified in *naux*, if the value specified is too small. It also indicates that no error messages should be issued.

```

.
.
.
    /*GLOBAL STATEMENTS FOR ESSL ERROR HANDLING*/
#define __ESVERR
#include <essl.h>
extern int enotrm();
.
.
.

    /*DECLARE THE VARIABLES*/
main ()
{
int (*iusadr) ();
int ierno,inoal,inomes,itrace,irc,dummy;
int naux;
.
.
.

    /*INITIALIZE THE POINTER TO THE ENOTRM ROUTINE*/
iusadr = enotrm;
.
.
.

    /*INITIALIZE THE ESSL ERROR OPTION TABLE*/
einfo (0,&dummy,&dummy);
.
.
.

    /*MAKE ERROR CODE 2015 A RECOVERABLE ERROR AND
    SUPPRESS PRINTING ALL ERROR MESSAGES FOR IT*/
ierno = 2015;
inoal = 0;
inomes = -1;
itrace = 0;
irange = 2015;
errset (&ierno,&inoal,&inomes,&itrace,&iusadr,&irange);
.
.
.

    /*CALL ESSL SUBROUTINE SWLEV. NAUX IS PASSED BY
    REFERENCE. IF THE NAUX INPUT IS TOO SMALL,
    ERROR 2015 OCCURS. THE MINIMUM VALUE REQUIRED
    IS STORED IN THE NAUX INPUT ARGUMENT, AND THE
    RETURN CODE OF 1 IS SET IN IRC.*/
irc = swlev (x,incx,u,incu,y,incy,n,aux,&naux);
if irc == 1
{
.
.
    /*CHECK THE RESULTING INPUT ARGUMENT VALUE
    IN NAUX AND TAKE THE DESIRED ACTION*/
.
.
}

.
.
.
}

```

## Computational Errors in C

To obtain information about an ESSL computational error in a C program, add the statements in the following steps to your program. Steps 4 and 9 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary. For a list of those computational errors that return information and to which these steps apply, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008.

### Step 1. Code the Global Statements for ESSL Error Handling:

```
/* Code two underscores */
/* before the letters ESVERR */
#define __ESVERR
#include <essl.h>
```

These statements are coded with your global declares in the front of your program. The `#define` must be coded before the `#include` statement for the ESSL header file. **After the point where you code these statements in your program, you must pass by reference all ESSL calling sequence arguments that can potentially be altered by ESSL error handling.** This applies to all your ESSL call statements. The two types of arguments are:

- *n*aux arguments for auxiliary storage
- *n* arguments for transform lengths

### Step 2. Declare the Variables:

```
int ierno,inoal,inomes,itrace,iusadr,irange,irc;
int inf1,inf2,dummy;
char storarea[8];
```

These statements include declares for the variables used by the ESSL and Fortran error-handling subroutines. Note that *storarea* must be 8 characters long. These should be coded in the beginning of your program before any of the following statements.

### Step 3. Do Initialization for ESSL:

```
einfo (0,&dummy,&dummy);
```

This statement calls the EINFO subroutine to initialize the ESSL error option table, where *dummy* is a declared integer and is a placeholder. For a description of EINFO, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008. These statements should be coded only once in the beginning of your program before calls to ERRSET.

### Step 4. Call ERRSAV:

```
errsav (&ierno,storarea);
```

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *storarea*, which

is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 8, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56. For an example, see “Example 1” on page 143.

#### Step 5. Call ERRSET:

```
errset (&ierno,&inoal,&inomes,&itrace,&iusadr,&irange);
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For ESSL computational errors, you need to call ERRSET only if you want to change the default values in the ESSL error option table. For one error (*ierno*) or a range of errors (*irange*), you can specify:

- How many times each error can occur before execution terminates (*inoal*)
- How many times each error message can be printed (*inomes*)

ERRSET must be called for each error code for which you want to change the default values. For ESSL, *ierno* should be set to one of the eligible values listed in Table 182 on page 1008. To allow your program to continue after an error in the specified range occurs, *inoal* must be set to a value greater than 1. For ESSL, *iusadr* should be specified as either 0 or 1 in a 32-bit environment (0l or 1l in a 64-bit environment), so a user exit is not taken.

For a list of the default values set in the ESSL error option table, see Table 34 on page 54. For a description of the computational errors, see “Computational Error Messages(2100-2199)” on page 186. For a description of ERRSET, see Chapter 17, “Utilities,” on page 1005.

#### Step 6. Call ESSL:

```
irc = name (arg1,...,argn);  
if irc == rc1  
    {  
        .  
        .  
        .  
    }  
if irc == rc2  
    {  
        .  
        .  
        .  
    }
```

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- *name* specifies the ESSL subroutine.
- *arg1,...,argn* are the input and output arguments. As explained in step 1, all arguments that can potentially be altered by error handling must be coded by reference.
- *irc* is the integer variable containing the return code resulting from the computation performed by the ESSL subroutine.



- *rc1*, *rc2*, and so forth are the possible return code values that can be passed back from the ESSL subroutine to C. The values can be 0, 1, 2, and so forth. Return code values are described under “Error Conditions” in each ESSL subroutine description in Part 2 of this book.

The statements following each test of the return code can perform any desired action. This includes calling EINFO for more information about the error, as described in step 7.

**Step 7. Call EINFO for Information:**

```
einfo (ierno,&inf1,&inf2);
```

This calls the EINFO subroutine, which returns information about certain computational errors, where:

- *ierno* is the error code of interest.
- *inf1* and *inf2* are the integer variables used to receive the information, where *inf1* is assigned a value for all errors, and *inf2* is assigned a value for some errors. You must specify both arguments, as there are no optional arguments for C. Both arguments must be passed by reference, because they are output scalar arguments. For a description of EINFO, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008.

**Step 8. Check the Values in the Information Receivers:** These statements check the values returned in the output argument information receivers, *inf1* and *inf2*, which contain the information about the computational error.

**Step 9. Call ERRSTR:**

```
errstr (&ierno,storarea);
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *storarea*, which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 4, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56. For an example, see “Example 1.”

**Example 1**

This 32-bit environment example shows an error code 2105, which returns one piece of information: the index of the pivot element (*i*) near zero, causing factorization to fail. It uses ERRSAV and ERRSTR to insulate the effects of the error handling for error 2105 by this program.

```

.
.
        /*GLOBAL STATEMENTS FOR ESSL ERROR HANDLING*/
#define __ESVERR
#include <essl.h>
.
.
        /*DECLARE THE VARIABLES*/
main ()
{
int ierno,inoal,inomes,itrace,iusadr,irange,irc;
int inf1,inf2,dummy;
char sav2105[8];
.
.
        /*INITIALIZE THE ESSL ERROR OPTION TABLE*/
einfo (0,&dummy,&dummy);
        /*SAVE THE EXISTING ERROR OPTION TABLE ENTRY
        FOR ERROR CODE 2105*/
ierno = 2105;
errsav (&ierno,sav2105);
.
.
        /*MAKE ERROR CODES 2101 THROUGH 2105 RECOVERABLE
        ERRORS AND SUPPRESS PRINTING ALL ERROR MESSAGES
        FOR THEM. THIS SHOWS HOW YOU CODE THE
        ERRSET ARGUMENTS FOR A RANGE OF ERRORS. */
ierno = 2101;
inoal = 0;
inomes = 0; /*A DUMMY ARGUMENT*/
itrace = 0; /*A DUMMY ARGUMENT*/
iusadr = 0; /*A DUMMY ARGUMENT*/
irange = 2105
errset (&ierno,&inoal,&inomes,&itrace, &iusadr,&irange);
.
.
        /*CALL ESSL SUBROUTINE DGEICD. IF THE INPUT MATRIX
        IS SINGULAR OR NEARLY SINGULAR, ERROR 2105
        OCCURS. A RETURN CODE OF 2 IS SET IN IRC.*/
irc = dgeicd (a,lda,n,iopt,&rcond,det,aux,&naux);
if irc == 2
{
        /*CALL THE INFORMATION-HANDLER ROUTINE FOR ERROR
        CODE 2105 TO RETURN ONE PIECE OF INFORMATION
        IN VARIABLE INF1, THE INDEX OF THE PIVOT ELEMENT
        NEAR ZERO, CAUSING FACTORIZATION TO FAIL.
        INF2 IS NOT USED, BUT MUST BE SPECIFIED.
        BOTH INF1 AND INF2 ARE PASSED BY REFERENCE,
        BECAUSE THEY ARE OUTPUT SCALAR ARGUMENTS.*/
ierno = 2105;
einfo (ierno,&inf1,&inf2);
        /*CHECK THE VALUE IN VARIABLE INF1 AND TAKE THE
        DESIRED ACTION*/
.
.
}
.
.
        /*RESTORE THE PREVIOUS ERROR OPTION TABLE ENTRY
        FOR ERROR CODE 2105. ERROR PROCESSING
        RETURNS TO HOW IT WAS BEFORE IT WAS ALTERED BY
        THE ABOVE ERRSAV STATEMENT*/
ierno = 2105;
errstr (&ierno,sav2105);
.
.
}

```

---

## C++ Programs

This section describes how to code your C++ program.

### Calling ESSL Subroutines and Functions in C++

This section shows how to call ESSL subroutines and functions from your C++ program.

#### Before You Call ESSL

Before you can call the ESSL subroutines from your C++ program, you must have the appropriate ESSL header file installed on your system. The ESSL header file allows you to code your function calls as described in this section. It contains entries for all the ESSL subroutines. The ESSL header file is distributed with the ESSL package. The ESSL header file to be used with the C++ compiler is named `essl.h`.

In the beginning of your program, before you call any of the ESSL subroutines, **you must code the following statement for the ESSL header file:**

```
#include <essl.h>
```

If you are creating your own threads for the ESSL Thread-Safe or SMP Library, you must include the `pthread.h` header file in your C++ program. For an example, see “Creating Multiple Threads and Calling ESSL from Your C++ Program” on page 150.

#### Coding the Calling Sequences

In C++ programs, the ESSL subroutines, not returning a function value, are invoked with the following type of statement:

```
subroutine-name (argument-1, . . . , argument-n);
```

An example of a calling sequence for SAXPY might be:

```
saxpy (5,a,x,incx,y,1);
```

The ESSL subroutines returning a function value are invoked with the following type of statement:

```
function-value-name=subroutine-name (argument-1, . . . , argument-n);
```

An example of invoking DASUM might be:

```
sum = dasum (n,x,incx);
```

See the C++ publications for details about how to code the function calls.

### Passing Arguments in C++

This section describes how to pass arguments in your C++ program.

## About the Syntax Shown in This Book

The argument syntax shown in this book assumes that you have installed and are using the ESSL header file. For further details, see “Calling ESSL Subroutines and Functions in C++” on page 145.

## No Optional Arguments

In the ESSL calling sequences for C++, there are no optional arguments, as for some programming languages. You must code all the arguments listed in the syntax.

## Arguments That Must Be Passed by Value

All scalar arguments that are not modified must be passed by value in the ESSL calling sequence. (This refers to input-only scalar arguments, such as *incx*, *m*, and *lda*.)

## Arguments That Must Be Passed by Reference

Following are the instances in which you pass your arguments by reference (as a pointer) in the ESSL calling sequence:

**Arrays:** Arguments that are arrays are passed by reference, as usual.

**Subroutine Names:** Some ESSL subroutines call a user-supplied subroutine. The name is part of the ESSL calling sequence. It must be passed by reference.

**Output Scalar Arguments:** When an output scalar argument is a scalar data item, it must be passed by reference as shown below. This is true for all scalar data types: real, complex, and so forth.

The ESSL header file supports two alternatives:

- The arguments are declared to be type reference in the function prototype. This is the default. Following is an example of how you can call DURAND using this alternative:

```
durand (seed, n, x);
```

- The arguments are declared as pointers in the function prototype. If you wish to use this alternative, you must define `_ESVCPTR` using one of the following methods:

- Define `_ESVCPTR` in your program using a `#define` statement, as shown below:

```
#define _ESVCPTR
```

This statement is coded with your global declares and must be coded before the `#include` statement for the ESSL header file.

- Define `_ESVCPTR` at compile time by using the job processing procedure described in “C++ Program Procedures on AIX” on page 165.

Following is an example of how you can call DURAND using this alternative:

```
durand (&seed, n, x);
```

**Character Arguments:** Character arguments must be passed as strings, by reference. You specify the character, in upper- or lowercase, in the ESSL calling sequence with double quotation marks around it, as in “t”. Following is an example of how you can call SGEADD, specifying the *transa* and *transb* arguments as strings *n* and *t*, respectively:

```
sgeadd (a,5,"n",b,3,"t",c,4,4,3);
```

## Setting Up a User-Supplied Subroutine for ESSL in C++

Some ESSL numerical quadrature subroutines call a user-supplied subroutine, *subf*, identified in the ESSL calling sequence. If your program that calls the numerical quadrature subroutines is coded in C++, there are some coding rules you must follow for the *subf* subroutine:

- You can code the *subf* subroutine using only C, C++, or Fortran.
- You must declare *subf* as an external subroutine in your application program.
- You should code the *subf* subroutine to the specifications given in “Programming Considerations for the SUBF Subroutine” on page 966. For an example of coding a *subf* subroutine in C++, see “Example 1” on page 978.

## Setting Up Scalar Data in C++

Table 37 lists the scalar data types in C++ that are used for ESSL. Only those types and lengths used by ESSL are listed.

Table 37. Scalar Data Types in C++ Programs

Terminology Used by ESSL	C++ Equivalent
Character item <sup>1</sup> 'N', 'T', 'C' or 'n', 't', 'c'	char * "n", "t", "c"
Logical item .TRUE., .FALSE.	int For additional information, see “Using Logical Data in C++” on page 150. <sup>2</sup>
32-bit environment integer 12345, -12345	int
64-bit environment integer <sup>3</sup> 12345l, -12345l	long
Short-precision real number <sup>4</sup> 12.345	float
Long-precision real number <sup>4</sup> 12.345	double
Short-precision complex number <sup>4</sup> (123.45, -54321.0)	complex <float> <sup>5</sup> , or as described in “On AIX—Setting Up Short-Precision Complex Data Types If You Are Using the IBM Open Class Complex Mathematics Library in C++” on page 148.
Long-precision complex number <sup>4</sup> (123.45, -54321.0)	complex <double> <sup>5</sup> or complex <sup>6</sup>

Table 37. Scalar Data Types in C++ Programs (continued)

Terminology Used by ESSL	C++ Equivalent
<p><b>Notes:</b></p> <ol style="list-style-type: none"> <li>1. ESSL accepts character data in either upper- or lowercase in its calling sequences.</li> <li>2. There are no equivalent data types for logical data in C++. These require special procedures. For details, see the referenced section.</li> <li>3. In accordance with the LP64 data model, all ESSL integer arguments remain 32-bits except for the <b>iusadr</b> argument for ERRSET.</li> <li>4. Short- and long-precision numbers look the same in this book.</li> <li>5. This data type is defined in file &lt;complex&gt;.</li> <li>6. This data type is defined in file &lt;complex.h&gt; (supported only on AIX).</li> </ol>	

## Using Complex Data in C++

On AIX, the ESSL header file supports both the IBM Open Class<sup>®</sup> Complex Mathematics Library (<complex.h>) and the Standard Numerics Library facilities for complex arithmetic (<complex>). On Linux, only the Standard Numerics Library is supported.

The following sections explain how to handle the two choices available on AIX.

### On AIX—Selecting the <complex> or <complex.h> Header File

Although the header files <complex> and <complex.h> are similar in purpose, they are mutually incompatible and cannot be simultaneously used.

If you wish to use the Standard Numerics Library facilities for complex arithmetic, you must do one of the following:

- Code the #include statement for the Standard Numerics Library facilities for complex arithmetic (#include <complex>) in your program prior to coding the #include statement for the ESSL header file.
- Define `_ESV_COMPLEX_`, using one of the following methods:
  - Define `_ESV_COMPLEX_` in your program using a #define statement, as shown below:
 

```
#define _ESV_COMPLEX_
```

 This statement is coded with your global declares and must be coded before the #include statement for the ESSL header file.
  - Define `_ESV_COMPLEX_` at compile time by using the job processing procedures described in Chapter 5, “Processing Your Program,” on page 163.

If you take none of the preceding steps, the ESSL header file will use the IBM Open Class Complex Mathematics Library. The ESSL header file will also use the IBM Open Class Complex Mathematics Library if you:

- Code the #include statement for the IBM Open Class Complex Mathematics Library (#include <complex.h>) in your program prior to coding the #include statement for the ESSL header file.

### On AIX—Setting Up Short-Precision Complex Data Types If You Are Using the IBM Open Class Complex Mathematics Library in C++

Short-precision complex data types are not part of the C++ language; however, some ESSL subroutines require arguments of these data types.

**Short-Precision Complex Data:** ESSL provides an identifier, `cmplx`, for the short-precision complex data type, defined in the ESSL header file, as well as two member functions, `sreal` and `simag`, for handling the real and imaginary parts of short-precision complex numbers:

```
#ifndef _CMPLX
class cmplx
{
private:
float _re,_im;
public:
cmplx() { _re = 0.0; _im = 0.0; }
cmplx(float r, float i = 0.0) { _re = r; _im = i; }
friend inline float sreal(const cmplx& a) { return a._re; }
friend inline float simag(const cmplx& a) { return a._im; }
};
#endif
```

You must, therefore, code an include statement for the ESSL header file in the beginning of your program to use these definitions. For details, see “Calling ESSL Subroutines and Functions in C++” on page 145.

Assuming you are using the ESSL header file, if you declare data items to be of type `cmplx` or `complex`, you can pass them as short- or long-precision complex data to ESSL, respectively. Following is an example of how you might code your program:

```
#include <complex.h>
#include <essl.h>
main()
{
cmplx alpha,t[3],s[5];
complex beta,td[3],sd[5];
.
.
alpha = cmplx(2.0,3.0);
caxpy (3,alpha,s,1,t,2);
.
.
beta = complex(2.0,3.0);
zaxpy (3,beta,sd,1,td,2);
.
.
}
```

If you choose to use your own definition for short-precision complex data, instead of that provided in the ESSL header file, your definition must conform to the following rules:

- The definition must have exactly two variables of type `float` representing the real and imaginary parts of the short-precision complex data. For example:  

```
struct cmplx { float _re, _im; };
```
- The definition cannot include an explicit destructor.

In addition, you must do one of the following:

- Define `_CMPLX` in your program using the `#define` statement. This statement is coded with your global declares in the front of your program and must be coded before the `#include` statement for the ESSL header file, as follows:

```
#define _CMPLX
```

- Use the job processing procedures described in Chapter 5, “Processing Your Program,” on page 163 to define your short-precision complex data at compile time.

## Using Logical Data in C++

Logical data types are not part of the C++ language; however, some ESSL subroutines require arguments of these data types.

By coding the following simple macro definitions in your program, you can then use TRUE or FALSE in assigning values to or specifying any logical arguments passed to ESSL:

```
#define FALSE 0
#define TRUE 1
```

## Setting Up Arrays in C++

C++ arrays are arranged in storage in row-major order. This means that the last subscript expression increases most rapidly, the next-to-the-last subscript expression increases less rapidly, and so forth, with the first subscript expression increasing least rapidly. ESSL subroutines require that arrays passed as arguments be in column-major order. This is the array storage convention used by Fortran, described in “Setting Up Arrays in Fortran” on page 112. To pass an array from your C++ program to ESSL, to have ESSL process the data correctly, and to get a result that is in the proper form for your C++ program, you can do any of the following:

- Build and process the matrix, logically transposed from the outset, and transpose the results as necessary.
- Before the ESSL call, transpose the input arrays. Then, following the ESSL call, transpose any arrays updated as output.
- If there are arguments in the ESSL calling sequence indicating whether the arrays are to be processed in normal or transposed form, such as the *transa* and *transb* arguments in the `_GEMM` subroutines, use these arguments in combination with the matrix equivalence rules to avoid having to transpose your data in separate operations. For further detail, see “SGEMMS, DGEMMS, CGEMMS, and ZGEMMS — Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes Using Winograd’s Variation of Strassen’s Algorithm” on page 398.

## Creating Multiple Threads and Calling ESSL from Your C++ Program

The example shown below shows how to create two threads, where each thread calls the ISAMAX subroutine. To use the pthreads library, you must remember to code the `pthread.h` header file in your C++ program.

**Note:** Be sure to compile this program with the `xlc_r` command.



```

#include "essl.h"
#ifdef __linux
#include <iostream>
#else
#include <iostream.h>
#endif

/* Define prototype for thread routine */
void *Thread(void *v);

/* Define prototype for thread library routine, which is in C */
extern "C" {
#include <pthread.h>
#include <stdlib.h>
int pthread_create(pthread_t *tid, const pthread_attr_t *attr,
void *(*start_routine)(void *), void *arg);
}
extern "Fortran" int isamax(const int &, float *, const int &);
/* Create structure for argument list */
struct arg_list {
int n;
float *x;
int incx;
};
void main()
{
float sx1[9] = { 1., 2., 7., -8., -5., -10., -9., 10., 6. };
float sx2[8] = { 1.,12., 7., -8., -5., -10., -9., 19.};
pthread_t first_th;
pthread_t second_th;
int rc;
struct arg_list a_l,b_l;

a_l.n = 9;
a_l.incx = 1;
a_l.x = sx1;

b_l.n = 8;
b_l.incx = 1;
b_l.x = sx2;

/* Creating argument list for first thread */
rc = pthread_create(&first_th, NULL, Thread, (void *) &a_l);
if (rc) exit(-1);

/* Creating argument list for second thread */
rc = pthread_create(&second_th, NULL, Thread, (void *) &b_l);
if (rc) exit(-1);

sleep(20);
exit(0);
}
/* Thread routine which calls the ESSL subroutine ISAMAX */
void* Thread(void *v)
{
struct arg_list *al;
float *t;
int n,incx;
int i;

al = (struct arg_list *) (v);
t = al->x;
n = al->n;
incx = al->incx;

```

```

/* Calling the ESSL subroutine ISAMAX */
i = isamax(n,t,incx);
if ( i == 8)
    cout << "max for sx2 should be 8 = " << i << "\n";
else
    cout << "max for sx1 should be 6 = " << i << "\n";
return NULL;
}

```

## Handling Errors in Your C++ Program

ESSL provides you with flexibilities in handling both input-argument errors and computational errors:

- For input-argument errors 2015, 2030, and 2200 which are optionally-recoverable errors, ESSL allows you to obtain corrected input-argument values and react at run time.

**Note:** In the case where error 2015 is unrecoverable, you have the option of dynamic allocation for most of the *aux* arguments. For details see the subroutine descriptions in Part 2 of this book.

- For computational errors, ESSL provides a return code and additional information to help you analyze the problem in your program and react at run time.

“Input-Argument Errors in C++” and “Computational Errors in C++” on page 157 explain how to use these facilities by describing the additional statements you must code in your program.

For multithreaded application programs, if you want to initialize the error option table and change the default settings for input-argument and computational errors, you need to implement the steps shown in “Input-Argument Errors in C++” and “Computational Errors in C++” on page 157 on each thread that calls ESSL.

### Input-Argument Errors in C++

To obtain corrected input-argument values in a C++ program and to avert program termination for the optionally-recoverable input-argument errors 2015, 2030, and 2200, add the statements in the following steps to your program. Steps 4 and 8 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary.

### Step 1. Code the Global Statements for ESSL Error Handling:

```
/* Code one underscore */
/* before the letters ESVERR */
#define _ESVERR
#ifdef __linux
#include <iostream>
#else
#include <iostream.h>
#endif
#include <stdio.h>
#include <essl.h>
extern "Fortran" int enotrm(int &,int &);
extern "Fortran" typedef int (*FN) (int &,int &);
```

These statements are coded with your global declares in the front of your program. The `#define` must be coded before the `#include` statements for the ESSL header file. The `extern` statements are required to call the ESSL error exit routine `ENOTRM` as an external reference in your program.

### Step 2. Declare the Variables:

```
FN iusadr;
int ierno,inoal,inomes,itrace,irange,irc,dummy;
char storarea[8];
```

This declares a pointer, *iusadr*, to be used for the ESSL error exit routine `ENOTRM`. Also included are declares for the variables used by the ESSL and Fortran error-handling subroutines. Note that *storarea* must be 8 characters long. These should be coded in the beginning of your program before any of the following statements.

### Step 3. Do Initialization for ESSL:

```
iusadr = enotrm;
dummy = 0;
einfo (0,dummy,dummy);
```

The first statement sets the function pointer, *iusadr*, to `ENOTRM`, the ESSL error exit routine. The last statement calls the `EINFO` subroutine to initialize the ESSL error option table, where *dummy* is a declared integer and is a placeholder. For a description of `EINFO`, see “`EINFO` — ESSL Error Information-Handler Subroutine” on page 1008. These statements should be coded only once in the beginning of your program before calls to `ERRSET`.

### Step 4. Call ERRSAV:

```
errsav (ierno,storarea);
```

(This is an optional step.) This calls the `ERRSAV` subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *storarea*, which is accessible to your program. `ERRSAV` must be called for each entry you want to

save. This step is used, along with step 8, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56. For an example, see “Example” on page 159, as the use is the same as for computational errors.

#### Step 5. Call ERRSET:

```
errset (ierno,inoal,inomes,itrace,iusadr,irange);
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For optionally-recoverable ESSL input-argument errors, you need to call ERRSET only if you want to avoid terminating your program and you want the input arguments associated with this error to be assigned correct values in your program when the error occurs. For one error (*ierno*) or a range of errors (*irange*), you can specify:

- How many times each error can occur before execution terminates (*inoal*)
- How many times each error message can be printed (*inomes*)
- The ESSL exit routine ENOTRM, to be invoked for the error indicated (*iusadr*)

ERRSET must be called for each error code you want to indicate as being recoverable. For ESSL, *ierno* should have a value of 2015, 2030, or 2200. If you want to eliminate error messages, you should indicate a negative number for *inomes*; otherwise, you should specify 0 for this argument. All the other ERRSET arguments should be specified as 0.

For a list of the default values set in the ESSL error option table, see Table 34 on page 54. For a description of the input-argument errors, see “Input-Argument Error Messages(2001-2099)” on page 180. For a description of ERRSET, see Chapter 17, “Utilities,” on page 1005.

#### Step 6. Call ESSL:

```
irc = name (arg1,...,argn);  
if irc == rc1  
{  
    .  
    .  
    .  
}  
if irc == rc2  
{  
    .  
    .  
    .  
}
```

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- *name* specifies the ESSL subroutine.
- *arg1,...,argn* are the input and output arguments.
- *irc* is the integer variable containing the return code resulting from the computation performed by the ESSL subroutine.

- *rc1*, *rc2*, and so forth are the possible return code values that can be passed back from the ESSL subroutine to C++. The values can be 0, 1, 2, and so forth. Return code values are described under “Error Conditions” in each ESSL subroutine description in Part 2 of this book.

**Step 7. Perform the Desired Action:** These are the statements following the test for each value of the return code, returned in *irc* in step 6. These statements perform whatever action is desired when the recoverable error occurs. These statements may check the new values set in the input arguments to determine whether adequate program storage is available, and then decide whether to continue or terminate the program. Otherwise, these statements may check that the size of the working storage arrays or the length of the transform agrees with other data in the program. The program may also store this corrected input argument value for future reference.

**Step 8. Call ERRSTR:**

```
errstr (ierno,storarea);
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *storarea*, which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 4, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56. For an example, see “Example” on page 159, as the use is the same as for computational errors.

**Example**

This example shows an error code 2015, which resets the size of the work area *aux*, specified in *naux*, if the value specified is too small. It also indicates that no error messages should be issued.

```

.
.
.
    /*GLOBAL STATEMENTS FOR ESSL ERROR HANDLING*/
#define _ESVERR
#include <essl.h>
#ifdef __linux
#include <iostream>
#else
#include <iostream.h>
#endif
#include <stdio.h>
extern "Fortran" int enotrm(int &,int &);
extern "Fortran" typedef int (*FN) (int &,int &);
.
.
.
    /*DECLARE THE VARIABLES*/
main ()
{
FN iusadr;
int ierno,inoal,inomes,itrace,irc,dummy;
int naux;
.
.
.
    /*INITIALIZE THE POINTER TO THE ENOTRM ROUTINE*/
iusadr = enotrm;
.
.
.
/*INITIALIZE THE ESSL ERROR OPTION TABLE*/
dummy = 0;
einfo (0,dummy,dummy);
.
.
.
    /*MAKE ERROR CODE 2015 A RECOVERABLE ERROR AND
    SUPPRESS PRINTING ALL ERROR MESSAGES FOR IT*/
ierno = 2015;
inoal = 0;
inomes = -1;
itrace = 0;
irange = 2015;
errset (ierno,inoal,inomes,itrace,iusadr,irange);
.
.
.
    /*CALL ESSL SUBROUTINE SWLEV. NAUX IS PASSED BY
    REFERENCE. IF THE NAUX INPUT IS TOO SMALL,
    ERROR 2015 OCCURS. THE MINIMUM VALUE REQUIRED
    IS STORED IN THE NAUX INPUT ARGUMENT, AND THE
    RETURN CODE OF 1 IS SET IN IRC.*/
irc = swlev (x,incx,u,incu,y,incy,n,aux,naux);
if irc == 1
{
.
.
.
    /*CHECK THE RESULTING INPUT ARGUMENT VALUE
    IN NAUX AND TAKE THE DESIRED ACTION*/
.
.
.
}
.
.
.
}

```

## Computational Errors in C++

To obtain information about an ESSL computational error in a C++ program, add the statements in the following steps to your program. Steps 4 and 9 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary. For a list of those computational errors that return information and to which these steps apply, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008.

### Step 1. Code the Global Statements for ESSL Error Handling:

```
/* Code one underscore */
/* before the letters ESVERR */
#define _ESVERR
#ifdef __linux
#include <iostream>
#else
#include <iostream.h>
#endif
#include <stdio.h>
#include <essl.h>
```

These statements are coded with your global declares in the front of your program. The #define must be coded before the #include statement for the ESSL header file.

### Step 2. Declare the Variables:

```
int ierno,inoal,inomes,itrace,iusadr,irange,irc;
int inf1,inf2,dummy;
char storarea[8];
```

These statements include declares for the variables used by the ESSL and Fortran error-handling subroutines. Note that *storarea* must be 8 characters long. These should be coded in the beginning of your program before any of the following statements.

### Step 3. Do Initialization for ESSL:

```
dummy = 0;
einfo (0,dummy,dummy);
```

The last statement calls the EINFO subroutine to initialize the ESSL error option table, where *dummy* is a declared integer and is a placeholder. For a description of EINFO, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008. These statements should be coded only once in the beginning of your program before calls to ERRSET.

### Step 4. Call ERRSAV:

```
errsav (iern,storarea);
```

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *storablea*, which is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 8, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56. For an example, see “Example” on page 159.

#### Step 5. Call ERRSET:

```
errset (ierno,inoal,inomes,itrace,iusadr,irange);
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For ESSL computational errors, you need to call ERRSET only if you want to change the default values in the ESSL error option table. For one error (*ierno*) or a range of errors (*irange*), you can specify:

- How many times each error can occur before execution terminates (*inoal*)
- How many times each error message can be printed (*inomes*)

ERRSET must be called for each error code for which you want to change the default values. For ESSL, *ierno* should be set to one of the eligible values listed in Table 182 on page 1008. To allow your program to continue after an error in the specified range occurs, *inoal* must be set to a value greater than 1. For ESSL, *iusadr* should be specified as either 0 or 1 in a 32-bit environment (0l or 1l in a 64-bit environment), so a user exit is not taken.

For a list of the default values set in the ESSL error option table, see Table 34 on page 54. For a description of the computational errors, see “Computational Error Messages(2100-2199)” on page 186. For a description of ERRSET, see Chapter 17, “Utilities,” on page 1005.

#### Step 6. Call ESSL:

```
irc = name (arg1,...,argn);  
if irc == rc1  
{  
  .  
  .  
  .  
}  
if irc == rc2  
{  
  .  
  .  
  .  
}
```

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- *name* specifies the ESSL subroutine.
- *arg1*,...,*argn* are the input and output arguments.
- *irc* is the integer variable containing the return code resulting from the computation performed by the ESSL subroutine.



- *rc1*, *rc2*, and so forth are the possible return code values that can be passed back from the ESSL subroutine to C++. The values can be 0, 1, 2, and so forth. Return code values are described under “Error Conditions” in each ESSL subroutine description in Part 2 of this book.

The statements following each test of the return code can perform any desired action. This includes calling EINFO for more information about the error, as described in step 7.

**Step 7. Call EINFO for Information:**

```
einfo (ierno, inf1, inf2);
```

This calls the EINFO subroutine, which returns information about certain computational errors, where:

- *ierno* is the error code of interest.
- *inf1* and *inf2* are the integer variables used to receive the information, where *inf1* is assigned a value for all errors, and *inf2* is assigned a value for some errors. You must specify both arguments, as there are no optional arguments for C. For a description of EINFO, see “EINFO — ESSL Error Information-Handler Subroutine” on page 1008.

**Step 8. Check the Values in the Information Receivers:** These statements check the values returned in the output argument information receivers, *inf1* and *inf2*, which contain the information about the computational error.

**Step 9. Call ERRSTR:**

```
errstr (ierno, storarea);
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *storarea*, which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 4, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see “How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?” on page 56. For an example, see “Example.”

**Example**

This 32-bit environment example shows an error code 2105, which returns one piece of information: the index of the pivot element (*i*) near zero, causing factorization to fail. It uses ERRSAV and ERRSTR to insulate the effects of the error handling for error 2105 by this program.

```

.
.
        /*GLOBAL STATEMENTS FOR ESSL ERROR HANDLING*/
#define _ESVERR
#include <essl.h>
#if defined(__linux) || defined(__blrts)
#include <iostream>
#else
#include <iostream.h>
#endif
#include <stdio.h>
.
.
        /*DECLARE THE VARIABLES*/
main ()
{
int ierno,inoal,inomes,itrace,iusadr,irange,irc;
int inf1,inf2,dummy;
char sav2105[8];
.
.
        /*INITIALIZE THE ESSL ERROR OPTION TABLE*/
dummy = 0;
einfo (0,dummy,dummy);
        /*SAVE THE EXISTING ERROR OPTION TABLE ENTRY
        FOR ERROR CODE 2105*/
ierno = 2105;
errsav (ierno,sav2105);
.
.
        /*MAKE ERROR CODES 2101 THROUGH 2105 RECOVERABLE
        ERRORS AND SUPPRESS PRINTING ALL ERROR MESSAGES
        FOR THEM. THIS SHOWS HOW YOU CODE THE
        ERRSET ARGUMENTS FOR A RANGE OF ERRORS. */
ierno = 2101;
inoal = 0;
inomes = 0; /*A DUMMY ARGUMENT*/
itrace = 0; /*A DUMMY ARGUMENT*/
iusadr = 0; /*A DUMMY ARGUMENT*/
irange = 2105
errset (ierno,inoal,inomes,itrace, iusadr,irange);
.
.
        /*CALL ESSL SUBROUTINE DGEICD. IF THE INPUT MATRIX
        IS SINGULAR OR NEARLY SINGULAR, ERROR 2105
        OCCURS. A RETURN CODE OF 2 IS SET IN IRC.*/
irc = dgeicd (a,lda,n,iopt,rcond,det,aux,naux);
if irc == 2
{
        /*CALL THE INFORMATION-HANDLER ROUTINE FOR ERROR
        CODE 2105 TO RETURN ONE PIECE OF INFORMATION
        IN VARIABLE INF1, THE INDEX OF THE PIVOT ELEMENT
        NEAR ZERO, CAUSING FACTORIZATION TO FAIL.
        INF2 IS NOT USED, BUT MUST BE SPECIFIED.
        BOTH INF1 AND INF2 ARE PASSED BY REFERENCE,
        BECAUSE THEY ARE OUTPUT SCALAR ARGUMENTS.*/
ierno = 2105;
einfo (ierno,inf1,inf2);
        /*CHECK THE VALUE IN VARIABLE INF1 AND TAKE THE
        DESIRED ACTION*/
.
.
}
}

```

```
.  
.      /*RESTORE THE PREVIOUS ERROR OPTION TABLE ENTRY  
      FOR ERROR CODE 2105.  ERROR PROCESSING  
      RETURNS TO HOW IT WAS BEFORE IT WAS ALTERED BY  
      THE ABOVE ERRSAV STATEMENT*/  
ierno = 2105;  
errstr (ierno,sav2105);  
.      }  
}
```



---

## Chapter 5. Processing Your Program

This section describes the **ESSL-specific changes** you need to make to your job procedures for compiling, linking, and running your program.

You can use any procedures you are currently using to compile, link, and run your Fortran, C, and C++ programs, as long as you make the necessary modifications required by ESSL.

---

### Processing Your Program on AIX

The following notes apply to processing your program on AIX.

#### Notes:

1. The default search path for the ESSL libraries is: **/usr/lib**. (Note that **/lib** is a symbolic link to **/usr/lib**.)

If the libraries are installed somewhere else, add the path name of that directory to the beginning of the **LIBPATH** environment variable, being careful to keep **/usr/lib** in the path. The correct **LIBPATH** setting is needed both for linking and executing the program.

For example, if you installed the ESSL libraries in **/home/me/lib** you would issue ksh commands similar to the following in order to compile and link a program:

```
LIBPATH=/home/me/lib:/usr/lib
export LIBPATH
xlf -o myprog myprog.f -lessl
```

After setting the **LIBPATH** command, the **/home/me/lib** directory is the directory that gets searched first for the necessary libraries. This same search criterion is used at both compile and link time and run time.

2. For the ESSL SMP Library, you can use the XL Fortran **XL SMP OPTS** or **OMP\_NUM\_THREADS** environment variable to specify options which affect SMP execution. For details, see the Fortran publications.
3. If you are accessing ESSL from a 64-bit-environment program, you must add the **-q64** compiler option.
4. ESSL supports the XL Fortran compile-time option **-qextname**. For details, see the Fortran manuals.
5. Fortran 90 programmers may be interested in the **-qessl** compiler option which allows the use of ESSL routines in place of Fortran 90 intrinsic procedures. For details, see the Fortran manuals.
6. In your job procedures, you must use only the allowable compilers and libraries listed in Table 4 on page 9.

### Dynamic Linking Versus Static Linking on AIX

Only dynamic linking is supported for programs using ESSL.

### Fortran Program Procedures on AIX

You do not need to modify your existing Fortran compilation procedures when using ESSL.

When linking and running your program, you must modify your existing job procedures for ESSL in order to set up the necessary libraries.

If you are accessing ESSL from a Fortran program, you can compile and link using the commands shown in the table below.

ESSL Library Name		Command
SMP	32-bit	<code>xlf_r -O -qnosave xyz.f -lesslsm</code>
	64-bit	<code>xlf_r -O -qnosave -q64 xyz.f -lesslsm</code>
Serial	32-bit	<code>xlf_r -O -qnosave xyz.f -lessl</code>
	64-bit	<code>xlf_r -O -qnosave -q64 xyz.f -lessl</code>
Serial	32-bit	<code>xlf -O xyz.f -lessl</code>
	64-bit	<code>xlf -O -q64 xyz.f -lessl</code>

where *xyz.f* is the name of your Fortran program.

ESSL supports the XL Fortran compile-time option **-qextname**. For details, see the Fortran manuals.

## C Program Procedures on AIX

The ESSL header file `essl.h`, used for C and C++ programs, is installed in the `<usr>include` directory. You do not need to modify your existing C compilation procedures when using ESSL, unless you want to specify your own definitions for complex data.

If you do want to specify your own definitions for short- and long-precision complex data, add **-D\_CMPLX** and **-D\_DCMPLX**, respectively, to your compile and link command. Otherwise, you automatically use the definitions of short- and long-precision complex data provided in the ESSL header file (as shown in the table below).

When linking and running your program, you must modify your existing job procedures for ESSL, to set up the necessary libraries.

If you are accessing ESSL from a C program, you can compile and link using the commands also shown in the table below.

ESSL Library Name		Command
SMP	32-bit	<code>cc_r -O xyz.c -lesslsm</code>
		<code>cc_r -O -D_CMPLX -D_DCMPLX xyz.c -lesslsm</code>
	64-bit	<code>cc_r -O -q64 xyz.c -lesslsm</code>
		<code>cc_r -O -D_CMPLX -D_DCMPLX -q64 xyz.c -lesslsm</code>
Serial	32-bit	<code>cc_r -O xyz.c -lessl</code>
		<code>cc_r -O -D_CMPLX -D_DCMPLX xyz.c -lessl</code>
	64-bit	<code>cc_r -O -q64 xyz.c -lessl</code>
		<code>cc_r -O -D_CMPLX -D_DCMPLX -q64 xyz.c -lessl</code>
Serial	32-bit	<code>cc -O xyz.c -lessl</code>
		<code>cc -O -D_CMPLX -D_DCMPLX xyz.c -lessl</code>
	64-bit	<code>cc -O -q64 xyz.c -lessl</code>
		<code>cc -O -D_CMPLX -D_DCMPLX -q64 xyz.c -lessl</code>

## C++ Program Procedures on AIX

The ESSL header file `essl.h`, used for C and C++ programs, is installed in the `<usr>/include` directory. When using ESSL, the compiler option `-qnocinc=/usr/include/essl` must be specified.

If you are using the IBM Open Class Complex Mathematics Library, you automatically use the definition of short-precision complex data provided in the ESSL header file. If you prefer to specify your own definition for short-precision complex data, add `-D_CMLPX` to your commands (as shown in the table below). Otherwise, ESSL will use the IBM Open Class Complex Mathematics Library or the Standard Numerics Library, as described in “On AIX—Selecting the `<complex>` or `<complex.h>` Header File” on page 148.

If you prefer to explicitly specify that you want to use the Standard Numerics Library facilities for complex arithmetic, add `-D_ESV_COMPLEX_` to your command as shown in the table below.

The ESSL header file supports two alternatives for declaring scalar output arguments. By default, the arguments are declared to be type reference. If you prefer for them to be declared as pointers, add `-D_ESVCPTR` to your commands as shown in the table below.

When linking and running your program, you must modify your existing job procedures for ESSL, to set up the necessary libraries.

If you are accessing ESSL from a C++ program, you can compile and link using the commands shown in the table below.

ESSL Library Name		Command
SMP	32-bit	<code>x1C_r -O xyz.C -lesslsmpl -qnocinc=/usr/include/essl</code>
		<code>x1C_r -O -D_CMLPX xyz.C -lesslsmpl -qnocinc=/usr/include/essl</code>
		<code>x1C_r -O -D_ESV_COMPLEX_ xyz.C -lesslsmpl -qnocinc=/usr/include/essl</code>
		<code>x1C_r -O -D_ESVCPTR xyz.C -lesslsmpl -qnocinc=/usr/include/essl</code>
	64-bit	<code>x1C_r -O -q64 xyz.C -lesslsmpl -qnocinc=/usr/include/essl</code>
		<code>x1C_r -O -D_CMLPX -q64 xyz.C -lesslsmpl -qnocinc=/usr/include/essl</code>
		<code>x1C_r -O -D_ESV_COMPLEX_ -q64 xyz.C -lesslsmpl -qnocinc=/usr/include/essl</code>
		<code>x1C_r -O -D_ESVCPTR -q64 xyz.C -lesslsmpl -qnocinc=/usr/include/essl</code>

ESSL Library Name		Command
Serial	32-bit	x1C_r -O xyz.C -lessl -qnocinc=/usr/include/essl
		x1C_r -O -D_CMPLX xyz.C -lessl -qnocinc=/usr/include/essl
		x1C_r -O -D_ESV_COMPLEX_ xyz.C -lessl -qnocinc=/usr/include/essl
		x1C_r -O -D_ESVCPTR xyz.C -lessl -qnocinc=/usr/include/essl
	64-bit	x1C_r -O -q64 xyz.C -lessl -qnocinc=/usr/include/essl
		x1C_r -O -D_CMPLX -q64 xyz.C -lessl -qnocinc=/usr/include/essl
		x1C_r -O -D_ESV_COMPLEX_ -q64 xyz.C -lessl -qnocinc=/usr/include/essl
		x1C_r -O -D_ESVCPTR -q64 xyz.C -lessl -qnocinc=/usr/include/essl
Serial	32-bit	x1C -O xyz.C -lessl -qnocinc=/usr/include/essl
		x1C -O -D_CMPLX xyz.C -lessl -qnocinc=/usr/include/essl
		x1C -O -D_ESV_COMPLEX_ xyz.C -lessl -qnocinc=/usr/include/essl
		x1C -O -D_ESVCPTR xyz.C -lessl -qnocinc=/usr/include/essl
	64-bit	x1C -O -q64 xyz.C -lessl -qnocinc=/usr/include/essl
		x1C -O -D_CMPLX -q64 xyz.C -lessl -qnocinc=/usr/include/essl
		x1C -O -D_ESV_COMPLEX_ -q64 xyz.C -lessl -qnocinc=/usr/include/essl
		x1C -O -D_ESVCPTR -q64 xyz.C -lessl -qnocinc=/usr/include/essl

## Processing Your Program on Linux

The following notes apply to processing your program on Linux.

### Notes:

1. The default search paths for the ESSL shared libraries are as follows:

**32-bit libraries**                      The default search path is: **/usr/lib**

**64-bit libraries**                      The default search path is: **/usr/lib64**

If the shared libraries are installed somewhere else, you need to set the link-time and run-time library search paths. There are two ways to set these search paths:

- Use one of the following compile/link options:

**-R** (or **-rpath**)      Writes the specified run-time library search paths into the executable program.

**-L**                      Searches the library search paths at link time, but does not write them into the executable as run-time library search paths.

—or—

- Use one of the following environment variables:

**LD\_LIBRARY\_PATH**                      Specifies the directories that are to be searched for libraries at run time.



**LD\_RUN\_PATH** Specifies the directories that are to be searched for libraries at both link and run time.

For example, if you installed the ESSL 32-bit libraries in `/home/me/lib`, you would issue ksh commands similar to the following in order to compile and link a program:

```
LD_LIBRARY_PATH=/home/me/lib: $LD_LIBRARY_PATH
LD_RUN_PATH=/home/me/lib: $LD_RUN_PATH
export LD_LIBRARY_PATH
export LD_RUN_PATH
xlf_r -o myprog myprog.f -lessl
```

The result would be that the `/home/me/lib` directory is the directory that gets searched at link time and run time.

For more information on link options and environment variables, see the manpage for the `ld` command

2. For the ESSL SMP Library, you can use the XL Fortran **XLSMPOPTS** or **OMP\_NUM\_THREADS** environment variable to specify options which affect SMP execution. For details, see the Fortran publications.
3. If you are accessing ESSL from a 64-bit-environment program, you must add the **-q64** compiler option.
4. ESSL supports the XL Fortran compile-time option **-qextname**. For details, see the Fortran publications.
5. Fortran 90 programmers may be interested in the **-qessl** compiler option which allows the use of ESSL routines in place of Fortran 90 intrinsic procedures. For details, see the Fortran manuals.
6. The commands in the table below assume that you installed the IBM compilers in the default directory, `/opt/ibmcomp`. If you used different directories, you need to make the appropriate changes to the **-L** and **-R** options.
7. The commands in the table below assume that you installed ESSL in the default directory `/opt/ibmmath`. If you used different directories, you need to make the appropriate changes to the **-I**, **-L**, and **-R** options.
8. In your job procedures, you must use only the allowable compilers and libraries listed in Table 5 on page 9.

## Dynamic Linking Versus Static Linking on Linux

The following list explains which type of linking is supported for programs using ESSL, depending on the type of ESSL library you are using:

### ESSL Serial Library and ESSL SMP Library

For the ESSL Serial Library and the ESSL SMP Library, only dynamic linking is supported.

### ESSL Blue Gene library

For the ESSL Blue Gene Library, only static linking is supported, and you must specify the **-L** option to identify the location of the library.

## Fortran Program Procedures on Linux

You do not need to modify your existing Fortran compilation procedures when using ESSL.

When linking and running your program, you must modify your existing job procedures for ESSL in order to set up the necessary libraries.

If you are accessing ESSL from a Fortran program, you can compile and link using the commands shown in the table below.

ESSL Library Name		Command
SMP	32-bit	xlf_r -0 -qnosave -qsmp xyz.f -lesslsmp xlf_r -0 -qnosave xyz.f -lesslsmp -lxlsmp
	64-bit	xlf_r -0 -qnosave -q64 -qsmp xyz.f -lesslsmp xlf_r -0 -qnosave -q64 xyz.f -lesslsmp -lxlsmp
Serial	32-bit	xlf_r -0 -qnosave xyz.f -lessl
	64-bit	xlf_r -0 -qnosave -q64 xyz.f -lessl
Blue Gene	32-bit	blrts_xlf -0 -qnosave -qbg1 xyz.f -lesslbg -L/opt/ibmmath/lib

where *xyz.f* is the name of your Fortran program.

ESSL supports the XL Fortran compile-time option **-qextname**. For details, see the Fortran manuals.

## C Program Procedures on Linux

If you want to specify your own definitions for short- and long-precision complex data, add **-D\_CMLX** and **-D\_DCMPLX**, respectively, to your compile and link command. Otherwise, you automatically use the definitions of short- and long-precision complex data provided in the ESSL header file.

For the ESSL Blue Gene Library, you must specify the **-I** option to identify the location of the ESSL header file.

When linking and running your program, you must modify your existing job procedures for ESSL in order to set up the necessary libraries.

If you are accessing ESSL from a C program, you can compile and link using the commands also shown in the table below.

ESSL Library Name		Command
SMP	32-bit	cc_r -0 xyz.c -lesslsmp -lxlf90_r -lxlsmp -lxlfmath -L/opt/ibmcmp/xlf/9.1/lib -R/opt/ibmcmp/xlf/9.1/lib
	64-bit	cc_r -0 -q64 xyz.c -lesslsmp -lxlf90_r -lxlsmp -lxlfmath -L/opt/ibmcmp/xlf/9.1/lib64 -R/opt/ibmcmp/xlf/9.1/lib64
Serial	32-bit	cc_r -0 xyz.c -lessl -lxlf90_r -lxlomp_ser -lxlfmath -L/opt/ibmcmp/xlf/9.1/lib -R/opt/ibmcmp/xlf/9.1/lib
	64-bit	cc_r -0 -q64 xyz.c -lessl -lxlf90_r -lxlomp_ser -lxlfmath -L/opt/ibmcmp/xlf/9.1/lib64 -R/opt/ibmcmp/xlf/9.1/lib64
Blue Gene	32-bit	blrts_cc -0 -qbg1 xyz.c -lesslbg -lxlf90 -lxlfmath -L/opt/ibmmath/lib -I/opt/ibmmath/include -L/opt/ibmcmp/xlf/9.1/blrts_lib

## C++ Program Procedures on Linux

The ESSL header file supports two alternatives for declaring scalar output arguments. By default, the arguments are declared to be type reference. If you prefer for them to be declared as pointers, add **-D\_ESVCPTR** to your commands.

For the ESSL Blue Gene Library, you must specify the **-I** option to identify the location of the ESSL header file.

When linking and running your program, you must modify your existing job procedures for ESSL, to set up the necessary libraries.

If you are accessing ESSL from a C++ program, you can compile and link using the commands shown in the table below.

ESSL Library Name		Command
SMP	32-bit	xlC_r -O xyz.C -lesslsmpl -lxlf90_r -lxlsmpl -lxlfmath -L/opt/ibmcmp/xlf/9.1/lib -R/opt/ibmcmp/xlf/9.1/lib
	64-bit	xlC_r -O -q64 xyz.C -lesslsmpl -lxlf90_r -lxlsmpl -lxlfmath -L/opt/ibmcmp/xlf/9.1/lib64 -R/opt/ibmcmp/xlf/9.1/lib64
Serial	32-bit	xlC_r -O xyz.C -lessl -lxlf90_r -xlomp_ser -lxlfmath -L/opt/ibmcmp/xlf/9.1/lib -R/opt/ibmcmp/xlf/9.1/lib
	64-bit	xlC_r -O -q64 xyz.C -lessl -lxlf90_r -xlomp_ser -lxlfmath -L/opt/ibmcmp/xlf/9.1/lib64 -R/opt/ibmcmp/xlf/9.1/lib64
Blue Gene	32-bit	blrts_xlC -O -qbg1 xyz.C -lesslbg -lxlf90 -lxlfmath -L/opt/ibmmath/lib -I/opt/ibmmath/include -L/opt/ibmcmp/xlf/9.1/blrts_lib



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## Chapter 6. Migrating Your Programs

This chapter explains many aspects of migrating your application programs to use the ESSL subroutines. It covers:

- “Migrating ESSL Version 4 Release 1 Programs to Version 4 Release 2”
- “Migrating ESSL Version 3 Release 3 Programs to Version 4 Release 1” on page 172
- “Planning for Future Migration” on page 172
- “Migrating From One Hardware Platform to Another” on page 172
- “Migrating from Other Libraries to ESSL” on page 173

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### Migrating ESSL Version 4 Release 2.1 Programs to Version 4 Release 2.2

In the ESSL Blue Gene Library, the Fourier Transform subroutines and the Convolutions and Correlations subroutines require that the alignments of certain arrays do not change between initialization and computation. If the array alignment does change, in some cases error message 2152 will be issued and your program will terminate. If you want your program to continue processing with degraded performance, use ERRSET with an ESSL error exit routine, ENOTRM, to make error 2152 recoverable.

For all other subroutines, the calling sequences for the subroutines in ESSL Version 4 Release 2.1 and ESSL Version 4 Release 2.2 are identical; therefore, no changes to your application programs are required.

---

### Migrating ESSL Version 4 Release 2 Programs to Version 4 Release 2.1

The calling sequences for the subroutines in ESSL Version 4 Release 2 and ESSL Version 4 Release 2.1 are identical; therefore, no changes to your application programs are required.

---

### Migrating ESSL Version 4 Release 1 Programs to Version 4 Release 2

The calling sequences for the subroutines in ESSL Version 4 Release 1 and ESSL Version 4 Release 2 are identical; therefore, no changes to your application programs are required.

ESSL Version 4 Release 2 does not support SLES8. In most cases, binary compatibility does not exist between SLES8 and SLES9. Therefore, SLES8 applications must be recompiled and rebuilt on SLES9.

On Linux, if you are accessing ESSL from a C or C++ program, you must change your compile and link commands so that they specify IBM XL Fortran Enterprise Edition Version 9.1 for Linux. See “C Program Procedures on Linux” on page 168 and “C++ Program Procedures on Linux” on page 168.

---

## Migrating ESSL Version 3 Release 3 Programs to Version 4 Release 1

The Symmetric Indefinite Matrix Factorization and Multiple Right-Hand Side Solve subroutine, DBSSV, has been modified so that the matrix is factored in the case where  $n$  is greater than zero and  $nrhs$  is zero. Previously, this was a quick-return condition and the matrix was not factored. (See the subroutine description on page 524.)

For all other subroutines, no changes to your application programs are required if you are migrating from ESSL Version 3 Release 3 to ESSL Version 4 Release 1.

**Note:** If you are migrating from a release earlier than ESSL Version 3 Release 3, see the documentation for ESSL Version 3 Release 3 (which is available from the Web sites listed in Table 7 on page 11).

### ESSL Subroutines

The calling sequences for the subroutines in ESSL Version 3 Release 3 and ESSL Version 4 Release 1 are identical.

---

## Planning for Future Migration

With respect to planning for the future, if working storage does not need to persist after the subroutine call, you should use dynamic allocation. Otherwise, you should use the processor-independent formulas or simple formulas for calculating the values for the *naux* arguments in the ESSL calling sequences. Two things may occur that could cause the minimum values of *naux*, returned by ESSL error handling, to increase in the future:

- If changes are made to the ESSL subroutines to improve performance
- If changes are necessary to support future processors

The formulas allow you to specify your auxiliary storage large enough to accommodate any future improvements to ESSL and any future processors. If you do not provide, at least, these amounts of storage, your program may not run in the future.

You should use the following rule of thumb: To protect your application from having to be recoded in the future because of possible increased requirements for auxiliary storage, use dynamic allocation if possible. If the working storage must persist after the subroutine call, then you should provide as much storage as possible in your current application. In determining the right amount to specify, you should weigh your storage constraints against the inconvenience of making future changes, then specify what you think is best. If possible, you should provide this larger amount of storage to prevent future migration problems.

---

## Migrating From One Hardware Platform to Another

This section describes all the aspects of migrating your ESSL application programs from one hardware platform to another.

### Auxiliary Storage

The minimum amount of auxiliary storage returned by ESSL error handling may vary from one hardware platform to another for the following subroutines:

- all the Fourier transform subroutines
- SCONF

- SCORF
- SACORF

Therefore, to guarantee that your application programs always migrate from any platform to any other platform, you should use the processor-independent formulas to determine the amount of auxiliary storage to use.

## Bitwise-Identical Results

Because of hardware and ESSL design differences, the results you obtain when migrating from one ESSL Library to another or from one hardware platform to another may not be bitwise identical. The results, however, are mathematically equivalent.

---

## Migrating from Other Libraries to ESSL

This section describes some general aspects of moving from an IBM or non-IBM engineering and scientific library to ESSL.

### Migrating from ESSL/370

There is a high degree of compatibility between ESSL/370 and ESSL. However you may need to make some coding changes for certain subroutines.

### Migrating from Another IBM Subroutine Library

If you are migrating from other IBM library products—such as Subroutine Library—Mathematics (SL MATH) or Scientific Subroutine Package (SSP), which have some functions similar to ESSL—the ESSL calling sequences differ from the calling sequences you are currently using. Your program must be modified to add the ESSL calling sequences and make the other ESSL-related coding changes.

If you are migrating from the Basic Linear Algebra Subroutine Library provided with AIX, your calling sequences do not need to be changed.

### Migrating from LAPACK

ESSL contains some subroutines that conform to the LAPACK interface. If you are using these subroutines, no coding changes are needed to migrate to ESSL.

**Note:** You should be aware that there are some ESSL subroutines whose names match those of existing LAPACK subroutines, but whose calling-sequence arguments and functionality are different from those LAPACK subroutines. (See Appendix B, “LAPACK,” on page 1043.)

Additionally, you may be interested in using the Call Conversion Interface (CCI) that is available with LAPACK. The CCI substitutes a call to an ESSL subroutine in place of an LAPACK subroutine whenever an ESSL subroutine provides either functional or near-functional equivalence. Using the CCI allows LAPACK users to obtain the optimized performance of ESSL for an additional subset of LAPACK subroutines. For details, see reference [42].

### Migrating from a Non-IBM Subroutine Library

If you are using a non-IBM library, ESSL may provide subroutines corresponding to those you are currently using. You may choose to migrate your program to benefit from the increased performance offered by the ESSL subroutines. In this case, you may have to recode your program to use the ESSL calling sequences,

because the names and arguments used by ESSL may be different from those used by the non-IBM library. On the other hand, if you are using any of the standard Level 1, 2, and 3 BLAS or LAPACK routines that correspond to ESSL subroutines, you do not need to recode the calling sequences. The ESSL calling sequences are the same as the public domain code.



---

## Chapter 7. Handling Problems

This chapter provides the following information for your use when dealing with errors:

- How to obtain IBM support.
- What to do about NLS (National Language Support) problems.
- A description of the different types of errors that can occur in ESSL. It explains what happens when an error occurs and, in some instances, how you can use error handling to obtain further information.
- All of the ESSL error messages are categorized into the different error types. There is also a description of the error message format.

---

### Where to Find More Information About Errors

Specific errors associated with each ESSL subroutine are listed under "Error Conditions" in each subroutine description in Part 3 of this book.

---

### Getting Help from IBM Support

Should you require help from IBM in resolving an ESSL problem, report it and provide the following information, if available and appropriate.

1. Your customer number
2. The ESSL program number:

**ESSL for AIX**                      5765-F82

**ESSL for Linux**                    5765-G17

This is important information that speeds up the correct routing of your call.

3. The version and release of the operating system that you are running on.

**On AIX**            Enter the following command:

**oslevel**

**On Linux**        Enter the following command:

**uname -a**

This is important information that speeds up the correct routing of your call.

4. The names and versions of key products being run.

**On AIX**            Enter the following command:

**lslpp -h *product***

where the appropriate values of *product* are listed in Table 38 on page 176.

**On Linux**        Enter the following command:

**rpm -q *package***

where the appropriate values of *package* are listed in Table 38.

Table 38. Product File Set and Package Names

Product File Sets on AIX	Product Packages on Linux	Descriptive Name
essl.*	essl.rte	ESSL
xlfrte	xlfrte	XL Fortran Run-Time Environment
xlsmp.rte	xlsmp.rte	SMP Run-Time Environment
xlfcmp	xlfcmp	XL Fortran compiler
vac.C	vac.cmp	XL C compiler
vacpp.cmp.C	vacpp.cmp	XL C++ compiler

5. The message that is returned when an error is detected.
6. Any error message relating to core dumps.
7. The compiler listings, including compiler options in effect, and any run-time listings produced
8. Program changes made in comparison with a previous successful run
9. A small test case demonstrating the problem using the minimum number of statements and variables, including input data

Consult your IBM Service representative for more assistance.

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## National Language Support

For National Language Support (NLS), all ESSL subroutines display messages located in externalized message catalogs. English versions of the message catalogs are shipped with the product, but your site may be using its own translated message catalogs. The environment variable **NLSPATH** is used by the various ESSL subroutines to find the appropriate message catalog. **NLSPATH** specifies a list of directories to search for message catalogs. The directories are searched, in the order listed, to locate the message catalog. In resolving the path to the message catalog, **NLSPATH** is affected by the value of the environment variables **LC\_MESSAGES** and **LANG**.

The ESSL message catalogs are in English, and are located in the following directories:

**On AIX**            /usr/lib/nls/msg/C  
                      /usr/lib/nls/msg/En\_US  
                      /usr/lib/nls/msg/en\_US

**On Linux**        /usr/share/locale/en\_US/LC\_MESSAGES  
                      /usr/share/locale/C

If your site is using its own translations of the message catalogs, consult your system administrator for the appropriate value of **NLSPATH** or **LANG**. For additional information on NLS and message catalogs, see *AIX General Programming Concepts: Writing and Debugging Programs*.

---

## Dealing with Errors

At run time, you can encounter a number of different types of errors that are specifically related to the use of the ESSL subroutines:

- Program exceptions
- Input-argument errors (2001-2099) and (2200-2299)
- Computational errors (2100-2199)
- Resource errors (2401-2499)
- Informational and Attention messages (2600-2699)
- Miscellaneous errors (2700-2799)

### Program Exceptions

The program exceptions you can encounter in ESSL are described in *ANSI/IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Standard 754-1985*.

### ESSL Input-Argument Error Messages

If you receive an error message in the form 2538-20 $nn$  or 2538-22 $nn$ , you have an input-argument error in the calling sequence for an ESSL subroutine. Your program terminated at this point unless you did one of the following:

- Specified the ESSL user exit routine, ENOTRM, with ERRSET to determine the correct input argument values in your program for the optionally-recoverable ESSL errors 2015, 2030 or 2200. For details on how to do this, see Chapter 4, “Coding Your Program,” on page 111.
- Reset the number of allowable errors (2099) during ESSL installation or using ERRSET in your program. **This is not recommended for input-argument errors.**

**Note:** For many of the ESSL subroutines requiring auxiliary storage, you can avoid program termination due to error 2015 by allowing ESSL to dynamically allocate auxiliary storage for you. You do this by setting  $naux = 0$  and making error 2015 unrecoverable. For details on which *aux* arguments allow dynamic allocation and how to specify them, see the subroutine descriptions in Part 2 of this book.

The name of the ESSL subroutine detecting the error is listed as part of the message. The argument number(s) involved in the error appears in the message text. See “Input-Argument Error Messages(2001-2099)” on page 180 for a complete description of the information contained in each message and for an indication of which messages correspond to optionally-recoverable errors. Regardless of whether the name in the message is a user-callable ESSL subroutine or an internal ESSL routine, the message-text and its unique parts apply to the user-callable ESSL subroutine. Return code values are described under “Error Conditions” for each ESSL subroutine in Part 2 of this book.

You may get more than one error message, because most of the arguments are checked by ESSL for possible errors during each call to the subroutine. The ESSL subroutine returns as many messages as there are errors detected. As a result, fewer runs are necessary to diagnose your program.

Fix the error(s), recompile, relink, and rerun your program.

## ESSL Computational Error Messages

If you receive an error message in the form 2538-21*nn*, you have a computational error in the ESSL subroutine. A computational error is any error occurring in the ESSL subroutine while using the computational data (that is, scalar and array data). The name of the ESSL subroutine detecting the error is listed as part of the message. Regardless of whether the name in the message is a user-callable ESSL subroutine or an internal ESSL routine, the message-text and its unique parts apply to the user-callable ESSL subroutine. A nonzero return code is returned when the ESSL subroutine encounters a computational error. See “Computational Error Messages(2100-2199)” on page 186 for a complete description of the information in each message. Return code values are described under “Error Conditions” for each ESSL subroutine in Part 2 of this book.

Your program terminates for some computational errors unless you have called ERRSET to reset the number of allowable errors for that particular error, and the number has not been exceeded. A message is issued for each computational error. You should use the message to determine where the error occurred in your program.

If you called ERRSET and you have not reached the limit of errors you had set, you can check the return code. If it is not 0, you should call the EINFO subroutine to obtain information about the data involved in the error. EINFO provides the same information provided in the messages; however, it is provided to your program so your program can check the information during run time. Depending on what you want to do, you may choose to continue processing or terminate your program after the error occurs. For information on how to make these changes in your program to reset the number of allowable errors, how to diagnose the error, and how to decide whether to continue or terminate your program, see Chapter 4, “Coding Your Program,” on page 111.

If you are unable to solve the problem, report it and provide the following information, if available and appropriate:

- The message number and the module that detected an error
- The system dump, system error code, and system log of this job
- The compiler listings, including compiler options in effect, and any run-time listings produced
- Program changes made in comparison with a previous successful run
- A small test case demonstrating the problem using the minimum number of statements and variables, including input data
- A brief description of the problem

## ESSL Resource Error Messages

If you receive a message in the form 2538-24*nn*, it means that ESSL issued a resource error message.

A resource error occurs when a buffer storage allocation request fails in a ESSL subroutine. In general, the ESSL subroutines allocate internal auxiliary storage dynamically as needed. Without sufficient storage, the subroutine cannot complete the computation.

When a buffer storage allocation request fails, a resource error message is issued, and the application program is terminated. You need to reduce the memory constraint on the system or increase the amount of memory available before rerunning the application program.

The following ways may reduce memory constraints:

- Investigate the load of your process and run in a more dedicated environment.
- Increase your processor's paging space.
- Select a machine with more memory.
- For a 32-bit environment application on AIX, consider specifying the `-bmaxdata` binder option when linking your program. For details see the Fortran publications.
- Check the setting of your user ID's user limit (`ulimit`). (See the *AIX Commands Reference*).

## ESSL Informational and Attention Messages

If you receive a message in the form `2538-26nn`, it means that ESSL issued an informational or attention message.

### Informational Messages

When you receive an informational message, check your application to determine why the condition was detected.

### ESSL Attention Messages

An attention message is issued to describe a condition that occurred. ESSL is able to continue processing, but performance may be degraded.

One condition that may produce an attention message is when enough work area was available to continue processing, but was not the amount initially requested. ESSL does not terminate your application program, but performance may be degraded. If you want to reduce the memory constraint on the system or increase the amount of memory available to eliminate the attention message, see the suggestions in "ESSL Resource Error Messages" on page 178.

## Miscellaneous Error Messages

If you receive a message in the form `2538-27nn`, it means that ESSL issued a miscellaneous error message.

A miscellaneous error is an error that does not fall under any other categories.

When ESSL detects a miscellaneous error, you receive an error message with information on how to proceed and your application program is terminated.

---

## Messages

This section explains the conventions used for the ESSL messages and lists all the ESSL messages. For a description of each of the four types of ESSL messages, see "Dealing with Errors" on page 177.

## Message Conventions

This section describes the message conventions for the ESSL product.

## About Upper- and Lowercase

The literals, such as 'N', 'T', 'U', and so forth, appear in the messages in this book in uppercase; however, they may be specified in your ESSL calling sequence in either upper- or lowercase, for example, 'n', 't', and 'u'.

## Message Format

The ESSL messages are issued in your output in the following format:

```
rtn-name : 2538-mmnn  
message-text
```

Figure 10. Message Format

The parts of the ESSL message are as follows:

*rtn-name*

gives the name of the ESSL subroutine that encountered the error.

**2538** is the ESSL component identification number.

*mm* indicates the type of ESSL error message:

- 20—Input-argument error message
- 21—Computational error message
- 22—Input-argument error message
- 24—Resource error message
- 26—Information and attention message
- 27—Miscellaneous error message

*nn* is the message identification number.

*message-text*

describes the nature of the error. Where one of several possible message-texts can be issued for a particular ESSL error, they are listed in this book with an "or" between them. The possible unique parts are:

- The argument number of each argument involved in the error is included in the message description as (ARG NO. \_)
- Additional information about the error is included in the message. The placement of this information is shown in the messages as (\_)

## Input-Argument Error Messages(2001-2099)

2538-2001	The number of elements (ARG NO. _) in a vector must be greater than or equal to zero.	2538-2005	The size of the leading dimension (ARG NO. _) of an array must be greater than zero.
2538-2002	The stride (ARG NO. _) for a vector must be nonzero.	2538-2006	The number of rows (ARG NO. _) of a matrix must be less than or equal to the size of the leading dimension (ARG NO. _) of its array.
2538-2003	The number of rows (ARG NO. _) in a matrix must be greater than or equal to zero.	2538-2007	The degree of a polynomial (ARG NO. _) must be greater than or equal to zero.
2538-2004	The number of columns (ARG NO. _) in a matrix must be greater than or equal to zero.		

2538-2008	The number of elements (ARG NO. _) to be scanned must be greater than or equal to 2.	2538-2021	The storage control switch (ARG NO. _) must be 1, 2, 3, or 4.
2538-2009	The number of elements (ARG NO. _) in a vector to be processed must be greater than or equal to 3.	2538-2022	(ARG NO. _) must be less than (_).
2538-2010	The transform length (ARG NO. _) must be a power of 2.	2538-2023	The outer loop increment (ARG NO. _) must be greater than or equal to zero.
2538-2011	The number of points used in the interpolation (ARG NO. _) must be greater than or equal to zero and less than or equal to the number of data points (ARG NO. _).	2538-2024	The stride (ARG NO. _) for a vector must be greater than or equal to zero.
2538-2012	The transform length (ARG NO. _) must be less than or equal to (_).	2538-2025	The stride (ARG NO. _) for a vector must be greater than zero.
2538-2013	The transform length (ARG NO. _) must be greater than or equal to (_).	2538-2026	The stride (ARG NO. _) for a vector must be greater than or equal to (_).
2538-2014	The routine must be initialized with the present value of (ARG NO. _).	2538-2027	The order (ARG NO. _) of a matrix must be greater than or equal to zero.
2538-2015	The number of elements (ARG NO. _) in a work array must be greater than or equal to (_).	2538-2028	The job option argument (ARG NO. _) must be 0, 1, or 2.  or The job option argument (ARG NO. _) must be 0, 1, 2, or 3.  or The job option argument (ARG NO. _) must be 0, 1, 2, 10, 11, or 12.  or The job option argument (ARG NO. _) must be 0, 1, 10, or 11.  or The job option argument (ARG NO. _) must be 0, 1, 20, or 21.  or The job option argument (ARG NO. _) must be 0, 1, 10, 11, 20, 21, 30, or 31.  or The job option argument (ARG NO. _) must be 0, 1, 2, 3, or 4.
2538-2016	The form (ARG NO. _) of a matrix must be 'N' or 'T'. or The form (ARG NO. _) of a matrix must be 'N', 'T', or 'C'. or The form (ARG NO. _) of a matrix must be 'N' or 'C'.		
2538-2017	The dimension (ARG NO. _) of the matrices must be greater than or equal to zero.		
2538-2018	The matrix form is specified by (ARG NO. _); therefore, the leading dimension (ARG NO. _) of its array must be greater than or equal to the number of its rows (ARG NO. _).		
2538-2019	The number of sequences (ARG NO. _) must be greater than zero.		
2538-2020	(ARG NO. _) must be nonzero.		

2538-2029	The job option argument (ARG NO. _) must be 0 or 1.	2538-2043	(ARG NO. _) must be greater than ().
2538-2030	The transform length (ARG NO. _) is not an allowed value. The next higher allowed value is ().	2538-2044	The number of initialized coefficients (ARG NO. _) cannot exceed the size of the coefficient vector (ARG NO. _).
2538-2031	The resulting convolution length obtained from ARG NO. 10 = (), ARG NO. 11 = (), ARG NO. 13 = (), and ARG NO. 14 = () must be less than ().	2538-2045	The order specified (ARG NO. _) is not supported for this quadrature method. The nearest supported order is ().
2538-2032	The size of the leading dimension (ARG NO. _) of the matrix must be greater than or equal to (), the bandwidth constraint.	2538-2046	The scaling parameter (ARG NO. _) must be greater than zero for this quadrature method.
2538-2033	The lower bandwidth (ARG NO. _) must be greater than or equal to zero.	2538-2047	The scaling parameter (ARG NO. _) must be nonzero for this quadrature method.
2538-2034	The upper bandwidth (ARG NO. _) must be greater than or equal to zero.	2538-2048	The sum of (ARG NO. _) and (ARG NO. _) must be nonzero for this quadrature method.
2538-2035	The half-band bandwidth (ARG NO. _) must be greater than or equal to zero.	2538-2049	The number of data points (ARG NO. _) must be greater than one in order to perform numerical quadrature.
2538-2036	The lower bandwidth (ARG NO. _) must be less than the order (ARG NO. _) of the matrix.	2538-2050	The number of columns specified for the arrays to store the matrix in compressed matrix mode (ARG NO. _) must be greater than or equal to ().
2538-2037	The upper bandwidth (ARG NO. _) must be less than the order (ARG NO. _) of the matrix.	2538-2051	The number of columns (ARG NO. _) specified for the matrix used to store the sparse matrix in compressed mode must be greater than zero.
2538-2038	The half-band bandwidth (ARG NO. _) must be less than the order (ARG NO. _) of the matrix.	2538-2052	The total number of non-zero elements of the input sparse matrix stored by rows, obtained from element () of the row pointers array (ARG NO. _), must be greater than or equal to zero.
2538-2039	(ARG NO. _) must be greater than zero.	2538-2053	The number of non-zero elements in row () obtained from the row pointer array (ARG NO. _) is less than zero.
2538-2040	Insufficient storage allocated for positive definite solve. () additional bytes required.	2538-2054	The number of diagonals (ARG NO. _) specified for the matrix used to store the sparse matrix in compressed diagonal mode must be greater than zero.
2538-2041	The resulting correlation length obtained from ARG NO. 8 = () and ARG NO. 10 = () must be less than ().		
2538-2042	(ARG NO. _) must be greater than or equal to zero.		



---

2538-2055 Element ( ) of the vector used to store the diagonal numbers (ARG NO. \_) is incompatible with the order of the sparse matrix (ARG NO. \_).

---

2538-2056 The matrix is singular because the number of non-zero entries (ARG NO. \_) is zero.

---

2538-2057 Element ( ) in the integer parameter vector (ARG NO. \_) must be greater than or equal to zero.

---

2538-2058 Element ( ) in the integer parameter vector (ARG NO. \_) must be ( ),( ), or ( ).

---

2538-2059 Element ( ) in the real parameter vector (ARG NO. \_) must be greater than zero.

---

2538-2060 The size of the leading dimension (ARG NO. \_) of an array must be greater than or equal to the maximum of (ARG NO. \_) and (ARG NO. \_).

---

2538-2061 Parameter (ARG NO. \_), which specifies the number of columns of the input sparse matrix (ARG NO. \_ and ARG NO. \_), must be greater than or equal to ( ).

---

2538-2062 The number of random numbers generated (ARG NO. \_) must be even and greater than or equal to zero.

---

2538-2063 SIDE (ARG NO. \_), which specifies whether the triangular input matrix (ARG NO. \_) appears on the left or right of the other input matrix, must be 'L' or 'R'.

---

2538-2064 UPLO (ARG NO. \_), which specifies whether an input matrix (ARG NO. \_) is upper or lower triangular, must be 'U' or 'L'.

---

2538-2065 DIAG (ARG NO. \_), which specifies whether an input matrix (ARG NO. \_) is unit triangular, must be 'U' or 'N'.

---

2538-2066 Given the value which has been assigned to SIDE (ARG NO. \_), the leading dimension (ARG NO. \_) for the triangular input matrix must be greater than or equal to (ARG NO. \_).

---

2538-2067 TRANSA (ARG NO. \_) specifies whether an input matrix (ARG NO. \_), its transpose, or its conjugate transpose should be used. TRANSA must be 'N', 'T', or 'C'.

---

2538-2068 The size of the leading dimension (ARG NO. \_) of an array must be greater than or equal to zero.

---

2538-2070 Element ( ) in (ARG NO. \_) must be 0 or 1.

or

Element ( ) in (ARG NO. \_) must be greater than zero.

or

Element ( ) in (ARG NO. \_) must be greater than or equal to zero.

or

Element ( ) in (ARG NO. \_) must be greater than or equal to zero and less than or equal to 1.

or

Element ( ) in (ARG NO. \_) must be greater than the preceding element.

or

Element ( ) in (ARG NO. \_) must be greater than or equal to 1 and less than or equal to n.

or

Element ( ) in (ARG NO. \_) must be -1 or 1.

or

Element ( ) in (ARG NO. \_) must be nonzero.

or

Element ( ) in (ARG NO. \_) must be

<p>0, 1, 2, 10, or 11.</p> <p>or</p> <p>Element ( ) in (ARG NO. _) must be 0, 1, 2, 10, 11, 100, 102, or 110.</p> <p>or</p> <p>Element ( ) in (ARG NO. _) must be 0.</p> <p>or</p> <p>Element ( ) in (ARG NO. _) must be 1.</p> <p>or</p> <p>Element ( ) in (ARG NO. _) must be 0, 1, 2, 10, 11, 100, 101, 102, 110, or 111.</p> <p>or</p> <p>Element ( ) in (ARG NO. _) must be 1, 2, 3, or 4.</p> <p>or</p> <p>Element ( ) in (ARG NO. _) must be 1, 2, 3, 4, or 5.</p>	<p>2538-2076 (ARG NO. _) must be greater than or equal to ( ) and smaller than ( ).</p> <hr/> <p>2538-2077 The matrix is singular. Column ( ) is empty in the matrix specified by (ARG NO. _), (ARG NO. _), and (ARG NO. _).</p> <hr/> <p>2538-2078 The matrix is singular. Row ( ) is empty in the matrix specified by (ARG NO. _), (ARG NO. _), and (ARG NO. _).</p> <hr/> <p>2538-2079 The matrix, specified by (ARG NO. _), (ARG NO. _), and (ARG NO. _), contains at least one duplicate column index in row ( ).</p> <hr/> <p>2538-2080 Element ( ) in (ARG NO. _) must be greater than or equal to ( ) and less than or equal to ( ).</p> <p>or</p> <p>Element ( ) in (ARG NO. _) must be greater than or equal to ( ) and less than or equal to (ARG NO. _).</p> <p>or</p> <p>Element ( ) in (ARG NO. _) must be greater than or equal to element ( ) and less than or equal to ( ).</p> <p>or</p> <p>Element ( ) in (ARG NO. _) must be zero or must be greater than or equal to ( ).</p>
<p>2538-2071 The number of eigenvalues (ARG NO. _) must be less than or equal to the order of the matrix (ARG NO. _).</p>	
<p>2538-2072 The work area (ARG NO. _) does not contain a valid vector seed. The routine must be called with a nonzero value of ISEED (ARG NO. _).</p>	
<p>2538-2073 (ARG NO. _) must be a double precision whole number greater than or equal to 1.0 and less than 2147483647.0.</p>	<p>2538-2081 Element ( ) in (ARG NO. _) must be less than or equal to ( ).</p>
<p>2538-2074 Performance can be improved by using a larger work array. For best performance, specify the number of elements (ARG NO. _) in the work array to be greater than or equal to ( ).</p>	<p>2538-2082 Element ( ) in (ARG NO. _) may cause incorrect or misleading results. A nonzero number with absolute value less than or equal to 1 is recommended.</p> <p>or</p> <p>Element ( ) in (ARG NO. _) may cause incorrect or misleading results. A positive number less than or equal to 1 is recommended.</p>
<p>2538-2075 The data type parameter (ARG NO. _) must be 'S', 'D', 'C', or 'Z'.</p>	

---

2538-2083 The pivot tolerance (element  $()$  in (ARG NO.  $_{}$ ) may cause incorrect or misleading results. A number greater than or equal to 0 and less than or equal to 1 is recommended.

---

2538-2084 The dimension (ARG NO.  $_{}$ ) of the array (ARG NO.  $_{}$ ) must be greater than or equal to  $()$ .

---

2538-2085 The number of steps after which the generalized minimum residual method is restarted, element  $()$  in (ARG NO.  $_{}$ ), must be greater than 0.

---

2538-2086 The acceleration parameter, element  $()$  in (ARG NO.  $_{}$ ), must be greater than 0 when using the SSOR preconditioner.

---

2538-2087 STOR (ARG NO.  $_{}$ ), which specifies the storage variation used to represent the input sparse matrix, must be 'G', 'L', or 'U'.

---

2538-2088 INIT (ARG NO.  $_{}$ ), which specifies the type of computation to be performed, must be 'I' or 'S'.

---

2538-2089 Element  $()$  in (ARG NO.  $_{}$ ) must be greater than or equal to  $()$ .

or  
Element  $()$  in (ARG NO.  $_{}$ ) must be greater than or equal to element  $()$ .

---

2538-2090 For level  $()$ , the number of grid points for dimension  $()$  must be an odd number greater than 1.

---

2538-2091 Since the mesh spacing (ARG NO.  $_{}$ ) here is not constant, the second order prolongation method must be used. That is, element  $()$  of (ARG NO.  $_{}$ ) must be  $()$ .

---

2538-2092 The index into (ARG NO.  $_{}$ ) is out of range. This index is element  $()$  of (ARG NO.  $_{}$ ).

---

2538-2093 The index into (ARG NO.  $_{}$ ) is out of range. This index is element  $()$  of (ARG NO.  $_{}$ ).

---

2538-2094 For dimension  $()$  on level  $()$ , the mesh spacing must be changed to a positive value.

---

2538-2095 Excess space in (ARG NO.  $_{}$ ) has been decreased and may be inadequate. To avoid this, specify the coarse level matrix as the final item in this argument.

---

2538-2096 For level  $()$ , the matrix type, solver, and preconditioner are incompatible.

---

2538-2097 The solver requested for level  $()$  requires a square matrix. Elements  $()$  and  $()$  in (ARG NO.  $_{}$ ) must be equal.

---

2538-2098 Element  $()$  of (ARG NO.  $_{}$ ) must be greater than or equal to  $()$ .

---

2538-2099 End of input argument error reporting. For more information, refer to Engineering and Scientific Subroutine Library Guide and Reference (SA22-7904).

**Note:** There are more input-argument error messages listed in "Input-Argument Error Messages(2200-2299)" on page 187

## Computational Error Messages(2100-2199)

2538-2100	The computed index of a vector is out of the range ( ) to ( ).	2538-2113	Unexpected nonzero vector mask detected in ESSL scalar routine. Contact your IBM Service Representative.
2538-2101	Eigenvalue ( ) failed to converge after ( ) iterations.	2538-2114	Eigenvalue ( ) failed to converge after ( ) iterations.
2538-2102	Eigenvector ( ) failed to converge after ( ) iterations.	2538-2115	The matrix (ARG NO. _) is not positive definite. The leading minor of order ( ) has a nonpositive determinant.
2538-2103	The matrix (ARG NO. _) is singular. Zero diagonal element ( ) has been detected.	2538-2116	The matrix specified by (ARG NO. _) and (ARG NO. _) is singular.
2538-2104	The matrix (ARG NO. _) is not positive definite. The last diagonal element with nonpositive value is ( ).	2538-2117	The pivot element in column ( ) is smaller than the first element in (ARG NO. _).
2538-2105	Factorization failed due to near zero pivot number ( ).	2538-2118	The pivot element in row ( ) is smaller than the first element in (ARG NO. _).
2538-2106	Vector boundary misalignment detected in ESSL scalar library.	2538-2119	The storage space, specified by (ARG NO. _), is insufficient.
2538-2107	Singular value ( ) failed to converge after ( ) iterations.	2538-2120	The matrix is singular. The last row processed in the matrix was row ( ).
2538-2108	The matrix specified by (ARG NO. _) and (ARG NO. _) is not definite because the diagonal is not of constant sign.	2538-2121	The matrix is singular. the last column processed was column ( ).
2538-2109	The matrix specified by (ARG NO. _) and (ARG NO. _) is not definite and the iterative process is stopped at iteration number ( ).	2538-2122	The factorization failed. No pivot element was found in the active submatrix.
2538-2110	The maximum allowed number of iterations, element number ( ) of (ARG NO. _), were performed but the iterative process did not converge to a solution according to the stopping procedure.	2538-2123	Performance can be improved by specifying a larger value for (ARG NO. _). ( ) compressions were performed.
2538-2111	The factorization matrix (ARG NO. _) is not consistent with the sparse matrix specified by (ARG NO. _) and (ARG NO. _).	2538-2124	The data contained in AUX1, (ARG NO. _), was computed for a different algorithm.
2538-2112	The incomplete factorization of the sparse matrix specified by (ARG NO. _) and (ARG NO. _) is not stable.	2538-2126	The pivot value at row ( ) is not acceptable based on pivot criteria ((ARG NO. _) and (ARG NO. _)). No fixup was applicable to this pivot. The matrix (ARG NO. _) may be singular or not definite.

2538-2127	The pivot value at row ( ) was replaced with element ( ) in (ARG NO. ). The matrix (ARG NO. ) may be singular or not definite.	2538-2146	The input matrix (ARG NO. ) is singular. The first diagonal element found to be exactly zero was in column ( ).
2538-2128	Internal ESSL error. contact your IBM service representative.	2538-2147	The matrix (ARG NO. ) is singular. Zero diagonal element ( ) has been detected.
2538-2129	The matrix specified by (ARG NO. ), (ARG NO. ), and (ARG NO. ) is not definite because the diagonal is not of constant sign or some diagonal element is zero.	2538-2148	The matrix (ARG NO. ) is not positive definite. The leading minor of order ( ) has a nonpositive determinant.
2538-2130	The incomplete factorization of the sparse matrix specified by (ARG NO. ), (ARG NO. ), and (ARG NO. ) is not stable.	2538-2149	Factorization failed due to near zero pivot number ( ).
2538-2131	The matrix specified by (ARG NO. ), (ARG NO. ), and (ARG NO. ) is singular.	2538-2150	The inverse of matrix (ARG NO. ) could not be computed. The first diagonal element of the factored matrix found to be exactly zero was in column ( ).
2538-2132	Element ( ) in (ARG NO. ) indicates that factorization was done on a previous call. The data passed is not the result of a prior valid factorization.	2538-2151	The inverse of matrix (ARG NO. ) could not be computed. The first diagonal element of the factored matrix found to be exactly zero was in column ( ).
2538-2133	An error occurred on level ( ) in the user-supplied subroutine specified by (ARG NO. ).	2538-2152	The alignment of (ARG NO. ) changed after initialization. Performance may be significantly degraded.
2538-2134	The data contained in (ARG NO. ) is not consistent with the sparse matrix specified by (ARG NO. ), (ARG NO. ), and (ARG NO. ).	2538-2199	End of computational error reporting. For more information, refer to Engineering and Scientific Subroutine Library Guide and Reference (SA22-7904).
2538-2135	For level ( ), loss of orthogonality occurred in a minimum residual solver because the input matrix (element ( ) of (ARG NO. )) is inappropriate. Choose one of the other non-symmetric solvers.		
2538-2136	For level ( ), the main diagonal element for row ( ) of a matrix is 0.		
2538-2145	The input matrix (ARG NO. ) is singular. The first diagonal element found to be exactly zero was in column ( ).		

## Input-Argument Error Messages(2200-2299)

---

2538-2200 The dimension (ARG NO. \_) of the array (ARG NO. \_) must be greater than or equal to (\_).

---

---

2538-2207 The number of elements in the array (ARG NO. \_) must be less than or equal to (\_).

---

2538-2201 The number of elements (ARG NO. \_) in a work array (ARG NO. \_) must be zero, to indicate dynamic allocation, minus one, to indicate workspace query, or greater than or equal to ( ) if a work array is being supplied.

## Resource Error Messages(2400-2499)

---

2538-2400 An internal buffer allocation has failed due to insufficient memory.

## Informational and Attention Error Messages(2600-2699)

---

2538-2600 Performance may be degraded due to limited buffer space availability.

---

---

2538-2607 Serial execution is taking place since the input array is equal to the output array and either:

---

2538-2601 Execution terminating due to error count for error number ( ) Message summary: Message number - Count

---

INC2X (ARG NO. \_) is not equal to INC2Y (ARG NO. \_) or INC3X (ARG NO. \_) is not equal to INC3Y (ARG NO. \_).

---

2538-2602 User error corrective routine entered. User corrective action taken. Execution continuing.

---

---

2538-2608 Performance may be improved by using a larger work array. For best performance, specify the number of elements (ARG NO. \_) in the work array to be greater than or equal to ( ).

---

---

2538-2603 Standard corrective action taken. Execution continuing.

---

---

2538-2604 Execution terminating due to error count for error number \_.

---

---

2538-2609 Performance may be improved by specifying a larger value for (ARG NO. \_). ( ) compressions were performed.

---

---

2538-2605 Message summary: \_ - \_

---

---

2538-2606 Serial execution is taking place since the input array is equal to the output array and either:

---

2538-2610 Performance may be degraded due to the alignment of (ARG NO. \_).

---

INC2X (ARG NO. \_) is not equal to 2 times INC2Y (ARG NO. \_) or INC3X (ARG NO. \_) is not equal to 2 times INC3Y (ARG NO. \_).

---

2538-2611 Performance may be improved by specifying an even value for (ARG NO. \_).

---

## Miscellaneous Error Messages(2700-2799)

---

2538-2700 Internal ESSL error number ( ). Contact your IBM service representative.

---

2538-2703 Internal ESSL error: message number requested ( ) is outside of the valid range. Contact your IBM service representative.

---

2538-2799    Unable to locate message number ( ).  
Please refer to the chapter entitled  
'Using Error Handling' in the ESSL  
Guide and Reference (SA22-7904) for the  
full message text.





---

## Part 2. Reference Information

This part of the book is organized into ten areas, providing reference information for coding the ESSL calling sequences. It is organized as follows:

- Linear Algebra Subprograms
- Matrix Operations
- Linear Algebraic Equations
- Eigensystem Analysis
- Fourier Transforms, Convolutions and Correlations, and Related Computations
- Sorting and Searching
- Interpolation
- Numerical Quadrature
- Random Number Generation
- Utilities



---

## Chapter 8. Linear Algebra Subprograms

The linear algebra subprograms, provided in four areas, are described in this chapter.

---

### Overview of the Linear Algebra Subprograms

This section describes the subprograms in each of the four linear algebra subprogram areas:

- Vector-scalar linear algebra subprograms (Table 39)
- Sparse vector-scalar linear algebra subprograms (Table 40)
- Matrix-vector linear algebra subprograms (Table 41)
- Sparse matrix-vector linear algebra subprograms (Table 42)

**Notes:**

1. The term **subprograms** is used to be consistent with the Basic Linear Algebra Subprograms (BLAS), because many of these subprograms correspond to the BLAS.
2. Some of the linear algebra subprograms were designed in accordance with the Level 1 and Level 2 BLAS de facto standard. If these subprograms do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subprograms, the updates could require modifications of the calling application program.

### Vector-Scalar Linear Algebra Subprograms

The vector-scalar linear algebra subprograms include a subset of the standard set of Level 1 BLAS. For details on the BLAS, see reference [82]. The remainder of the vector-scalar linear algebra subprograms are commonly used computations provided for your applications. Both real and complex versions of the subprograms are provided.

*Table 39. List of Vector-Scalar Linear Algebra Subprograms*

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Position of the First or Last Occurrence of the Vector Element Having the Largest Magnitude	ISAMAX <sup>+</sup> ICAMAX <sup>+</sup>	IDAMAX <sup>+</sup> IZAMAX <sup>+</sup>	199
Position of the First or Last Occurrence of the Vector Element Having Minimum Absolute Value	ISAMIN <sup>+</sup>	IDAMIN <sup>+</sup>	202
Position of the First or Last Occurrence of the Vector Element Having Maximum Value	ISMAX <sup>+</sup>	IDMAX <sup>+</sup>	205
Position of the First or Last Occurrence of the Vector Element Having Minimum Value	ISMIN <sup>+</sup>	IDMIN <sup>+</sup>	208
Sum of the Magnitudes of the Elements in a Vector	SASUM <sup>+</sup> SCASUM <sup>+</sup>	DASUM <sup>+</sup> DZASUM <sup>+</sup>	211
Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y	SAXPY <sup>*</sup> CAXPY <sup>*</sup>	DAXPY <sup>*</sup> ZAXPY <sup>*</sup>	214
Copy a Vector	SCOPY <sup>*</sup> CCOPY <sup>*</sup>	DCOPY <sup>*</sup> ZCOPY <sup>*</sup>	217

Table 39. List of Vector-Scalar Linear Algebra Subprograms (continued)

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Dot Product of Two Vectors	SDOT <sup>†*</sup> CDOTU <sup>†*</sup> CDOTC <sup>†*</sup>	DDOT <sup>†*</sup> ZDOTU <sup>†*</sup> ZDOTC <sup>†*</sup>	220
Compute SAXPY or DAXPY N Times	SNAXPY	DNAXPY	224
Compute Special Dot Products N Times	SNDOT	DNDOT	229
Euclidean Length of a Vector with Scaling of Input to Avoid Destructive Underflow and Overflow	SNRM2 <sup>†*</sup> SCNRM2 <sup>†*</sup>	DNRM2 <sup>†*</sup> DZNRM2 <sup>†*</sup>	234
Euclidean Length of a Vector with No Scaling of Input	SNORM2 <sup>†</sup> CNORM2 <sup>†</sup>	DNORM2 <sup>†</sup> ZNORM2 <sup>†</sup>	237
Construct a Givens Plane Rotation	SROTG <sup>*</sup> CROTG <sup>*</sup>	DROTG <sup>*</sup> ZROTG <sup>*</sup>	240
Apply a Plane Rotation	SROT <sup>*</sup> CROT <sup>*</sup> CSROT <sup>*</sup>	DROT <sup>*</sup> ZROT <sup>*</sup> ZDROT <sup>*</sup>	247
Multiply a Vector X by a Scalar and Store in the Vector X	SSCAL <sup>*</sup> CSCAL <sup>*</sup> CSSCAL <sup>*</sup>	DSCAL <sup>*</sup> ZSCAL <sup>*</sup> ZDSCAL <sup>*</sup>	251
Interchange the Elements of Two Vectors	SSWAP <sup>*</sup> CSWAP <sup>*</sup>	DSWAP <sup>*</sup> ZSWAP <sup>*</sup>	254
Add a Vector X to a Vector Y and Store in a Vector Z	SVEA CVEA	DVEA ZVEA	257
Subtract a Vector Y from a Vector X and Store in a Vector Z	SVES CVES	DVES ZVES	261
Multiply a Vector X by a Vector Y and Store in a Vector Z	SVEM CVEM	DVEM ZVEM	265
Multiply a Vector X by a Scalar and Store in a Vector Y	SYAX CYAX CSYAX	DYAX ZYAX ZDYAX	269
Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in a Vector Z	SZAXPY CZAXPY	DZAXPY ZZAXPY	272
<sup>†</sup> This subprogram is invoked as a function in a Fortran program. <sup>*</sup> Level 1 BLAS			

## Sparse Vector-Scalar Linear Algebra Subprograms

The sparse vector-scalar linear algebra subprograms operate on sparse vectors using optimized storage techniques; that is, only the nonzero elements of the vector are stored. These subprograms provide similar functions to the vector-scalar subprograms. These subprograms represent a subset of the sparse extensions to the Level 1 BLAS described in reference [31]. Both real and complex versions of the subprograms are provided.

Table 40. List of Sparse Vector-Scalar Linear Algebra Subprograms

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Scatter the Elements of a Sparse Vector X in Compressed-Vector Storage Mode into Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode	SSCTR CSCTR	DSCTR ZSCTR	277

Table 40. List of Sparse Vector-Scalar Linear Algebra Subprograms (continued)

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Gather Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode into a Sparse Vector X in Compressed-Vector Storage Mode	SGTHR CGTHR	DGTHR ZGTHR	280
Gather Specified Elements of a Sparse Vector Y in Full-Vector Mode into a Sparse Vector X in Compressed-Vector Mode, and Zero the Same Specified Elements of Y	SGTHRZ CGTHRZ	DGTHRZ ZGTHRZ	283
Multiply a Sparse Vector X in Compressed-Vector Storage Mode by a Scalar, Add to a Sparse Vector Y in Full-Vector Storage Mode, and Store in the Vector Y	SAXPYI CAXPYI	DAXPYI ZAXPYI	286
Dot Product of a Sparse Vector X in Compressed-Vector Storage Mode and a Sparse Vector Y in Full-Vector Storage Mode	SDOTI <sup>†</sup> CDOTCI <sup>†</sup> CDOTUI <sup>†</sup>	DDOTI <sup>†</sup> ZDOTCI <sup>†</sup> ZDOTUI <sup>†</sup>	289
<sup>†</sup> This subprogram is invoked as a function in a Fortran program.			

## Matrix-Vector Linear Algebra Subprograms

The matrix-vector linear algebra subprograms operate on a higher-level data structure—matrix-vector rather than vector-scalar—using optimized algorithms to improve performance. These subprograms represent a subset of the Level 2 BLAS described in references [36] and [37]. Both real and complex versions of the subprograms are provided.

Table 41. List of Matrix-Vector Linear Algebra Subprograms

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose	SGEMV <sup>†</sup> CGEMV <sup>†</sup> SGEMX <sup>§</sup> SGEMTX <sup>§</sup>	DGEMV <sup>†</sup> ZGEMV <sup>†</sup> DGEMX <sup>§</sup> DGEMTX <sup>§</sup>	294
Rank-One Update of a General Matrix	SGER <sup>†</sup> CGERU <sup>†</sup> CGERC <sup>†</sup>	DGER <sup>†</sup> ZGERU <sup>†</sup> ZGERC <sup>†</sup>	305
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Matrix	SSPMV <sup>†</sup> CHPMV <sup>†</sup> SSYMV <sup>†</sup> CHEMV <sup>†</sup> SSLMX <sup>§</sup>	DSPMV <sup>†</sup> ZHPMV <sup>†</sup> DSYMV <sup>†</sup> ZHEMV <sup>†</sup> DSLX <sup>§</sup>	312
Rank-One Update of a Real Symmetric or Complex Hermitian Matrix	SSPR <sup>†</sup> CHPR <sup>†</sup> SSYR <sup>†</sup> CHER <sup>†</sup> SSLR1 <sup>§</sup>	DSPR <sup>†</sup> ZHPR <sup>†</sup> DSYR <sup>†</sup> ZHER <sup>†</sup> DSL1 <sup>§</sup>	320
Rank-Two Update of a Real Symmetric or Complex Hermitian Matrix	SSPR2 <sup>†</sup> CHPR2 <sup>†</sup> SSYR2 <sup>†</sup> CHER2 <sup>†</sup> SSLR2 <sup>§</sup>	DSPR2 <sup>†</sup> ZHPR2 <sup>†</sup> DSYR2 <sup>†</sup> ZHER2 <sup>†</sup> DSL2 <sup>§</sup>	327
Matrix-Vector Product for a General Band Matrix, Its Transpose, or Its Conjugate Transpose	SGBMV <sup>†</sup> CGBMV <sup>†</sup>	DGBMV <sup>†</sup> ZGBMV <sup>†</sup>	336

Table 41. List of Matrix-Vector Linear Algebra Subprograms (continued)

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Band Matrix	SSBMV <sup>†</sup> CHBMV <sup>†</sup>	DSBMV <sup>†</sup> ZHBMV <sup>†</sup>	343
Matrix-Vector Product for a Triangular Matrix, Its Transpose, or Its Conjugate Transpose	STRMV <sup>†</sup> CTRMV <sup>†</sup> STPMV <sup>†</sup> CTPMV <sup>†</sup>	DTRMV <sup>†</sup> ZTRMV <sup>†</sup> DTPMV <sup>†</sup> ZTPMV <sup>†</sup>	348
Matrix-Vector Product for a Triangular Band Matrix, Its Transpose, or Its Conjugate Transpose	STBMV <sup>†</sup> CTBMV <sup>†</sup>	DTBMV <sup>†</sup> ZTBMV <sup>†</sup>	354
<sup>†</sup> Level 2 BLAS <sup>§</sup> These subroutines are provided only for migration from earlier releases of ESSL and are not intended for use in new programs.			

## Sparse Matrix-Vector Linear Algebra Subprograms

The sparse matrix-vector linear algebra subprograms operate on sparse matrices using optimized storage techniques; that is, only the nonzero elements of the vector are stored. These subprograms provide similar functions to the matrix-vector subprograms.

Table 42. List of Sparse Matrix-Vector Linear Algebra Subprograms

Descriptive Name	Long- Precision Subprogram	Page
Matrix-Vector Product for a Sparse Matrix in Compressed-Matrix Storage Mode	DSMMX	360
Transpose a Sparse Matrix in Compressed-Matrix Storage Mode	DSMTM	363
Matrix-Vector Product for a Sparse Matrix or Its Transpose in Compressed-Diagonal Storage Mode	DSDMX	367

## Use Considerations

If your program uses a sparse matrix stored by rows, as defined in “Storage-by-Rows” on page 100, you should first convert your sparse matrix to compressed-matrix storage mode by using the subroutine DSRSM on page 1026. DSRSM converts a matrix to compressed-matrix storage mode. To convert your sparse matrix to compressed-diagonal storage mode, you need to perform this conversion in your application program before calling the ESSL subroutine.

## Performance and Accuracy Considerations

1. In ESSL, the SSCAL and DSCAL subroutines provide the fastest way to zero out contiguous (stride 1) arrays, by specifying  $incx = 1$  and  $\alpha = 0$ .
2. Where possible, use the matrix-vector linear algebra subprograms, rather than the vector-scalar, to optimize performance. Because data is presented in matrices rather than vectors, multiple operations can be performed by a single ESSL subprogram.
3. Where possible, use subprograms that do multiple computations, such as SNDOT and SNXPY, rather than individual computations, such as SDOT and SAXPY. You get better performance.

4. Many of the short-precision subprograms provide increased accuracy by accumulating results in long precision. This is noted in the functional description of each subprogram.
5. In some of the subprograms, because implementation techniques vary to optimize performance, accuracy of the results may vary for different array sizes. In the subprograms in which this occurs, a general description of the implementation techniques is given in the functional description for each subprogram.
6. To select the sparse matrix subroutine that gives you the best performance, you must consider the layout of the data in your matrix. From this, you can determine the most efficient storage mode for your sparse matrix. ESSL provides two versions of each of its sparse matrix-vector subroutines that you can use. One operates on sparse matrices stored in compressed-matrix storage mode, and the other operates on sparse matrices stored in compressed-diagonal storage mode. These two storage modes are described in “Sparse Matrix” on page 94.

Compressed-matrix storage mode is generally applicable. It should be used when each row of the matrix contains approximately the same number of nonzero elements. However, if the matrix has a special form—that is, where the nonzero elements are concentrated along a few diagonals—compressed-diagonal storage mode gives improved performance.

7. There are some ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see “What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?” on page 48.

## Vector-Scalar Subprograms

This section contains the vector-scalar subprogram descriptions.



## ISAMAX, IDAMAX, ICAMAX, and IZAMAX — Position of the First or Last Occurrence of the Vector Element Having the Largest Magnitude

### Purpose

ISAMAX and IDAMAX find the position  $i$  of the first or last occurrence of a vector element having the maximum absolute value. ICAMAX and IZAMAX find the position  $i$  of the first or last occurrence of a vector element having the largest sum of the absolute values of the real and imaginary parts of the vector elements.

You get the position of the first or last occurrence of an element by specifying positive or negative stride, respectively, for vector  $x$ . Regardless of the stride, the position  $i$  is always relative to the location specified in the calling sequence for vector  $x$  (in argument  $x$ ).

Table 43. Data Types

$x$	Subprogram
Short-precision real	ISAMAX
Long-precision real	IDAMAX
Short-precision complex	ICAMAX
Long-precision complex	IZAMAX

### Syntax

Fortran	ISAMAX   IDAMAX   ICAMAX   IZAMAX ( $n, x, incx$ )
C and C++	isamax   idamax   icamax   izamax ( $n, x, incx$ );

### On Entry

- $n$  is the number of elements in vector  $x$ . Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 43.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.

### On Return

*Function value*

- is the position  $i$  of the element in the array, where:  
If  $incx \geq 0$ ,  $i$  is the position of the first occurrence.  
If  $incx < 0$ ,  $i$  is the position of the last occurrence.  
Returned as: a fullword integer;  $0 \leq i \leq n$ .

### Notes

Declare the ISAMAX, IDAMAX, ICAMAX, and IZAMAX functions in your program as returning a fullword integer value.

## Function

ICAMAX and IZAMAX find the first element  $x_k$ , where  $k$  is defined as the smallest index  $k$ , such that:

$$|a_k| + |b_k| = \max\{|a_j| + |b_j| \text{ for } j = 1, n\}$$

where  $x_k = (a_k, b_k)$

By specifying a positive or negative stride for vector  $x$ , the first or last occurrence, respectively, is found in the array. The position  $i$ , returned as the value of the function, is always figured relative to the location specified in the calling sequence for vector  $x$  (in argument  $x$ ). Therefore, depending on the stride specified for  $incx$ ,  $i$  has the following values:

For  $incx \geq 0$ ,  $i = k$   
 For  $incx < 0$ ,  $i = n - k + 1$

See reference [82]. The result is returned as a function value. If  $n$  is 0, then 0 is returned as the value of the function.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows a vector,  $x$ , with a stride of 1.

#### Function Reference and Input:

$$\text{IMAX} = \text{ISAMAX} \left( \begin{array}{ccc} \text{N} & \text{X} & \text{INCX} \\ | & | & | \\ 9 & \text{X} & 1 \end{array} \right)$$

$X = (1.0, 2.0, 7.0, -8.0, -5.0, -10.0, -9.0, 10.0, 6.0)$

#### Output:

$\text{IMAX} = 6$

### Example 2

This example shows a vector,  $x$ , with a stride greater than 1.

#### Function Reference and Input:

$$\text{IMAX} = \text{ISAMAX} \left( \begin{array}{ccc} \text{N} & \text{X} & \text{INCX} \\ | & | & | \\ 5 & \text{X} & 2 \end{array} \right)$$

$X = (1.0, ., 7.0, ., -5.0, ., -9.0, ., 6.0)$

#### Output:

$\text{IMAX} = 4$

**Example 3**

This example shows a vector,  $x$ , with a stride of 0.

**Function Reference and Input:**

$$\begin{array}{ccc} & N & X & INCX \\ & | & | & | \\ \text{IMAX} = \text{ISAMAX} & ( & 9, X, & 0 \end{array} )$$

$$X = (1.0, ., ., ., ., ., ., ., ., .)$$
**Output:**

$$\text{IMAX} = 1$$
**Example 4**

This example shows a vector,  $x$ , with a negative stride. Processing begins at element  $X(15)$ , which is 2.0.

**Function Reference and Input:**

$$\begin{array}{ccc} & N & X & INCX \\ & | & | & | \\ \text{IMAX} = \text{ISAMAX} & ( & 8, X, & -2 \end{array} )$$

$$X = (3.0, ., ., 5.0, ., ., -8.0, ., ., 6.0, ., ., 8.0, ., ., 4.0, ., ., 8.0, ., ., 2.0)$$
**Output:**

$$\text{IMAX} = 7$$
**Example 5**

This example shows a vector,  $x$ , containing complex numbers and having a stride of 1.

**Function Reference and Input:**

$$\begin{array}{ccc} & N & X & INCX \\ & | & | & | \\ \text{IMAX} = \text{ICAMAX} & ( & 5, X, & 1 \end{array} )$$

$$X = ((9.0, 2.0), (7.0, -8.0), (-5.0, -10.0), (-4.0, 10.0), (6.0, 3.0))$$
**Output:**

$$\text{IMAX} = 2$$

## ISAMIN and IDAMIN — Position of the First or Last Occurrence of the Vector Element Having Minimum Absolute Value

### Purpose

These subprograms find the position  $i$  of the first or last occurrence of a vector element having the minimum absolute value.

You get the position of the first or last occurrence of an element by specifying positive or negative stride, respectively, for vector  $x$ . Regardless of the stride, the position  $i$  is always relative to the location specified in the calling sequence for vector  $x$  (in argument  $x$ ).

Table 44. Data Types

$x$	Subprogram
Short-precision real	ISAMIN
Long-precision real	IDAMIN

### Syntax

Fortran	ISAMIN   IDAMIN ( $n, x, incx$ )
C and C++	isamin   idamin ( $n, x, incx$ );

### On Entry

- $n$  is the number of elements in vector  $x$ . Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 44.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.

### On Return

*Function value*

- is the position  $i$  of the element in the array, where:  
If  $incx \geq 0$ ,  $i$  is the position of the first occurrence.  
If  $incx < 0$ ,  $i$  is the position of the last occurrence.  
Returned as: a fullword integer;  $0 \leq i \leq n$ .

### Notes

Declare the ISAMIN and IDAMIN functions in your program as returning a fullword integer value.

### Function

These subprograms find the first element  $x_k$ , where  $k$  is defined as the smallest index  $k$ , such that:

$$|x_k| = \min\{|x_j| \text{ for } j = 1, n\}$$

By specifying a positive or negative stride for vector  $x$ , the first or last occurrence, respectively, is found in the array. The position  $i$ , returned as the value of the function, is always figured relative to the location specified in the calling sequence for vector  $x$  (in argument  $x$ ). Therefore, depending on the stride specified for  $incx$ ,  $i$  has the following values:

For  $incx \geq 0$ ,  $i = k$   
 For  $incx < 0$ ,  $i = n-k+1$

See reference [82]. The result is returned as a function value. If  $n$  is 0, then 0 is returned as the value of the function.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows a vector,  $x$ , with a stride of 1.

#### Function Reference and Input:

	N	X	INCX
IMIN = ISAMIN(	6	, X	, 1 )
X	=	(3.0, 4.0, 1.0, 8.0, 1.0, 3.0)	

#### Output:

IMIN = 3

### Example 2

This example shows a vector,  $x$ , with a stride greater than 1.

#### Function Reference and Input:

	N	X	INCX
IMIN = ISAMIN(	4	, X	, 2 )
X	=	(-3.0, . , -9.0, . , -8.0, . , 3.0)	

#### Output:

IMIN = 1

### Example 3

This example shows a vector,  $x$ , with a positive stride and two elements with the minimum absolute value. The position of the first occurrence is returned.

#### Function Reference and Input:

## ISAMIN and IDAMIN

```
      N  X  INCX
      |  |  |
IMIN = ISAMIN( 4 , X , 2 )
```

```
X      = (2.0, . , -1.0, . , 4.0, . , 1.0)
```

### Output:

```
IMIN   = 2
```

### Example 4

This example shows a vector,  $x$ , with a negative stride and two elements with the minimum absolute value. The position of the last occurrence is returned. Processing begins at element  $X(7)$ , which is 1.0.

### Function Reference and Input:

```
      N  X  INCX
      |  |  |
IMIN = ISAMIN( 4 , X , -2 )
```

```
X      = (2.0, . , -1.0, . , 4.0, . , 1.0)
```

### Output:

```
IMIN   = 4
```

## ISMAX and IDMAX — Position of the First or Last Occurrence of the Vector Element Having the Maximum Value

### Purpose

These subprograms find the position  $i$  of the first or last occurrence of a vector element having the maximum value.

You get the position of the first or last occurrence of an element by specifying positive or negative stride, respectively, for vector  $x$ . Regardless of the stride, the position  $i$  is always relative to the location specified in the calling sequence for vector  $x$  (in argument  $x$ ).

Table 45. Data Types

$x$	Subprogram
Short-precision real	ISMAX
Long-precision real	IDMAX

### Syntax

Fortran	ISMAX   IDMAX ( $n, x, incx$ )
C and C++	ismax   idmax ( $n, x, incx$ );

### On Entry

- $n$  is the number of elements in vector  $x$ . Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 45.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.

### On Return

*Function value*

- is the position  $i$  of the element in the array, where:  
If  $incx \geq 0$ ,  $i$  is the position of the first occurrence.  
If  $incx < 0$ ,  $i$  is the position of the last occurrence.  
Returned as: a fullword integer;  $0 \leq i \leq n$ .

### Notes

Declare the ISMAX and IDMAX functions in your program as returning a fullword integer value.

### Function

These subprograms find the first element  $x_k$ , where  $k$  is defined as the smallest index  $k$ , such that:

$$x_k = \max\{x_j \text{ for } j = 1, n\}$$

## ISMAX and IDMAX

By specifying a positive or negative stride for vector  $x$ , the first or last occurrence, respectively, is found in the array. The position  $i$ , returned as the value of the function, is always figured relative to the location specified in the calling sequence for vector  $x$  (in argument  $x$ ). Therefore, depending on the stride specified for  $incx$ ,  $i$  has the following values:

For  $incx \geq 0$ ,  $i = k$   
For  $incx < 0$ ,  $i = n-k+1$

See reference [82]. The result is returned as a function value. If  $n$  is 0, then 0 is returned as the value of the function.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

$n < 0$

### Examples

#### Example 1

This example shows a vector,  $x$ , with a stride of 1.

##### Function Reference and Input:

```
          N   X   INCX
          |   |   |
IMAX = ISMAX( 6 , X , 1 )
X          = (3.0, 4.0, 1.0, 8.0, 1.0, 8.0)
```

##### Output:

```
IMAX      = 4
```

#### Example 2

This example shows a vector,  $x$ , with a stride greater than 1.

##### Function Reference and Input:

```
          N   X   INCX
          |   |   |
IMAX = ISMAX( 4 , X , 2 )
X          = (-3.0, . , 9.0, . , -8.0, . , 3.0)
```

##### Output:

```
IMAX      = 2
```

#### Example 3

This example shows a vector,  $x$ , with a positive stride and two elements with the maximum value. The position of the first occurrence is returned.

##### Function Reference and Input:



$$\begin{array}{c} \text{N} \quad \text{X} \quad \text{INCX} \\ | \quad | \quad | \\ \text{IMAX} = \text{ISMAX}( 4, \text{X}, 2 ) \end{array}$$

$$\text{X} = (2.0, ., 4.0, ., 4.0, ., 1.0)$$
**Output:**

$$\text{IMAX} = 2$$
**Example 4**

This example shows a vector,  $x$ , with a negative stride and two elements with the maximum value. The position of the last occurrence is returned. Processing begins at element  $X(7)$ , which is 1.0.

**Function Reference and Input:**

$$\begin{array}{c} \text{N} \quad \text{X} \quad \text{INCX} \\ | \quad | \quad | \\ \text{IMAX} = \text{ISMAX}( 4, \text{X}, -2 ) \end{array}$$

$$\text{X} = (2.0, ., 4.0, ., 4.0, ., 1.0)$$
**Output:**

$$\text{IMAX} = 3$$

## ISMIN and IDMIN — Position of the First or Last Occurrence of the Vector Element Having Minimum Value

### Purpose

These subprograms find the position  $i$  of the first or last occurrence of a vector element having the minimum value.

You get the position of the first or last occurrence of an element by specifying positive or negative stride, respectively, for vector  $x$ . Regardless of the stride, the position  $i$  is always relative to the location specified in the calling sequence for vector  $x$  (in argument  $x$ ).

Table 46. Data Types

$x$	Subprogram
Short-precision real	ISMIN
Long-precision real	IDMIN

### Syntax

Fortran	ISMIN   IDMIN ( $n, x, incx$ )
C and C++	ismin   idmin ( $n, x, incx$ );

### On Entry

- $n$  is the number of elements in vector  $x$ . Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 46.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.

### On Return

*Function value*

- is the position  $i$  of the element in the array, where:  
 If  $incx \geq 0$ ,  $i$  is the position of the first occurrence.  
 If  $incx < 0$ ,  $i$  is the position of the last occurrence.  
 Returned as: a fullword integer;  $0 \leq i \leq n$ .

### Notes

Declare the ISMIN and IDMIN functions in your program as returning a fullword integer value.

### Function

These subprograms find the first element  $x_k$ , where  $k$  is defined as the smallest index  $k$ , such that:

$$x_k = \min\{x_j \text{ for } j = 1, n\}$$

By specifying a positive or negative stride for vector  $x$ , the first or last occurrence, respectively, is found in the array. The position  $i$ , returned as the value of the function, is always figured relative to the location specified in the calling sequence for vector  $x$  (in argument  $x$ ). Therefore, depending on the stride specified for  $incx$ ,  $i$  has the following values:

For  $incx \geq 0$ ,  $i = k$   
 For  $incx < 0$ ,  $i = n-k+1$

See reference [82]. The result is returned as a function value. If  $n$  is 0, then 0 is returned as the value of the function.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows a vector,  $x$ , with a stride of 1.

#### Function Reference and Input:

$$\begin{array}{rcccc} & & N & X & INCX \\ & & | & | & | \\ IMIN = ISMIN( & 6 & , & X & , & 1 & ) \\ \\ X & & = & (3.0, & 4.0, & 1.0, & 8.0, & 1.0, & 3.0) \end{array}$$

#### Output:

IMIN = 3

### Example 2

This example shows a vector,  $x$ , with a stride greater than 1.

#### Function Reference and Input:

$$\begin{array}{rcccc} & & N & X & INCX \\ & & | & | & | \\ IMIN = ISMIN( & 4 & , & X & , & 2 & ) \\ \\ X & & = & (-3.0, & . , & -9.0, & . , & -8.0, & . , & 3.0) \end{array}$$

#### Output:

IMIN = 2

### Example 3

This example shows a vector,  $x$ , with a positive stride and two elements with the minimum value. The position of the first occurrence is returned. Processing begins at element  $X(7)$ , which is 1.0.

#### Function Reference and Input:

## ISMIN and IDMIN

```
          N  X  INCX
          |  |  |
IMIN = ISMIN( 4 , X , 2 )
X          = (2.0, . , 1.0, . , 4.0, . , 1.0)
```

### Output:

```
IMIN      = 2
```

### Example 4

This example shows a vector,  $x$ , with a negative stride and two elements with the minimum value. The position of the last occurrence is returned. Processing begins at element  $X(7)$ , which is 1.0.

### Function Reference and Input:

```
          N  X  INCX
          |  |  |
IMIN = ISMIN( 4 , X , -2 )
X          = (2.0, . , 1.0, . , 4.0, . , 1.0)
```

### Output:

```
IMIN      = 4
```

## SASUM, DASUM, SCASUM, and DZASUM — Sum of the Magnitudes of the Elements in a Vector

### Purpose

SASUM and DASUM compute the sum of the absolute values of the elements in vector  $x$ . SCASUM and DZASUM compute the sum of the absolute values of the real and imaginary parts of the elements in vector  $x$ .

Table 47. Data Types

$x$	Result	Subprogram
Short-precision real	Short-precision real	SASUM
Long-precision real	Long-precision real	DASUM
Short-precision complex	Short-precision real	SCASUM
Long-precision complex	Long-precision real	DZASUM

### Syntax

<b>Fortran</b>	SASUM   DASUM   SCASUM   DZASUM ( $n, x, incx$ )
<b>C and C++</b>	sasum   dasum   scasum   dzasum ( $n, x, incx$ );

### On Entry

- $n$  is the number of elements in vector  $x$ . Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 47.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.

### On Return

- Function value* is the result of the summation. Returned as: a number of the data type indicated in Table 47.

### Notes

Declare this function in your program as returning a value of the type indicated in Table 47.

### Function

SASUM and DASUM compute the sum of the absolute values of the elements of  $x$ , which is expressed as follows:

$$\sum_{i=1}^n |x_i| = |x_1| + |x_2| + \dots + |x_n|$$

## SASUM, DASUM, SCASUM, and DZASUM

SCASUM and DZASUM compute the sum of the absolute values of the real and imaginary parts of the elements of  $x$ , which is expressed as follows:

$$\sum_{i=1}^n (|a_i| + |b_i|) = (|a_1| + |b_1|) + (|a_2| + |b_2|) + \dots + (|a_n| + |b_n|)$$

where  $x_i = (a_i, b_i)$

See reference [82]. The result is returned as a function value. If  $n$  is 0, then 0.0 is returned as the value of the function. For SASUM and SCASUM, intermediate results are accumulated in long precision.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

$n < 0$

### Examples

#### Example 1

This example shows a vector,  $x$ , with a stride of 1.

##### Function Reference and Input:

```
          N   X   INCX
          |   |   |
SUMM = SASUM( 7 , X , 1 )
```

X = (1.0, -3.0, -6.0, 7.0, 5.0, 2.0, -4.0)

##### Output:

SUMM = 28.0

#### Example 2

This example shows a vector,  $x$ , with a stride greater than 1.

##### Function Reference and Input:

```
          N   X   INCX
          |   |   |
SUMM = SASUM( 4 , X , 2 )
```

X = (1.0, . , -6.0, . , 5.0, . , -4.0)

##### Output:

SUMM = 16.0

#### Example 3

This example shows a vector,  $x$ , with negative stride. Processing begins at element  $x(7)$ , which is  $-4.0$ .

##### Function Reference and Input:

```

      N   X   INCX
      |   |   |
SUMM = SASUM( 4 , X , -2 )
X          = (1.0, . , -6.0, . , 5.0, . , -4.0)

```

**Output:**

SUMM = 16.0

**Example 4**

This example shows a vector,  $x$ , with a stride of 0. The result in SUMM is  $nx_1$ .

**Function Reference and Input:**

```

      N   X   INCX
      |   |   |
SUMM = SASUM( 7 , X , 0 )
X          = (-2.0, . , . , . , . , . , .)

```

**Output:**

SUMM = 14.0

**Example 5**

This example shows a vector,  $x$ , containing complex numbers and having a stride of 1.

**Function Reference and Input:**

```

      N   X   INCX
      |   |   |
SUMM = SCASUM( 5 , X , 1 )
X          = ((1.0, 2.0), (-3.0, 4.0), (5.0, -6.0), (-7.0, -8.0),
              (9.0, 10.0))

```

**Output:**

SUMM = 55.0

## SAXPY, DAXPY, CAXPY, and ZAXPY — Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y

### Purpose

These subprograms perform the following computation, using the scalar  $\alpha$  and vectors  $x$  and  $y$ :

$$y \leftarrow y + \alpha x$$

Table 48. Data Types

$\alpha, x, y$	Subprogram
Short-precision real	SAXPY
Long-precision real	DAXPY
Short-precision complex	CAXPY
Long-precision complex	ZAXPY

### Syntax

<b>Fortran</b>	CALL SAXPY   DAXPY   CAXPY   ZAXPY ( $n, \alpha, x, incx, y, incy$ )
<b>C and C++</b>	saxpy   daxpy   caxpy   zaxpy ( $n, \alpha, x, incx, y, incy$ );

### On Entry

- $n$  is the number of elements in vectors  $x$  and  $y$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $\alpha$  is the scalar  $\alpha$ .  
Specified as: a number of the data type indicated in Table 48.
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 48.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  is the vector  $y$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 48.
- $incy$  is the stride for vector  $y$ .  
Specified as: a fullword integer. It can have any value.

### On Return

- $y$  is the vector  $y$ , containing the results of the computation  $y + \alpha x$ .  
Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 48.

### Notes

1. If you specify the same vector for  $x$  and  $y$ ,  $incx$  and  $incy$  must be equal; otherwise, results are unpredictable.



2. If you specify different vectors for  $x$  and  $y$ , they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.

## Function

The computation is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

See reference [82]. If  $alpha$  or  $n$  is zero, no computation is performed. For CAXPY, intermediate results are accumulated in long precision.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows vectors  $x$  and  $y$  with positive strides.

#### Call Statement and Input:

```

          N ALPHA X INCX Y INCY
CALL SAXPY( 5 , 2.0 , X , 1 , Y , 2 )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (1.0, . , 1.0, . , 1.0, . , 1.0, . , 1.0)

```

#### Output:

```

Y      = (3.0, . , 5.0, . , 7.0, . , 9.0, . , 11.0)

```

### Example 2

This example shows vectors  $x$  and  $y$  having strides of opposite signs. For  $y$ , which has negative stride, processing begins at element  $Y(5)$ , which is 1.0.

#### Call Statement and Input:

```

          N ALPHA X INCX Y INCY
CALL SAXPY( 5 , 2.0 , X , 1 , Y , -1 )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (5.0, 4.0, 3.0, 2.0, 1.0)

```

#### Output:

```

Y      = (15.0, 12.0, 9.0, 6.0, 3.0)

```

## SAXPY, DAXPY, CAXPY, and ZAXPY

### Example 3

This example shows a vector,  $x$ , with 0 stride. Vector  $x$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $x$ .

#### Call Statement and Input:

```
          N ALPHA X INCX Y INCY
          |   |   |   |   |   |
CALL SAXPY( 5 , 2.0 , X , 0 , Y , 1 )
```

```
X      = (1.0)
Y      = (5.0, 4.0, 3.0, 2.0, 1.0)
```

#### Output:

```
Y      = (7.0, 6.0, 5.0, 4.0, 3.0)
```

### Example 4

This example shows how SAXPY can be used to compute a scalar value. In this case, vectors  $x$  and  $y$  contain scalar values and the strides for both vectors are 0. The number of elements to be processed,  $n$ , is 1.

#### Call Statement and Input:

```
          N ALPHA X INCX Y INCY
          |   |   |   |   |   |
CALL SAXPY( 1 , 2.0 , X , 0 , Y , 0 )
```

```
X      = (1.0)
Y      = (5.0)
```

#### Output:

```
Y      = (7.0)
```

### Example 5

This example shows how to use CAXPY, where vectors  $x$  and  $y$  contain complex numbers. In this case, vectors  $x$  and  $y$  have positive strides.

#### Call Statement and Input:

```
          N ALPHA X INCX Y INCY
          |   |   |   |   |   |
CALL CAXPY( 3 ,ALPHA, X , 1 , Y , 2 )
```

```
ALPHA  = (2.0, 3.0)
X      = ((1.0, 2.0), (2.0, 0.0), (3.0, 5.0))
Y      = ((1.0, 1.0), . , (0.0, 2.0), . , (5.0, 4.0))
```

#### Output:

```
Y      = ((-3.0, 8.0), . , (4.0, 8.0), . , (-4.0, 23.0))
```

## SCOPY, DCOPY, CCOPY, and ZCOPY — Copy a Vector

### Purpose

These subprograms copy vector  $x$  to another vector,  $y$ :

$$y \leftarrow x$$

Table 49. Data Types

$x, y$	Subprogram
Short-precision real	SCOPY
Long-precision real	DCOPY
Short-precision complex	CCOPY
Long-precision complex	ZCOPY

### Syntax

Fortran	CALL SCOPY   DCOPY   CCOPY   ZCOPY ( $n, x, incx, y, incy$ )
C and C++	scopy   dcopy   ccopy   zcopy ( $n, x, incx, y, incy$ );

### On Entry

- $n$  is the number of elements in vectors  $x$  and  $y$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 49.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  See “On Return.”
- $incy$  is the stride for vector  $y$ . Specified as: a fullword integer. It can have any value.

### On Return

- $y$  is the vector  $y$  of length  $n$ . Returned as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 49.

### Notes

1. If you specify the same vector for  $x$  and  $y$ ,  $incx$  and  $incy$  must be equal; otherwise, results are unpredictable.
2. If you specify different vectors for  $x$  and  $y$ , they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.

### Function

The copy is expressed as follows:

## SCOPY, DCOPY, CCOPY, and ZCOPY

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

See reference [82]. If  $n$  is 0, no copy is performed.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

$n < 0$

### Examples

#### Example 1

This example shows input vector  $x$  and output vector  $y$  with positive strides.

##### Call Statement and Input:

```
CALL SCOPY(  $\begin{matrix} N & X & INCX & Y & INCY \\ | & | & | & | & | \\ 5 & X & 1 & Y & 2 \end{matrix}$  )
```

$X = (1.0, 2.0, 3.0, 4.0, 5.0)$

##### Output:

$Y = (1.0, ., 2.0, ., 3.0, ., 4.0, ., 5.0)$

#### Example 2

This example shows how to obtain a reverse copy of the input vector  $x$  by specifying strides with the same absolute value, but with opposite signs, for input vector  $x$  and output vector  $y$ . For  $y$ , which has a negative stride, results are stored beginning at element  $Y(5)$ .

##### Call Statement and Input:

```
CALL SCOPY(  $\begin{matrix} N & X & INCX & Y & INCY \\ | & | & | & | & | \\ 5 & X & 1 & Y & -1 \end{matrix}$  )
```

$X = (1.0, 2.0, 3.0, 4.0, 5.0)$

##### Output:

$Y = (5.0, 4.0, 3.0, 2.0, 1.0)$

#### Example 3

This example shows an input vector,  $x$ , with 0 stride. Vector  $x$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $x$ . This is a technique for replicating an element of a vector.

##### Call Statement and Input:

```

      N   X   INCX  Y   INCY
      |   |   |    |   |
CALL SCOPY( 5 , X , 0 , Y , 1 )
X          = (13.0)

```

**Output:**

Y = (13.0, 13.0, 13.0, 13.0, 13.0)

**Example 4**

This example shows input vector  $x$  and output vector  $y$ , containing complex numbers and having positive strides.

**Call Statement and Input:**

```

      N   X   INCX  Y   INCY
      |   |   |    |   |
CALL CCOPY( 4 , X , 1 , Y , 2 )
X          = ((1.0, 1.0), (2.0, 2.0), (3.0, 3.0), (4.0, 4.0))

```

**Output:**

Y = ((1.0, 1.0), . . , (2.0, 2.0), . . , (3.0, 3.0), . . ,  
 (4.0, 4.0))

---

## SDOT, DDOT, CDOTU, ZDOTU, CDOTC, and ZDOTC — Dot Product of Two Vectors

### Purpose

SDOT, DDOT, CDOTU, and ZDOTU compute the dot product of vectors  $x$  and  $y$ :

$$x \bullet y$$

CDOTC and ZDOTC compute the dot product of the complex conjugate of vector  $x$  with vector  $y$ :

$$\bar{x} \bullet y$$

Table 50. Data Types

$x, y$ , Result	Subprogram
Short-precision real	SDOT
Long-precision real	DDOT
Short-precision complex	CDOTU and CDOTC
Long-precision complex	ZDOTU and ZDOTC

### Syntax

Fortran	SDOT   DDOT   CDOTU   ZDOTU   CDOTC   ZDOTC ( $n, x, incx, y, incy$ )
C and C++	sdot   ddot   cdotu   zdotu   cdotc   zdotc ( $n, x, incx, y, incy$ );

#### On Entry

- $n$  is the number of elements in vectors  $x$  and  $y$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 50.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  is the vector  $y$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 50.
- $incy$  is the stride for vector  $y$ .  
Specified as: a fullword integer. It can have any value.

#### On Return

- Function value* is the result of the dot product computation. Returned as: a number of the data type indicated in Table 50.

## Notes

Declare this function in your program as returning a value of the data type indicated in Table 50 on page 220.

## Function

SDOT, DDOT, CDOTU, and ZDOTU compute the dot product of the vectors  $x$  and  $y$ , which is expressed as follows:

$$x \bullet y = x_1y_1 + x_2y_2 + \dots + x_ny_n$$

CDOTC and ZDOTC compute the dot product of the complex conjugate of vector  $x$  with vector  $y$ , which is expressed as follows:

$$\bar{x} \bullet y = \bar{x}_1y_1 + \bar{x}_2y_2 + \dots + \bar{x}_ny_n$$

See reference [82]. The result is returned as a function value. If  $n$  is 0, then zero is returned as the value of the function.

For SDOT, CDOTU, and CDOTC, intermediate results are accumulated in long precision.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows how to compute the dot product of two vectors,  $x$  and  $y$ , having strides of 1.

#### Function Reference and Input:

```

          N  X  INCX  Y  INCY
          |  |  |    |  |
DOTT = SDOT( 5 , X , 1 , Y , 1 )

```

```

X      = (1.0, 2.0, -3.0, 4.0, 5.0)
Y      = (9.0, 8.0, 7.0, -6.0, 5.0)

```

#### Output:

```

DOTT   = (9.0 + 16.0 - 21.0 - 24.0 + 25.0) = 5.0

```

### Example 2

This example shows how to compute the dot product of a vector,  $x$ , with a stride of 1, and a vector,  $y$ , with a stride greater than 1.

#### Function Reference and Input:

## SDOT, DDOT, CDOTU, ZDOTU, CDOTC, ZDOTC

$$\text{DOTT} = \text{SDOT} \left( \begin{array}{c} \text{N} \\ | \\ 5 \end{array}, \begin{array}{c} \text{X} \\ | \\ \text{X} \end{array}, \begin{array}{c} \text{INCX} \\ | \\ 1 \end{array}, \begin{array}{c} \text{Y} \\ | \\ \text{Y} \end{array}, \begin{array}{c} \text{INCY} \\ | \\ 2 \end{array} \right)$$

X = (1.0, 2.0, -3.0, 4.0, 5.0)  
Y = (9.0, ., 7.0, ., 5.0, ., -3.0, ., 1.0)

### Output:

DOTT = (9.0 + 14.0 - 15.0 - 12.0 + 5.0) = 1.0

### Example 3

This example shows how to compute the dot product of a vector,  $x$ , with a negative stride, and a vector,  $y$ , with a stride greater than 1. For  $x$ , processing begins at element  $X(5)$ , which is 5.0.

### Function Reference and Input:

$$\text{DOTT} = \text{SDOT} \left( \begin{array}{c} \text{N} \\ | \\ 5 \end{array}, \begin{array}{c} \text{X} \\ | \\ \text{X} \end{array}, \begin{array}{c} \text{INCX} \\ | \\ -1 \end{array}, \begin{array}{c} \text{Y} \\ | \\ \text{Y} \end{array}, \begin{array}{c} \text{INCY} \\ | \\ 2 \end{array} \right)$$

X = (1.0, 2.0, -3.0, 4.0, 5.0)  
Y = (9.0, ., 7.0, ., 5.0, ., -3.0, ., 1.0)

### Output:

DOTT = (45.0 + 28.0 - 15.0 - 6.0 + 1.0) = 53.0

### Example 4

This example shows how to compute the dot product of a vector,  $x$ , with a stride of 0, and a vector,  $y$ , with a stride of 1. The result in DOTT is  $x_1(y_1+\dots+y_n)$ .

### Function Reference and Input:

$$\text{DOTT} = \text{SDOT} \left( \begin{array}{c} \text{N} \\ | \\ 5 \end{array}, \begin{array}{c} \text{X} \\ | \\ \text{X} \end{array}, \begin{array}{c} \text{INCX} \\ | \\ 0 \end{array}, \begin{array}{c} \text{Y} \\ | \\ \text{Y} \end{array}, \begin{array}{c} \text{INCY} \\ | \\ 1 \end{array} \right)$$

X = (1.0, ., ., ., .)  
Y = (9.0, 8.0, 7.0, -6.0, 5.0)

### Output:

DOTT = (1.0) × (9.0 + 8.0 + 7.0 - 6.0 + 5.0) = 23.0

### Example 5

This example shows how to compute the dot product of two vectors,  $x$  and  $y$ , with strides of 0. The result in DOTT is  $nx_1y_1$ .

### Function Reference and Input:

$$\text{DOTT} = \text{SDOT} \left( \begin{array}{c} \text{N} \\ | \\ 5 \end{array}, \begin{array}{c} \text{X} \\ | \\ \text{X} \end{array}, \begin{array}{c} \text{INCX} \\ | \\ 0 \end{array}, \begin{array}{c} \text{Y} \\ | \\ \text{Y} \end{array}, \begin{array}{c} \text{INCY} \\ | \\ 0 \end{array} \right)$$

X = (1.0, ., ., ., .)  
Y = (9.0, ., ., ., .)

### Output:

DOTT = (5) × (1.0) × (9.0) = 45.0



**Example 6**

This example shows how to compute the dot product of two vectors,  $x$  and  $y$ , containing complex numbers, where  $x$  has a stride of 1, and  $y$  has a stride greater than 1.

**Function Reference and Input:**

$$\begin{array}{cccccc} & N & X & INCX & Y & INCY \\ & | & | & | & | & | \\ \text{DOTT} = \text{CDOTU} & ( & 3 & , & X & , & 1 & , & Y & , & 2 & ) \end{array}$$

$$\begin{aligned} X &= ((1.0, 2.0), (3.0, -4.0), (-5.0, 6.0)) \\ Y &= ((10.0, 9.0), ., (-6.0, 5.0), ., (2.0, 1.0)) \end{aligned}$$
**Output:**

$$\begin{aligned} \text{DOTT} &= ((10.0 - 18.0 - 10.0) - (18.0 - 20.0 + 6.0), \\ &\quad (9.0 + 15.0 - 5.0) + (20.0 + 24.0 + 12.0)) \\ &= (-22.0, 75.0) \end{aligned}$$
**Example 7**

This example shows how to compute the dot product of the conjugate of a vector,  $x$ , with vector  $y$ , both containing complex numbers, where  $x$  has a stride of 1, and  $y$  has a stride greater than 1.

**Function Reference and Input:**

$$\begin{array}{cccccc} & N & X & INCX & Y & INCY \\ & | & | & | & | & | \\ \text{DOTT} = \text{CDOTC} & ( & 3 & , & X & , & 1 & , & Y & , & 2 & ) \end{array}$$

$$\begin{aligned} X &= ((1.0, 2.0), (3.0, -4.0), (-5.0, 6.0)) \\ Y &= ((10.0, 9.0), ., (-6.0, 5.0), ., (2.0, 1.0)) \end{aligned}$$
**Output:**

$$\begin{aligned} \text{DOTT} &= ((10.0 - 18.0 - 10.0) + (18.0 - 20.0 + 6.0), \\ &\quad (9.0 + 15.0 - 5.0) - (20.0 + 24.0 + 12.0)) \\ &= (-14.0, -37.0) \end{aligned}$$

---

## SNAXPY and DNAXPY — Compute SAXPY or DAXPY N Times

### Purpose

These subprograms compute SAXPY or DAXPY, respectively,  $n$  times:

$$y_i \leftarrow y_i + \alpha_i x_i \quad \text{for } i = 1, n$$

where each  $\alpha_i$  is a scalar value, contained in the vector  $a$ , and each  $x_i$  and  $y_i$  are vectors, contained in vectors (or matrices)  $x$  and  $y$ , respectively. For an explanation of the SAXPY and DAXPY computations, see “SAXPY, DAXPY, CAXPY, and ZAXPY — Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y” on page 214.

Table 51. Data Types

$a, x, y$	Subprogram
Short-precision real	SNAXPY
Long-precision real	DNAXPY

### Syntax

Fortran	CALL SNAXPY   DNAXPY ( $n, m, a, inca, x, incxi, incxo, y, incyi, incyo$ )
C and C++	snaxpy   dnaxpy ( $n, m, a, inca, x, incxi, incxo, y, incyi, incyo$ );

### On Entry

- $n$  is the number of SAXPY or DAXPY computations to be performed and the number of elements in vector  $a$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $m$  is the number of elements in vectors  $x_i$  and  $y_i$  for each SAXPY or DAXPY computation.  
Specified as: a fullword integer;  $m \geq 0$ .
- $a$  is the vector  $a$  of length  $n$ , containing the scalar values  $\alpha_i$ , used in each computation of  $y_i + \alpha_i x_i$ .  
Specified as: a one-dimensional array of (at least) length  $1+(n-1)|inca|$ , containing numbers of the data type indicated in Table 51.
- $inca$  is the stride for vector  $a$ .  
Specified as: a fullword integer. It can have any value.
- $x$  is the vector (or matrix)  $x$ , containing the  $x_i$  vectors of length  $m$ , used in the  $n$  computations of  $y_i + \alpha_i x_i$ . Specified as: a one- or two-dimensional array of (at least) length  $(1+(n-1)(incxo)) + (m-1)|incxi|$ , containing numbers of the data type indicated in Table 51.
- $incxi$  is the stride for  $x$  in the inner loop—that is, the stride identifying the elements in each vector  $x_i$ .  
Specified as: a fullword integer. It can have any value.

<i>incxo</i>	is the stride for $x$ in the outer loop—that is, the stride identifying each vector $x_i$ in $x$ . Specified as: a fullword integer; $incxo \geq 0$ .
$y$	is the vector (or matrix) $y$ , containing the $y_i$ vectors of length $m$ , used in the $n$ computations of $y_i + \alpha_i x_i$ . Specified as: a one- or two-dimensional array of (at least) length $(1+(n-1)(incyo)) + (m-1) incyi $ , containing numbers of the data type indicated in Table 51 on page 224.
<i>incyi</i>	is the stride for $y$ in the inner loop—that is, the stride identifying the elements in each vector $y_i$ in $y$ . Specified as: a fullword integer; $incyi > 0$ or $incyi < 0$ .
<i>incyo</i>	is the stride for $y$ in the outer loop—that is, the stride identifying each vector $y_i$ in $y$ . Specified as: a fullword integer; $incyo \geq 0$ .

### On Return

$y$	is the vector (or matrix) $y$ , containing the $y_i$ vectors of length $m$ , which contain the results of the $n$ SAXPY or DAXPY computations, $y_i + \alpha_i x_i$ for $i = 1, n$ . Returned as: a one- or two-dimensional array, containing numbers of the data type indicated in Table 51 on page 224.
-----	---

### Notes

Vector  $y$  must have no common elements with vector  $a$  or vector  $x$ ; otherwise, results are unpredictable. See “Concepts” on page 59.

### Function

The SAXPY or DAXPY computations:

$$y \leftarrow y + \alpha x$$

are performed  $n$  times. This is expressed as follows:

$$y_i \leftarrow y_i + \alpha_i x_i \quad \text{for } i = 1, n$$

where each  $\alpha_i$  is a scalar value, contained in the vector  $a$ , and each  $x_i$  and  $y_i$  are vectors, contained in vectors (or matrices)  $x$  and  $y$ , respectively.

Each computation of SAXPY or DAXPY on page 214 uses the length of the  $x_i$  and  $y_i$  vectors,  $m$ , for its input argument,  $n$ . It also uses the strides for the inner loop,  $incxi$  and  $incyi$ , for its parameters  $incx$  and  $incy$ , respectively. See “Function” on page 215 for a description of how the computation is done.

The outer loop of the SNAXPY or DNAXPY computation uses the strides of  $inca$ ,  $incxo$ , and  $incyo$  to locate the elements in  $a$  and vectors in  $x$  and  $y$  for each  $i$ -th computation. These are:

For  $i = 1, n$ :

## SNAXPY and DNAXPY

$$\begin{aligned} &\alpha_{((i-1)inca+1)} && \text{for } inca \geq 0 \\ &\alpha_{((i-n)inca+1)} && \text{for } inca < 0 \\ &X_{((i-1)incxo+1)} \\ &Y_{((i-1)incyo+1)} \end{aligned}$$

If  $m$  or  $n$  is 0, no computation is performed.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

1.  $n < 0$
2.  $m < 0$
3.  $incxo < 0$
4.  $incyi = 0$
5.  $incyo < 0$

### Examples

#### Example 1

This example shows vectors, contained in matrices, with the stride of the inner loops  $incxi$  and  $incyi$  equal to 1.

#### Call Statement and Input:

```
CALL SNAXPY( N, M, A, INCA, X, INCXI, INCXO, Y, INCYI, INCYO )
```

|   |   |   |   |   |   |   |   |   |   |

3 , 4 , A , 1 , X , 1 , 10 , Y , 1 , 5 )

A = (3.0, 2.0, 4.0)

X =  $\begin{bmatrix} 1.0 & 4.0 & 3.0 \\ 2.0 & 3.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 1.0 & 1.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$

Y =  $\begin{bmatrix} 4.0 & 1.0 & 3.0 \\ 3.0 & 2.0 & 4.0 \\ 2.0 & 3.0 & 2.0 \\ 1.0 & 4.0 & 1.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$

#### Output:

Y =  $\begin{bmatrix} 7.0 & 9.0 & 15.0 \\ 9.0 & 8.0 & 20.0 \\ 11.0 & 7.0 & 10.0 \\ 13.0 & 6.0 & 5.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$

**Example 2**

This example shows vectors, contained in matrices, with a stride of the inner loop *incxi* greater than 1.

**Call Statement and Input:**

```

          N   M   A   INCA  X   INCXI  INCXO  Y   INCYI  INCYO
          |   |   |   |    |   |       |   |   |       |
CALL SNAXPY( 3 , 4 , A , 1 , X , 2 , 10 , Y , 1 , 5 )
    
```

A = (3.0, 2.0, 4.0)

$$X = \begin{bmatrix} 1.0 & 4.0 & 3.0 \\ \cdot & \cdot & \cdot \\ 2.0 & 3.0 & 4.0 \\ \cdot & \cdot & \cdot \\ 3.0 & 2.0 & 2.0 \\ \cdot & \cdot & \cdot \\ 4.0 & 1.0 & 1.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$Y = \begin{bmatrix} 4.0 & 1.0 & 3.0 \\ 3.0 & 2.0 & 4.0 \\ 2.0 & 3.0 & 2.0 \\ 1.0 & 4.0 & 1.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

Y =(same as output Y in Example 1)

**Example 3**

This example shows vectors, contained in matrices, with a negative stride, *incyi*, for the inner loop.

**Call Statement and Input:**

```

          N   M   A   INCA  X   INCXI  INCXO  Y   INCYI  INCYO
          |   |   |   |    |   |       |   |   |       |
CALL SNAXPY( 3 , 4 , A , 1 , X , 1 , 10 , Y , -1 , 5 )
    
```

A = (3.0, 2.0, 4.0)

$$X = \begin{bmatrix} 1.0 & 4.0 & 3.0 \\ 2.0 & 3.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 1.0 & 1.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$\begin{bmatrix} 1.0 & 4.0 & 1.0 \\ 2.0 & 3.0 & 2.0 \end{bmatrix}$$

## SNAXPY and DNAXPY

$$Y = \begin{bmatrix} 3.0 & 2.0 & 4.0 \\ 4.0 & 1.0 & 3.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$Y = \begin{bmatrix} 13.0 & 6.0 & 5.0 \\ 11.0 & 7.0 & 10.0 \\ 9.0 & 8.0 & 20.0 \\ 7.0 & 9.0 & 15.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 4

This example shows vectors, contained in matrices, with a negative stride, *inca*, for vector *a*. For vector *a*, processing begins at element A(5), which is 3.0.

**Call Statement and Input:**

```
CALL SNAXPY( N, M, A, INCA, X, INCXI, INCXO, Y, INCYI, INCYO )
```

|   |   |   |   |   |   |   |   |   |   |  
3, 4, A, -2, X, 1, 10, Y, 1, 5

A = (4.0, . , 2.0, . , 3.0)

$$X = \begin{bmatrix} 1.0 & 4.0 & 3.0 \\ 2.0 & 3.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 1.0 & 1.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$Y = \begin{bmatrix} 4.0 & 1.0 & 3.0 \\ 3.0 & 2.0 & 4.0 \\ 2.0 & 3.0 & 2.0 \\ 1.0 & 4.0 & 1.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

Y = (same as output Y in Example 1)

## SNDOT and DNDOT — Compute Special Dot Products N Times

### Purpose

These subprograms compute one of the following special dot products  $n$  times:

$s_i \leftarrow x_i \cdot y_i$	Store positive dot product
$s_i \leftarrow -x_i \cdot y_i$	Store negative dot product
$s_i \leftarrow s_i + x_i \cdot y_i$	Accumulate positive dot product
$s_i \leftarrow s_i - x_i \cdot y_i$	Accumulate negative dot product
for $i = 1, n$	

where each  $s_i$  is an element in vector  $s$ , and each  $x_i$  and  $y_i$  are vectors contained in vectors (or matrices)  $x$  and  $y$ , respectively.

Table 52. Data Types

$s, x, y$	Subprogram
Short-precision real	SNDOT
Long-precision real	DNDOT

### Syntax

<b>Fortran</b>	CALL SNDOT   DNDOT ( $n, m, s, incs, isw, x, incxi, incxo, y, incyi, incyo$ )
<b>C and C++</b>	sndot   dndot ( $n, m, s, incs, isw, x, incxi, incxo, y, incyi, incyo$ );

### On Entry

$n$	is the number of dot product computations to be performed and the number of elements in the vector $s$ . Specified as: a fullword integer; $n \geq 0$ .
$m$	is the number of elements in vectors $x_i$ and $y_i$ for each dot product computation. Specified as: a fullword integer; $m \geq 0$ .
$s$	is the vector $s$ , containing the $n$ scalar values $s_i$ , where: If $isw = 1$ or $2$ , $s_i$ is not used in the computation (no input value specified.) If $isw = 3$ or $4$ , $s_i$ is used in the computation (input value specified.) Specified as: a one-dimensional array of (at least) length $1+(n-1) incs $ , containing numbers of the data type indicated in Table 52.
$incs$	is the stride for vector $s$ . Specified as: a fullword integer; $incs > 0$ or $incs < 0$ .
$isw$	indicates the type of computation to perform, depending on the value specified: If $isw = 1$ , $s_i \leftarrow x_i \cdot y_i$ If $isw = 2$ , $s_i \leftarrow -x_i \cdot y_i$ If $isw = 3$ , $s_i \leftarrow s_i + x_i \cdot y_i$

## SNDOT and DNDOT

If  $isw = 4$ ,  $s_i \leftarrow s_i - x_i \bullet y_i$

where  $i = 1, n$

Specified as: a fullword integer. Its value must be 1, 2, 3, or 4.

$x$  is the vector (or matrix)  $x$ , containing the  $x_i$  vectors of length  $m$ , used in the  $n$  dot product computations. Specified as: a one- or two-dimensional array of (at least) length  $(1+(n-1)(incxo))+(m-1)|incxi|$ , containing numbers of the data type indicated in Table 52 on page 229.

$incxi$  is the stride for  $x$  in the inner loop—that is, the stride identifying the elements in each vector  $x_i$ .

Specified as: a fullword integer. It can have any value.

$incxo$  is the stride for  $x$  in the outer loop—that is, the stride identifying each vector  $x_i$  in  $x$ .

Specified as: a fullword integer;  $incxo \geq 0$ .

$y$  is the vector (or matrix)  $y$ , containing the  $y_i$  vectors of length  $m$ , used in the  $n$  dot product computations. Specified as: a one- or two-dimensional array of (at least) length  $(1+(n-1)(incyo)) + (m-1)|incyi|$ , containing numbers of the data type indicated in Table 52 on page 229.

$incyi$  is the stride for  $y$  in the inner loop—that is, the stride identifying the elements in each vector  $y_i$ .

Specified as: a fullword integer. It can have any value.

$incyo$  is the stride for  $y$  in the outer loop—that is, the stride identifying each vector  $y_i$  in  $y$ .

Specified as: a fullword integer;  $incyo \geq 0$ .

### On Return

$s$  is the vector  $s$  of length  $n$ , containing the results of the  $n$  dot product computations. The type of dot product computation depends of the value specified for  $isw$ .

If  $isw = 1$ ,  $s_i \leftarrow x_i \bullet y_i$

If  $isw = 2$ ,  $s_i \leftarrow -x_i \bullet y_i$

If  $isw = 3$ ,  $s_i \leftarrow s_i + x_i \bullet y_i$

If  $isw = 4$ ,  $s_i \leftarrow s_i - x_i \bullet y_i$

where  $i = 1, n$

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 52 on page 229.

## Function

The four possible computations that can be performed by these subprograms are:

$s_i \leftarrow x_i \bullet y_i$

Store positive dot product

$s_i \leftarrow -x_i \bullet y_i$

Store negative dot product



```

si ← si+xi • yi           Accumulate positive dot
                             product
si ← si-xi • yi           Accumulate negative dot
                             product
for i = 1, n

```

where each  $s_i$  is a scalar element in the vector  $s$  of length  $n$ , and each of the  $n$   $x_i$  and  $y_i$  vectors of length  $m$  are contained in vectors (or matrices)  $x$  and  $y$ , respectively. Each computation uses the dot product, which is expressed:

$$x_i \cdot y_i = u_1v_1 + u_2v_2 + \dots + u_mv_m$$

where  $u_i$  and  $v_i$  are elements of  $x_i$  and  $y_i$ , respectively. To find the elements for the computation, it uses:

- The strides for the inner loops, *incxi* and *incy<sub>i</sub>*, to locate the elements in vectors  $x_i$  and  $y_i$ , respectively.
- The strides for the outer loops, *incs*, *incxo*, and *incyo*, to locate the element  $s_i$  in vector  $s$  and the vectors  $x_i$  and  $y_i$  in vectors (or matrices)  $x$  and  $y$ , respectively.

If  $m$  or  $n$  is 0, no computation is performed. For SNDOT, intermediate results are accumulated in long precision.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $n < 0$
2.  $m < 0$
3.  $incs = 0$
4.  $isw < 1$  or  $isw > 4$
5.  $incxo < 0$
6.  $incyo < 0$

## Examples

### Example 1

This example shows a store positive dot product computation using vectors with positive strides.

#### Call Statement and Input:

```

          N  M  S  INCS ISW  X  INCXI INCXO  Y  INCYI INCYO
CALL SNDOT( 3 , 4 , S , 1 , 1 , X , 1 , 4 , Y , 1 , 4 )

```

$$X = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 2.0 & 3.0 & 4.0 \\ 3.0 & 4.0 & 5.0 \\ 4.0 & 5.0 & 6.0 \end{bmatrix}$$

$$\begin{bmatrix} 4.0 & 3.0 & 2.0 \end{bmatrix}$$

## SNDOT and DNDOT

$$Y = \begin{bmatrix} 3.0 & 2.0 & 1.0 \\ 2.0 & 1.0 & 4.0 \\ 1.0 & 4.0 & 3.0 \end{bmatrix}$$

### Output:

$$S = (20.0, 36.0, 48.0)$$

### Example 2

This example shows a store negative dot product computation using vectors with positive and negative strides.

### Call Statement and Input:

```
CALL SNDOT( N, M, S, INCS, ISW, X, INCXI, INCXO, Y, INCYI, INCYO )
           | | | | | | | | | | |
           3, 4, S, -1, 2, X, 2, 10, Y, -1, 6 )
```

$$X = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ \cdot & \cdot & \cdot \\ 2.0 & 3.0 & 4.0 \\ \cdot & \cdot & \cdot \\ 3.0 & 4.0 & 5.0 \\ \cdot & \cdot & \cdot \\ 4.0 & 5.0 & 6.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$Y = \begin{bmatrix} 4.0 & 3.0 & 2.0 \\ 3.0 & 2.0 & 1.0 \\ 2.0 & 1.0 & 4.0 \\ 1.0 & 4.0 & 3.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

### Output:

$$S = (-42.0, -34.0, -30.0)$$

### Example 3

This example shows an accumulative positive dot product using vectors with positive and negative strides.

### Call Statement and Input:

```
CALL SNDOT( N, M, S, INCS, ISW, X, INCXI, INCXO, Y, INCYI, INCYO )
           | | | | | | | | | | |
           3, 4, S, 1, 3, X, -2, 10, Y, 2, 10 )
```

$$S = (2.0, 5.0, 8.0)$$

$$X = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ \cdot & \cdot & \cdot \\ 2.0 & 3.0 & 4.0 \\ \cdot & \cdot & \cdot \\ 3.0 & 4.0 & 5.0 \\ \cdot & \cdot & \cdot \\ 4.0 & 5.0 & 6.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$Y = \begin{bmatrix} 4.0 & 3.0 & 2.0 \\ \cdot & \cdot & \cdot \\ 3.0 & 2.0 & 1.0 \\ \cdot & \cdot & \cdot \\ 2.0 & 1.0 & 4.0 \\ \cdot & \cdot & \cdot \\ 1.0 & 4.0 & 3.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

S = (32.0, 39.0, 50.0)

**Example 4**

This example shows an accumulative negative dot product using vectors with positive and negative strides.

**Call Statement and Input:**

```

CALL SNDOT( N, M, S, INCS, ISW, X, INCXI, INCXO, Y, INCYI, INCYO )
           |  |  |  |  |  |  |  |  |  |  |  |
           3, 4, S, -1, 4, X, 1, 6, Y, 2, 10 )
S         = (3.0, 6.0, 9.0)

```

$$X = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 2.0 & 3.0 & 4.0 \\ 3.0 & 4.0 & 5.0 \\ 4.0 & 5.0 & 6.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$Y = \begin{bmatrix} 4.0 & 3.0 & 2.0 \\ \cdot & \cdot & \cdot \\ 3.0 & 2.0 & 1.0 \\ \cdot & \cdot & \cdot \\ 2.0 & 1.0 & 4.0 \\ \cdot & \cdot & \cdot \\ 1.0 & 4.0 & 3.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

S = (-45.0, -30.0, -11.0)

## SNRM2, DNRM2, SCNRM2, and DZNRM2 — Euclidean Length of a Vector with Scaling of Input to Avoid Destructive Underflow and Overflow

### Purpose

These subprograms compute the Euclidean length ( $l_2$  norm) of vector  $x$ , with scaling of input to avoid destructive underflow and overflow.

Table 53. Data Types

$x$	Result	Subprogram
Short-precision real	Short-precision real	SNRM2
Long-precision real	Long-precision real	DNRM2
Short-precision complex	Short-precision real	SCNRM2
Long-precision complex	Long-precision real	DZNRM2

**Note:** If there is a possibility that your data will cause the computation to overflow or underflow, you should use these subroutines instead of SNORM2, DNORM2, CNORM2, and ZNORM2, because the intermediate computational results may exceed the maximum or minimum limits of the machine. “Notes” on page 237 explains how to estimate whether your data will cause an overflow or underflow.

### Syntax

Fortran	SNRM2   DNRM2   SCNRM2   DZNRM2 ( $n, x, incx$ )
C and C++	snrm2   dnrm2   scnrm2   dznrm2 ( $n, x, incx$ );

#### On Entry

- $n$  is the number of elements in vector  $x$ . Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ , whose Euclidean length is to be computed.  
Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 53.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.

#### On Return

- Function value* is the Euclidean length ( $l_2$  norm) of the vector  $x$ . Returned as: a number of the data type indicated in Table 53.

### Notes

Declare this function in your program as returning a value of the data type indicated in Table 53.

## Function

The Euclidean length ( $l_2$  norm) of vector  $x$  is expressed as follows, with scaling of input to avoid destructive underflow and overflow:

$$\sqrt{|x_1|^2 + |x_2|^2 + \dots + |x_n|^2}$$

See reference [82]. The result is returned as the function value. If  $n$  is 0, then 0.0 is returned as the value of the function.

For SNRM2 and SCNRM2, the sum of the squares of the absolute values of the elements is accumulated in long precision. The square root of this long-precision sum is then computed and, if necessary, is unscaled.

Although these subroutines eliminate destructive underflow, nondestructive underflows may occur if the input elements differ greatly in magnitude. This does not affect accuracy, but it degrades performance. The system default is to mask underflow, which improves the performance of these subroutines.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

### Important Information About the Following Examples

Workstations use workstation architecture precisions: ANSI/IEEE 32-bit and 64-bit binary floating-point format. The ranges are:

- For short-precision:  $3.37 \times 10^{-38}$  to  $3.37 \times 10^{38}$
- For long-precision:  $1.67 \times 10^{-308}$  to  $1.67 \times 10^{308}$

## Examples

### Example 1

This example shows a vector,  $x$ , whose elements must be scaled to prevent overflow.

#### Function Reference and Input:

```

      N   X   INCX
      |   |   |
DNORM = DNRM2( 6 , X , 1 )

```

```

X      = (0.68056D+200, 0.25521D+200, 0.34028D+200,
          0.85071D+200, 0.25521D+200, 0.85071D+200)

```

#### Output:

```

DNORM   = 0.1469D+201

```

### Example 2

This example shows a vector,  $x$ , whose elements must be scaled to prevent destructive underflow.

#### Function Reference and Input:

## SNRM2, DNRM2, SCNRM2, and DZNRM2

$$\text{DNORM} = \text{DNRM2} \left( \begin{array}{c} N \\ | \\ 4 \end{array}, \begin{array}{c} X \\ | \\ X \end{array}, \begin{array}{c} \text{INCX} \\ | \\ 2 \end{array} \right)$$
$$X = (0.10795\text{D}-200, \dots, 0.10795\text{D}-200, \dots, 0.10795\text{D}-200, \dots, 0.10795\text{D}-200)$$

### Output:

$$\text{DNORM} = 0.21590\text{D}-200$$

### Example 3

This example shows a vector,  $x$ , with a stride of 0. The result in SNORM is:

$$\sqrt{nx_1^2}$$

### Function Reference and Input:

$$\text{SNORM} = \text{SNRM2} \left( \begin{array}{c} N \\ | \\ 4 \end{array}, \begin{array}{c} X \\ | \\ X \end{array}, \begin{array}{c} \text{INCX} \\ | \\ 0 \end{array} \right)$$
$$X = (4.0)$$

### Output:

$$\text{SNORM} = 8.0$$

### Example 4

This example shows a vector,  $x$ , containing complex numbers, and whose elements must be scaled to prevent overflow.

### Function Reference and Input:

$$\text{DZNORM} = \text{DZNRM2} \left( \begin{array}{c} N \\ | \\ 3 \end{array}, \begin{array}{c} X \\ | \\ X \end{array}, \begin{array}{c} \text{INCX} \\ | \\ 1 \end{array} \right)$$
$$X = ((0.68056\text{D}+200, 0.25521\text{D}+200), (0.34028\text{D}+200, 0.85071\text{D}+200), (0.25521\text{D}+200, 0.85071\text{D}+200))$$

### Output:

$$\text{DZNORM} = 0.1469\text{D}+201$$

### Example 5

This example shows a vector,  $x$ , containing complex numbers, and whose elements must be scaled to prevent destructive underflow.

### Function Reference and Input:

$$\text{DZNORM} = \text{DZNRM2} \left( \begin{array}{c} N \\ | \\ 2 \end{array}, \begin{array}{c} X \\ | \\ X \end{array}, \begin{array}{c} \text{INCX} \\ | \\ 2 \end{array} \right)$$
$$X = ((0.10795\text{D}-200, 0.10795\text{D}-200), \dots, (0.10795\text{D}-200, 0.10795\text{D}-200))$$

### Output:

$$\text{DZNORM} = 0.2159\text{D}-200$$

## SNORM2, DNORM2, CNORM2, and ZNORM2 — Euclidean Length of a Vector with No Scaling of Input

### Purpose

These subprograms compute the euclidean length ( $l_2$  norm) of vector  $x$  with no scaling of input.

Table 54. Data Types

$x$	Result	Subprogram
Short-precision real	Short-precision real	SNORM2
Long-precision real	Long-precision real	DNORM2
Short-precision complex	Short-precision real	CNORM2
Long-precision complex	Long-precision real	ZNORM2

### Syntax

<b>Fortran</b>	SNORM2   DNORM2   CNORM2   ZNORM2 ( $n, x, incx$ )
<b>C and C++</b>	snorm2   dnorm2   cnorm2   znorm2 ( $n, x, incx$ );

### On Entry

- $n$  is the number of elements in vector  $x$ . Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ , whose euclidean length is to be computed.  
Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 54.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.

### On Return

- Function value* is the euclidean length ( $l_2$  norm) of the vector  $x$ . Returned as: a number of the data type indicated in Table 54.

### Notes

- This subroutine does not underflow or overflow if the values of the elements in vector  $x$  conform to the following conditions. If these conditions are violated, overflow or destructive underflow may occur:
  - For short-precision numbers:  
Any valid short-precision number.
  - For long-precision numbers:  
 $|x_i| = 0$  or  $0.10010E-145 < |x_i| < 0.13408E+155$  for  $i = 1, n$
- Declare this function in your program as returning a value of the data type indicated in Table 54.

## Function

The euclidean length ( $l_2$  norm) of vector  $x$  is expressed as follows with no scaling of input:

$$\sqrt{|x_1|^2 + |x_2|^2 + \dots + |x_n|^2}$$

See reference [82]. The result is returned as the function value. If  $n$  is 0, then 0.0 is returned as the value of the function.

For SNORM2 and CNORM2, the sum of the squares of the absolute values of the elements is accumulated in long-precision. The square root of this long-precision sum is then computed.

This subroutine should not be used if the values in vector  $x$  do not conform to the restriction given in "Notes" on page 237.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows a vector,  $x$ , with a stride of 1.

#### Function Reference and Input:

```

          N   X   INCX
          |   |   |
SNORM = SNORM2( 6 , X , 1 )
    
```

X = (3.0, 4.0, 1.0, 8.0, 1.0, 3.0)

#### Output:

SNORM = 10.0

### Example 2

This example shows a vector,  $x$ , with a stride greater than 1.

#### Function Reference and Input:

```

          N   X   INCX
          |   |   |
SNORM = SNORM2( 6 , X , 2 )
    
```

X = (3.0, . , 4.0, . , 1.0, . , 8.0, . , 1.0, . , 3.0)

#### Output:

SNORM = 10.0



**Example 3**

This example shows a vector,  $x$ , with a stride of 0. The result in SNORM is:

$$\sqrt{nx_1^2}$$

**Function Reference and Input:**

```

          N  X  INCX
          |  |  |
SNORM = SNORM2( 4 , X , 0 )

```

X = (4.0)

**Output:**

SNORM = 8.0

**Example 4**

This example shows a vector,  $x$ , containing complex numbers and having a stride of 1.

**Function Reference and Input:**

```

          N  X  INCX
          |  |  |
CNORM = CNORM2( 3 , X , 1 )

```

X = ((3.0, 4.0), (1.0, 8.0), (-1.0, 3.0))

**Output:**

CNORM = 10.0

## SROTG, DROTG, CROTG, and ZROTG — Construct a Givens Plane Rotation

### Purpose

SROTG and DROTG construct a real Givens plane rotation, and CROTG and ZROTG construct a complex Givens plane rotation. The computations use rotational elimination parameters  $a$  and  $b$ . Values are returned for  $r$ , as well as the cosine  $c$  and the sine  $s$  of the angle of rotation. SROTG and DROTG also return a value for  $z$ .

**Note:** Throughout this description, the symbols  $r$  and  $z$  are used to represent two of the output values returned for this computation. It is important to note that the values for  $r$  and  $z$  are actually returned in the input-output arguments  $a$  and  $b$ , respectively, overwriting the original values passed in  $a$  and  $b$ .

Table 55. Data Types

$a, b, r, s$	$c$	$z$	Subprogram
Short-precision real	Short-precision real	Short-precision real	SROTG
Long-precision real	Long-precision real	Long-precision real	DROTG
Short-precision complex	Short-precision real	(No value returned)	CROTG
Long-precision complex	Long-precision real	(No value returned)	ZROTG

### Syntax

Fortran	CALL SROTG   DROTG   CROTG   ZROTG ( $a, b, c, s$ )
C and C++	srotg   drotg   crotg   zrotg ( $a, b, c, s$ );

### On Entry

- $a$  is the rotational elimination parameter  $a$ .  
Specified as: a number of the data type indicated in Table 55.
- $b$  is the rotational elimination parameter  $b$ .  
Specified as: a number of the data type indicated in Table 55.
- $c$  See "On Return."
- $s$  See "On Return."

### On Return

- $a$  is the value computed for  $r$ .  
For SROTG and DROTG:

$$r = \sigma \sqrt{a^2 + b^2}$$

where:

$$\begin{aligned} \sigma &= \text{SIGN}(a) \text{ if } |a| > |b| \\ \sigma &= \text{SIGN}(b) \text{ if } |a| \leq |b| \end{aligned}$$

For CROTG and ZROTG:

$$r = \psi \sqrt{|a|^2 + |b|^2} \quad \text{if } |a| \neq 0$$

$$r = b \quad \text{if } |a| = 0$$

where:

$$\psi = a / |a|$$

Returned as: a number of the data type indicated in Table 55 on page 240.

*b* is the value computed for *z*.

For SROTG and DROTG:

$$\begin{aligned} z &= s && \text{if } |a| > |b| \\ z &= 1/c && \text{if } |a| \leq |b| \text{ and } c \neq 0 \text{ and } r \neq 0 \\ z &= 1 && \text{if } |a| \leq |b| \text{ and } c = 0 \text{ and } r \neq 0 \\ z &= 0 && \text{if } r = 0 \end{aligned}$$

For CROTG and ZROTG: no value is returned, and the input value is not changed.

Returned as: a number of the data type indicated in Table 55 on page 240.

*c* is the cosine *c* of the angle of (Givens) rotation. For SROTG and DROTG:

$$\begin{aligned} c &= a/r && \text{if } r \neq 0 \\ c &= 1 && \text{if } r = 0 \end{aligned}$$

For CROTG and ZROTG:

$$c = \frac{|a|}{\sqrt{|a|^2 + |b|^2}} \quad \text{if } |a| \neq 0$$

$$c = 0 \quad \text{if } |a| = 0$$

Returned as: a number of the data type indicated in Table 55 on page 240.

*s* is the sine *s* of the angle of (Givens) rotation.

For SROTG and DROTG:

$$\begin{aligned} s &= b/r && \text{if } r \neq 0 \\ s &= 0 && \text{if } r = 0 \end{aligned}$$

## SROTG, DROTG, CROTG, and ZROTG

For CROTG and ZROTG:

$$s = \frac{\psi \bar{b}}{\sqrt{|a|^2 + |b|^2}} \quad \text{if } |a| \neq 0$$

$$s = (1.0, 0.0) \quad \text{if } |a| = 0$$

where  $\psi = a / |a|$

Returned as: a number of the data type indicated in Table 55 on page 240.

### Notes

In your C program, arguments  $a$ ,  $b$ ,  $c$ , and  $s$  must be passed by reference.

### Function

#### SROTG and DROTG

A real Givens plane rotation is constructed for values  $a$  and  $b$  by computing values for  $r$ ,  $c$ ,  $s$ , and  $z$ , where:

$$r = \sigma \sqrt{a^2 + b^2}$$

where:

$$\sigma = \text{SIGN}(a) \quad \text{if } |a| > |b|$$

$$\sigma = \text{SIGN}(b) \quad \text{if } |a| \leq |b|$$

$$c = a/r \quad \text{if } r \neq 0$$

$$c = 1 \quad \text{if } r = 0$$

$$s = b/r \quad \text{if } r \neq 0$$

$$s = 0 \quad \text{if } r = 0$$

$$z = s \quad \text{if } |a| > |b|$$

$$z = 1/c \quad \text{if } |a| \leq |b| \text{ and } c \neq 0 \text{ and } r \neq 0$$

$$z = 1 \quad \text{if } |a| \leq |b| \text{ and } c = 0 \text{ and } r \neq 0$$

$$z = 0 \quad \text{if } r = 0$$

See reference [82].

Following are some important points about the computation:

1. The numbers for  $c$ ,  $s$ , and  $r$  satisfy:

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

2. Where necessary, scaling is used to avoid overflow and destructive underflow in the computation of  $r$ , which is expressed as follows:

$$r = \sigma(|a|+|b|) \sqrt{\left(\frac{a}{|a|+|b|}\right)^2 + \left(\frac{b}{|a|+|b|}\right)^2}$$

3.  $\sigma$  is not essential to the computation of a Givens rotation matrix, but its use permits later stable reconstruction of  $c$  and  $s$  from just one stored number,  $z$ . See reference [95].  $c$  and  $s$  are reconstructed from  $z$  as follows:

For  $z = 1$ ,  $c = 0$  and  $s = 1$

For  $|z| < 1$ ,  $c = \sqrt{1-z^2}$  and  $s = z$

For  $|z| > 1$ ,  $c = 1/z$  and  $s = \sqrt{1-c^2}$

### CROTG and ZROTG

A complex Givens plane rotation is constructed for values  $a$  and  $b$  by computing values for  $r$ ,  $c$ , and  $s$ , where:

$$r = \psi \sqrt{|a|^2 + |b|^2} \quad \text{if } |a| \neq 0$$

$$r = b \quad \text{if } |a| = 0$$

where:

$$\psi = a/|a|$$

$$c = \frac{|a|}{\sqrt{|a|^2 + |b|^2}} \quad \text{if } |a| \neq 0$$

$$c = 0 \quad \text{if } |a| = 0$$

## SROTG, DROTG, CROTG, and ZROTG

$$s = \frac{\psi \bar{b}}{\sqrt{|a|^2 + |b|^2}} \quad \text{if } |a| \neq 0$$

$$s = (1.0, 0.0) \quad \text{if } |a| = 0$$

See reference [82].

Following are some important points about the computation:

1. The numbers for  $c$ ,  $s$ , and  $r$  satisfy:

$$\begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

2. Where necessary, scaling is used to avoid overflow and destructive underflow in the computation of  $r$ , which is expressed as follows:

$$r = \psi (|a| + |b|) \sqrt{\left| \frac{a}{|a| + |b|} \right|^2 + \left| \frac{b}{|a| + |b|} \right|^2}$$

## Error conditions

### Computational Errors

None

### Input-Argument Errors

None

## Examples

### Example 1

This example shows the construction of a real Givens plane rotation, where  $r$  is 0.

#### Call Statement and Input:

```
CALL SROTG( A , B , C , S )
           |   |   |   |
           0.0 , 0.0 , C , S )
```

#### Output:

```
A      = 0.0
B      = 0.0
C      = 1.0
S      = 0.0
```

### Example 2

This example shows the construction of a real Givens plane rotation, where  $c$  is 0.

#### Call Statement and Input:

```

      A   B   C   S
      |   |   |   |
CALL SROTG( 0.0 , 2.0 , C , S )

```

**Output:**

```

A      = 2.0
B      = 1.0
C      = 0.0
S      = 1.0

```

**Example 3**

This example shows the construction of a real Givens plane rotation, where  $|b| > |a|$ .

**Call Statement and Input:**

```

      A   B   C   S
      |   |   |   |
CALL SROTG( 6.0 , -8.0 , C , S )

```

**Output:**

```

A      = -10.0
B      = -1.666̄
C      = -0.6
S      = 0.8

```

**Example 4**

This example shows the construction of a real Givens plane rotation, where  $|a| > |b|$ .

**Call Statement and Input:**

```

      A   B   C   S
      |   |   |   |
CALL SROTG( 8.0 , 6.0 , C , S )

```

**Output:**

```

A      = 10.0
B      = 0.6
C      = 0.8
S      = 0.6

```

**Example 5**

This example shows the construction of a complex Givens plane rotation, where  $|a| = 0$ .

**Call Statement and Input:**

```

      A   B   C   S
      |   |   |   |
CALL CROTG( A , B , C , S )

```

```

A      = (0.0, 0.0)
B      = (1.0, 0.0)

```

**Output:**

```

A      = (1.0, 0.0)
C      = 0.0
S      = (1.0, 0.0)

```

## SROTG, DROTG, CROTG, and ZROTG

### Example 6

This example shows the construction of a complex Givens plane rotation, where  $|a| \neq 0$ .

#### Call Statement and Input:

```
          A  B  C  S
          |  |  |  |
CALL CROTG( A , B , C , S )
```

```
A      = (3.0, 4.0)
B      = (4.0, 6.0)
```

#### Output:

```
A      = (5.26, 7.02)
C      = 0.57
S      = (0.82, -0.05)
```



## SROT, DROT, CROT, ZROT, CSROT, and ZDROT — Apply a Plane Rotation

### Purpose

SROT and DROT apply a real plane rotation to real vectors; CROT and ZROT apply a complex plane rotation to complex vectors; and CSROT and ZDROT apply a real plane rotation to complex vectors. The plane rotation is applied to  $n$  points, where the points to be rotated are contained in vectors  $x$  and  $y$ , and where the cosine and sine of the angle of rotation are  $c$  and  $s$ , respectively.

Table 56. Data Types

$x, y$	$c$	$s$	Subprogram
Short-precision real	Short-precision real	Short-precision real	SROT
Long-precision real	Long-precision real	Long-precision real	DROT
Short-precision complex	Short-precision real	Short-precision complex	CROT
Long-precision complex	Long-precision real	Long-precision complex	ZROT
Short-precision complex	Short-precision real	Short-precision real	CSROT
Long-precision complex	Long-precision real	Long-precision real	ZDROT

### Syntax

Fortran	CALL SROT   DROT   CROT   ZROT   CSROT   ZDROT ( $n, x, incx, y, incy, c, s$ )
C and C++	srot   drot   crot   zrot   csrot   zdrot ( $n, x, incx, y, incy, c, s$ );

### On Entry

- $n$  is the number of points to be rotated—that is, the number of elements in vectors  $x$  and  $y$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ , containing the  $x_i$  coordinates of the points to be rotated.  
Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 56.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  is the vector  $y$  of length  $n$ , containing the  $y_i$  coordinates of the points to be rotated.  
Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 56.
- $incy$  is the stride for vector  $y$ .  
Specified as: a fullword integer. It can have any value.
- $c$  the cosine,  $c$ , of the angle of rotation.  
Specified as: a number of the data type indicated in Table 56.

## SROT, DROT, CROT, ZROT, CSROT, ZDROT

$s$  the sine,  $s$ , of the angle of rotation.  
Specified as: a number of the data type indicated in Table 56 on page 247.

### On Return

$x$  is the vector  $x$  of length  $n$ , containing the rotated  $x_i$  coordinates, where:

$$x_i \leftarrow cx_i + sy_i \quad \text{for } i = 1, n$$

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 56 on page 247.

$y$  is the vector  $y$  of length  $n$ , containing the rotated  $y_i$  coordinates, where:

For SROT, DROT, CSROT, and ZDROT:

$$y_i \leftarrow -sx_i + cy_i \quad \text{for } i = 1, n$$

For CROT and ZROT:

$$y_i \leftarrow -\bar{s}x_i + cy_i \quad \text{for } i = 1, n$$

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 56 on page 247.

## Notes

The vectors  $x$  and  $y$  must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.

## Function

Applying a plane rotation to  $n$  points, where the points to be rotated are contained in vectors  $x$  and  $y$ , is expressed as follows, where  $c$  and  $s$  are the cosine and sine of the angle of rotation, respectively. For SROT, DROT, CSROT, and ZDROT:

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} \leftarrow \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} \quad \text{for } i = 1, n$$

For CROT and ZROT:

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} \leftarrow \begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} \quad \text{for } i = 1, n$$

See references [59] and [82]. No computation is performed if  $n$  is 0 or if  $c$  is 1.0 and  $s$  is zero. For SROT, CROT, and CSROT, intermediate results are accumulated in long precision.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows how to apply a real plane rotation to real vectors  $x$  and  $y$  having positive strides.

#### Call Statement and Input:

```

      N   X   INCX  Y   INCY   C   S
      |   |   |    |   |    |   |
CALL SROT( 5 , X , 1 , Y , 2 , 0.5 , S )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (-1.0, . , -2.0, . , -3.0, . , -4.0, . , -5.0)

```

$$S = \frac{\sqrt{3.0}}{2.0}$$

#### Output:

```

X      = (-0.366, -0.732, -1.098, -1.464, -1.830)
Y      = (-1.366, -2.732, -4.098, -5.464, -6.830)

```

### Example 2

This example shows how to apply a real plane rotation to real vectors  $x$  and  $y$  having strides of opposite sign.

#### Call Statement and Input:

```

      N   X   INCX  Y   INCY   C   S
      |   |   |    |   |    |   |
CALL SROT( 5 , X , 1 , Y , -1 , 0.5 , S )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (-5.0, -4.0, -3.0, -2.0, -1.0)

```

$$S = \frac{\sqrt{3.0}}{2.0}$$

#### Output:

```

X      =(same as output X in Example 1)
Y      = (-6.830, -5.464, -4.098, -2.732, -1.366)

```

### Example 3

This example shows how scalar values in vectors  $x$  and  $y$  can be processed by specifying 0 strides and the number of elements to be processed,  $n$ , equal to 1.

## SROT, DROT, CROT, ZROT, CSROT, ZDROT

### Call Statement and Input:

```
          N  X  INCX  Y  INCY  C  S
          |  |  |     |  |     |  |
CALL SROT( 1 , X , 0 , Y , 0 , 0.5 , S )
```

```
X      = (1.0)
Y      = (-1.0)
```

$$S = \frac{\sqrt{3.0}}{2.0}$$

### Output:

```
X      = (-0.366)
Y      = (-1.366)
```

### Example 4

This example shows how to apply a complex plane rotation to complex vectors  $x$  and  $y$  having positive strides.

### Call Statement and Input:

```
          N  X  INCX  Y  INCY  C  S
          |  |  |     |  |     |  |
CALL CROT( 3 , X , 1 , Y , 2 , 0.5 , S )
```

```
X      = ((1.0, 2.0), (2.0, 3.0), (3.0, 4.0))
Y      = ((-1.0, 5.0), . , (-2.0, 4.0), . , (-3.0, 3.0))
S      = (0.75, 0.50)
```

### Output:

```
X      = ((-2.750, 4.250), (-2.500, 3.500), (-2.250, 2.750))
Y      = ((-2.250, 1.500), . , (-4.000, 0.750), . ,
          (-5.750, 0.000))
```

### Example 5

This example shows how to apply a real plane rotation to complex vectors  $x$  and  $y$  having positive strides.

### Call Statement and Input:

```
          N  X  INCX  Y  INCY  C  S
          |  |  |     |  |     |  |
CALL CSROT( 3 , X , 1 , Y , 2 , 0.5 , S )
```

```
X      = ((1.0, 2.0), (2.0, 3.0), (3.0, 4.0))
Y      = ((-1.0, 5.0), . , (-2.0, 4.0), . , (-3.0, 3.0))
```

$$S = \frac{\sqrt{3.0}}{2.0}$$

### Output:

```
X      = ((-0.366, 5.330), (-0.732, 4.964), (-1.098, 4.598))
Y      = ((-1.366, 0.768), . , (-2.732, -0.598), . ,
          (-4.098, -1.964))
```

## SSCAL, DSCAL, CSCAL, ZSCAL, CSSCAL, and ZDSCAL — Multiply a Vector X by a Scalar and Store in the Vector X

### Purpose

These subprograms perform the following computation, using the scalar  $\alpha$  and the vector  $x$ :

$$x \leftarrow \alpha x$$

Table 57. Data Types

$\alpha$	$x$	Subprogram
Short-precision real	Short-precision real	SSCAL
Long-precision real	Long-precision real	DSCAL
Short-precision complex	Short-precision complex	CSCAL
Long-precision complex	Long-precision complex	ZSCAL
Short-precision real	Short-precision complex	CSSCAL
Long-precision real	Long-precision complex	ZDSCAL

### Syntax

<b>Fortran</b>	CALL SSCAL   DSCAL   CSCAL   ZSCAL   CSSCAL   ZDSCAL ( $n$ , $alpha$ , $x$ , $incx$ )
<b>C and C++</b>	sscal   dscal   cscal   zscal   csscal   zdscal ( $n$ , $alpha$ , $x$ , $incx$ );

#### On Entry

- $n$  is the number of elements in vector  $x$ . Specified as: a fullword integer;  $n \geq 0$ .
- $alpha$  is the scalar  $\alpha$ .  
Specified as: a number of the data type indicated in Table 57.
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 57.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.

#### On Return

- $x$  is the vector  $x$  of length  $n$ , containing the result of the computation  $\alpha x$ . Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 57.

### Notes

The fastest way in ESSL to zero out contiguous (stride 1) arrays is to call SSCAL or DSCAL, specifying  $incx = 1$  and  $\alpha = 0$ .

### Function

The computation is expressed as follows:

$$\begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \leftarrow \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

See reference [82]. If  $n$  is 0, no computation is performed. For CSCAL, intermediate results are accumulated in long precision.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows a vector,  $x$ , with a stride of 1.

#### Call Statement and Input:

```

          N ALPHA X INCX
          |   |   |   |
CALL SSSCAL( 5 , 2.0 , X , 1 )

```

$X = (1.0, 2.0, 3.0, 4.0, 5.0)$

#### Output:

$X = (2.0, 4.0, 6.0, 8.0, 10.0)$

### Example 2

This example shows vector,  $x$ , with a stride greater than 1.

#### Call Statement and Input:

```

          N ALPHA X INCX
          |   |   |   |
CALL SSSCAL( 5 , 2.0 , X , 2 )

```

$X = (1.0, . , 2.0, . , 3.0, . , 4.0, . , 5.0)$

#### Output:

$X = (2.0, . , 4.0, . , 6.0, . , 8.0, . , 10.0)$

### Example 3

This example illustrates that when the strides for two similar computations (Example 1 and Example 3) have the same absolute value but have opposite signs, the output is the same. This example is the same as Example 1, except the stride for  $x$  is negative ( $-1$ ). For performance reasons, it is better to specify the positive stride. For  $x$ , processing begins at element  $X(5)$ , which is 5.0, and results are stored beginning at the same element.

#### Call Statement and Input:

```

          N ALPHA X INCX
          |   |   |   |
CALL SSCAL( 5 , 2.0 , X , -1 )

X      = (1.0, 2.0, 3.0, 4.0, 5.0)

```

**Output:**

```
X      = (2.0, 4.0, 6.0, 8.0, 10.0)
```

**Example 4**

This example shows how SSCAL can be used to compute a scalar value. In this case, input vector  $x$  contains a scalar value, and the stride is 0. The number of elements to be processed,  $n$ , is 1.

**Call Statement and Input:**

```

          N ALPHA X INCX
          |   |   |   |
CALL SSCAL( 1 , 2.0 , X , 0 )

X      = (1.0)

```

**Output:**

```
X      = (2.0)
```

**Example 5**

This example shows a scalar,  $\alpha$ , and a vector,  $x$ , containing complex numbers, where vector  $x$  has a stride of 1.

**Call Statement and Input:**

```

          N ALPHA X INCX
          |   |   |   |
CALL CSCAL( 3 ,ALPHA, X , 1 )

ALPHA  = (2.0, 3.0)
X      = ((1.0, 2.0), (2.0, 0.0), (3.0, 5.0))

```

**Output:**

```
X      = ((-4.0, 7.0), (4.0, 6.0), (-9.0, 19.0))
```

**Example 6**

This example shows a scalar,  $\alpha$ , containing a real number, and a vector,  $x$ , containing complex numbers, where vector  $x$  has a stride of 1.

**Call Statement and Input:**

```

          N ALPHA X INCX
          |   |   |   |
CALL CSSCAL( 3 , 2.0 , X , 1 )

X      = ((1.0, 2.0), (2.0, 0.0), (3.0, 5.0))

```

**Output:**

```
X      = ((2.0, 4.0), (4.0, 0.0), (6.0, 10.0))
```

## SSWAP, DSWAP, CSWAP, and ZSWAP — Interchange the Elements of Two Vectors

### Purpose

These subprograms interchange the elements of vectors  $x$  and  $y$ :

$$y \leftrightarrow x$$

Table 58. Data Types

$x, y$	Subprogram
Short-precision real	SSWAP
Long-precision real	DSWAP
Short-precision complex	CSWAP
Long-precision complex	ZSWAP

### Syntax

Fortran	CALL SSWAP   DSWAP   CSWAP   ZSWAP ( $n, x, incx, y, incy$ )
C and C++	sswap   dswap   cswap   zswap ( $n, x, incx, y, incy$ );

### On Entry

- $n$  is the number of elements in vectors  $x$  and  $y$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 58.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  is the vector  $y$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 58.
- $incy$  is the stride for vector  $y$ .  
Specified as: a fullword integer. It can have any value.

### On Return

- $x$  is the vector  $x$  of length  $n$ , containing the elements that were swapped from vector  $y$ . Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 58.
- $y$  is the vector  $y$  of length  $n$ , containing the elements that were swapped from vector  $x$ . Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 58.

### Notes

1. If you specify the same vector for  $x$  and  $y$ , then  $incx$  and  $incy$  must be equal; otherwise, results are unpredictable.



2. If you specify different vectors for  $x$  and  $y$ , they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.

## Function

The elements of vectors  $x$  and  $y$  are interchanged as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftrightarrow \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

See reference [82]. If  $n$  is 0, no elements are interchanged.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows vectors  $x$  and  $y$  with positive strides.

#### Call Statement and Input:

```

          N   X   INCX  Y   INCY
          |   |   |     |   |
CALL SSWAP( 5 , X , 1 , Y , 2 )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (-1.0, . , -2.0, . , -3.0, . , -4.0, . , -5.0)

```

#### Output:

```

X      = (-1.0, -2.0, -3.0, -4.0, -5.0)
Y      = (1.0, . , 2.0, . , 3.0, . , 4.0, . , 5.0)

```

### Example 2

This example shows how to obtain output vectors  $x$  and  $y$  that are reverse copies of the input vectors  $y$  and  $x$ . You must specify strides with the same absolute value, but with opposite signs. For  $y$ , which has negative stride, processing begins at element  $Y(5)$ , which is  $-5.0$ , and the results of the swap are stored beginning at the same element.

#### Call Statement and Input:

```

          N   X   INCX  Y   INCY
          |   |   |     |   |
CALL SSWAP( 5 , X , 1 , Y , -1 )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (-1.0, -2.0, -3.0, -4.0, -5.0)

```

#### Output:

## SSWAP, DSWAP, CSWAP, and ZSWAP

```
X      = (-5.0, -4.0, -3.0, -2.0, -1.0)
Y      = (5.0, 4.0, 3.0, 2.0, 1.0)
```

### Example 3

This example shows how SSWAP can be used to interchange scalar values in vectors  $x$  and  $y$  by specifying 0 strides and the number of elements to be processed as 1.

#### Call Statement and Input:

```
          N  X  INCX  Y  INCY
          |  |  |     |  |
CALL SSWAP( 1 , X , 0 , Y , 0 )
```

```
X      = (1.0)
Y      = (-4.0)
```

#### Output:

```
X      = (-4.0)
Y      = (1.0)
```

### Example 4

This example shows vectors  $x$  and  $y$ , containing complex numbers and having positive strides.

#### Call Statement and Input:

```
          N  X  INCX  Y  INCY
          |  |  |     |  |
CALL CSWAP( 4 , X , 1 , Y , 2 )
```

```
X      = ((1.0, 6.0), (2.0, 7.0), (3.0, 8.0), (4.0, 9.0))
Y      = ((-1.0, -1.0), . . , (-2.0, -2.0), . . , (-3.0, -3.0), . . ,
          (-4.0, -4.0))
```

#### Output:

```
X      = ((-1.0, -1.0), (-2.0, -2.0), (-3.0, -3.0), (-4.0, -4.0))
Y      = ((1.0, 6.0), . . , (2.0, 7.0), . . , (3.0, 8.0), . . ,
          (4.0, 9.0))
```

## SVEA, DVEA, CVEA, and ZVEA — Add a Vector X to a Vector Y and Store in a Vector Z

### Purpose

These subprograms perform the following computation, using vectors  $x$ ,  $y$ , and  $z$ :

$$z \leftarrow x + y$$

Table 59. Data Types

$x, y, z$	Subprogram
Short-precision real	SVEA
Long-precision real	DVEA
Short-precision complex	CVEA
Long-precision complex	ZVEA

### Syntax

<b>Fortran</b>	CALL SVEA   DVEA   CVEA   ZVEA ( $n, x, incx, y, incy, z, incz$ )
<b>C and C++</b>	svea   dvea   cvea   zvea ( $n, x, incx, y, incy, z, incz$ );

### On Entry

- $n$  is the number of elements in vectors  $x$ ,  $y$ , and  $z$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 59.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  is the vector  $y$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 59.
- $incy$  is the stride for vector  $y$ .  
Specified as: a fullword integer. It can have any value.
- $z$  See "On Return."
- $incz$  is the stride for vector  $z$ .  
Specified as: a fullword integer. It can have any value.

### On Return

- $z$  is the vector  $z$  of length  $n$ , containing the result of the computation. Returned as: a one-dimensional array of (at least) length  $1+(n-1)|incz|$ , containing numbers of the data type indicated in Table 59.

## Notes

1. If you specify the same vector for  $x$  and  $z$ , then  $incx$  and  $incz$  must be equal; otherwise, results are unpredictable. The same is true for  $y$  and  $z$ .
2. If you specify different vectors for  $x$  and  $z$ , they must have no common elements; otherwise, results are unpredictable. The same is true for  $y$  and  $z$ . See “Concepts” on page 59.

## Function

The computation is expressed as follows:

$$\begin{bmatrix} z_1 \\ \cdot \\ \cdot \\ \cdot \\ z_n \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} + \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix}$$

If  $n$  is 0, no computation is performed.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows vectors  $x$ ,  $y$ , and  $z$ , with positive strides.

#### Call Statement and Input:

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |    |  |    |  |
CALL SVEA( 5 , X , 1  , Y , 2  , Z , 1  )
    
```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (1.0, . , 1.0, . , 1.0, . , 1.0, . , 1.0)
    
```

#### Output:

```

Z      = (2.0, 3.0, 4.0, 5.0, 6.0)
    
```

### Example 2

This example shows vectors  $x$  and  $y$  having strides of opposite sign, and an output vector  $z$  having a positive stride. For  $y$ , which has negative stride, processing begins at element  $Y(5)$ , which is 1.0.

#### Call Statement and Input:

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |    |  |    |  |
CALL SVEA( 5 , X , 1  , Y , -1 , Z , 2  )
    
```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (5.0, 4.0, 3.0, 2.0, 1.0)
    
```

**Output:**

Z = (2.0, . , 4.0, . , 6.0, . , 8.0, . , 10.0)

**Example 3**

This example shows a vector,  $x$ , with 0 stride and a vector,  $z$ , with negative stride.  $x$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $x$ . For vector  $z$ , results are stored beginning in element Z(5).

**Call Statement and Input:**

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVEA( 5 , X , 0  , Y , 1  , Z , -1 )

```

X = (1.0)  
Y = (5.0, 4.0, 3.0, 2.0, 1.0)

**Output:**

Z = (2.0, 3.0, 4.0, 5.0, 6.0)

**Example 4**

This example shows a vector,  $y$ , with 0 stride.  $y$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $y$ .

**Call Statement and Input:**

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVEA( 5 , X , 1  , Y , 0  , Z , 1 )

```

X = (1.0, 2.0, 3.0, 4.0, 5.0)  
Y = (5.0)

**Output:**

Z = (6.0, 7.0, 8.0, 9.0, 10.0)

**Example 5**

This example shows the output vector,  $z$ , with 0 stride, where the vector  $x$  has positive stride, and the vector  $y$  has 0 stride. The number of elements to be processed,  $n$ , is greater than 1.

**Call Statement and Input:**

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVEA( 5 , X , 1  , Y , 0  , Z , 0 )

```

X = (1.0, 2.0, 3.0, 4.0, 5.0)  
Y = (5.0)

**Output:**

Z = (10.0)

**Example 6**

This example shows the output vector  $z$ , with 0 stride, where the vector  $x$  has 0 stride, and the vector  $y$  has negative stride. The number of elements to be processed,  $n$ , is greater than 1.

**Call Statement and Input:**

## SVEA, DVEA, CVEA, and ZVEA

```
          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVEA( 5 , X , 0  , Y , -1 , Z , 0  )
```

```
X          = (1.0)
Y          = (5.0, 4.0, 3.0, 2.0, 1.0)
```

### Output:

```
Z          = (6.0)
```

### Example 7

This example shows how SVEA can be used to compute a scalar value. In this case, vectors  $x$  and  $y$  contain scalar values. The strides of all vectors,  $x$ ,  $y$ , and  $z$ , are 0. The number of elements to be processed,  $n$ , is 1.

### Call Statement and Input:

```
          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVEA( 1 , X , 0  , Y , 0  , Z , 0  )
```

```
X          = (1.0)
Y          = (5.0)
```

### Output:

```
Z          = (6.0)
```

### Example 8

This example shows vectors  $x$  and  $y$ , containing complex numbers and having positive strides.

### Call Statement and Input:

```
          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL CVEA( 3 , X , 1  , Y , 2  , Z , 1  )
```

```
X          = ((1.0, 2.0), (3.0, 4.0), (5.0, 6.0))
Y          = ((7.0, 8.0), . , (9.0, 10.0), . , (11.0, 12.0))
```

### Output:

```
Z          = ((8.0, 10.0), (12.0, 14.0), (16.0, 18.0))
```

## SVES, DVES, CVES, and ZVES — Subtract a Vector Y from a Vector X and Store in a Vector Z

### Purpose

These subprograms perform the following computation, using vectors  $x$ ,  $y$ , and  $z$ :

$$z \leftarrow x - y$$

Table 60. Data Types

$x, y, z$	Subprogram
Short-precision real	SVES
Long-precision real	DVES
Short-precision complex	CVES
Long-precision complex	ZVES

### Syntax

<b>Fortran</b>	CALL SVES   DVES   CVES   ZVES ( $n, x, incx, y, incy, z, incz$ )
<b>C and C++</b>	sves   dves   cves   zves ( $n, x, incx, y, incy, z, incz$ );

### On Entry

- $n$  is the number of elements in vectors  $x$ ,  $y$ , and  $z$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 60.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  is the vector  $y$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 60.
- $incy$  is the stride for vector  $y$ .  
Specified as: a fullword integer. It can have any value.
- $z$  See On Return.
- $incz$  is the stride for vector  $z$ .  
Specified as: a fullword integer. It can have any value.

### On Return

- $z$  is the vector  $z$  of length  $n$ , containing the result of the computation. Returned as: a one-dimensional array of (at least) length  $1+(n-1)|incz|$ , containing numbers of the data type indicated in Table 60.

## Notes

1. If you specify the same vector for  $x$  and  $z$ , then  $incx$  and  $incz$  must be equal; otherwise, results are unpredictable. The same is true for  $y$  and  $z$ .
2. If you specify different vectors for  $x$  and  $z$ , they must have no common elements; otherwise, results are unpredictable. The same is true for  $y$  and  $z$ . See "Concepts" on page 59.

## Function

The computation is expressed as follows:

$$\begin{bmatrix} z_1 \\ \cdot \\ \cdot \\ \cdot \\ z_n \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} - \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix}$$

If  $n$  is 0, no computation is performed.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows vectors  $x$ ,  $y$ , and  $z$ , with positive strides.

#### Call Statement and Input:

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |    |  |    |  |
CALL SVES( 5 , X , 1  , Y , 2  , Z , 1  )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (1.0, . , 1.0, . , 1.0, . , 1.0, . , 1.0)

```

#### Output:

```
Z      = (0.0, 1.0, 2.0, 3.0, 4.0)
```

### Example 2

This example shows vectors  $x$  and  $y$  having strides of opposite sign, and an output vector  $z$  having a positive stride. For  $y$ , which has negative stride, processing begins at element  $Y(5)$ , which is 1.0.

#### Call Statement and Input:

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |    |  |    |  |
CALL SVES( 5 , X , 1  , Y , -1 , Z , 2  )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (5.0, 4.0, 3.0, 2.0, 1.0)

```



**Output:**

Z = (0.0, . , 0.0, . , 0.0, . , 0.0, . , 0.0)

**Example 3**

This example shows a vector,  $x$ , with 0 stride, and a vector,  $z$ , with negative stride.  $x$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $x$ . For vector  $z$ , results are stored beginning in element  $Z(5)$ .

**Call Statement and Input:**

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVES( 5 , X , 0  , Y , 1  , Z , -1 )

```

X = (1.0)  
Y = (5.0, 4.0, 3.0, 2.0, 1.0)

**Output:**

Z = (0.0, -1.0, -2.0, -3.0, -4.0)

**Example 4**

This example shows a vector,  $y$ , with 0 stride.  $y$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $y$ .

**Call Statement and Input:**

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVES( 5 , X , 1  , Y , 0  , Z , 1 )

```

X = (1.0, 2.0, 3.0, 4.0, 5.0)  
Y = (5.0)

**Output:**

Z = (-4.0, -3.0, -2.0, -1.0, 0.0)

**Example 5**

This example shows the output vector  $z$ , with 0 stride, where the vector  $x$  has positive stride, and the vector  $y$  has 0 stride. The number of elements to be processed,  $n$ , is greater than 1.

**Call Statement and Input:**

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVES( 5 , X , 1  , Y , 0  , Z , 0 )

```

X = (1.0, 2.0, 3.0, 4.0, 5.0)  
Y = (5.0)

**Output:**

Z = (0.0)

**Example 6**

This example shows the output vector  $z$ , with 0 stride, where the vector  $x$  has 0 stride, and the vector  $y$  has negative stride. The number of elements to be processed,  $n$ , is greater than 1.

**Call Statement and Input:**

## SVES, DVES, CVES, and ZVES

```
          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVES( 5 , X , 0 , Y , -1 , Z , 0 )
```

```
X      = (1.0)
Y      = (5.0, 4.0, 3.0, 2.0, 1.0)
```

### Output:

```
Z      = (-4.0)
```

### Example 7

This example shows how SVES can be used to compute a scalar value. In this case, vectors  $x$  and  $y$  contain scalar values. The strides of all vectors,  $x$ ,  $y$ , and  $z$ , are 0. The number of elements to be processed,  $n$ , is 1.

### Call Statement and Input:

```
          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVES( 1 , X , 0 , Y , 0 , Z , 0 )
```

```
X      = (1.0)
Y      = (5.0)
```

### Output:

```
Z      = (-4.0)
```

### Example 8

This example shows vectors  $x$  and  $y$ , containing complex numbers and having positive strides.

### Call Statement and Input:

```
          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL CVES( 3 , X , 1 , Y , 2 , Z , 1 )
```

```
X      = ((1.0, 2.0), (3.0, 4.0), (5.0, 6.0))
Y      = ((7.0, 8.0), . , (9.0, 10.0), . , (11.0, 12.0))
```

### Output:

```
Z      = ((-6.0, -6.0), (-6.0, -6.0), (-6.0, -6.0))
```

## SVEM, DVEM, CVEM, and ZVEM — Multiply a Vector X by a Vector Y and Store in a Vector Z

### Purpose

These subprograms perform the following computation, using vectors  $x$ ,  $y$ , and  $z$ :

$$z \leftarrow xy$$

Table 61. Data Types

$x, y, z$	Subprogram
Short-precision real	SVEM
Long-precision real	DVEM
Short-precision complex	CVEM
Long-precision complex	ZVEM

### Syntax

Fortran	CALL SVEM   DVEM   CVEM   ZVEM ( $n, x, incx, y, incy, z, incz$ )
C and C++	svem   dvem   cvem   zvem ( $n, x, incx, y, incy, z, incz$ );

### On Entry

$n$  is the number of elements in vectors  $x$ ,  $y$ , and  $z$ .

Specified as: a fullword integer;  $n \geq 0$ .

$x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 61.

$incx$  is the stride for vector  $x$ .

Specified as: a fullword integer. It can have any value.

$y$  is the vector  $y$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 61.

$incy$  is the stride for vector  $y$ .

Specified as: a fullword integer. It can have any value.

$z$  See "On Return."

$incz$  is the stride for vector  $z$ .

Specified as: a fullword integer. It can have any value.

### On Return

$z$  is the vector  $z$  of length  $n$ , containing the result of the computation. Returned as: a one-dimensional array of (at least) length  $1+(n-1)|incz|$ , containing numbers of the data type indicated in Table 61.

## Notes

1. If you specify the same vector for  $x$  and  $z$ , then  $incx$  and  $incz$  must be equal; otherwise, results are unpredictable. The same is true for  $y$  and  $z$ .
2. If you specify different vectors for  $x$  and  $z$ , they must have no common elements; otherwise, results are unpredictable. The same is true for  $y$  and  $z$ . See “Concepts” on page 59.

## Function

The computation is expressed as follows:

$$z_i \leftarrow x_i y_i \quad \text{for } i = 1, n$$

If  $n$  is 0, no computation is performed. For CVEM, intermediate results are accumulated in long precision (short-precision Multiply followed by a long-precision Add), with the final result truncated to short precision.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows vectors  $x$ ,  $y$ , and  $z$ , with positive strides.

#### Call Statement and Input:

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |    |  |    |  |
CALL SVEM( 5 , X , 1  , Y , 2  , Z , 1  )

```

X = (1.0, 2.0, 3.0, 4.0, 5.0)

Y = (1.0, . , 1.0, . , 1.0, . , 1.0, . , 1.0)

#### Output:

Z = (1.0, 2.0, 3.0, 4.0, 5.0)

### Example 2

This example shows vectors  $x$  and  $y$  having strides of opposite sign, and an output vector  $z$  having a positive stride. For  $y$ , which has negative stride, processing begins at element  $Y(5)$ , which is 1.0.

#### Call Statement and Input:

```

          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |    |  |    |  |
CALL SVEM( 5 , X , 1  , Y , -1 , Z , 2  )

```

X = (1.0, 2.0, 3.0, 4.0, 5.0)

Y = (5.0, 4.0, 3.0, 2.0, 1.0)

#### Output:

Z = (1.0, . , 4.0, . , 9.0, . , 16.0, . , 25.0)

**Example 3**

This example shows a vector,  $x$ , with 0 stride, and a vector,  $z$ , with negative stride.  $x$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $x$ . For vector  $z$ , results are stored beginning in element  $Z(5)$ .

**Call Statement and Input:**

```

      N  X  INCX  Y  INCY  Z  INCZ
      |  |  |    |  |    |  |
CALL SVEM( 5 , X , 0 , Y , 1 , Z , -1 )

```

```

X      = (1.0)
Y      = (5.0, 4.0, 3.0, 2.0, 1.0)

```

**Output:**

```

Z      = (1.0, 2.0, 3.0, 4.0, 5.0)

```

**Example 4**

This example shows a vector,  $y$ , with 0 stride.  $y$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $y$ .

**Call Statement and Input:**

```

      N  X  INCX  Y  INCY  Z  INCZ
      |  |  |    |  |    |  |
CALL SVEM( 5 , X , 1 , Y , 0 , Z , 1 )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (5.0)

```

**Output:**

```

Z      = (5.0, 10.0, 15.0, 20.0, 25.0)

```

**Example 5**

This example shows the output vector,  $z$ , with 0 stride, where the vector  $x$  has positive stride, and the vector  $y$  has 0 stride. The number of elements to be processed,  $n$ , is greater than 1.

**Call Statement and Input:**

```

      N  X  INCX  Y  INCY  Z  INCZ
      |  |  |    |  |    |  |
CALL SVEM( 5 , X , 1 , Y , 0 , Z , 0 )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (5.0)

```

**Output:**

```

Z      = (25.0)

```

**Example 6**

This example shows the output vector  $z$ , with 0 stride, where the vector  $x$  has 0 stride, and the vector  $y$  has negative stride. The number of elements to be processed,  $n$ , is greater than 1.

**Call Statement and Input:**

```

      N  X  INCX  Y  INCY  Z  INCZ
      |  |  |    |  |    |  |
CALL SVEM( 5 , X , 0 , Y , -1 , Z , 0 )

```

```

X      = (1.0)
Y      = (5.0, 4.0, 3.0, 2.0, 1.0)

```

## SVEM, DVEM, CVEM, and ZVEM

### Output:

Z = (5.0)

### Example 7

This example shows how SVEM can be used to compute a scalar value. In this case, vectors  $x$  and  $y$  contain scalar values. The strides of all vectors,  $x$ ,  $y$ , and  $z$ , are 0. The number of elements to be processed,  $n$ , is 1.

### Call Statement and Input:

```
          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL SVEM( 1 , X , 0  , Y , 0  , Z , 0  )
```

X = (1.0)

Y = (5.0)

### Output:

Z = (5.0)

### Example 8

This example shows vectors  $x$  and  $y$ , containing complex numbers and having positive strides.

### Call Statement and Input:

```
          N  X  INCX  Y  INCY  Z  INCZ
          |  |  |     |  |     |  |
CALL CVEM( 3 , X , 1  , Y , 2  , Z , 1  )
```

X = ((1.0, 2.0), (3.0, 4.0), (5.0, 6.0))

Y = ((7.0, 8.0), . , (9.0, 10.0), . , (11.0, 12.0))

### Output:

Z = ((-9.0, 22.0), (-13.0, 66.0), (-17.0, 126.0))

## SYAX, DYAX, CYAX, ZYAX, CSYAX, and ZDYAX — Multiply a Vector X by a Scalar and Store in a Vector Y

### Purpose

These subprograms perform the following computation, using the scalar  $\alpha$  and vectors  $x$  and  $y$ :

$$y \leftarrow \alpha x$$

Table 62. Data Types

$\alpha$	$x, y$	Subprogram
Short-precision real	Short-precision real	SYAX
Long-precision real	Long-precision real	DYAX
Short-precision complex	Short-precision complex	CYAX
Long-precision complex	Long-precision complex	ZYAX
Short-precision real	Short-precision complex	CSYAX
Long-precision real	Long-precision complex	ZDYAX

### Syntax

<b>Fortran</b>	CALL SYAX   DYAX   CYAX   ZYAX   CSYAX   ZDYAX ( $n, \alpha, x, incx, y, incy$ )
<b>C and C++</b>	syax   dyax   cyax   zyax   csyax   zdyax ( $n, \alpha, x, incx, y, incy$ );

#### On Entry

- $n$  is the number of elements in vector  $x$  and  $y$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $\alpha$  is the scalar  $\alpha$ .  
Specified as: a number of the data type indicated in Table 62.
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 62.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  See "On Return."
- $incy$  is the stride for vector  $y$ .  
Specified as: a fullword integer. It can have any value.

#### On Return

- $y$  is the vector  $y$  of length  $n$ , containing the result of the computation  $\alpha x$ . Returned as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 62.

## Notes

1. If you specify the same vector for  $x$  and  $y$ , then  $incx$  and  $incy$  must be equal; otherwise, results are unpredictable.
2. If you specify different vectors for  $x$  and  $y$ , they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.

## Function

The computation is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

See reference [82]. If  $n$  is 0, no computation is performed. For CYAX, intermediate results are accumulated in long precision.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows vectors  $x$  and  $y$  with positive strides.

#### Call Statement and Input:

```

          N ALPHA X INCX Y INCY
          |   |   |   |   |   |
CALL SYAX( 5 , 2.0 , X , 1 , Y , 2 )

```

X = (1.0, 2.0, 3.0, 4.0, 5.0)

#### Output:

Y = (2.0, . , 4.0, . , 6.0, . , 8.0, . , 10.0)

### Example 2

This example shows vectors  $x$  and  $y$  that have strides of opposite signs. For  $y$ , which has negative stride, results are stored beginning in element Y(5).

#### Call Statement and Input:

```

          N ALPHA X INCX Y INCY
          |   |   |   |   |   |
CALL SYAX( 5 , 2.0 , X , 1 , Y , -1 )

```

X = (1.0, 2.0, 3.0, 4.0, 5.0)

#### Output:



Y = (10.0, 8.0, 6.0, 4.0, 2.0)

### Example 3

This example shows a vector,  $x$ , with 0 stride.  $x$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $x$ .

#### Call Statement and Input:

```

          N ALPHA X INCX Y INCY
          |   |   |   |   |   |
CALL SYAX( 5 , 2.0 , X , 0 , Y , 1 )

```

X = (1.0)

#### Output:

Y = (2.0, 2.0, 2.0, 2.0, 2.0)

### Example 4

This example shows how SYAX can be used to compute a scalar value. In this case both vectors  $x$  and  $y$  contain scalar values, and the strides for both vectors are 0. The number of elements to be processed,  $n$ , is 1.

#### Call Statement and Input:

```

          N ALPHA X INCX Y INCY
          |   |   |   |   |   |
CALL SYAX( 1 , 2.0 , X , 0 , Y , 0 )

```

X = (1.0)

#### Output:

Y = (2.0)

### Example 5

This example shows a scalar,  $\alpha$ , and vectors  $x$  and  $y$ , containing complex numbers, where both vectors have a stride of 1.

#### Call Statement and Input:

```

          N ALPHA X INCX Y INCY
          |   |   |   |   |   |
CALL CYAX( 3 ,ALPHA, X , 1 , Y , 1 )

```

ALPHA = (2.0, 3.0)

X = ((1.0, 2.0), (2.0, 0.0), (3.0, 5.0))

#### Output:

Y = ((-4.0, 7.0), (4.0, 6.0), (-9.0, 19.0))

### Example 6

This example shows a scalar,  $\alpha$ , containing a real number, and vectors  $x$  and  $y$ , containing complex numbers, where both vectors have a stride of 1.

#### Call Statement and Input:

```

          N ALPHA X INCX Y INCY
          |   |   |   |   |   |
CALL CSYAX( 3 , 2.0 , X , 1 , Y , 1 )

```

X = ((1.0, 2.0), (2.0, 0.0), (3.0, 5.0))

#### Output:

Y = ((2.0, 4.0), (4.0, 0.0), (6.0, 10.0))

## SZAXPY, DZAXPY, CZAXPY, and ZZAXPY — Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in a Vector Z

### Purpose

These subprograms perform the following computation, using the scalar  $\alpha$  and vectors  $x$ ,  $y$ , and  $z$ :

$$z \leftarrow y + \alpha x$$

Table 63. Data Types

$\alpha$ , $x$ , $y$ , $z$	Subprogram
Short-precision real	SZAXPY
Long-precision real	DZAXPY
Short-precision complex	CZAXPY
Long-precision complex	ZZAXPY

### Syntax

<b>Fortran</b>	CALL SZAXPY   DZAXPY   CZAXPY   ZZAXPY ( $n$ , $alpha$ , $x$ , $incx$ , $y$ , $incy$ , $z$ , $incz$ )
<b>C and C++</b>	szaxpy   dzaxpy   czaxpy   zzaxpy ( $n$ , $alpha$ , $x$ , $incx$ , $y$ , $incy$ , $z$ , $incz$ );

### On Entry

- $n$  is the number of elements in vectors  $x$ ,  $y$ , and  $z$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $alpha$  is the scalar  $\alpha$ .  
Specified as: a number of the data type indicated in Table 63.
- $x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 63.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  is the vector  $y$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 63.
- $incy$  is the stride for vector  $y$ .  
Specified as: a fullword integer. It can have any value.
- $z$  See "On Return."
- $incz$  is the stride for vector  $z$ .  
Specified as: a fullword integer. It can have any value.

### On Return

- $z$  is the vector  $z$  of length  $n$ , containing the result of the computation

$y+\alpha x$ . Returned as: a one-dimensional array of (at least) length  $1+(n-1)|incz|$ , containing numbers of the data type indicated in Table 63 on page 272.

## Notes

1. If you specify the same vector for  $x$  and  $z$ , then  $incx$  and  $incz$  must be equal; otherwise, results are unpredictable. The same is true for  $y$  and  $z$ .
2. If you specify different vectors for  $x$  and  $z$ , they must have no common elements; otherwise, results are unpredictable. The same is true for  $y$  and  $z$ . See "Concepts" on page 59.

## Function

The computation is expressed as follows:

$$\begin{bmatrix} z_1 \\ \cdot \\ \cdot \\ \cdot \\ z_n \end{bmatrix} \leftarrow \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

See reference [82]. If  $n$  is 0, no computation is performed. For CZAXPY, intermediate results are accumulated in long precision.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows vectors  $x$  and  $y$  with positive strides.

#### Call Statement and Input:

```

          N ALPHA X INCX Y INCY Z INCZ
CALL SZAXPY( 5 , 2.0 , X , 1 , Y , 2 , Z , 1 )

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (1.0, . , 1.0, . , 1.0, . , 1.0, . , 1.0)

```

#### Output:

```
Z      = (3.0, 5.0, 7.0, 9.0, 11.0)
```

### Example 2

This example shows vectors  $x$  and  $y$  having strides of opposite sign, and an output vector  $z$  having a positive stride. For  $y$ , which has negative stride, processing begins at element  $Y(5)$ , which is 1.0.

#### Call Statement and Input:

## SZAXPY, DZAXPY, CZAXPY, and ZZAXPY

```
          N ALPHA X INCX Y INCY Z INCZ
          |   |   |   |   |   |   |
CALL SZAXPY( 5 , 2.0 , X , 1 , Y , -1 , Z , 2 )
```

```
X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (5.0, 4.0, 3.0, 2.0, 1.0)
```

### Output:

```
Z      = (3.0, . , 6.0, . , 9.0, . , 12.0, . , 15.0)
```

### Example 3

This example shows a vector,  $x$ , with 0 stride, and a vector,  $z$ , with negative stride.  $x$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $x$ . For vector  $z$ , results are stored beginning in element  $Z(5)$ .

### Call Statement and Input:

```
          N ALPHA X INCX Y INCY Z INCZ
          |   |   |   |   |   |   |
CALL SZAXPY( 5 , 2.0 , X , 0 , Y , 1 , Z , -1 )
```

```
X      = (1.0)
Y      = (5.0, 4.0, 3.0, 2.0, 1.0)
```

### Output:

```
Z      = (3.0, 4.0, 5.0, 6.0, 7.0)
```

### Example 4

This example shows a vector,  $y$ , with 0 stride.  $y$  is treated like a vector of length  $n$ , all of whose elements are the same as the single element in  $y$ .

### Call Statement and Input:

```
          N ALPHA X INCX Y INCY Z INCZ
          |   |   |   |   |   |   |
CALL SZAXPY( 5 , 2.0 , X , 1 , Y , 0 , Z , 1 )
```

```
X      = (1.0, 2.0, 3.0, 4.0, 5.0)
Y      = (5.0)
```

### Output:

```
Z      = (7.0, 9.0, 11.0, 13.0, 15.0)
```

### Example 5

This example shows how SZAXPY can be used to compute a scalar value. In this case, vectors  $x$  and  $y$  contain scalar values. The strides of all vectors,  $x$ ,  $y$ , and  $z$ , are 0. The number of elements to be processed,  $n$ , is 1.

### Call Statement and Input:

```
          N ALPHA X INCX Y INCY Z INCZ
          |   |   |   |   |   |   |
CALL SZAXPY( 1 , 2.0 , X , 0 , Y , 0 , Z , 0 )
```

```
X      = (1.0)
Y      = (5.0)
```

### Output:

```
Z      = (7.0)
```

**Example 6**

This example shows vectors  $x$  and  $y$ , containing complex numbers and having positive strides.

**Call Statement and Input:**

```

          N ALPHA X INCX Y INCY Z INCZ
          |   |   |   |   |   |   |
CALL CZAXPY( 3 ,ALPHA, X , 1 , Y , 2 , Z , 1 )

```

```

ALPHA    = (2.0, 3.0)
X        = ((1.0, 2.0), (2.0, 0.0), (3.0, 5.0))
Y        = ((1.0, 1.0), . , (0.0, 2.0), . , (5.0, 4.0))

```

**Output:**

```

Z        = ((-3.0, 8.0), (4.0, 8.0), (-4.0, 23.0))

```

## **Sparse Vector-Scalar Subprograms**

This section contains the sparse vector-scalar subprogram descriptions.

## SSCTR, DSCTR, CSCTR, ZSCTR — Scatter the Elements of a Sparse Vector X in Compressed-Vector Storage Mode into Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode

### Purpose

These subprograms scatter the elements of sparse vector  $x$ , stored in compressed-vector storage mode, into specified elements of sparse vector  $y$ , stored in full-vector storage mode.

Table 64. Data Types

$x, y$	Subprogram
Short-precision real	SSCTR
Long-precision real	DSCTR
Short-precision complex	CSCTR
Long-precision complex	ZSCTR

### Syntax

Fortran	CALL SSCTR   DSCTR   CSCTR   ZSCTR ( $nz, x, indx, y$ )
C and C++	ssctr   dsctr   csctr   zsctr ( $nz, x, indx, y$ );

### On Entry

- $nz$  is the number of elements in sparse vector  $x$ , stored in compressed-vector storage mode. Specified as: a fullword integer;  $nz \geq 0$ .
- $x$  is the sparse vector  $x$ , containing  $nz$  elements, stored in compressed-vector storage mode in an array, referred to as  $X$ . Specified as: a one-dimensional array of (at least) length  $nz$ , containing numbers of the data type indicated in Table 64.
- $indx$  is the array, referred to as  $INDX$ , containing the  $nz$  indices that indicate the positions of the elements of the sparse vector  $x$  when in full-vector storage mode. They also indicate the positions in vector  $y$  into which the elements are copied.  
Specified as: a one-dimensional array of (at least) length  $nz$ , containing fullword integers.
- $y$  See "On Return."

### On Return

- $y$  is the sparse vector  $y$ , stored in full-vector storage mode, of (at least) length  $\max(INDX(i))$  for  $i = 1, nz$ , into which  $nz$  elements of vector  $x$  are copied at positions indicated by the indices array  $INDX$ .  
Returned as: a one-dimensional array of (at least) length  $\max(INDX(i))$  for  $i = 1, nz$ , containing numbers of the data type indicated in Table 64.

## Notes

1. Each value specified in array *INDX* must be unique; otherwise, results are unpredictable.
2. Vectors *x* and *y* must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
3. For a description of how sparse vectors are stored, see “Sparse Vector” on page 64.

## Function

The copy is expressed as follows:

$$y_{\text{INDX}(i)} \leftarrow x_i \quad \text{for } i = 1, nz$$

where:

*x* is a sparse vector, stored in compressed-vector storage mode.

*INDX* is the indices array for sparse vector *x*.

*y* is a sparse vector, stored in full-vector storage mode.

See reference [31]. If *nz* is 0, no copy is performed.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$nz < 0$

## Examples

### Example 1

This example shows how to use SSCTR to copy a sparse vector *x* of length 5 into the following vector *y*, where the elements of array *INDX* are in ascending order:

$$Y = (6.0, 2.0, 4.0, 7.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)$$

#### Call Statement and Input:

```

           NZ  X   INDX  Y
           |   |   |     |
CALL SSCTR( 5 , X , INDX , Y )
    
```

*X* = (1.0, 2.0, 3.0, 4.0, 5.0)

*INDX* = (1, 3, 4, 7, 10)

#### Output:

*Y* = (1.0, 2.0, 2.0, 3.0, 6.0, 10.0, 4.0, 8.0, 9.0, 5.0)

### Example 2

This example shows how to use SSCTR to copy a sparse vector *x* of length 5 into the following vector *y*, where the elements of array *INDX* are in random order:

$$Y = (6.0, 2.0, 4.0, 7.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)$$

#### Call Statement and Input:



```

      NZ  X   INDX  Y
      |  |   |    |
CALL SSCTR( 5 , X , INDX , Y )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0)
INDX   = (4, 3, 1, 10, 7)

```

**Output:**

```

Y      = (3.0, 2.0, 2.0, 1.0, 6.0, 10.0, 5.0, 8.0, 9.0, 4.0)

```

**Example 3**

This example shows how to use CSCTR to copy a sparse vector  $x$  of length 3 into the following vector  $y$ , where the elements of array INDX are in random order:

```

Y = ((6.0, 5.0), (-2.0, 3.0), (15.0, 4.0), (9.0, 0.0))

```

**Call Statement and Input:**

```

      NZ  X   INDX  Y
      |  |   |    |
CALL CSCTR( 3 , X , INDX , Y )

```

```

X      = ((1.0, 2.0), (3.0, 4.0), (5.0, 6.0))
INDX   = (4, 1, 3)

```

**Output:**

```

Y      = ((3.0, 4.0), (-2.0, 3.0), (5.0, 6.0), (1.0, 2.0))

```

## SGTHR, DGTHR, CGTHR, and ZGTHR — Gather Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode into a Sparse Vector X in Compressed-Vector Storage Mode

### Purpose

These subprograms gather specified elements of vector  $y$ , stored in full-vector storage mode, into sparse vector  $x$ , stored in compressed-vector storage mode.

Table 65. Data Types

$x, y$	Subprogram
Short-precision real	SGTHR
Long-precision real	DGTHR
Short-precision complex	CGTHR
Long-precision complex	ZGTHR

### Syntax

Fortran	CALL SGTHR   DGTHR   CGTHR   ZGTHR ( $nz, y, x, indx$ )
C and C++	sgthr   dgthr   cgthr   zgthr ( $nz, y, x, indx$ );

### On Entry

- $nz$  is the number of elements in sparse vector  $x$ , stored in compressed-vector storage mode. Specified as: a fullword integer;  $nz \geq 0$ .
- $y$  is the sparse vector  $y$ , stored in full-vector storage mode, of (at least) length  $\max(\text{INDX}(i))$  for  $i = 1, nz$ , from which  $nz$  elements are copied from positions indicated by the indices array  $\text{INDX}$ .  
Specified as: a one-dimensional array of (at least) length  $\max(\text{INDX}(i))$  for  $i = 1, nz$ , containing numbers of the data type indicated in Table 65.
- $x$  See "On Return."
- $indx$  is the array, referred to as  $\text{INDX}$ , containing the  $nz$  indices that indicate the positions of the elements of the sparse vector  $x$  when in full-vector storage mode. They also indicate the positions in vector  $y$  from which elements are copied.  
Specified as: a one-dimensional array of (at least) length  $nz$ , containing fullword integers.

### On Return

- $x$  is the sparse vector  $x$ , containing  $nz$  elements, stored in compressed-vector storage mode in an array, referred to as  $X$ , into which are copied the elements of vector  $y$  from positions indicated by the indices array  $\text{INDX}$ .  
Returned as: a one-dimensional array of (at least) length  $nz$ , containing numbers of the data type indicated in Table 65.

## Notes

1. Vectors  $x$  and  $y$  must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
2. For a description of how sparse vectors are stored, see “Sparse Vector” on page 64.

## Function

The copy is expressed as follows:

$$x_i \leftarrow y_{\text{INDX}(i)} \quad \text{for } i = 1, \text{nz}$$

where:

$x$  is a sparse vector, stored in compressed-vector storage mode.

INDX is the indices array for sparse vector  $x$ .

$y$  is a sparse vector, stored in full-vector storage mode.

See reference [31]. If  $\text{nz}$  is 0, no copy is performed.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$\text{nz} < 0$

## Examples

### Example 1

This example shows how to use SGTHR to copy specified elements of a vector  $y$  into a sparse vector  $x$  of length 5, where the elements of array INDX are in ascending order.

#### Call Statement and Input:

```

           NZ  Y   X   INDX
           |   |   |   |
CALL SGTHR( 5 , Y , X , INDX )

```

```

Y          = (6.0, 2.0, 4.0, 7.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)
INDX      = (1, 3, 4, 7, 9)

```

#### Output:

```

X          = (6.0, 4.0, 7.0, -2.0, 9.0)

```

### Example 2

This example shows how to use SGTHR to copy specified elements of a vector  $y$  into a sparse vector  $x$  of length 5, where the elements of array INDX are in random order. (Note that the element 0.0 occurs in output vector  $x$ . This does not produce an error.)

#### Call Statement and Input:

## SGTHR, DGTHR, CGTHR, and ZGTHR

```
          NZ  Y  X  INDX
          |  |  |  |
CALL SGTHR( 5 , Y , X , INDX )
```

```
Y          = (6.0, 2.0, 4.0, 7.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)
INDX       = (4, 3, 1, 10, 7)
```

### Output:

```
X          = (7.0, 4.0, 6.0, 0.0, -2.0)
```

### Example 3

This example shows how to use CGTHR to copy specified elements of a vector,  $y$ , into a sparse vector,  $x$ , of length 3, where the elements of array INDX are in random order.

### Call Statement and Input:

```
          NZ  Y  X  INDX
          |  |  |  |
CALL CGTHR( 3 , Y , X , INDX )
```

```
Y          = ((6.0, 5.0), (-2.0, 3.0), (15.0, 4.0), (9.0, 0.0))
INDX       = (4, 1, 3)
```

### Output:

```
X          = ((9.0, 0.0), (6.0, 5.0), (15.0, 4.0))
```

## SGTHRZ, DGTHRZ, CGTHRZ, and ZGTHRZ — Gather Specified Elements of a Sparse Vector $y$ in Full-Vector Mode into a Sparse Vector $x$ in Compressed-Vector Mode, and Zero the Same Specified Elements of $y$

### Purpose

These subprograms gather specified elements of sparse vector  $y$ , stored in full-vector storage mode, into sparse vector  $x$ , stored in compressed-vector storage mode, and zero the same specified elements of vector  $y$ .

Table 66. Data Types

$x, y$	Subprogram
Short-precision real	SGTHRZ
Long-precision real	DGTHRZ
Short-precision complex	CGTHRZ
Long-precision complex	ZGTHRZ

### Syntax

Fortran	CALL SGTHRZ   DGTHRZ   CGTHRZ   ZGTHRZ ( $nz, y, x, indx$ )
C and C++	sgthrz   dgthrz   cgthrz   zgthrz ( $nz, y, x, indx$ );

### On Entry

- $nz$  is the number of elements in sparse vector  $x$ , stored in compressed-vector storage mode. Specified as: a fullword integer;  $nz \geq 0$ .
- $y$  is the sparse vector  $y$ , stored in full-vector storage mode, of (at least) length  $\max(\text{INDX}(i))$  for  $i = 1, nz$ , from which  $nz$  elements are copied from positions indicated by the indices array  $\text{INDX}$ .  
Specified as: a one-dimensional array of (at least) length  $\max(\text{INDX}(i))$  for  $i = 1, nz$ , containing numbers of the data type indicated in Table 66.
- $x$  See “On Return.”
- $indx$  is the array, referred to as  $\text{INDX}$ , containing the  $nz$  indices that indicate the positions of the elements of the sparse vector  $x$  when in full-vector storage mode. They also indicate the positions in vector  $y$  from which elements are copied then set to zero.  
Specified as: a one-dimensional array of (at least) length  $nz$ , containing fullword integers.

### On Return

- $y$  is the sparse vector  $y$ , stored in full-vector storage mode, of (at least) length  $\max(\text{INDX}(i))$  for  $i = 1, nz$ , whose elements are set to zero at positions indicated by the indices array  $\text{INDX}$ .  
Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 66.

## SGTHRZ, DGTHRZ, CGTHRZ, and ZGTHRZ

$x$  is the sparse vector  $x$ , containing  $nz$  elements stored in compressed-vector storage mode in an array, referred to as  $X$ , into which are copied the elements of vector  $y$  from positions indicated by the indices array  $INDX$ .

Returned as: a one-dimensional array of (at least) length  $nz$ , containing numbers of the data type indicated in Table 66 on page 283.

### Notes

1. Each value specified in array  $INDX$  must be unique; otherwise, results are unpredictable.
2. Vectors  $x$  and  $y$  must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.
3. For a description of how sparse vectors are stored, see "Sparse Vector" on page 64.

### Function

The copy is expressed as follows:

$$\begin{aligned} x_i &\leftarrow y_{INDX(i)} \\ y_{INDX(i)} &\leftarrow 0.0 && \text{(for SGTHRZ and DGTHRZ)} \\ y_{INDX(i)} &\leftarrow (0.0, 0.0) && \text{(for CGTHRZ and ZGTHRZ)} \\ &\text{for } i = 1, nz \end{aligned}$$

where:

$x$  is a sparse vector, stored in compressed-vector storage mode.

$INDX$  is the indices array for sparse vector  $x$ .

$y$  is a sparse vector, stored in full-vector storage mode.

See reference [31]. If  $nz$  is 0, no computation is performed.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

$nz < 0$

### Examples

#### Example 1

This example shows how to use SGTHRZ to copy specified elements of a vector  $y$  into a sparse vector  $x$  of length 5, where the elements of array  $INDX$  are in ascending order.

#### Call Statement and Input:

```

          NZ  Y  X  INDX
          |  |  |  |
CALL SGTHRZ( 5 , Y , X , INDX )

Y        = (6.0, 2.0, 4.0, 7.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)
INDX     = (1, 3, 4, 7, 9)
```

**Output:**

Y = (0.0, 2.0, 0.0, 0.0, 6.0, 10.0, 0.0, 8.0, 0.0, 0.0)  
 X = (6.0, 4.0, 7.0, -2.0, 9.0)

**Example 2**

This example shows how to use SGTHRZ to copy specified elements of a vector  $y$  into a sparse vector  $x$  of length 5, where the elements of array INDX are in random order. (Note that the element 0.0 occurs in output vector  $x$ . This does not produce an error.)

**Call Statement and Input:**

```

          NZ  Y  X  INDX
          |  |  |  |
CALL SGTHRZ( 5 , Y , X , INDX )
    
```

Y = (6.0, 2.0, 4.0, 7.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)  
 INDX = (4, 3, 1, 10, 7)

**Output:**

Y = (0.0, 2.0, 0.0, 0.0, 6.0, 10.0, 0.0, 8.0, 9.0, 0.0)  
 X = (7.0, 4.0, 6.0, 0.0, -2.0)

**Example 3**

This example shows how to use CGTHRZ to copy specified elements of a vector  $y$  into a sparse vector  $x$  of length 3, where the elements of array INDX are in random order.

**Call Statement and Input:**

```

          NZ  Y  X  INDX
          |  |  |  |
CALL CGTHRZ( 3 , Y , X , INDX )
    
```

Y = ((6.0, 5.0), (-2.0, 3.0), (15.0, 4.0), (9.0, 0.0))  
 INDX = (4, 1, 3)

**Output:**

Y = ((0.0, 0.0), (-2.0, 3.0), (0.0, 0.0), (0.0, 0.0))  
 X = ((9.0, 0.0), (6.0, 5.0), (15.0, 4.0))

## SAXPYI, DAXPYI, CAXPYI, and ZAXPYI — Multiply a Sparse Vector X in Compressed-Vector Storage Mode by a Scalar, Add to a Sparse Vector Y in Full-Vector Storage Mode, and Store in the Vector Y

### Purpose

These subprograms multiply sparse vector  $x$ , stored in compressed-vector storage mode, by scalar  $\alpha$ , add it to sparse vector  $y$ , stored in full-vector storage mode, and store the result in vector  $y$ .

Table 67. Data Types

$\alpha, x, y$	Subprogram
Short-precision real	SAXPYI
Long-precision real	DAXPYI
Short-precision complex	CAXPYI
Long-precision complex	ZAXPYI

### Syntax

Fortran	CALL SAXPYI   DAXPYI   CAXPYI   ZAXPYI ( $nz, \alpha, x, indx, y$ )
C and C++	saxpyi   daxpyi   caxpyi   zaxpyi ( $nz, \alpha, x, indx, y$ );

### On Entry

- $nz$  is the number of elements in sparse vector  $x$ , stored in compressed-vector storage mode. Specified as: a fullword integer;  $nz \geq 0$ .
- $\alpha$  is the scalar  $\alpha$ . Specified as: a number of the data type indicated in Table 67.
- $x$  is the sparse vector  $x$ , containing  $nz$  elements, stored in compressed-vector storage mode in an array, referred to as  $X$ . Specified as: a one-dimensional array of (at least) length  $nz$ , containing numbers of the data type indicated in Table 67.
- $indx$  is the array, referred to as  $INDX$ , containing the  $nz$  indices that indicate the positions of the elements of the sparse vector  $x$  when in full-vector storage mode. They also indicate the positions of the elements in vector  $y$  that are used in the computation.  
Specified as: a one-dimensional array of (at least) length  $nz$ , containing fullword integers.
- $y$  is the sparse vector  $y$ , stored in full-vector storage mode, of (at least) length  $\max(INDX(i))$  for  $i = 1, nz$ . Specified as: a one-dimensional array of (at least) length  $\max(INDX(i))$  for  $i = 1, nz$ , containing numbers of the data type indicated in Table 67.

### On Return

- $y$  is the sparse vector  $y$ , stored in full-vector storage mode, of (at least) length  $\max(INDX(i))$  for  $i = 1, nz$  containing the results of the computation, stored at positions indicated by the indices array  $INDX$ .



Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 67 on page 286.

## Notes

1. Each value specified in array `INDX` must be unique; otherwise, results are unpredictable.
2. Vectors  $x$  and  $y$  must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
3. For a description of how sparse vectors are stored, see “Sparse Vector” on page 64.

## Function

The computation is expressed as follows:

$$y_{\text{INDX}(i)} \leftarrow y_{\text{INDX}(i)} + \alpha x_i \quad \text{for } i = 1, nz$$

where:

$x$  is a sparse vector, stored in compressed-vector storage mode.

`INDX` is the indices array for sparse vector  $x$ .

$y$  is a sparse vector, stored in full-vector storage mode.

See reference [31]. If  $\alpha$  or  $nz$  is zero, no computation is performed. For SAXPYI and CAXPYI, intermediate results are accumulated in long-precision.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$nz < 0$

## Examples

### Example 1

This example shows how to use SAXPYI to perform a computation using a sparse vector  $x$  of length 5, where the elements of array `INDX` are in ascending order.

#### Call Statement and Input:

```

           NZ ALPHA X   INDX  Y
           |   |   |   |   |
CALL SAXPYI( 5 , 2.0 , X , INDX , Y )

```

$X$  = (1.0, 2.0, 3.0, 4.0, 5.0)

$INDX$  = (1, 3, 4, 7, 10)

$Y$  = (1.0, 5.0, 4.0, 3.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)

#### Output:

$Y$  = (3.0, 5.0, 8.0, 9.0, 6.0, 10.0, 6.0, 8.0, 9.0, 10.0)

### Example 2

This example shows how to use SAXPYI to perform a computation using a sparse vector  $x$  of length 5, where the elements of array `INDX` are in random order.

## SAXPYI, DAXPYI, CAXPYI, and ZAXPYI

### Call Statement and Input:

```
          NZ ALPHA X   INDX Y  
          |   |   |   |   |  
CALL SAXPYI( 5 , 2.0 , X , INDX , Y )
```

```
X       = (1.0, 2.0, 3.0, 4.0, 5.0)  
INDX    = (4, 3, 1, 10, 7)  
Y       = (1.0, 5.0, 4.0, 3.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)
```

### Output:

```
Y       = (7.0, 5.0, 8.0, 5.0, 6.0, 10.0, 8.0, 8.0, 9.0, 8.0)
```

### Example 3

This example shows how to use CAXPYI to perform a computation using a sparse vector  $x$  of length 3, where the elements of array `INDX` are in random order.

### Call Statement and Input:

```
          NZ ALPHA X   INDX Y  
          |   |   |   |   |  
CALL CAXPYI( 3 , ALPHA , X , INDX , Y )
```

```
ALPHA   = (2.0, 3.0)  
X       = ((1.0, 2.0), (3.0, 4.0), (5.0, 6.0))  
INDX    = (4, 1, 3)  
Y       = ((6.0, 5.0), (-2.0, 3.0), (15.0, 4.0), (9.0, 0.0))
```

### Output:

```
Y       = ((0.0, 22.0), (-2.0, 3.0), (7.0, 31.0), (5.0, 7.0))
```

## SDOTI, DDOTI, CDOTUI, ZDOTUI, CDOTCI, and ZDOTCI — Dot Product of a Sparse Vector $x$ in Compressed-Vector Storage Mode and a Sparse Vector $y$ in Full-Vector Storage Mode

### Purpose

SDOTI, DDOTI, CDOTUI, and ZDOTUI compute the dot product of sparse vector  $x$ , stored in compressed-vector storage mode, and full vector  $y$ , stored in full-vector storage mode.

CDOTCI and ZDOTCI compute the dot product of the complex conjugate of sparse vector  $x$ , stored in compressed-vector storage mode, and full vector  $y$ , stored in full-vector storage mode.

Table 68. Data Types

$x, y$ , Result	Subprogram
Short-precision real	SDOTI
Long-precision real	DDOTI
Short-precision complex	CDOTUI
Long-precision complex	ZDOTUI
Short-precision complex	CDOTCI
Long-precision complex	ZDOTCI

### Syntax

<b>Fortran</b>	SDOTI   DDOTI   CDOTUI   ZDOTUI   CDOTCI   ZDOTCI ( $nz, x, indx, y$ )
<b>C and C++</b>	sdoti   ddoti   cdotui   zdotui   cdotci   zdotci ( $nz, x, indx, y$ );

### On Entry

- $nz$  is the number of elements in sparse vector  $x$ , stored in compressed-vector storage mode. Specified as: a fullword integer;  $nz \geq 0$ .
- $x$  is the sparse vector  $x$ , containing  $nz$  elements, stored in compressed-vector storage mode in an array, referred to as  $X$ . Specified as: a one-dimensional array of (at least) length  $nz$ , containing numbers of the data type indicated in Table 68.
- $indx$  is the array, referred to as  $INDX$ , containing the  $nz$  indices that indicate the positions of the elements of the sparse vector  $x$  when in full-vector storage mode. They also indicate the positions of elements in vector  $y$  that are used in the computation.  
Specified as: a one-dimensional array of (at least) length  $nz$ , containing fullword integers.
- $y$  is the sparse vector  $y$ , stored in full-vector storage mode, of (at least) length  $\max(INDX(i))$  for  $i = 1, nz$ . Specified as: a one-dimensional array of (at least) length  $\max(INDX(i))$  for  $i = 1, nz$ , containing numbers of the data type indicated in Table 68.

## SDOTI, DDOTI, CDOTUI, ZDOTUI, CDOTCI, and ZDOTCI

### On Return

*Function value*

is the result of the dot product computation.

Returned as: a number of the data type indicated in Table 68 on page 289.

### Notes

1. Declare this function in your program as returning a value of the data type indicated in Table 68 on page 289.
2. For a description of how sparse vectors are stored, see “Sparse Vector” on page 64.

### Function

For SDOTI, DDOTI, CDOTUI, and ZDOTUI, the dot product computation is expressed as follows:

$$\sum_{i=1}^{nz} x_i y_{\text{INDX}(i)} = x_1 y_{\text{INDX}(1)} + x_2 y_{\text{INDX}(2)} + \dots + x_{nz} y_{\text{INDX}(nz)}$$

For CDOTCI and ZDOTCI, the dot product computation is expressed as follows:

$$\sum_{i=1}^{nz} \bar{x}_i y_{\text{INDX}(i)} = \bar{x}_1 y_{\text{INDX}(1)} + \bar{x}_2 y_{\text{INDX}(2)} + \dots + \bar{x}_{nz} y_{\text{INDX}(nz)}$$

where:

$x$  is a sparse vector, stored in compressed-vector storage mode.

$\bar{x}$  is the complex conjugate of a sparse vector, stored in compressed - vector storage mode.

INDX is the indices array for sparse vector  $x$ .

$y$  is a sparse vector, stored in full-vector storage mode.

See reference [31]. The result is returned as the function value. If  $nz$  is 0, then zero is returned as the value of the function.

For SDOTI, CDOTUI, and CDOTCI, intermediate results are accumulated in long-precision.

### Error conditions

#### Computational Errors

None

**Input-Argument Errors** $nz < 0$ **Examples****Example 1**

This example shows how to use SDOTI to compute a dot product using a sparse vector  $x$  of length 5, where the elements of array `INDX` are in ascending order.

**Function Reference and Input:**

	NZ	X	INDX	Y

$$\text{DOTT} = \text{SDOTI}(5, X, \text{INDX}, Y)$$

X	=	(1.0, 2.0, 3.0, 4.0, 5.0)
INDX	=	(1, 3, 4, 7, 10)
Y	=	(1.0, 5.0, 4.0, 3.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)

**Output:**

$$\text{DOTT} = (1.0 + 8.0 + 9.0 - 8.0 + 0.0) = 10.0$$
**Example 2**

This example shows how to use SDOTI to compute a dot product using a sparse vector  $x$  of length 5, where the elements of array `INDX` are in random order.

**Function Reference and Input:**

	NZ	X	INDX	Y

$$\text{DOTT} = \text{SDOTI}(5, X, \text{INDX}, Y)$$

X	=	(1.0, 2.0, 3.0, 4.0, 5.0)
INDX	=	(4, 3, 1, 10, 7)
Y	=	(1.0, 5.0, 4.0, 3.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)

**Output:**

$$\text{DOTT} = (3.0 + 8.0 + 3.0 + 0.0 - 10.0) = 4.0$$
**Example 3**

This example shows how to use CDOTUI to compute a dot product using a sparse vector  $x$  of length 3, where the elements of array `INDX` are in ascending order.

**Function Reference and Input:**

	NZ	X	INDX	Y

$$\text{DOTT} = \text{CDOTUI}(3, X, \text{INDX}, Y)$$

X	=	((1.0, 2.0), (3.0, 4.0), (5.0, 6.0))
INDX	=	(1, 3, 4)
Y	=	((6.0, 5.0), (-2.0, 3.0), (15.0, 4.0), (9.0, 0.0))

**Output:**

$$\text{DOTT} = (70.0, 143.0)$$
**Example 4**

This example shows how to use CDOTCI to compute a dot product using the complex conjugate of a sparse vector  $x$  of length 3, where the elements of array `INDX` are in random order.

## SDOTI, DDOTI, CDOTUI, ZDOTUI, CDOTCI, and ZDOTCI

### Function Reference and Input:

	NZ	X	INDX	Y
DOTT = CDOTCI(	3	X	INDX	Y

X = ((1.0, 2.0), (3.0, 4.0), (5.0, 6.0))

INDX = (4, 1, 3)

Y = ((6.0, 5.0), (-2.0, 3.0), (15.0, 4.0), (9.0, 0.0))

### Output:

DOTT = (146.0, -97.0)

## Matrix-Vector Subprograms

This section contains the matrix-vector subprogram descriptions.

## SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX — Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose

### Purpose

SGEMV and DGEMV compute the matrix-vector product for either a real general matrix or its transpose, using the scalars  $\alpha$  and  $\beta$ , vectors  $x$  and  $y$ , and matrix  $A$  or its transpose:

$$y \leftarrow \beta y + \alpha Ax$$

$$y \leftarrow \beta y + \alpha A^T x$$

CGEMV and ZGEMV compute the matrix-vector product for either a complex general matrix, its transpose, or its conjugate transpose, using the scalars  $\alpha$  and  $\beta$ , vectors  $x$  and  $y$ , and matrix  $A$ , its transpose, or its conjugate transpose:

$$y \leftarrow \beta y + \alpha Ax$$

$$y \leftarrow \beta y + \alpha A^T x$$

$$y \leftarrow \beta y + \alpha A^H x$$

SGEMX and DGEMX compute the matrix-vector product for a real general matrix, using the scalar  $\alpha$ , vectors  $x$  and  $y$ , and matrix  $A$ :

$$y \leftarrow y + \alpha Ax$$

SGEMTX and DGEMTX compute the matrix-vector product for the transpose of a real general matrix, using the scalar  $\alpha$ , vectors  $x$  and  $y$ , and the transpose of matrix  $A$ :

$$y \leftarrow y + \alpha A^T x$$

Table 69. Data Types

$\alpha, \beta, x, y, A$	Subprogram
Short-precision real	SGEMV, SGEMX, and SGEMTX
Long-precision real	DGEMV, DGEMX, and DGEMTX
Short-precision complex	CGEMV
Long-precision complex	ZGEMV

**Note:** SGEMV and DGEMV are Level 2 BLAS subroutines. It is suggested that these subroutines be used instead of SGEMX, DGEMX, SGEMTX, and DGEMTX, which are provided only for compatibility with earlier releases of ESSL.

### Syntax

<b>Fortran</b>	CALL SGEMV   DGEMV   CGEMV   ZGEMV ( <i>transa, m, n, alpha, a, lda, x, incx, beta, y, incy</i> ) CALL SGEMX   DGEMX   SGEMTX   DGEMTX ( <i>m, n, alpha, a, lda, x, incx, y, incy</i> )
<b>C and C++</b>	sgemv   dgemv   cgemv   zgemv ( <i>transa, m, n, alpha, a, lda, x, incx, beta, y, incy</i> ); sgemx   dgemx   sgemtx   dgemtx ( <i>m, n, alpha, a, lda, x, incx, y, incy</i> );



### On Entry

*transa* indicates the form of matrix  $A$  to use in the computation, where:  
 If  $transa = 'N'$ ,  $A$  is used in the computation.  
 If  $transa = 'T'$ ,  $A^T$  is used in the computation.  
 If  $transa = 'C'$ ,  $A^H$  is used in the computation.  
 Specified as: a single character. It must be 'N', 'T', or 'C'.

*m* is the number of rows in matrix  $A$ , and:  
 For SGEMV, DGEMV, CGEMV, and ZGEMV:  
 If  $transa = 'N'$ , it is the length of vector  $y$ .  
 If  $transa = 'T'$  or 'C', it is the length of vector  $x$ .  
 For SGEMX and DGEMX, it is the length of vector  $y$ .  
 For SGEMTX and DGEMTX, it is the length of vector  $x$ .  
 Specified as: a fullword integer;  $0 \leq m \leq lda$ .

*n* is the number of columns in matrix  $A$ , and:  
 For SGEMV, DGEMV, CGEMV, and ZGEMV:  
 If  $transa = 'N'$ , it is the length of vector  $x$ .  
 If  $transa = 'T'$  or 'C', it is the length of vector  $y$ .  
 For SGEMX and DGEMX, it is the length of vector  $x$ .  
 For SGEMTX and DGEMTX, it is the length of vector  $y$ .  
 Specified as: a fullword integer;  $n \geq 0$ .

*alpha* is the scaling constant  $\alpha$ .  
 Specified as: a number of the data type indicated in Table 69 on page 294.

*a* is the  $m$  by  $n$  matrix  $A$ , where:  
 For SGEMV, DGEMV, CGEMV, and ZGEMV:  
 If  $transa = 'N'$ ,  $A$  is used in the computation.  
 If  $transa = 'T'$ ,  $A^T$  is used in the computation.  
 If  $transa = 'C'$ ,  $A^H$  is used in the computation.  
 For SGEMX and DGEMX,  $A$  is used in the computation.  
 For SGEMTX and DGEMTX,  $A^T$  is used in the computation.  
**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix  $A$  should always be stored in its untransposed form.  
 Specified as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 69 on page 294.

## SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX

*lda* is the leading dimension of the array specified for *a*.  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq m$ .

*x* is the vector *x*, where:  
For SGEMV, DGEMV, CGEMV, and ZGEMV:  
If *transa* = 'N', it has length *n*.  
If *transa* = 'T' or 'C', it has length *m*.  
For SGEMX and DGEMX, it has length *n*.  
For SGEMTX and DGEMTX, it has length *m*.  
Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 69 on page 294, where:  
For SGEMV, DGEMV, CGEMV, and ZGEMV:  
If *transa* = 'N', it must have at least  $1+(n-1)|incx|$  elements.  
If *transa* = 'T' or 'C', it must have at least  $1+(m-1)|incx|$  elements.  
For SGEMX and DGEMX, it must have at least  $1+(n-1)|incx|$  elements.  
For SGEMTX and DGEMTX, it must have at least  $1+(m-1)|incx|$  elements.

*incx* is the stride for vector *x*.  
Specified as: a fullword integer; It can have any value.

*beta* is the scaling constant  $\beta$ .  
Specified as: a number of the data type indicated in Table 69 on page 294.

*y* is the vector *y*, where:  
For SGEMV, DGEMV, CGEMV, and ZGEMV:  
If *transa* = 'N', it has length *m*.  
If *transa* = 'T' or 'C', it has length *n*.  
For SGEMX and DGEMX, it has length *m*.  
For SGEMTX and DGEMTX, it has length *n*.  
Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 69 on page 294, where:  
For SGEMV, DGEMV, CGEMV, and ZGEMV:  
If *transa* = 'N', it must have at least  $1+(m-1)|incy|$  elements.  
If *transa* = 'T' or 'C', it must have at least  $1+(n-1)|incy|$  elements.  
For SGEMX and DGEMX, it must have at least  $1+(m-1)|incy|$  elements.

## SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX

For SGEMTX and DGEMTX, it must have at least  $1+(n-1)|incy|$  elements.

*incy*

is the stride for vector  $y$ .

Specified as: a fullword integer;  $incy > 0$  or  $incy < 0$ .

### On Return

$y$

is the vector  $y$ , containing the result of the computation, where:

For SGEMV, DGEMV, CGEMV, and ZGEMV:

If *transa* = 'N', it has length  $m$ .

If *transa* = 'T' or 'C', it has length  $n$ .

For SGEMX and DGEMX, it has length  $m$ .

For SGEMTX and DGEMTX, it has length  $n$ .

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 69 on page 294.

### Notes

1. For SGEMV and DGEMV, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
2. The SGEMV, DGEMV, CGEMV, and ZGEMV subroutines accept lowercase letters for the *transa* argument.
3. In the SGEMV, DGEMV, CGEMV, and ZGEMV subroutines,  $incx = 0$  is valid; however, the Level 2 BLAS standard considers  $incx = 0$  to be invalid. See references [36] and [37].
4. Vector  $y$  must have no common elements with matrix  $A$  or vector  $x$ ; otherwise, results are unpredictable. See "Concepts" on page 59.

### Function

The possible computations that can be performed by these subroutines are described in the following sections. Varying implementation techniques are used for this computation to improve performance. As a result, accuracy of the computational result may vary for different computations.

For SGEMV, CGEMV, SGEMX, and SGEMTX, intermediate results are accumulated in long precision. Occasionally, for performance reasons, these intermediate results are stored.

See references [36], [37], [40], [48], and [82]. No computation is performed if  $m$  or  $n$  is 0 or if  $\alpha$  is zero and  $\beta$  is one.

#### General Matrix

For SGEMV, DGEMV, CGEMV, and ZGEMV, the matrix-vector product for a general matrix:

$$y \leftarrow \beta y + \alpha Ax$$

is expressed as follows:

## SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_m \end{bmatrix} \leftarrow \beta \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_m \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

For SGEMX and DGEMX, the matrix-vector product for a real general matrix:

$$y \leftarrow y + \alpha Ax$$

is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_m \end{bmatrix} \leftarrow \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_m \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

In these expressions:

$y$  is a vector of length  $m$ .

$\alpha$  is a scalar.

$\beta$  is a scalar.

$A$  is an  $m$  by  $n$  matrix.

$x$  is a vector of length  $n$ .

### Transpose of a General Matrix

For SGEMV, DGEMV, CGEMV and ZGEMV, the matrix-vector product for the transpose of a general matrix:

$$y \leftarrow \beta y + \alpha A^T x$$

is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \beta \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{m1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{1n} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_m \end{bmatrix}$$

For SGEMTX and DGEMTX, the matrix-vector product for the transpose of a real general matrix:

$$y \leftarrow y + \alpha A^T x$$

is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \cdots & a_{m1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{1n} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_m \end{bmatrix}$$

In these expressions:

$y$  is a vector of length  $n$ .

$\alpha$  is a scalar.

$\beta$  is a scalar.

$A^T$  is the transpose of matrix  $A$ , where  $A$  is an  $m$  by  $n$  matrix.

$x$  is a vector of length  $m$ .

### Conjugate Transpose of a General Matrix

For CGEMV and ZGEMV, the matrix-vector product for the conjugate transpose of a general matrix:

$$y \leftarrow \beta y + \alpha A^H x$$

is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \beta \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} \bar{a}_{11} & \cdots & \bar{a}_{m1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \bar{a}_{1n} & \cdots & \bar{a}_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_m \end{bmatrix}$$

where:

$y$  is a vector of length  $n$ .

$\alpha$  is a scalar.

$\beta$  is a scalar.

$A^H$  is the conjugate transpose of matrix  $A$ , where  $A$  is an  $m$  by  $n$  matrix.

$x$  is a vector of length  $m$ .

## Error conditions

### Resource Errors

Unable to allocate internal work area (for SGEMV, DGEMV, CGEMV, and ZGEMV).

### Computational Errors

None

### Input-Argument Errors

1.  $transa \neq 'N', 'T', \text{ or } 'C'$
2.  $m < 0$
3.  $m > lda$
4.  $n < 0$
5.  $lda \leq 0$
6.  $incy = 0$

## Examples

### Example 1

This example shows the computation for TRANS equal to 'N', where the real general matrix *A* is used in the computation. Because *lda* is 10 and *n* is 3, array *A* must be declared as *A*(E1:E2,F1:F2), where E2-E1+1=10 and F2-F1+1 ≥ 3. In this example, array *A* is declared as *A*(1:10,0:2).

#### Call Statement and Input:

```

          TRANS M  N  ALPHA  A      LDA  X  INCX  BETA  Y  INCY
          |      |  |      |      |    |  |    |    |  |
CALL SGEMV( 'N' , 4 , 3 , 1.0 , A(1,0) , 10 , X , 1 , 1.0 , Y , 2 )
    
```

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 2.0 & 2.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 2.0 & 1.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

X = (3.0, 2.0, 1.0)  
 Y = (4.0, . , 5.0, . , 2.0, . , 3.0)

#### Output:

Y = (14.0, . , 19.0, . , 17.0, . , 20.0)

### Example 2

This example shows the computation for TRANS equal to 'T', where the transpose of the real general matrix *A* is used in the computation. Array *A* must follow the same rules as given in Example 1. In this example, array *A* is declared as *A*(-1:8,1:3).

#### Call Statement and Input:

```

          TRANS M  N  ALPHA  A      LDA  X  INCX  BETA  Y  INCY
          |      |  |      |      |    |  |    |    |  |
CALL SGEMV( 'T' , 4 , 3 , 1.0 , A(-1,1) , 10 , X , 1 , 2.0 , Y , 2 )
    
```

A = (same as input *A* in Example 1)  
 X = (3.0, 2.0, 1.0, 4.0)  
 Y = (1.0, . , 2.0, . , 3.0)

#### Output:

Y = (28.0, . , 24.0, . , 29.0)

### Example 3

This example shows the computation for TRANS equal to 'N', where the complex general matrix *A* is used in the computation.

#### Call Statement and Input:

```

          TRANS M  N  ALPHA  A      LDA  X  INCX  BETA  Y  INCY
          |      |  |      |      |    |  |    |    |  |
CALL CGEMV( 'N' , 5 , 3 , ALPHA , A , 10 , X , 1 , BETA , Y , 1 )
    
```

ALPHA = (1.0, 0.0)

## SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX

$$A = \begin{bmatrix} (1.0, 2.0) & (3.0, 5.0) & (2.0, 0.0) \\ (2.0, 3.0) & (7.0, 9.0) & (4.0, 8.0) \\ (7.0, 4.0) & (1.0, 4.0) & (6.0, 0.0) \\ (8.0, 2.0) & (2.0, 5.0) & (8.0, 0.0) \\ (9.0, 1.0) & (3.0, 6.0) & (1.0, 0.0) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$\begin{aligned} X &= ((1.0, 2.0), (4.0, 0.0), (1.0, 1.0)) \\ \text{BETA} &= (1.0, 0.0) \\ Y &= ((1.0, 2.0), (4.0, 0.0), (1.0, -1.0), (3.0, 4.0), \\ &\quad (2.0, 0.0)) \end{aligned}$$

### Output:

$$Y = ((12.0, 28.0), (24.0, 55.0), (10.0, 39.0), (23.0, 50.0), (22.0, 44.0))$$

### Example 4

This example shows the computation for TRANSA equal to 'T', where the transpose of complex general matrix  $A$  is used in the computation. Because  $\beta$  is zero, the result of the computation is  $\alpha A^T x$

#### Call Statement and Input:

```

          TRANSA M  N  ALPHA  A  LDA  X  INCX  BETA  Y  INCY
          |      |  |      |  |    |  |    |      |  |
CALL CGEMV( 'T' , 5 , 3 , ALPHA , A , 10 , X , 1 , BETA , Y , 1 )

```

$$\begin{aligned} \text{ALPHA} &= (1.0, 0.0) \\ A &= \text{(same as input } A \text{ in Example 3)} \\ X &= ((1.0, 2.0), (4.0, 0.0), (1.0, 1.0), (3.0, 4.0), \\ &\quad (2.0, 0.0)) \\ \text{BETA} &= (0.0, 0.0) \\ Y &= \text{(not relevant)} \end{aligned}$$

### Output:

$$Y = ((42.0, 67.0), (10.0, 87.0), (50.0, 74.0))$$

### Example 5

This example shows the computation for TRANSA equal to 'C', where the conjugate transpose of the complex general matrix  $A$  is used in the computation.

#### Call Statement and Input:

```

          TRANSA M  N  ALPHA  A  LDA  X  INCX  BETA  Y  INCY
          |      |  |      |  |    |  |    |      |  |
CALL CGEMV( 'C' , 5 , 3 , ALPHA , A , 10 , X , 1 , BETA , Y , 1 )

```

$$\begin{aligned} \text{ALPHA} &= (-1.0, 0.0) \\ A &= \text{(same as input } A \text{ in Example 3)} \\ X &= ((1.0, 2.0), (4.0, 0.0), (1.0, 1.0), (3.0, 4.0), \\ &\quad (2.0, 0.0)) \\ \text{BETA} &= (1.0, 0.0) \\ Y &= ((1.0, 2.0), (4.0, 0.0), (1.0, -1.0)) \end{aligned}$$

### Output:

$$Y = ((-73.0, -13.0), (-74.0, 57.0), (-49.0, -11.0))$$

### Example 6

This example shows a matrix,  $A$ , contained in a larger array,  $A$ . The strides of vectors  $x$  and  $y$  are positive. Because  $lda$  is 10 and  $n$  is 3, array  $A$  must be declared as  $A(E1:E2,F1:F2)$ , where  $E2-E1+1=10$  and  $F2-F1+1 \geq 3$ . For this example, array  $A$  is declared as  $A(1:10,0:2)$ .

#### Call Statement and Input:

```

          M  N  ALPHA  A  LDA  X  INCX  Y  INCY
          |  |  |      |  |   |   |   |   |
CALL SGEMX( 4 , 3 , 1.0 , A(1,0) , 10 , X , 1 , Y , 2 )
    
```

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 2.0 & 2.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 2.0 & 1.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$X = (3.0, 2.0, 1.0)$   
 $Y = (4.0, \cdot, 5.0, \cdot, 2.0, \cdot, 3.0)$

#### Output:

$Y = (14.0, \cdot, 19.0, \cdot, 17.0, \cdot, 20.0)$

### Example 7

This example shows a matrix,  $A$ , contained in a larger array,  $A$ . The strides of vectors  $x$  and  $y$  are of opposite sign. For  $y$ , which has negative stride, processing begins at element  $Y(7)$ , which is 4.0. Array  $A$  must follow the same rules as given in Example 6. For this example, array  $A$  is declared as  $A(-1:8,1:3)$ .

#### Call Statement and Input:

```

          M  N  ALPHA  A  LDA  X  INCX  Y  INCY
          |  |  |      |  |   |   |   |   |
CALL SGEMX( 4 , 3 , 1.0 , A(-1,1) , 10 , X , 1 , Y , -2 )
    
```

$A =$  (same as input  $A$  in Example 6)  
 $X = (3.0, 2.0, 1.0)$   
 $Y = (3.0, \cdot, 2.0, \cdot, 5.0, \cdot, 4.0)$

#### Output:

$Y = (20.0, \cdot, 17.0, \cdot, 19.0, \cdot, 14.0)$

### Example 8

This example shows a matrix,  $A$ , contained in a larger array,  $A$ , and the first element of the matrix is not the first element of the array. Array  $A$  must follow the same rules as given in Example 6. For this example, array  $A$  is declared as  $A(1:10,1:3)$ .

#### Call Statement and Input:

```

          M  N  ALPHA  A  LDA  X  INCX  Y  INCY
          |  |  |      |  |   |   |   |   |
CALL SGEMX( 4 , 3 , 1.0 , A(5,1) , 10 , X , 1 , Y , 1 )
    
```



## SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX

$$A = \begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1.0 & 2.0 & 3.0 \\ 2.0 & 2.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 2.0 & 1.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$\begin{aligned} X &= (3.0, 2.0, 1.0) \\ Y &= (4.0, 5.0, 2.0, 3.0) \end{aligned}$$

### Output:

$$Y = (14.0, 19.0, 17.0, 20.0)$$

### Example 9

This example shows a matrix,  $A$ , and an array,  $A$ , having the same number of rows. For this case,  $m$  and  $lda$  are equal. Because  $lda$  is 4 and  $n$  is 3, array  $A$  must be declared as  $A(E1:E2,F1:F2)$ , where  $E2-E1+1=4$  and  $F2-F1+1 \geq 3$ . For this example, array  $A$  is declared as  $A(1:4,0:2)$ .

### Call Statement and Input:

	M	N	ALPHA	A	LDA	X	INCX	Y	INCY
CALL SGEMX(	4	3	1.0	A(1,0)	4	X	1	Y	1

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 2.0 & 2.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 2.0 & 1.0 \end{bmatrix}$$

$$\begin{aligned} X &= (3.0, 2.0, 1.0) \\ Y &= (4.0, 5.0, 2.0, 3.0) \end{aligned}$$

### Output:

$$Y = (14.0, 19.0, 17.0, 20.0)$$

### Example 10

This example shows a matrix,  $A$ , and an array,  $A$ , having the same number of rows. For this case,  $m$  and  $lda$  are equal. Because  $lda$  is 4 and  $n$  is 3, array  $A$  must be declared as  $A(E1:E2,F1:F2)$ , where  $E2-E1+1=4$  and  $F2-F1+1 \geq 3$ . For this example, array  $A$  is declared as  $A(1:4,0:2)$ .

### Call Statement and Input:

	M	N	ALPHA	A	LDA	X	INCX	Y	INCY
CALL SGEMTX(	4	3	1.0	A(1,0)	4	X	1	Y	1

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 2.0 & 2.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 2.0 & 1.0 \end{bmatrix}$$

$$\begin{aligned} X &= (3.0, 2.0, 1.0, 4.0) \\ Y &= (1.0, 2.0, 3.0) \end{aligned}$$

## SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX

### Output:

Y = (27.0, 22.0, 26.0)

### Example 11

This example shows a computation in which *alpha* is greater than 1. Array A must follow the same rules as given in Example 10. For this example, array A is declared as A(-1:2,1:3).

### Call Statement and Input:

```
          M  N  ALPHA      A      LDA  X  INCX  Y  INCY
          |  |  |         |      |    |    |  |    |
CALL SGEMTX( 4 , 3 , 2.0 , A(-1,1) , 4 , X , 1 , Y , 1 )
```

A = (same as input A in Example 10)

X = (3.0, 2.0, 1.0, 4.0)

Y = (1.0, 2.0, 3.0)

### Output:

Y = (53.0, 42.0, 49.0)

## SGER, DGER, CGERU, ZGERU, CGERC, and ZGERC — Rank-One Update of a General Matrix

### Purpose

SGER, DGER, CGERU, and ZGERU compute the rank-one update of a general matrix, using the scalar  $\alpha$ , matrix  $A$ , vector  $x$ , and the transpose of vector  $y$ :

$$A \leftarrow A + \alpha xy^T$$

CGERC and ZGERC compute the rank-one update of a general matrix, using the scalar  $\alpha$ , matrix  $A$ , vector  $x$ , and the conjugate transpose of vector  $y$ :

$$A \leftarrow A + \alpha xy^H$$

Table 70. Data Types

$\alpha, A, x, y$	Subprogram
Short-precision real	SGER
Long-precision real	DGER
Short-precision complex	CGERU and CGERC
Long-precision complex	ZGERU and ZGERC

**Note:** For compatibility with earlier releases of ESSL, you can use the names SGER1 and DGER1 for SGER and DGER, respectively.

### Syntax

Fortran	CALL SGER   DGER   CGERU   ZGERU   CGERC   ZGERC ( $m, n, alpha, x, incx, y, incy, a, lda$ )
C and C++	sger   dger   cgeru   zgeru   cgerc   zgerc ( $m, n, alpha, x, incx, y, incy, a, lda$ );

### On Entry

- $m$  is the number of rows in matrix  $A$  and the number of elements in vector  $x$ .  
Specified as: a fullword integer;  $0 \leq m \leq lda$ .
- $n$  is the number of columns in matrix  $A$  and the number of elements in vector  $y$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $alpha$  is the scaling constant  $\alpha$ .  
Specified as: a number of the data type indicated in Table 70.
- $x$  is the vector  $x$  of length  $m$ .  
Specified as: a one-dimensional array of (at least) length  $1+(m-1)|incx|$ , containing numbers of the data type indicated in Table 70.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  is the vector  $y$  of length  $n$ , whose transpose or conjugate transpose is used in the computation.

## SGER, DGER, CGERU, ZGERU, CGERC, ZGERC

**Note:** No data should be moved to form  $y^T$  or  $y^H$ ; that is, the vector  $y$  should always be stored in its untransposed form.

Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 70 on page 305.

*incy* is the stride for vector  $y$ .

Specified as: a fullword integer. It can have any value.

*a* is the  $m$  by  $n$  matrix  $A$ . Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 70 on page 305.

*lda* is the size of the leading dimension of the array specified for  $a$ .  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq m$ .

### On Return

*a* is the  $m$  by  $n$  matrix  $A$ , containing the result of the computation.

Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 70 on page 305.

### Notes

1. In these subroutines,  $incx = 0$  and  $incy = 0$  are valid; however, the Level 2 BLAS standard considers  $incx = 0$  and  $incy = 0$  to be invalid. See references [36] and [37].
2. Matrix  $A$  can have no common elements with vectors  $x$  and  $y$ ; otherwise, results are unpredictable. See "Concepts" on page 59.

### Function

SGER, DGER, CGERU, and ZGERU compute the rank-one update of a general matrix:

$$A \leftarrow A + \alpha x y^T$$

where:

$A$  is an  $m$  by  $n$  matrix.

$\alpha$  is a scalar.

$x$  is a vector of length  $m$ .

$y^T$  is the transpose of vector  $y$  of length  $n$ .

It is expressed as follows:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_m \end{bmatrix} [y_1 \dots y_n]$$

It can also be expressed as:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} + \alpha x_1 y_1 & \dots & a_{1n} + \alpha x_1 y_n \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} + \alpha x_m y_1 & \dots & a_{mn} + \alpha x_m y_n \end{bmatrix}$$

CGERC and ZGERC compute a slightly different rank-one update of a general matrix:

$$A \leftarrow A + \alpha x y^H$$

where:

$A$  is an  $m$  by  $n$  matrix.

$\alpha$  is a scalar.

$x$  is a vector of length  $m$ .

$y^H$  is the conjugate transpose of vector  $y$  of length  $n$ .

It is expressed as follows:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_m \end{bmatrix} [\bar{y}_1 \dots \bar{y}_n]$$

It can also be expressed as:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} + \alpha x_1 \bar{y}_1 & \dots & a_{1n} + \alpha x_1 \bar{y}_n \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} + \alpha x_m \bar{y}_1 & \dots & a_{mn} + \alpha x_m \bar{y}_n \end{bmatrix}$$

See references [36], [37], and [82]. No computation is performed if  $m$ ,  $n$ , or  $\alpha$  is zero. For CGERU and CGERC, intermediate results are accumulated in long precision. For SGER, intermediate results are accumulated in long precision on some platforms.

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

None

### Input-Argument Errors

1.  $m < 0$
2.  $n < 0$

## SGER, DGER, CGERU, ZGERU, CGERC, ZGERC

3.  $lda \leq 0$
4.  $m > lda$

### Examples

#### Example 1

This example shows a matrix,  $A$ , contained in a larger array,  $A$ . The strides of vectors  $x$  and  $y$  are positive. Because  $lda$  is 10 and  $n$  is 3, array  $A$  must be declared as  $A(E1:E2,F1:F2)$ , where  $E2-E1+1=10$  and  $F2-F1+1 \geq 3$ . For this example, array  $A$  is declared as  $A(1:10,0:2)$ .

#### Call Statement and Input:

```
          M  N  ALPHA  X  INCX  Y  INCY  A  LDA
CALL SGER( 4 , 3 , 1.0 , X , 1 , Y , 2 , A(1,0) , 10 )
```

```
X      = (3.0, 2.0, 1.0, 4.0)
Y      = (1.0, . , 2.0, . , 3.0)
```

```
A =  $\begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 2.0 & 2.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 2.0 & 1.0 \\ . & . & . \\ . & . & . \\ . & . & . \\ . & . & . \\ . & . & . \\ . & . & . \end{bmatrix}$ 
```

#### Output:

```
A =  $\begin{bmatrix} 4.0 & 8.0 & 12.0 \\ 4.0 & 6.0 & 10.0 \\ 4.0 & 4.0 & 5.0 \\ 8.0 & 10.0 & 13.0 \\ . & . & . \\ . & . & . \\ . & . & . \\ . & . & . \\ . & . & . \\ . & . & . \end{bmatrix}$ 
```

#### Example 2

This example shows a matrix,  $A$ , contained in a larger array,  $A$ . The strides of vectors  $x$  and  $y$  are of opposite sign. For  $y$ , which has negative stride, processing begins at element  $Y(5)$ , which is 1.0. Array  $A$  must follow the same rules as given in Example 1. For this example, array  $A$  is declared as  $A(-1:8,1:3)$ .

#### Call Statement and Input:

```
          M  N  ALPHA  X  INCX  Y  INCY  A  LDA
CALL SGER( 4 , 3 , 1.0 , X , 1 , Y , -2 , A(-1,1) , 10 )
```

```
X      = (3.0, 2.0, 1.0, 4.0)
Y      = (3.0, . , 2.0, . , 1.0)
A      =(same as input A in Example 1)
```

**Output:**

A = (same as input A in Example 1)

**Example 3**

This example shows a matrix, *A*, contained in a larger array, *A*, and the first element of the matrix is not the first element of the array. Array *A* must follow the same rules as given in Example 1. For this example, array *A* is declared as *A*(1:10,1:3).

**Call Statement and Input:**

```

          M  N  ALPHA  X  INCX  Y  INCY  A  LDA
          |  |  |      |  |      |  |  |
CALL SGER( 4 , 3 , 1.0 , X , 3 , Y , 1 , A(4,1) , 10 )
    
```

X = (3.0, . . . , 2.0, . . . , 1.0, . . . , 4.0)  
 Y = (1.0, 2.0, 3.0)

$$A = \begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1.0 & 2.0 & 3.0 \\ 2.0 & 2.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 2.0 & 1.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 4.0 & 8.0 & 12.0 \\ 4.0 & 6.0 & 10.0 \\ 4.0 & 4.0 & 5.0 \\ 8.0 & 10.0 & 13.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Example 4**

This example shows a matrix, *A*, and array, *A*, having the same number of rows. For this case, *m* and *lda* are equal. Because *lda* is 4 and *n* is 3, array *A* must be declared as *A*(*E1*:*E2*,*F1*:*F2*), where *E2*-*E1*+1=4 and *F2*-*F1*+1 ≥ 3. For this example, array *A* is declared as *A*(1:4,0:2).

**Call Statement and Input:**

```

          M  N  ALPHA  X  INCX  Y  INCY  A  LDA
          |  |  |      |  |      |  |  |
CALL SGER( 4 , 3 , 1.0 , X , 1 , Y , 1 , A(1,0) , 4 )
    
```

X = (3.0, 2.0, 1.0, 4.0)  
 Y = (1.0, 2.0, 3.0)

## SGER, DGER, CGERU, ZGERU, CGERC, ZGERC

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 2.0 & 2.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 2.0 & 1.0 \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} 4.0 & 8.0 & 12.0 \\ 4.0 & 6.0 & 10.0 \\ 4.0 & 4.0 & 5.0 \\ 8.0 & 10.0 & 13.0 \end{bmatrix}$$

### Example 5

This example shows a computation in which scalar value for *alpha* is greater than 1. Array A must follow the same rules as given in Example 4. For this example, array A is declared as A(-1:2,1:3).

**Call Statement and Input:**

```

           M  N  ALPHA  X  INCX  Y  INCY  A  LDA
           |  |  |      |  |     |  |   |  |
CALL SGER( 4 , 3 , 2.0 , X , 1 , Y , 1 , A(-1,1) , 4 )

```

```

X          = (3.0, 2.0, 1.0, 4.0)
Y          = (1.0, 2.0, 3.0)
A          =(same as input A in Example 4)

```

**Output:**

$$A = \begin{bmatrix} 7.0 & 14.0 & 21.0 \\ 6.0 & 10.0 & 16.0 \\ 5.0 & 6.0 & 8.0 \\ 12.0 & 18.0 & 25.0 \end{bmatrix}$$

### Example 6

This example shows a rank-one update in which all data items contain complex numbers, and the transpose  $y^T$  is used in the computation. Matrix A is contained in a larger array, A. The strides of vectors *x* and *y* are positive. The Fortran DIMENSION statement for array A must follow the same rules as given in Example 1. For this example, array A is declared as A(1:10,0:2).

**Call Statement and Input:**

```

           M  N  ALPHA  X  INCX  Y  INCY  A  LDA
           |  |  |      |  |     |  |   |  |
CALL CGERU( 5 , 3 , ALPHA , X , 1 , Y , 1 , A(1,0) , 10 )

```

```

ALPHA      = (1.0, 0.0)
X          = ((1.0, 2.0), (4.0, 0.0), (1.0, 1.0), (3.0, 4.0),
              (2.0, 0.0))
Y          = ((1.0, 2.0), (4.0, 0.0), (1.0, -1.0))

```

$$A = \begin{bmatrix} (1.0, 2.0) & (3.0, 5.0) & (2.0, 0.0) \\ (2.0, 3.0) & (7.0, 9.0) & (4.0, 8.0) \\ (7.0, 4.0) & (1.0, 4.0) & (6.0, 0.0) \\ (8.0, 2.0) & (2.0, 5.0) & (8.0, 0.0) \\ (9.0, 1.0) & (3.0, 6.0) & (1.0, 0.0) \\ \vdots & \vdots & \vdots \end{bmatrix}$$



$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} (-2.0, 6.0) & (7.0, 13.0) & (5.0, 1.0) \\ (6.0, 11.0) & (23.0, 9.0) & (8.0, 4.0) \\ (6.0, 7.0) & (5.0, 8.0) & (8.0, 0.0) \\ (3.0, 12.0) & (14.0, 21.0) & (15.0, 1.0) \\ (11.0, 5.0) & (11.0, 6.0) & (3.0, -2.0) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Example 7**

This example shows a rank-one update in which all data items contain complex numbers, and the conjugate transpose  $y^H$  is used in the computation. Matrix  $A$  is contained in a larger array, A. The strides of vectors  $x$  and  $y$  are positive. The Fortran DIMENSION statement for array A must follow the same rules as given in Example 1. For this example, array A is declared as A(1:10,0:2).

**Call Statement and Input:**

```

          M  N  ALPHA  X  INCX  Y  INCY  A  LDA
CALL CGERC( 5 , 3 , ALPHA , X , 1 , Y , 1 , A(1,0) , 10 )
    
```

```

ALPHA  = (1.0, 0.0)
X      = ((1.0, 2.0), (4.0, 0.0), (1.0, 1.0), (3.0, 4.0),
          (2.0, 0.0))
Y      = ((1.0, 2.0), (4.0, 0.0), (1.0, -1.0))
A      =(same as input A in Example 6 )
    
```

**Output:**

$$A = \begin{bmatrix} (6.0, 2.0) & (7.0, 13.0) & (1.0, 3.0) \\ (6.0, -5.0) & (23.0, 9.0) & (8.0, 12.0) \\ (10.0, 3.0) & (5.0, 8.0) & (6.0, 2.0) \\ (19.0, 0.0) & (14.0, 21.0) & (7.0, 7.0) \\ (11.0, -3.0) & (11.0, 6.0) & (3.0, 2.0) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

## SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, ZHEMV, SSLMX, and DSLMX — Matrix-Vector Product for a Real Symmetric or Complex Hermitian Matrix

### Purpose

SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, and ZHEMV compute the matrix-vector product for either a real symmetric matrix or a complex Hermitian matrix, using the scalars  $\alpha$  and  $\beta$ , matrix  $A$ , and vectors  $x$  and  $y$ :

$$y \leftarrow \beta y + \alpha Ax$$

SSLMX and DSLMX compute the matrix-vector product for a real symmetric matrix, using the scalar  $\alpha$ , matrix  $A$ , and vectors  $x$  and  $y$ :

$$y \leftarrow y + \alpha Ax$$

The following storage modes are used:

- For SSPMV, DSPMV, CHPMV, and ZHPMV, matrix  $A$  is stored in upper- or lower-packed storage mode.
- For SSYMV, DSYMV, CHEMV, and ZHEMV, matrix  $A$  is stored in upper or lower storage mode.
- For SSLMX and DSLMX, matrix  $A$  is stored in lower-packed storage mode.

Table 71. Data Types

$\alpha, \beta, A, x, y$	Subprogram
Short-precision real	SSPMV, SSYMV, and SSLMX
Long-precision real	DSPMV, DSYMV, and DSLMX
Short-precision complex	CHPMV and CHEMV
Long-precision complex	ZHPMV and ZHEMV

**Note:** SSPMV and DSPMV are Level 2 BLAS subroutines. You should use these subroutines instead of SSLMX and DSLMX, which are provided only for compatibility with earlier releases of ESSL.

### Syntax

<b>Fortran</b>	CALL SSPMV   DSPMV   CHPMV   ZHPMV ( <i>uplo, n, alpha, ap, x, incx, beta, y, incy</i> ) CALL SSYMV   DSYMV   CHEMV   ZHEMV ( <i>uplo, n, alpha, a, lda, x, incx, beta, y, incy</i> ) CALL SSLMX   DSLMX ( <i>n, alpha, ap, x, incx, y, incy</i> )
<b>C and C++</b>	sspmv   dspmv   chpmv   zhpmv ( <i>uplo, n, alpha, ap, x, incx, beta, y, incy</i> ); ssymv   dsymv   chemv   zhemv ( <i>uplo, n, alpha, a, lda, x, incx, beta, y, incy</i> ); sslmx   dslmx ( <i>n, alpha, ap, x, incx, y, incy</i> );

### On Entry

*uplo* indicates the storage mode used for matrix  $A$ , where:  
If *uplo* = 'U',  $A$  is stored in upper-packed or upper storage mode.

If *uplo* = 'L', *A* is stored in lower-packed or lower storage mode.  
 Specified as: a single character. It must be 'U' or 'L'.

*n* is the number of elements in vectors *x* and *y* and the order of matrix *A*.  
 Specified as: a fullword integer;  $n \geq 0$ .

*alpha* is the scaling constant  $\alpha$ .  
 Specified as: a number of the data type indicated in Table 71 on page 312.

*ap* has the following meaning:  
 For SSPMV and DSPMV, *ap* is the real symmetric matrix *A* of order *n*, stored in upper- or lower-packed storage mode.  
 For CHPMV and ZHPMV, *ap* is the complex Hermitian matrix *A* of order *n*, stored in upper- or lower-packed storage mode.  
 For SSLMX and DSLMX, *ap* is the real symmetric matrix *A* of order *n*, stored in lower-packed storage mode.  
 Specified as: a one-dimensional array of (at least) length  $n(n+1)/2$ , containing numbers of the data type indicated in Table 71 on page 312.

*a* has the following meaning:  
 For SSYMV and DSYMV, *a* is the real symmetric matrix *A* of order *n*, stored in upper or lower storage mode.  
 For CHEMV and ZHEMV, *a* is the complex Hermitian matrix *A* of order *n*, stored in upper or lower storage mode.  
 Specified as: an *lda* by (at least) *n* array, containing numbers of the data type indicated in Table 71 on page 312.

*lda* is the leading dimension of the array specified for *a*.  
 Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .

*x* is the vector *x* of length *n*.  
 Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 71 on page 312.

*incx* is the stride for vector *x*.  
 Specified as: a fullword integer, where:  
 For SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, and ZHEMV,  $incx < 0$  or  $incx > 0$ .  
 For SSLMX and DSLMX, *incx* can have any value.

*beta* is the scaling constant  $\beta$ .  
 Specified as: a number of the data type indicated in Table 71 on page 312.

*y* is the vector *y* of length *n*.  
 Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 71 on page 312.

*incy* is the stride for vector *y*.  
Specified as: a fullword integer; *incy* > 0 or *incy* < 0.

### On Return

*y* is the vector *y* of length *n*, containing the result of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 71 on page 312.

### Notes

1. All subroutines accept lowercase letters for the *uplo* argument.
2. The vector *y* must have no common elements with vector *x* or matrix *A*; otherwise, results are unpredictable. See “Concepts” on page 59.
3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix *A* are assumed to be zero, so you do not have to set these values.
4. For a description of how symmetric matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see “Symmetric Matrix” on page 69. For a description of how complex Hermitian matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see “Complex Hermitian Matrix” on page 73.

### Function

These subroutines perform the computations described in the two sections below. See references [36], [37], and [82]. For SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, and ZHEMV, if *n* is zero or if  $\alpha$  is zero and  $\beta$  is one, no computation is performed. For SSLMX and DSLMX, if *n* or  $\alpha$  is zero, no computation is performed.

For SSLMX, SSPMV, SSYMV, CHPMV, and CHEMV, intermediate results are accumulated in long precision. However, several intermediate stores may occur for each element of the vector *y*.

#### For SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, and ZHEMV

These subroutines compute the matrix-vector product for either a real symmetric matrix or a complex Hermitian matrix:

$$y \leftarrow \beta y + \alpha Ax$$

where:

*y* is a vector of length *n*.

$\alpha$  is a scalar.

$\beta$  is a scalar.

*A* is a real symmetric or complex Hermitian matrix of order *n*.

*x* is a vector of length *n*.

It is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \beta \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

### For SSLMX and DSLMX

These subroutines compute the matrix-vector product for a real symmetric matrix stored in lower-packed storage mode:

$$y \leftarrow y + \alpha Ax$$

where:

$y$  is a vector of length  $n$ .

$\alpha$  is a scalar.

$A$  is a real symmetric matrix of order  $n$ .

$x$  is a vector of length  $n$ .

It is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $uplo \neq 'L'$  or  $'U'$
2.  $n < 0$
3.  $lda < n$
4.  $lda \leq 0$
5.  $incx = 0$
6.  $incy = 0$

## Examples

### Example 1

This example shows vectors  $x$  and  $y$  with positive strides and a real symmetric matrix  $A$  of order 3, stored in lower-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 8.0 & 4.0 & 2.0 \\ 4.0 & 6.0 & 7.0 \\ 2.0 & 7.0 & 3.0 \end{bmatrix}$$

**Call Statement and Input:**

```

          UPLO N  ALPHA AP  X  INCX BETA Y  INCY
          |   |   |   |   |   |   |   |
CALL SSPMV( 'L' , 3 , 1.0 , AP , X , 1 , 1.0 , Y , 2 )
    
```

```

AP      = (8.0, 4.0, 2.0, 6.0, 7.0, 3.0)
X       = (3.0, 2.0, 1.0)
Y       = (5.0, . , 3.0, . , 2.0)
    
```

**Output:**

```

Y       = (39.0, . , 34.0, . , 25.0)
    
```

**Example 2**

This example shows vector  $x$  and  $y$  having strides of opposite signs. For  $x$ , which has negative stride, processing begins at element  $x(5)$ , which is 1.0. The real symmetric matrix  $A$  of order 3 is stored in upper-packed storage mode. It uses the same input matrix  $A$  as in Example 1.

**Call Statement and Input:**

```

          UPLO N  ALPHA AP  X  INCX BETA Y  INCY
          |   |   |   |   |   |   |   |
CALL SSPMV( 'U' , 3 , 1.0 , AP , X , -2 , 2.0 , Y , 1 )
    
```

```

AP      = (8.0, 4.0, 6.0, 2.0, 7.0, 3.0)
X       = (4.0, . , 2.0, . , 1.0)
Y       = (6.0, 5.0, 4.0)
    
```

**Output:**

```

Y       = (36.0, 54.0, 36.0)
    
```

**Example 3**

This example shows vector  $x$  and  $y$  with positive stride and a complex Hermitian matrix  $A$  of order 3, stored in lower-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} (1.0, 0.0) & (3.0, 5.0) & (2.0, -3.0) \\ (3.0, -5.0) & (7.0, 0.0) & (4.0, -8.0) \\ (2.0, 3.0) & (4.0, 8.0) & (6.0, 0.0) \end{bmatrix}$$

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values.

**Call Statement and Input:**

```

          UPLO N  ALPHA AP  X  INCX BETA Y  INCY
          |   |   |   |   |   |   |   |
CALL CHPMV( 'L' , 3 , ALPHA , AP , X , 1 , BETA , Y , 2 )
    
```

```

ALPHA   = (1.0, 0.0)
AP      = ((1.0, . ), (3.0, -5.0), (2.0, 3.0), (7.0, . ),
          (4.0, 8.0), (6.0, . ))
X       = ((1.0, 2.0), (4.0, 0.0), (3.0, 4.0))
BETA    = (1.0, 0.0)
Y       = ((1.0, 0.0), . , (2.0, -1.0), . , (2.0, 1.0))
    
```

**Output:**

```

Y       = ((32.0, 21.0), . , (87.0, -8.0), . , (32.0, 64.0))
    
```

**Example 4**

This example shows vector  $x$  and  $y$  having strides of opposite signs. For  $x$ , which has negative stride, processing begins at element  $X(5)$ , which is (1.0, 2.0). The complex Hermitian matrix  $A$  of order 3 is stored in upper-packed storage mode. It uses the same input matrix  $A$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values.

**Call Statement and Input:**

```

          UPLO N  ALPHA  AP  X  INCX  BETA  Y  INCY
          |   |   |     |   |   |     |   |
CALL CHPMV( 'U' , 3 , ALPHA , AP , X , -2 , BETA , Y , 2 )

```

```

ALPHA    = (1.0, 0.0)
AP       = ((1.0, . ), (3.0, 5.0), (7.0, . ), (2.0, -3.0),
           (4.0, -8.0), (6.0, . ))
X        = ((3.0, 4.0), . , (4.0, 0.0), . , (1.0, 2.0))
BETA     = (0.0, 0.0)
Y        =(not relevant)

```

**Output:**

```

Y        = ((31.0, 21.0), . , (85.0, -7.0), . , (30.0, 63.0))

```

**Example 5**

This example shows vectors  $x$  and  $y$  with positive strides and a real symmetric matrix  $A$  of order 3, stored in lower storage mode. It uses the same input matrix  $A$  as in Example 1.

**Call Statement and Input:**

```

          UPLO N  ALPHA  A  LDA  X  INCX  BETA  Y  INCY
          |   |   |     |   |   |   |     |   |
CALL SSYMV( 'L' , 3 , 1.0 , A , 3 , X , 1 , 1.0 , Y , 2 )

```

$$A = \begin{bmatrix} 8.0 & . & . \\ 4.0 & 6.0 & . \\ 2.0 & 7.0 & 3.0 \end{bmatrix}$$

```

X        = (3.0, 2.0, 1.0)
Y        = (5.0, . , 3.0, . , 2.0)

```

**Output:**

```

Y        = (39.0, . , 34.0, . , 25.0)

```

**Example 6**

This example shows vector  $x$  and  $y$  having strides of opposite signs. For  $x$ , which has negative stride, processing begins at element  $X(5)$ , which is 1.0. The real symmetric matrix  $A$  of order 3 is stored in upper storage mode. It uses the same input matrix  $A$  as in Example 1.

**Call Statement and Input:**

```

          UPLO N  ALPHA  A  LDA  X  INCX  BETA  Y  INCY
          |   |   |     |   |   |   |     |   |
CALL SSYMV( 'U' , 3 , 1.0 , A , 4 , X , -2 , 2.0 , Y , 1 )

```

$$A = \begin{bmatrix} 8.0 & 4.0 & 2.0 \\ . & 6.0 & 7.0 \\ . & . & 3.0 \\ . & . & . \end{bmatrix}$$

$$X = (4.0, ., 2.0, ., 1.0)$$

$$Y = (6.0, 5.0, 4.0)$$

**Output:**

$$A = (36.0, 54.0, 36.0)$$

**Example 7**

This example shows vector  $x$  and  $y$  with positive stride and a complex Hermitian matrix  $A$  of order 3, stored in lower storage mode. It uses the same input matrix  $A$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values.

**Call Statement and Input:**

```

          UPLO N  ALPHA  A  LDA  X  INCX BETA  Y  INCY
          |   |   |     |   |   |   |   |   |   |
CALL CHEMV( 'L' , 3 , ALPHA , A , 3 , X , 1 , BETA , Y , 2 )
    
```

$$ALPHA = (1.0, 0.0)$$

$$A = \begin{bmatrix} (1.0, .) & . & . \\ (3.0, -5.0) & (7.0, .) & . \\ (2.0, 3.0) & (4.0, 8.0) & (6.0, .) \end{bmatrix}$$

$$X = ((1.0, 2.0), (4.0, 0.0), (3.0, 4.0))$$

$$BETA = (1.0, 0.0)$$

$$Y = ((1.0, 0.0), ., (2.0, -1.0), ., (2.0, 1.0))$$

**Output:**

$$Y = ((32.0, 21.0), ., (87.0, -8.0), ., (32.0, 64.0))$$

**Example 8**

This example shows vector  $x$  and  $y$  having strides of opposite signs. For  $x$ , which has negative stride, processing begins at element  $X(5)$ , which is  $(1.0, 2.0)$ . The complex Hermitian matrix  $A$  of order 3 is stored in upper storage mode. It uses the same input matrix  $A$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values.

**Call Statement and Input:**

```

          UPLO N  ALPHA  A  LDA  X  INCX BETA  Y  INCY
          |   |   |     |   |   |   |   |   |   |
CALL CHEMV( 'U' , 3 , ALPHA , A , 3 , X , -2 , BETA , Y , 2 )
    
```

$$ALPHA = (1.0, 0.0)$$



$$A = \begin{bmatrix} (1.0, \dots) & (3.0, 5.0) & (2.0, -3.0) \\ \cdot & (7.0, \dots) & (4.0, -8.0) \\ \cdot & \cdot & (6.0, \dots) \end{bmatrix}$$

X = ((3.0, 4.0), . . , (4.0, 0.0), . . , (1.0, 2.0))  
 BETA = (0.0, 0.0)  
 Y =(not relevant)

**Output:**

Y = ((31.0, 21.0), . . , (85.0, -7.0), . . , (30.0, 63.0))

**Example 9**

This example shows vectors *x* and *y* with positive strides and a real symmetric matrix *A* of order 3. Matrix *A* is:

$$\begin{bmatrix} 8.0 & 4.0 & 2.0 \\ 4.0 & 6.0 & 7.0 \\ 2.0 & 7.0 & 3.0 \end{bmatrix}$$

**Call Statement and Input:**

```

          N ALPHA AP X INCX Y INCY
          |   |   | | |   |   |
CALL SSLMX( 3 , 1.0 , AP , X , 1 , Y , 2 )
    
```

AP = (8.0, 4.0, 2.0, 6.0, 7.0, 3.0)  
 X = (3.0, 2.0, 1.0)  
 Y = (5.0, . . , 3.0, . . , 2.0)

**Output:**

Y = (39.0, . . , 34.0, . . , 25.0)

## SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, ZHER, SSLR1, and DSLR1 — Rank-One Update of a Real Symmetric or Complex Hermitian Matrix

### Purpose

SSPR, DSPR, SSYR, DSYR, SSLR1, and DSLR1 compute the rank-one update of a real symmetric matrix, using the scalar  $\alpha$ , matrix  $A$ , vector  $x$ , and its transpose  $x^T$ :

$$A \leftarrow A + \alpha x x^T$$

CHPR, ZHPR, CHER, and ZHER compute the rank-one update of a complex Hermitian matrix, using the scalar  $\alpha$ , matrix  $A$ , vector  $x$ , and its conjugate transpose  $x^H$ :

$$A \leftarrow A + \alpha x x^H$$

The following storage modes are used:

- For SSPR, DSPR, CHPR, and ZHPR, matrix  $A$  is stored in upper- or lower-packed storage mode.
- For SSYR, DSYR, CHER, and ZHER, matrix  $A$  is stored in upper or lower storage mode.
- For SSLR1 and DSLR1, matrix  $A$  is stored in lower-packed storage mode.

Table 72. Data Types

$A, x$	$\alpha$	Subprogram
Short-precision real	Short-precision real	SSPR, SSYR, and SSLR1
Long-precision real	Long-precision real	DSPR, DSYR, and DSLR1
Short-precision complex	Short-precision real	CHPR and CHER
Long-precision complex	Long-precision real	ZHPR and ZHER

**Note:** SSPR and DSPR are Level 2 BLAS subroutines. You should use these subroutines instead of SSLR1 and DSLR1, which are only provided for compatibility with earlier releases of ESSL.

### Syntax

<b>Fortran</b>	CALL SSPR   DSPR   CHPR   ZHPR ( <i>uplo, n, alpha, x, incx, ap</i> ) CALL SSYR   DSYR   CHER   ZHER ( <i>uplo, n, alpha, x, incx, a, lda</i> ) CALL SSLR1   DSLR1 ( <i>n, alpha, x, incx, ap</i> )
<b>C and C++</b>	sspr   dspr   chpr   zhpr ( <i>uplo, n, alpha, x, incx, ap</i> ); ssyr   dsyr   cher   zher ( <i>uplo, n, alpha, x, incx, a, lda</i> ); sslr1   dslr1 ( <i>n, alpha, x, incx, ap</i> );

### On Entry

*uplo* indicates the storage mode used for matrix  $A$ , where:  
If *uplo* = 'U',  $A$  is stored in upper-packed or upper storage mode.

## SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, ZHER, SSLR1, and DSLR1

	If <i>uplo</i> = 'L', <i>A</i> is stored in lower-packed or lower storage mode. Specified as: a single character. It must be 'U' or 'L'.
<i>n</i>	is the number of elements in vector <i>x</i> and the order of matrix <i>A</i> . Specified as: a fullword integer; $n \geq 0$ .
<i>alpha</i>	is the scaling constant $\alpha$ . Specified as: a number of the data type indicated in Table 72 on page 320.
<i>x</i>	is the vector <i>x</i> of length <i>n</i> . Specified as: a one-dimensional array of (at least) length $1+(n-1) incx $ , containing numbers of the data type indicated in Table 72 on page 320.
<i>incx</i>	is the stride for vector <i>x</i> . Specified as: a fullword integer, where: For SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, and ZHER, $incx < 0$ or $incx > 0$ . For SSLR1 and DSLR1, <i>incx</i> can have any value.
<i>ap</i>	has the following meaning: For SSPR and DSPR, <i>ap</i> is the real symmetric matrix <i>A</i> of order <i>n</i> , stored in upper- or lower-packed storage mode. For CHPR and ZHPR, <i>ap</i> is the complex Hermitian matrix <i>A</i> of order <i>n</i> , stored in upper- or lower-packed storage mode. For SSLR1 and DSLR1, <i>ap</i> is the real symmetric matrix <i>A</i> of order <i>n</i> , stored in lower-packed storage mode. Specified as: a one-dimensional array of (at least) length $n(n+1)/2$ , containing numbers of the data type indicated in Table 72 on page 320.
<i>a</i>	has the following meaning: For SSYR and DSYR, <i>a</i> is the real symmetric matrix <i>A</i> of order <i>n</i> , stored in upper or lower storage mode. For CHER and ZHER, <i>a</i> is the complex Hermitian matrix <i>A</i> of order <i>n</i> , stored in upper or lower storage mode. Specified as: an <i>lda</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 72 on page 320.
<i>lda</i>	is the leading dimension of the array specified for <i>a</i> . Specified as: a fullword integer; $lda > 0$ and $lda \geq n$ .

### On Return

<i>ap</i>	is the matrix <i>A</i> of order <i>n</i> , containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 72 on page 320.
<i>a</i>	is the matrix <i>A</i> of order <i>n</i> , containing the results of the computation. Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 72 on page 320.

## Notes

1. All subroutines accept lowercase letters for the *uplo* argument.
2. The vector  $x$  must have no common elements with matrix  $A$ ; otherwise, results are unpredictable. See “Concepts” on page 59.
3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq 0.0$ , they are set to zero.
4. For a description of how symmetric matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see “Symmetric Matrix” on page 69. For a description of how complex Hermitian matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see “Complex Hermitian Matrix” on page 73.

## Function

These subroutines perform the computations described in the two sections below. See references [36], [37], and [82]. If  $n$  or  $\alpha$  is 0, no computation is performed.

For CHPR and CHER, intermediate results are accumulated in long precision. For SSPR, SSYR, and SSLR1, intermediate results are accumulated in long precision on some platforms.

### For SSPR, DSPR, SSYR, DSYR, SSLR1, and DSLR1

These subroutines compute the rank-one update of a real symmetric matrix:

$$A \leftarrow A + \alpha x x^T$$

where:

$A$  is a real symmetric matrix of order  $n$ .

$\alpha$  is a scalar.

$x$  is a vector of length  $n$ .

$x^T$  is the transpose of vector  $x$ .

It is expressed as follows:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \begin{bmatrix} x_1 & \dots & x_n \end{bmatrix}$$

### For CHPR, ZHPR, CHER, and ZHER

These subroutines compute the rank-one update of a complex Hermitian matrix:

$$A \leftarrow A + \alpha x x^H$$

where:

$A$  is a complex Hermitian matrix of order  $n$ .

$\alpha$  is a scalar.

$x$  is a vector of length  $n$ .

$x^H$  is the conjugate transpose of vector  $x$ .

It is expressed as follows:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \begin{bmatrix} \bar{x}_1 & \dots & \bar{x}_n \end{bmatrix}$$

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1. *uplo* ≠ 'L' or 'U'
2. *n* < 0
3. *incx* = 0
4. *lda* ≤ 0
5. *lda* < *n*

## Examples

### Example 1

This example shows a vector *x* with a positive stride, and a real symmetric matrix *A* of order 3, stored in lower-packed storage mode. Matrix *A* is:

$$\begin{bmatrix} 8.0 & 4.0 & 2.0 \\ 4.0 & 6.0 & 7.0 \\ 2.0 & 7.0 & 3.0 \end{bmatrix}$$

#### Call Statement and Input:

```

          UPLO  N  ALPHA  X  INCX  AP
          |    |    |    |    |    |
CALL SSPR( 'L' , 3 , 1.0 , X , 1 , AP )

```

```

X          = (3.0, 2.0, 1.0)
AP         = (8.0, 4.0, 2.0, 6.0, 7.0, 3.0)

```

#### Output:

```

AP         = (17.0, 10.0, 5.0, 10.0, 9.0, 4.0)

```

### Example 2

This example shows a vector *x* with a negative stride, and a real symmetric matrix *A* of order 3, stored in upper-packed storage mode. It uses the same input matrix *A* as in Example 1.

#### Call Statement and Input:

```

          UPLO  N  ALPHA  X  INCX  AP
          |    |    |    |    |    |
CALL SSPR( 'U' , 3 , 1.0 , X , -2 , AP )

```

```

X          = (1.0, . , 2.0, . , 3.0)
AP         = (8.0, 4.0, 6.0, 2.0, 7.0, 3.0)

```

#### Output:

## SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, ZHER, SSLR1, and DSLR1

AP = (17.0, 10.0, 10.0, 5.0, 9.0, 4.0)

### Example 3

This example shows a vector  $x$  with a positive stride, and a complex Hermitian matrix  $A$  of order 3, stored in lower-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} (1.0, 0.0) & (3.0, 5.0) & (2.0, -3.0) \\ (3.0, -5.0) & (7.0, 0.0) & (4.0, -8.0) \\ (2.0, 3.0) & (4.0, 8.0) & (6.0, 0.0) \end{bmatrix}$$

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq 0.0$ , they are set to zero.

#### Call Statement and Input:

```
          UPLO N ALPHA X INCX AP
          |   |   |   |   |   |
CALL CHPR( 'L' , 3 , 1.0 , X , 1 , AP )
```

```
X      = ((1.0, 2.0), (4.0, 0.0), (3.0, 4.0))
AP     = ((1.0, . ), (3.0, -5.0), (2.0, 3.0), (7.0, . ),
          (4.0, 8.0), (6.0, . ))
```

#### Output:

```
AP     = ((6.0, 0.0), (7.0, -13.0), (13.0, 1.0), (23.0, 0.0),
          (16.0, 24.0), (31.0, 0.0))
```

### Example 4

This example shows a vector  $x$  with a negative stride, and a complex Hermitian matrix  $A$  of order 3, stored in upper-packed storage mode. It uses the same input matrix  $A$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq 0.0$ , they are set to zero.

#### Call Statement and Input:

```
          UPLO N ALPHA X INCX AP
          |   |   |   |   |   |
CALL CHPR( 'U' , 3 , 1.0 , X , -2 , AP )
```

```
X      = ((3.0, 4.0), . , (4.0, 0.0), . , (1.0, 2.0))
AP     = ((1.0, . ), (3.0, 5.0), (7.0, . ), (2.0, -3.0),
          (4.0, -8.0), (6.0, . ))
```

#### Output:

```
AP     = ((6.0, 0.0), (7.0, 13.0), (23.0, 0.0), (13.0, -1.0),
          (16.0, -24.0), (31.0, 0.0))
```

### Example 5

This example shows a vector  $x$  with a positive stride, and a real symmetric matrix  $A$  of order 3, stored in lower storage mode. It uses the same input matrix  $A$  as in Example 1.

#### Call Statement and Input:

```
          UPLO N ALPHA X INCX A LDA
          |   |   |   |   |   |   |
CALL SSYR( 'L' , 3 , 1.0 , X , 1 , A , 3 )
```

$$X = (3.0, 2.0, 1.0)$$

$$A = \begin{bmatrix} 8.0 & . & . \\ 4.0 & 6.0 & . \\ 2.0 & 7.0 & 3.0 \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} 17.0 & . & . \\ 10.0 & 10.0 & . \\ 5.0 & 9.0 & 4.0 \end{bmatrix}$$

### Example 6

This example shows a vector  $x$  with a negative stride, and a real symmetric matrix  $A$  of order 3, stored in upper storage mode. It uses the same input matrix  $A$  as in Example 1.

**Call Statement and Input:**

```

          UPLO  N  ALPHA  X  INCX  A  LDA
          |    |    |    |    |    |
CALL SSYR( 'U' , 3 , 1.0 , X , -2 , A , 4 )

```

$$X = (1.0, . , 2.0, . , 3.0)$$

$$A = \begin{bmatrix} 8.0 & 4.0 & 2.0 \\ . & 6.0 & 7.0 \\ . & . & 3.0 \\ . & . & . \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} 17.0 & 10.0 & 5.0 \\ . & 10.0 & 9.0 \\ . & . & 4.0 \\ . & . & . \end{bmatrix}$$

### Example 7

This example shows a vector  $x$  with a positive stride, and a complex Hermitian matrix  $A$  of order 3, stored in lower storage mode. It uses the same input matrix  $A$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq 0.0$ , they are set to zero.

**Call Statement and Input:**

```

          UPLO  N  ALPHA  X  INCX  A  LDA
          |    |    |    |    |    |
CALL CHER( 'L' , 3 , 1.0 , X , 1 , A , 3 )

```

$$X = ((1.0, 2.0), (4.0, 0.0), (3.0, 4.0))$$

$$\begin{bmatrix} (1.0, .) & . & . \end{bmatrix}$$

## SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, ZHER, SSLR1, and DSLR1

$$A = \begin{bmatrix} (3.0, -5.0) & (7.0, .) \\ (2.0, 3.0) & (4.0, 8.0) & (6.0, .) \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} (6.0, 0.0) & . & . \\ (7.0, -13.0) & (23.0, 0.0) & . \\ (13.0, 1.0) & (16.0, 24.0) & (31.0, 0.0) \end{bmatrix}$$

### Example 8

This example shows a vector  $x$  with a negative stride, and a complex Hermitian matrix  $A$  of order 3, stored in upper storage mode. It uses the same input matrix  $A$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq 0.0$ , they are set to zero.

**Call Statement and Input:**

```
          UPLO  N  ALPHA  X  INCX  A  LDA
          |    |    |    |    |    |
CALL CHER( 'U' , 3 , 1.0 , X , -2 , A , 3 )
```

$$X = ((3.0, 4.0), . , (4.0, 0.0), . , (1.0, 2.0))$$

$$A = \begin{bmatrix} (1.0, .) & (3.0, 5.0) & (2.0, -3.0) \\ . & (7.0, .) & (4.0, -8.0) \\ . & . & (6.0, .) \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} (6.0, 0.0) & (7.0, 13.0) & (13.0, -1.0) \\ . & (23.0, 0.0) & (16.0, -24.0) \\ . & . & (31.0, 0.0) \end{bmatrix}$$

### Example 9

This example shows a vector  $x$  with a positive stride, and a real symmetric matrix  $A$  of order 3, stored in lower-packed storage mode. It uses the same input matrix  $A$  as in Example 1.

**Call Statement and Input:**

```
          N  ALPHA  X  INCX  AP
          |    |    |    |    |
CALL SSLR1( 3 , 1.0 , X , 1 , AP )
```

$$X = (3.0, 2.0, 1.0)$$
$$AP = (8.0, 4.0, 2.0, 6.0, 7.0, 3.0)$$

**Output:**

$$AP = (17.0, 10.0, 5.0, 10.0, 9.0, 4.0)$$



## SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, ZHER2, SSLR2, and DSLR2 — Rank-Two Update of a Real Symmetric or Complex Hermitian Matrix

### Purpose

SSPR2, DSPR2, SSYR2, DSYR2, SSLR2, and DSLR2 compute the rank-two update of a real symmetric matrix, using the scalar  $\alpha$ , matrix  $A$ , vectors  $x$  and  $y$ , and their transposes  $x^T$  and  $y^T$ :

$$A \leftarrow A + \alpha xy^T + \alpha yx^T$$

CHPR2, ZHPR2, CHER2, and ZHER2, compute the rank-two update of a complex Hermitian matrix, using the scalar  $\alpha$ , matrix  $A$ , vectors  $x$  and  $y$ , and their conjugate transposes  $x^H$  and  $y^H$ :

$$A \leftarrow A + \alpha xy^H + \bar{\alpha} yx^H$$

The following storage modes are used:

- For SSPR2, DSPR2, CHPR2, and ZHPR2, matrix  $A$  is stored in upper- or lower-packed storage mode.
- For SSYR2, DSYR2, CHER2, and ZHER2, matrix  $A$  is stored in upper or lower storage mode.
- For SSLR2 and DSLR2, matrix  $A$  is stored in lower-packed storage mode.

Table 73. Data Types

$\alpha, A, x, y$	Subprogram
Short-precision real	SSPR2, SSYR2, and SSLR2
Long-precision real	DSPR2, DSYR2, and DSLR2
Short-precision complex	CHPR2 and CHER2
Long-precision complex	ZHPR2 and ZHER2

**Note:** SSPR2 and DSPR2 are Level 2 BLAS subroutines. You should use these subroutines instead of SSLR2 and DSLR2, which are only provided for compatibility with earlier releases of ESSL.

### Syntax

<b>Fortran</b>	CALL SSPR2   DSPR2   CHPR2   ZHPR2 ( <i>uplo, n, alpha, x, incx, y, incy, ap</i> ) CALL SSYR2   DSYR2   CHER2   ZHER2 ( <i>uplo, n, alpha, x, incx, y, incy, a, lda</i> ) CALL SSLR2   DSLR2 ( <i>n, alpha, x, incx, y, incy, ap</i> )
<b>C and C++</b>	sspr2   dspr2   chpr2   zhpr2 ( <i>uplo, n, alpha, x, incx, y, incy, ap</i> ); ssyr2   dsyr2   cher2   zher2 ( <i>uplo, n, alpha, x, incx, y, incy, a, lda</i> ); sslr2   dslr2 ( <i>n, alpha, x, incx, y, incy, ap</i> );

**On Entry**

<i>uplo</i>	<p>indicates the storage mode used for matrix <i>A</i>, where:</p> <p>If <i>uplo</i> = 'U', <i>A</i> is stored in upper-packed or upper storage mode.</p> <p>If <i>uplo</i> = 'L', <i>A</i> is stored in lower-packed or lower storage mode.</p> <p>Specified as: a single character. It must be 'U' or 'L'.</p>
<i>n</i>	<p>is the number of elements in vectors <i>x</i> and <i>y</i> and the order of matrix <i>A</i>.</p> <p>Specified as: a fullword integer; <math>n \geq 0</math>.</p>
<i>alpha</i>	<p>is the scaling constant <math>\alpha</math>.</p> <p>Specified as: a number of the data type indicated in Table 73 on page 327.</p>
<i>x</i>	<p>is the vector <i>x</i> of length <i>n</i>.</p> <p>Specified as: a one-dimensional array of (at least) length <math>1+(n-1) incx </math>, containing numbers of the data type indicated in Table 73 on page 327.</p>
<i>incx</i>	<p>is the stride for vector <i>x</i>.</p> <p>Specified as: a fullword integer, where:</p> <p>For SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, and ZHER2, <math>incx &lt; 0</math> or <math>incx &gt; 0</math>.</p> <p>For SSLR2 and DSLR2, <i>incx</i> can have any value.</p>
<i>y</i>	<p>is the vector <i>y</i> of length <i>n</i>.</p> <p>Specified as: a one-dimensional array of (at least) length <math>1+(n-1) incy </math>, containing numbers of the data type indicated in Table 73 on page 327.</p>
<i>incy</i>	<p>is the stride for vector <i>y</i>.</p> <p>Specified as: a fullword integer, where:</p> <p>For SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, and ZHER2, <math>incy &lt; 0</math> or <math>incy &gt; 0</math>.</p> <p>For SSLR2 and DSLR2, <i>incy</i> can have any value.</p>
<i>ap</i>	<p>has the following meaning:</p> <p>For SSPR2 and DSPR2, <i>ap</i> is the real symmetric matrix <i>A</i> of order <i>n</i>, stored in upper- or lower-packed storage mode.</p> <p>For CHPR2 and ZHPR2, <i>ap</i> is the complex Hermitian matrix <i>A</i> of order <i>n</i>, stored in upper- or lower-packed storage mode.</p> <p>For SSLR2 and DSLR2, <i>ap</i> is the real symmetric matrix <i>A</i> of order <i>n</i>, stored in lower-packed storage mode.</p> <p>Specified as: a one-dimensional array of (at least) length <math>n(n+1)/2</math>, containing numbers of the data type indicated in Table 73 on page 327.</p>
<i>a</i>	<p>has the following meaning:</p> <p>For SSYR2 and DSYR2, <i>a</i> is the real symmetric matrix <i>A</i> of order <i>n</i>, stored in upper or lower storage mode.</p>

## SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, ZHER2, SSLR2, and DSLR2

For CHER2 and ZHER2,  $a$  is the complex Hermitian matrix  $A$  of order  $n$ , stored in upper or lower storage mode.

Specified as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 73 on page 327.

$lda$  is the leading dimension of the array specified for  $a$ .  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .

### On Return

$ap$  is the matrix  $A$  of order  $n$ , containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 73 on page 327.

$a$  is the matrix  $A$  of order  $n$ , containing the results of the computation. Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 73 on page 327.

### Notes

1. All subroutines accept lowercase letters for the *uplo* argument.
2. The vectors  $x$  and  $y$  must have no common elements with matrix  $A$ ; otherwise, results are unpredictable. See “Concepts” on page 59.
3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq$  zero, the imaginary parts of the diagonal elements are set to zero.
4. For a description of how symmetric matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see “Symmetric Matrix” on page 69. For a description of how complex Hermitian matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see “Complex Hermitian Matrix” on page 73.

### Function

These subroutines perform the computation described in the two sections below. See references [36], [37], and [82]. If  $n$  or  $\alpha$  is zero, no computation is performed.

For SSPR2, SSYR2, SSLR2, CHPR2, and CHER2, intermediate results are accumulated in long precision.

### SSPR2, DSPR2, SSYR2, DSYR2, SSLR2, and DSLR2

These subroutines compute the rank-two update of a real symmetric matrix:

$$A \leftarrow A + \alpha xy^T + \alpha yx^T$$

where:

$A$  is a real symmetric matrix of order  $n$ .

$\alpha$  is a scalar.

$x$  is a vector of length  $n$ .

$x^T$  is the transpose of vector  $x$ .

$y$  is a vector of length  $n$ .

$y^T$  is the transpose of vector  $y$ .

It is expressed as follows:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} [y_1 \dots y_n] \\ + \alpha \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} [x_1 \dots x_n]$$

### CHPR2, ZHPR2, CHER2, and ZHER2

These subroutines compute the rank-two update of a complex Hermitian matrix:

$$A \leftarrow A + \alpha xy^H + \bar{\alpha}yx^H$$

where:

$A$  is a complex Hermitian matrix of order  $n$ .

$\alpha$  is a scalar.

$x$  is a vector of length  $n$ .

$x^H$  is the conjugate transpose of vector  $x$ .

$y$  is a vector of length  $n$ .

$y^H$  is the conjugate transpose of vector  $y$ .

It is expressed as follows:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} [\bar{y}_1 \dots \bar{y}_n] \\ + \bar{\alpha} \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} [\bar{x}_1 \dots \bar{x}_n]$$

## Error conditions

### Computational Errors

None

**Input-Argument Errors**

1.  $uplo \neq 'L'$  or  $'U'$
2.  $n < 0$
3.  $incx = 0$
4.  $incy = 0$
5.  $lda \leq 0$
6.  $lda < n$

**Examples****Example 1**

This example shows vectors  $x$  and  $y$  with positive strides and a real symmetric matrix  $A$  of order 3, stored in lower-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 8.0 & 4.0 & 2.0 \\ 4.0 & 6.0 & 7.0 \\ 2.0 & 7.0 & 3.0 \end{bmatrix}$$

**Call Statement and Input:**

```

          UPLO N ALPHA X INCX Y INCY AP
          |   |   |   |   |   |   |
CALL SSPR2( 'L' , 3 , 1.0 , X , 1 , Y , 2 , AP )

```

```

X      = (3.0, 2.0, 1.0)
Y      = (5.0, . , 3.0, . , 2.0)
AP     = (8.0, 4.0, 2.0, 6.0, 7.0, 3.0)

```

**Output:**

```
AP     = (38.0, 23.0, 13.0, 18.0, 14.0, 7.0)
```

**Example 2**

This example shows vector  $x$  and  $y$  having strides of opposite signs. For  $x$ , which has negative stride, processing begins at element  $X(5)$ , which is 3.0. The real symmetric matrix  $A$  of order 3 is stored in upper-packed storage mode. It uses the same input matrix  $A$  as in Example 1.

**Call Statement and Input:**

```

          UPLO N ALPHA X INCX Y INCY AP
          |   |   |   |   |   |   |
CALL SSPR2( 'U' , 3 , 1.0 , X , -2 , Y , 2 , AP )

```

```

X      = (1.0, . , 2.0, . , 3.0)
Y      = (5.0, . , 3.0, . , 2.0)
AP     = (8.0, 4.0, 6.0, 2.0, 7.0, 3.0)

```

**Output:**

```
AP     = (38.0, 23.0, 18.0, 13.0, 14.0, 7.0)
```

**Example 3**

This example shows vector  $x$  and  $y$  with positive stride and a complex Hermitian matrix  $A$  of order 3, stored in lower-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} (1.0, 0.0) & (3.0, 5.0) & (2.0, -3.0) \\ (3.0, -5.0) & (7.0, 0.0) & (4.0, -8.0) \\ (2.0, 3.0) & (4.0, 8.0) & (6.0, 0.0) \end{bmatrix}$$



$$A = \begin{bmatrix} 8.0 & . & . \\ 4.0 & 6.0 & . \\ 2.0 & 7.0 & 3.0 \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} 38.0 & . & . \\ 23.0 & 18.0 & . \\ 13.0 & 14.0 & 7.0 \end{bmatrix}$$

### Example 6

This example shows vector  $x$  and  $y$  having strides of opposite signs. For  $x$ , which has negative stride, processing begins at element  $x(5)$ , which is 3.0. The real symmetric matrix  $A$  of order 3 is stored in upper storage mode. It uses the same input matrix  $A$  as in Example 1.

**Call Statement and Input:**

```

                UPLO N  ALPHA X  INCX Y  INCY A  LDA
                |  |  |    |  |   |  |   |  |
CALL SSYR2( 'U' , 3 , 1.0 , X , -2 , Y , 2 , A , 4 )
    
```

$X = (1.0, ., 2.0, ., 3.0)$   
 $Y = (5.0, ., 3.0, ., 2.0)$

$$A = \begin{bmatrix} 8.0 & 4.0 & 2.0 \\ . & 6.0 & 7.0 \\ . & . & 3.0 \\ . & . & . \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} 38.0 & 23.0 & 13.0 \\ . & 18.0 & 14.0 \\ . & . & 7.0 \\ . & . & . \end{bmatrix}$$

### Example 7

This example shows vector  $x$  and  $y$  with positive stride, and a complex Hermitian matrix  $A$  of order 3, stored in lower storage mode. It uses the same input matrix  $A$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq$  zero, the imaginary parts of the diagonal elements are set to zero.

**Call Statement and Input:**

```

                UPLO N  ALPHA X  INCX Y  INCY A  LDA
                |  |  |    |  |   |  |   |  |
CALL CHER2( 'L' , 3 , ALPHA , X , 1 , Y , 2 , A , 3 )
    
```

$ALPHA = (1.0, 0.0)$   
 $X = ((1.0, 2.0), (4.0, 0.0), (3.0, 4.0))$   
 $Y = ((1.0, 0.0), ., (2.0, -1.0), ., (2.0, 1.0))$

$$A = \begin{bmatrix} (1.0, .) & . & . \\ (3.0, -5.0) & (7.0, .) & . \\ (2.0, 3.0) & (4.0, 8.0) & (6.0, .) \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} (3.0, 0.0) & . & . \\ (7.0, -10.0) & (23.0, 0.0) & . \\ (9.0, 4.0) & (14.0, 23.0) & (26.0, 0.0) \end{bmatrix}$$

### Example 8

This example shows vector  $x$  and  $y$  having strides of opposite signs. For  $x$ , which has negative stride, processing begins at element  $x(5)$ , which is  $(1.0, 2.0)$ . The complex Hermitian matrix  $A$  of order 3 is stored in upper storage mode. It uses the same input matrix  $A$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq$  zero, the imaginary parts of the diagonal elements are set to zero.

**Call Statement and Input:**

```

          UPLO N  ALPHA X  INCX Y  INCY A  LDA
CALL CHER2( 'U' , 3 , ALPHA , X , -2 , Y , 2 , A , 3 )

ALPHA   = (1.0, 0.0)
X       = ((3.0, 4.0), . , (4.0, 0.0), . , (1.0, 2.0))
Y       = ((1.0, 0.0), . , (2.0, -1.0), . , (2.0, 1.0))

```

$$A = \begin{bmatrix} (1.0, .) & (3.0, 5.0) & (2.0, -3.0) \\ . & (7.0, .) & (4.0, -8.0) \\ . & . & (6.0, .) \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} (3.0, 0.0) & (7.0, 10.0) & (9.0, -4.0) \\ . & (23.0, 0.0) & (14.0, -23.0) \\ . & . & (26.0, 0.0) \end{bmatrix}$$

### Example 9

This example shows vectors  $x$  and  $y$  with positive strides and a real symmetric matrix  $A$  of order 3, stored in lower-packed storage mode. It uses the same input matrix  $A$  as in Example 1.

**Call Statement and Input:**

```

          N ALPHA X  INCX Y  INCY AP
CALL SSLR2( 3 , 1.0 , X , 1 , Y , 2 , AP )

X       = (3.0, 2.0, 1.0)
Y       = (5.0, . , 3.0, . , 2.0)
AP      = (8.0, 4.0, 2.0, 6.0, 7.0, 3.0)

```

**Output:**



**SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, ZHER2, SSLR2, and DSLR2**

AP = (38.0, 23.0, 13.0, 18.0, 14.0, 7.0)

## SGBMV, DGBMV, CGBMV, and ZGBMV — Matrix-Vector Product for a General Band Matrix, Its Transpose, or Its Conjugate Transpose

### Purpose

SGBMV and DGBMV compute the matrix-vector product for either a real general band matrix or its transpose, where the general band matrix is stored in BLAS-general-band storage mode. It uses the scalars  $\alpha$  and  $\beta$ , vectors  $x$  and  $y$ , and general band matrix  $A$  or its transpose:

$$y \leftarrow \beta y + \alpha Ax$$

$$y \leftarrow \beta y + \alpha A^T x$$

CGBMV and ZGBMV compute the matrix-vector product for either a complex general band matrix, its transpose, or its conjugate transpose, where the general band matrix is stored in BLAS-general-band storage mode. It uses the scalars  $\alpha$  and  $\beta$ , vectors  $x$  and  $y$ , and general band matrix  $A$ , its transpose, or its conjugate transpose:

$$y \leftarrow \beta y + \alpha Ax$$

$$y \leftarrow \beta y + \alpha A^T x$$

$$y \leftarrow \beta y + \alpha A^H x$$

Table 74. Data Types

$\alpha, \beta, x, y, A$	Subprogram
Short-precision real	SGBMV
Long-precision real	DGBMV
Short-precision complex	CGBMV
Long-precision complex	ZGBMV

### Syntax

Fortran	CALL SGBMV   DGBMV   CGBMV   ZGBMV ( <i>transa, m, n, ml, mu, alpha, a, lda, x, incx, beta, y, incy</i> )
C and C++	sgbmv   dgbmv   cgbmv   zgbmv ( <i>transa, m, n, ml, mu, alpha, a, lda, x, incx, beta, y, incy</i> );

### On Entry

*transa* indicates the form of matrix  $A$  to use in the computation, where:

- If *transa* = 'N',  $A$  is used in the computation.
- If *transa* = 'T',  $A^T$  is used in the computation.
- If *transa* = 'C',  $A^H$  is used in the computation.

Specified as: a single character. It must be 'N', 'T', or 'C'.

*m* is the number of rows in matrix  $A$ , and:

- If *transa* = 'N', it is the length of vector  $y$ .
- If *transa* = 'T' or 'C', it is the length of vector  $x$ .

Specified as: a fullword integer;  $m \geq 0$ .

<i>n</i>	<p>is the number of columns in matrix <i>A</i>, and:            If <i>transa</i> = 'N', it is the length of vector <i>x</i>.            If <i>transa</i> = 'T' or 'C', it is the length of vector <i>y</i>.            Specified as: a fullword integer; <math>n \geq 0</math>.</p>
<i>ml</i>	<p>is the lower band width <i>ml</i> of the matrix <i>A</i>.            Specified as: a fullword integer; <math>ml \geq 0</math>.</p>
<i>mu</i>	<p>is the upper band width <i>mu</i> of the matrix <i>A</i>.            Specified as: a fullword integer; <math>mu \geq 0</math>.</p>
<i>alpha</i>	<p>is the scaling constant <math>\alpha</math>.            Specified as: a number of the data type indicated in Table 74 on page 336.</p>
<i>a</i>	<p>is the <i>m</i> by <i>n</i> general band matrix <i>A</i>, stored in BLAS-general-band storage mode. It has an upper band width <i>mu</i> and a lower band width <i>ml</i>. Also:            If <i>transa</i> = 'N', <i>A</i> is used in the computation.            If <i>transa</i> = 'T', <math>A^T</math> is used in the computation.            If <i>transa</i> = 'C', <math>A^H</math> is used in the computation.</p> <p><b>Note:</b> No data should be moved to form <math>A^T</math> or <math>A^H</math>; that is, the matrix <i>A</i> should always be stored in its untransposed form in BLAS-general-band storage mode.</p> <p>Specified as: an <i>lda</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 74 on page 336, where <math>lda \geq ml+mu+1</math>.</p>
<i>lda</i>	<p>is the leading dimension of the array specified for <i>a</i>.            Specified as: a fullword integer; <math>lda &gt; 0</math> and <math>lda \geq ml+mu+1</math>.</p>
<i>x</i>	<p>is the vector <i>x</i>, where:            If <i>transa</i> = 'N', it has length <i>n</i>.            If <i>transa</i> = 'T' or 'C', it has length <i>m</i>.</p> <p>Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 74 on page 336, where:            If <i>transa</i> = 'N', it must have at least <math>1+(n-1) incx </math> elements.            If <i>transa</i> = 'T' or 'C', it must have at least <math>1+(m-1) incx </math> elements.</p>
<i>incx</i>	<p>is the stride for vector <i>x</i>.            Specified as: a fullword integer; <math>incx &gt; 0</math> or <math>incx &lt; 0</math>.</p>
<i>beta</i>	<p>is the scaling constant <math>\beta</math>.            Specified as: a number of the data type indicated in Table 74 on page 336.</p>
<i>y</i>	<p>is the vector <i>y</i>, where:            If <i>transa</i> = 'N', it has length <i>m</i>.            If <i>transa</i> = 'T' or 'C', it has length <i>n</i>.</p>

## SGBMV, DGBMV, CGBMV, and ZGBMV

Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 74 on page 336, where:

If  $transa = 'N'$ , it must have at least  $1+(m-1)|incy|$  elements.

If  $transa = 'T'$  or  $'C'$ , it must have at least  $1+(n-1)|incy|$  elements.

$incy$  is the stride for vector  $y$ .

Specified as: a fullword integer;  $incy > 0$  or  $incy < 0$ .

### On Return

$y$  is the vector  $y$ , containing the result of the computation, where:

If  $transa = 'N'$ , it has length  $m$ .

If  $transa = 'T'$  or  $'C'$ , it has length  $n$ .

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 74 on page 336.

### Notes

1. For SGBMV and DGBMV, if you specify 'C' for the  $transa$  argument, it is interpreted as though you specified 'T'.
2. All subroutines accept lowercase letters for the  $transa$  argument.
3. Vector  $y$  must have no common elements with matrix  $A$  or vector  $x$ ; otherwise, results are unpredictable. See “Concepts” on page 59.
4. To achieve optimal performance, use  $lda = mu+ml+1$ .
5. For general band matrices, if you specify  $ml \geq m$  or  $mu \geq n$ , ESSL assumes, **only for purposes of the computation**, that the lower band width is  $m-1$  or the upper band width is  $n-1$ , respectively. However, ESSL uses the original values for  $ml$  and  $mu$  **for the purposes of finding the locations** of element  $a_{11}$  and all other elements in the array specified for  $A$ , as described in “General Band Matrix” on page 80. For an illustration of this technique, see “Example 4” on page 341.
6. For a description of how a general band matrix is stored in BLAS-general-band storage mode in an array, see “General Band Matrix” on page 80.

### Function

The possible computations that can be performed by these subroutines are described in the following sections. Varying implementation techniques are used for this computation to improve performance. As a result, accuracy of the computational result may vary for different computations.

In all the computations, general band matrix  $A$  is stored in its untransposed form in an array, using BLAS-general-band storage mode.

For SGBMV and CGBMV, intermediate results are accumulated in long precision. Occasionally, for performance reasons, these intermediate results are truncated to short precision and stored.

See references [36], [37], [40], [48], and [82]. No computation is performed if  $m$  or  $n$  is 0 or if  $\alpha$  is zero and  $\beta$  is one.

### General Band Matrix

For SGBMV, DGBMV, CGBMV, and ZGBMV, the matrix-vector product for a general band matrix is expressed as follows:

$$y \leftarrow \beta y + \alpha Ax$$

where:

$x$  is a vector of length  $n$ .

$y$  is a vector of length  $m$ .

$\alpha$  is a scalar.

$\beta$  is a scalar.

$A$  is an  $m$  by  $n$  general band matrix, having a lower band width of  $ml$  and an upper band width of  $mu$ .

### Transpose of a General Band Matrix

For SGBMV, DGBMV, CGBMV, and ZGBMV, the matrix-vector product for the transpose of a general band matrix is expressed as:

$$y \leftarrow \beta y + \alpha A^T x$$

where:

$x$  is a vector of length  $m$ .

$y$  is a vector of length  $n$ .

$\alpha$  is a scalar.

$\beta$  is a scalar.

$A^T$  is the transpose of an  $m$  by  $n$  general band matrix  $A$ , having a lower band width of  $ml$  and an upper band width of  $mu$ .

### Conjugate Transpose of a General Band Matrix

For CGBMV and ZGBMV, the matrix-vector product for the conjugate transpose of a general band matrix is expressed as follows:

$$y \leftarrow \beta y + \alpha A^H x$$

where:

$x$  is a vector of length  $m$ .

$y$  is a vector of length  $n$ .

$\alpha$  is a scalar.

$\beta$  is a scalar.

$A^H$  is the conjugate transpose of an  $m$  by  $n$  general band matrix  $A$  of order  $n$ , having a lower band width of  $ml$  and an upper band width of  $mu$ .

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1. *transa* ≠ 'N', 'T', or 'C'
2. *m* < 0
3. *n* < 0
4. *ml* < 0
5. *mu* < 0
6. *lda* ≤ 0
7. *lda* < *ml*+*mu*+1
8. *incx* = 0
9. *incy* = 0

## Examples

### Example 1

This example shows how to use SGBMV to perform the computation  $y \leftarrow \beta y + \alpha Ax$ , where TRANS is equal to 'N', and the following real general band matrix *A* is used in the computation. Matrix *A* is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 0.0 \\ 2.0 & 2.0 & 2.0 & 2.0 \\ 3.0 & 3.0 & 3.0 & 3.0 \\ 4.0 & 4.0 & 4.0 & 4.0 \\ 0.0 & 5.0 & 5.0 & 5.0 \end{bmatrix}$$

### Call Statement and Input:

```

          TRANS  M    N    ML  MU  ALPHA  A  LDA  X  INCX  BETA  Y  INCY
          |      |    |    |   |   |      |  |   |   |   |   |   |
CALL SGBMV( 'N' , 5 , 4 , 3 , 2 , 2.0 , A , 8 , X , 1 , 10.0 , Y , 2 )
    
```

$$A = \begin{bmatrix} . & . & 1.0 & 2.0 \\ . & 1.0 & 2.0 & 3.0 \\ 1.0 & 2.0 & 3.0 & 4.0 \\ 2.0 & 3.0 & 4.0 & 5.0 \\ 3.0 & 4.0 & 5.0 & . \\ 4.0 & 5.0 & . & . \\ . & . & . & . \\ . & . & . & . \end{bmatrix}$$

X = (1.0, 2.0, 3.0, 4.0)  
 Y = (1.0, . , 2.0, . , 3.0, . , 4.0, . , 5.0, . )

### Output:

Y = (22.0, . , 60.0, . , 90.0, . , 120.0, . , 140.0, . )

### Example 2

This example shows how to use SGBMV to perform the computation  $y \leftarrow \beta y + \alpha A^T x$ , where TRANS is equal to 'T', and the transpose of a real general band matrix *A* is used in the computation. It uses the same input as Example 1.

### Call Statement and Input:

```

          TRANSA M  N  ML  MU  ALPHA  A  LDA  X  INCX  BETA  Y  INCY
          |      |  |  |  |  |      |  |  |  |  |  |  |
CALL SGBMV( 'T' , 5 , 4 , 3 , 2 , 2.0 , A , 8 , X , 1 , 10.0 , Y , 2 )
    
```

**Output:**

Y = (70.0, . , 130.0, . , 140.0, . , 148.0, . )

**Example 3**

This example shows how to use CGBMV to perform the computation  $y \leftarrow \beta y + \alpha A^H x$ , where TRANSA is equal to 'C', and the complex conjugate of the following general band matrix  $A$  is used in the computation. Matrix  $A$  is:

$$\begin{bmatrix}
 (1.0, 1.0) & (1.0, 1.0) & (1.0, 1.0) & (0.0, 0.0) \\
 (2.0, 2.0) & (2.0, 2.0) & (2.0, 2.0) & (2.0, 2.0) \\
 (3.0, 3.0) & (3.0, 3.0) & (3.0, 3.0) & (3.0, 3.0) \\
 (4.0, 4.0) & (4.0, 4.0) & (4.0, 4.0) & (4.0, 4.0) \\
 (0.0, 0.0) & (5.0, 5.0) & (5.0, 5.0) & (0.0, 0.0)
 \end{bmatrix}$$

**Call Statement and Input:**

```

          TRANSA M  N  ML  MU  ALPHA  A  LDA  X  INCX  BETA  Y  INCY
          |      |  |  |  |  |      |  |  |  |  |  |  |
CALL CGBMV( 'C' , 5 , 4 , 3 , 2 , ALPHA , A , 8 , X , 1 , BETA , Y , 2 )
    
```

$$A = \begin{bmatrix}
 . & . & (1.0, 1.0) & (2.0, 2.0) \\
 . & (1.0, 1.0) & (2.0, 2.0) & (3.0, 3.0) \\
 (1.0, 1.0) & (2.0, 2.0) & (3.0, 3.0) & (4.0, 4.0) \\
 (2.0, 2.0) & (3.0, 3.0) & (4.0, 4.0) & (5.0, 5.0) \\
 (3.0, 3.0) & (4.0, 4.0) & (5.0, 5.0) & . \\
 (4.0, 4.0) & (5.0, 5.0) & . & . \\
 . & . & . & . \\
 . & . & . & .
 \end{bmatrix}$$

X = ((1.0, 2.0), (2.0, 3.0), (3.0, 4.0), (4.0, 5.0), (5.0, 6.0))  
 ALPHA = (1.0, 1.0)  
 BETA = (10.0, 0.0)  
 Y = ((1.0, 2.0), . , (2.0, 3.0), . , (3.0, 4.0), . , (4.0, 5.0), . )

**Output:**

Y = ((70.0, 100.0), . , (130.0, 170.0), . , (140.0, 180.0), . , (148.0, 186.0), . )

**Example 4**

This example shows how to use SGBMV to perform the computation  $y \leftarrow \beta y + \alpha Ax$ , where  $ml \geq m$  and  $mu \geq n$ , TRANSA is equal to 'N', and the following real general band matrix  $A$  is used in the computation. Matrix  $A$  is:

$$\begin{bmatrix}
 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\
 2.0 & 2.0 & 2.0 & 2.0 & 2.0 \\
 3.0 & 3.0 & 3.0 & 3.0 & 3.0 \\
 4.0 & 4.0 & 4.0 & 4.0 & 4.0
 \end{bmatrix}$$

**Call Statement and Input:**

```

          TRANSA M  N  ML  MU  ALPHA  A  LDA  X  INCX  BETA  Y  INCY
          |      |  |  |  |  |      |  |  |  |  |  |  |
CALL SGBMV( 'N' , 4 , 5 , 6 , 5 , 2.0 , A , 12 , X , 1 , 10.0 , Y , 2 )
    
```

## SGBMV, DGBMV, CGBMV, and ZGBMV

$$A = \begin{bmatrix} . & . & . & . & . \\ . & . & . & . & 1.0 \\ . & . & . & 1.0 & 2.0 \\ . & . & 1.0 & 2.0 & 3.0 \\ . & 1.0 & 2.0 & 3.0 & 4.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & . \\ 2.0 & 3.0 & 4.0 & . & . \\ 3.0 & 4.0 & . & . & . \\ 4.0 & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \end{bmatrix}$$

$$\begin{aligned} X &= (1.0, 2.0, 3.0, 4.0, 5.0) \\ Y &= (1.0, ., 2.0, ., 3.0, ., 4.0, .) \end{aligned}$$

### Output:

$$Y = (40.0, ., 80.0, ., 120.0, ., 160.0, .)$$



## SSBMV, DSBMV, CHBMV, and ZHBMV — Matrix-Vector Product for a Real Symmetric or Complex Hermitian Band Matrix

### Purpose

SSBMV and DSBMV compute the matrix-vector product for a real symmetric band matrix. CHBMV and ZHBMV compute the matrix-vector product for a complex Hermitian band matrix. The band matrix  $A$  is stored in either upper- or lower-band-packed storage mode. It uses the scalars  $\alpha$  and  $\beta$ , vectors  $x$  and  $y$ , and band matrix  $A$ :

$$y \leftarrow \beta y + \alpha Ax$$

$$y \leftarrow \beta y + \alpha Ax$$

Table 75. Data Types

$\alpha, \beta, x, y, A$	Subprogram
Short-precision real	SSBMV
Long-precision real	DSBMV
Short-precision complex	CHBMV
Long-precision complex	ZHBMV

### Syntax

<b>Fortran</b>	CALL SSBMV   DSBMV   CHBMV   ZHBMV ( <i>uplo, n, k, alpha, a, lda, x, incx, beta, y, incy</i> )
<b>C and C++</b>	ssbmv   dsbmv   chbmv   zhbmv ( <i>uplo, n, k, alpha, a, lda, x, incx, beta, y, incy</i> );

### On Entry

- uplo* indicates the storage mode used for matrix  $A$ , where either the upper or lower triangle can be stored:  
 If *uplo* = 'U',  $A$  is stored in upper-band-packed storage mode.  
 If *uplo* = 'L',  $A$  is stored in lower-band-packed storage mode.  
 Specified as: a single character. It must be 'U' or 'L'.
- n* is the order of matrix  $A$  and the number of elements in vectors  $x$  and  $y$ .  
 Specified as: a fullword integer;  $n \geq 0$ .
- k* is the half band width  $k$  of the matrix  $A$ .  
 Specified as: a fullword integer;  $k \geq 0$ .
- alpha* is the scaling constant  $\alpha$ .  
 Specified as: a number of the data type indicated in Table 75.
- a* is the real symmetric or complex Hermitian band matrix  $A$  of order  $n$ , having a half band width of  $k$ , where:  
 If *uplo* = 'U',  $A$  is stored in upper-band-packed storage mode.  
 If *uplo* = 'L',  $A$  is stored in lower-band-packed storage mode.  
 Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 75, where  $lda \geq k+1$ .

## SSBMV, DSBMV, CHBMV, and ZHBMV

<i>lda</i>	is the leading dimension of the array specified for <i>a</i> . Specified as: a fullword integer; $lda > 0$ and $lda \geq k+1$ .
<i>x</i>	is the vector <i>x</i> of length <i>n</i> . Specified as: a one-dimensional array of (at least) length $1+(n-1) incx $ , containing numbers of the data type indicated in Table 75 on page 343.
<i>incx</i>	is the stride for vector <i>x</i> . Specified as: a fullword integer; $incx > 0$ or $incx < 0$ .
<i>beta</i>	is the scaling constant $\beta$ . Specified as: a number of the data type indicated in Table 75 on page 343.
<i>y</i>	is the vector <i>y</i> of length <i>n</i> . Specified as: a one-dimensional array of (at least) length <i>n</i> , containing numbers of the data type indicated in Table 75 on page 343.
<i>incy</i>	is the stride for vector <i>y</i> . Specified as: a fullword integer; $incy > 0$ or $incy < 0$ .

### On Return

<i>y</i>	is the vector <i>y</i> of length <i>n</i> , containing the result of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 75 on page 343.
----------	--

## Notes

1. All subroutines accept lowercase letters for the *uplo* argument.
2. Vector *y* must have no common elements with matrix *A* or vector *x*; otherwise, results are unpredictable. See “Concepts” on page 59.
3. To achieve optimal performance in these subroutines, use  $lda = k+1$ .
4. The imaginary parts of the diagonal elements of the complex Hermitian matrix *A* are assumed to be zero, so you do not have to set these values.
5. For real symmetric and complex Hermitian band matrices, if you specify  $k \geq n$ , ESSL assumes, **only for purposes of the computation**, that the half band width of matrix *A* is  $n-1$ ; that is, it processes matrix *A*, of order *n*, as though it is a (nonbanded) real symmetric or complex Hermitian matrix. However, ESSL uses the original value for *k* **for the purposes of finding the locations** of element  $a_{11}$  and all other elements in the array specified for *A*, as described in the storage modes referenced in the next note. For an illustration of this technique, see “Example 3” on page 346.
6. For a description of how a real symmetric band matrix is stored, see “Upper-Band-Packed Storage Mode” on page 86 or “Lower-Band-Packed Storage Mode” on page 87. For a description of how a complex Hermitian band matrix is stored, see “Complex Hermitian Matrix” on page 73.

## Function

These subroutines perform the following matrix-vector product, using a real symmetric or complex Hermitian band matrix *A*, stored in either upper- or lower-band-packed storage mode:

$$y \leftarrow \beta y + \alpha Ax$$

where:

$x$  and  $y$  are vectors of length  $n$ .

$\alpha$  and  $\beta$  are scalars.

$A$  is a real symmetric or complex Hermitian band matrix of order  $n$ , having a half bandwidth of  $k$ .

For SSBMV and CHBMV, intermediate results are accumulated in long precision. Occasionally, for performance reasons, these intermediate results are truncated to short precision and stored.

See references [36], [40], [48], and [82]. No computation is performed if  $n$  is 0 or if  $\alpha$  is zero and  $\beta$  is one.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $uplo \neq 'U'$  or  $'L'$
2.  $n < 0$
3.  $k < 0$
4.  $lda \leq 0$
5.  $lda < k+1$
6.  $incx = 0$
7.  $incy = 0$

## Examples

### Example 1

This example shows how to use SSBMV to perform the matrix-vector product, where the real symmetric band matrix  $A$  of order 7 and half band width of 3 is stored in upper-band-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 2.0 & 2.0 & 2.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 3.0 & 3.0 & 3.0 & 3.0 & 0.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 4.0 & 4.0 & 4.0 \\ 0.0 & 2.0 & 3.0 & 4.0 & 5.0 & 5.0 & 5.0 \\ 0.0 & 0.0 & 3.0 & 4.0 & 5.0 & 6.0 & 6.0 \\ 0.0 & 0.0 & 0.0 & 4.0 & 5.0 & 6.0 & 7.0 \end{bmatrix}$$

### Call Statement and Input:

```

          UPLO  N   K ALPHA  A  LDA  X  INCX  BETA  Y  INCY
          |    |   |      |  |    |  |    |    |   |   |
CALL SSBMV( 'U' , 7 , 3 , 2.0 , A , 5 , X , 1 , 10.0 , Y , 2 )

```

$$A = \begin{bmatrix} . & . & . & 1.0 & 2.0 & 3.0 & 4.0 \\ . & . & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \\ . & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 \end{bmatrix}$$

## SSBMV, DSBMV, CHBMV, and ZHBMV

$$\left[ \begin{array}{cccccccc} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{array} \right]$$

X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0)  
 Y = (1.0, . , 2.0, . , 3.0, . , 4.0, . , 5.0, . , 6.0, . , 7.0)

### Output:

Y = (30.0, . , 78.0, . , 148.0, . , 244.0, . , 288.0, . ,  
 316.0, . , 322.0)

### Example 2

This example shows how to use CHBMV to perform the matrix-vector product, where the complex Hermitian band matrix *A* of order 7 and half band width of 3 is stored in lower-band-packed storage mode. Matrix *A* is:

$$\left[ \begin{array}{ccccccc} (1.0, 0.0) & (1.0, 1.0) & (1.0, 1.0) & (1.0, 1.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) \\ (1.0, -1.0) & (2.0, 0.0) & (2.0, 2.0) & (2.0, 2.0) & (2.0, 2.0) & (0.0, 0.0) & (0.0, 0.0) \\ (1.0, -1.0) & (2.0, -2.0) & (3.0, 0.0) & (3.0, 3.0) & (3.0, 3.0) & (3.0, 3.0) & (0.0, 0.0) \\ (1.0, -1.0) & (2.0, -2.0) & (3.0, -3.0) & (4.0, 0.0) & (4.0, 4.0) & (4.0, 4.0) & (4.0, 4.0) \\ (0.0, 0.0) & (2.0, -2.0) & (3.0, -3.0) & (4.0, -4.0) & (5.0, 0.0) & (5.0, 5.0) & (5.0, 5.0) \\ (0.0, 0.0) & (0.0, 0.0) & (3.0, -3.0) & (4.0, -4.0) & (5.0, -5.0) & (6.0, 0.0) & (6.0, 6.0) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (4.0, -4.0) & (5.0, -5.0) & (6.0, -6.0) & (7.0, 0.0) \end{array} \right]$$

**Note:** The imaginary parts of the diagonal elements of a complex Hermitian matrix are assumed to be zero, so you do not need to set these values.

### Call Statement and Input:

```

          UPLO N  K  ALPHA  A  LDA  X  INCX  BETA  Y  INCY
CALL CHBMV( 'L' , 7 , 3 , ALPHA , A , 5 , X , 1 , BETA , Y , 2 )

ALPHA = (2.0, 0.0)
BETA  = (10.0, 0.0)

```

$$A = \left[ \begin{array}{ccccccc} (1.0, .) & (2.0, .) & (3.0, .) & (4.0, .) & (5.0, .) & (6.0, .) & (7.0, .) \\ (1.0, 1.0) & (2.0, 2.0) & (3.0, 3.0) & (4.0, 4.0) & (5.0, 5.0) & (6.0, 6.0) & . \\ (1.0, 1.0) & (2.0, 2.0) & (3.0, 3.0) & (4.0, 4.0) & (5.0, 5.0) & . & . \\ (1.0, 1.0) & (2.0, 2.0) & (3.0, 3.0) & (4.0, 4.0) & . & . & . \\ . & . & . & . & . & . & . \end{array} \right]$$

X = ((1.0, 1.0), (2.0, 2.0), (3.0, 3.0), (4.0, 4.0),  
 (5.0, 5.0), (6.0, 6.0), (7.0, 7.0))  
 Y = ((1.0, 1.0), . , (2.0, 2.0), . , (3.0, 3.0), . ,  
 (4.0, 4.0), . , (5.0, 5.0), . , (6.0, 6.0), . ,  
 (7.0, 7.0))

### Output:

Y = ((48.0, 12.0), . , (124.0, 32.0), . , (228.0, 68.0), . ,  
 (360.0, 128.0), . , (360.0, 216.0), . ,  
 (300.0, 332.0), . , (168.0, 476.0))

### Example 3

This example shows how to use SSBMV to perform the matrix-vector product, where  $n \geq k$ . Matrix *A* is a real 5 by 5 symmetric band matrix with a half band width of 5, stored in upper-band-packed storage mode. Matrix *A* is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 1.0 & 2.0 & 2.0 & 2.0 & 2.0 \\ 1.0 & 2.0 & 3.0 & 3.0 & 3.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 4.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \end{bmatrix}$$

**Call Statement and Input:**

```

          UPLO N  K ALPHA  A  LDA  X  INCX  BETA  Y  INCY
          |   |  |   |    |   |   |   |   |   |   |
CALL SSBMV( 'U' , 5 , 5 , 2.0 , A , 7 , X , 1 , 10.0 , Y , 2 )
    
```

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1.0 & 2.0 \\ \cdot & \cdot & 1.0 & 2.0 & 3.0 \\ \cdot & 1.0 & 2.0 & 3.0 & 4.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

X = (1.0, 2.0, 3.0, 4.0, 5.0)  
 Y = (1.0, . , 2.0, . , 3.0, . , 4.0, . , 5.0, . )

**Output:**

Y = (40.0, . , 78.0, . , 112.0, . , 140.0, . , 160.0, . )

## STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, and ZTPMV — Matrix-Vector Product for a Triangular Matrix, Its Transpose, or Its Conjugate Transpose

### Purpose

STRMV, DTRMV, STPMV, and DTPMV compute one of the following matrix-vector products, using the vector  $x$  and triangular matrix  $A$  or its transpose:

$$x \leftarrow Ax$$

$$x \leftarrow A^T x$$

CTRMV, ZTRMV, CTPMV, and ZTPMV compute one of the following matrix-vector products, using the vector  $x$  and triangular matrix  $A$ , its transpose, or its conjugate transpose:

$$x \leftarrow Ax$$

$$x \leftarrow A^T x$$

$$x \leftarrow A^H x$$

Matrix  $A$  can be either upper or lower triangular, where:

- For the `_TRMV` subroutines, it is stored in upper- or lower-triangular storage mode, respectively.
- For the `_TPMV` subroutines, it is stored in upper- or lower-triangular-packed storage mode, respectively.

Table 76. Data Types

$A, x$	Subprogram
Short-precision real	STRMV and STPMV
Long-precision real	DTRMV and DTPMV
Short-precision complex	CTRMV and CTPMV
Long-precision complex	ZTRMV and ZTPMV

### Syntax

Fortran	CALL STRMV   DTRMV   CTRMV   ZTRMV ( <i>uplo, transa, diag, n, a, lda, x, incx</i> )
	CALL STPMV   DTPMV   CTPMV   ZTPMV ( <i>uplo, transa, diag, n, ap, x, incx</i> )
C and C++	strmv   dtrmv   ctrmv   ztrmv ( <i>uplo, transa, diag, n, a, lda, x, incx</i> ); stpmv   dtpmv   ctpmv   ztpmv ( <i>uplo, transa, diag, n, ap, x, incx</i> );

### On Entry

*uplo* indicates whether matrix  $A$  is an upper or lower triangular matrix, where:

If *uplo* = 'U',  $A$  is an upper triangular matrix.

If *uplo* = 'L',  $A$  is a lower triangular matrix.

Specified as: a single character. It must be 'U' or 'L'.

*transa* indicates the form of matrix  $A$  to use in the computation, where:

## STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, and ZTPMV

	If <i>transa</i> = 'N', <i>A</i> is used in the computation.
	If <i>transa</i> = 'T', $A^T$ is used in the computation.
	If <i>transa</i> = 'C', $A^H$ is used in the computation.
	Specified as: a single character. It must be 'N', 'T', or 'C'.
<i>diag</i>	indicates the characteristics of the diagonal of matrix <i>A</i> , where: If <i>diag</i> = 'U', <i>A</i> is a unit triangular matrix. If <i>diag</i> = 'N', <i>A</i> is not a unit triangular matrix. Specified as: a single character. It must be 'U' or 'N'.
<i>n</i>	is the order of triangular matrix <i>A</i> . Specified as: a fullword integer; $0 \leq n \leq lda$ .
<i>a</i>	is the upper or lower triangular matrix <i>A</i> of order <i>n</i> , stored in upper- or lower-triangular storage mode, respectively.  <b>Note:</b> No data should be moved to form $A^T$ or $A^H$ ; that is, the matrix <i>A</i> should always be stored in its untransposed form. Specified as: an <i>lda</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 76 on page 348.
<i>lda</i>	is the leading dimension of the array specified for <i>a</i> . Specified as: a fullword integer; $lda > 0$ and $lda \geq n$ .
<i>ap</i>	is the upper or lower triangular matrix <i>A</i> of order <i>n</i> , stored in upper- or lower-triangular-packed storage mode, respectively. Specified as: a one-dimensional array of (at least) length $n(n+1)/2$ , containing numbers of the data type indicated in Table 76 on page 348.
<i>x</i>	is the vector <i>x</i> of length <i>n</i> . Specified as: a one-dimensional array of (at least) length $1+(n-1) incx $ , containing numbers of the data type indicated in Table 76 on page 348.
<i>incx</i>	is the stride for vector <i>x</i> . Specified as: a fullword integer; $incx > 0$ or $incx < 0$ .

### On Return

<i>x</i>	is the vector <i>x</i> of length <i>n</i> , containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 76 on page 348.
----------	---

### Notes

1. These subroutines accept lowercase letters for the *uplo*, *transa*, and *diag* arguments.
2. For STRMV, DTRMV, STPMV, and DTPMV if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
3. Matrix *A* and vector *x* must have no common elements; otherwise, results are unpredictable.
4. ESSL assumes certain values in your array for parts of a triangular matrix. As a result, you do not have to set these values. For unit triangular matrices, the

## STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, and ZTPMV

elements of the diagonal are assumed to be 1.0 for real matrices and (1.0, 0.0) for complex matrices. When using upper- or lower-triangular storage, the unreferenced elements in the lower and upper triangular part, respectively, are assumed to be zero.

5. For a description of triangular matrices and how they are stored in upper- and lower-triangular storage mode and in upper- and lower-triangular-packed storage mode, see “Triangular Matrix” on page 77.

### Function

These subroutines can perform the following matrix-vector product computations, using the triangular matrix  $A$ , its transpose, or its conjugate transpose, where  $A$  can be either upper or lower triangular:

$$\begin{aligned}x &\leftarrow Ax \\x &\leftarrow A^T x \\x &\leftarrow A^H x \quad (\text{for CTRMV, ZTRMV, CTPMV, and ZTPMV only})\end{aligned}$$

where:

$x$  is a vector of length  $n$ .

$A$  is an upper or lower triangular matrix of order  $n$ . For `_TRMV`, it is stored in upper- or lower-triangular storage mode, respectively. For `_TPMV`, it is stored in upper- or lower-triangular-packed storage mode, respectively.

See references [34] and [40]. If  $n$  is 0, no computation is performed.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

1.  $uplo \neq 'L'$  or  $'U'$
2.  $transa \neq 'T', 'N',$  or  $'C'$
3.  $diag \neq 'N'$  or  $'U'$
4.  $n < 0$
5.  $lda \leq 0$
6.  $lda < n$
7.  $incx = 0$

### Examples

#### Example 1

This example shows the computation  $x \leftarrow Ax$ . Matrix  $A$  is a real 4 by 4 lower triangular matrix that is unit triangular, stored in lower-triangular storage mode. Vector  $x$  is a vector of length 4. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & . & . & . \\ 1.0 & 1.0 & . & . \\ 2.0 & 3.0 & 1.0 & . \\ 3.0 & 4.0 & 3.0 & 1.0 \end{bmatrix}$$

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.



## STRMV, DTRMV, CTRMV, ZTRMV, SPMV, DTPMV, CTPMV, and ZTPMV

### Call Statement and Input:

```

          UPLO  TRANSA  DIAG  N  A  LDA  X  INCX
          |      |      |      |  |  |  |  |
CALL STRMV( 'L' , 'N' , 'U' , 4 , A , 4 , X , 1 )

```

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ 1.0 & \cdot & \cdot & \cdot \\ 2.0 & 3.0 & \cdot & \cdot \\ 3.0 & 4.0 & 3.0 & \cdot \end{bmatrix}$$

$$X = (1.0, 2.0, 3.0, 4.0)$$

### Output:

$$X = (1.0, 3.0, 11.0, 24.0)$$

### Example 2

This example shows the computation  $x \leftarrow A^T x$ . Matrix  $A$  is a real 4 by 4 upper triangular matrix that is unit triangular, stored in upper-triangular storage mode. Vector  $x$  is a vector of length 4. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 2.0 & 3.0 & 2.0 \\ \cdot & 1.0 & 2.0 & 5.0 \\ \cdot & \cdot & 1.0 & 3.0 \\ \cdot & \cdot & \cdot & 1.0 \end{bmatrix}$$

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

### Call Statement and Input:

```

          UPLO  TRANSA  DIAG  N  A  LDA  X  INCX
          |      |      |      |  |  |  |  |
CALL STRMV( 'U' , 'T' , 'U' , 4 , A , 4 , X , 1 )

```

$$A = \begin{bmatrix} \cdot & 2.0 & 3.0 & 2.0 \\ \cdot & \cdot & 2.0 & 5.0 \\ \cdot & \cdot & \cdot & 3.0 \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$X = (5.0, 4.0, 3.0, 2.0)$$

### Output:

$$X = (5.0, 14.0, 26.0, 41.0)$$

### Example 3

This example shows the computation  $x \leftarrow A^H x$ . Matrix  $A$  is a complex 4 by 4 upper triangular matrix that is unit triangular, stored in upper-triangular storage mode. Vector  $x$  is a vector of length 4. Matrix  $A$  is:

$$\begin{bmatrix} (1.0, 0.0) & (2.0, 2.0) & (3.0, 3.0) & (2.0, 2.0) \\ \cdot & (1.0, 0.0) & (2.0, 2.0) & (5.0, 5.0) \\ \cdot & \cdot & (1.0, 0.0) & (3.0, 3.0) \\ \cdot & \cdot & \cdot & (1.0, 0.0) \end{bmatrix}$$

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of (1.0, 0.0) for the diagonal elements.

## STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, and ZTPMV

### Call Statement and Input:

```
          UPLO  TRANSA  DIAG  N   A   LDA  X   INCX
          |    |      |    |   |   |   |   |
CALL CTRMV( 'U' , 'C' , 'U' , 4 , A , 4 , X , 1 )
```

$$A = \begin{bmatrix} . & (2.0, 2.0) & (3.0, 3.0) & (2.0, 2.0) \\ . & . & (2.0, 2.0) & (5.0, 5.0) \\ . & . & . & (3.0, 3.0) \\ . & . & . & . \end{bmatrix}$$

$$X = ((5.0, 5.0), (4.0, 4.0), (3.0, 3.0), (2.0, 2.0))$$

### Output:

$$X = ((5.0, 5.0), (24.0, 4.0), (49.0, 3.0), (80.0, 2.0))$$

### Example 4

This example shows the computation  $x \leftarrow Ax$ . Matrix  $A$  is a real 4 by 4 lower triangular matrix that is unit triangular, stored in lower-triangular-packed storage mode. Vector  $x$  is a vector of length 4. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & . & . & . \\ 1.0 & 1.0 & . & . \\ 2.0 & 3.0 & 1.0 & . \\ 3.0 & 4.0 & 3.0 & 1.0 \end{bmatrix}$$

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

### Call Statement and Input:

```
          UPLO  TRANSA  DIAG  N   AP   X   INCX
          |    |      |    |   |   |   |
CALL STPMV( 'L' , 'N' , 'U' , 4 , AP , X , 1 )
```

$$\begin{aligned} AP &= ( . , 1.0, 2.0, 3.0, . , 3.0, 4.0, . , 3.0, . ) \\ X &= (1.0, 2.0, 3.0, 4.0) \end{aligned}$$

### Output:

$$X = (1.0, 3.0, 11.0, 24.0)$$

### Example 5

This example shows the computation  $x \leftarrow A^T x$ . Matrix  $A$  is a real 4 by 4 upper triangular matrix that is not unit triangular, stored in upper-triangular-packed storage mode. Vector  $x$  is a vector of length 4. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 2.0 & 3.0 & 2.0 \\ . & 2.0 & 2.0 & 5.0 \\ . & . & 3.0 & 3.0 \\ . & . & . & 1.0 \end{bmatrix}$$

### Call Statement and Input:

```
          UPLO  TRANSA  DIAG  N   AP   X   INCX
          |    |      |    |   |   |   |
CALL STPMV( 'U' , 'T' , 'N' , 4 , AP , X , 1 )
```

$$\begin{aligned} AP &= (1.0, 2.0, 2.0, 3.0, 2.0, 3.0, 2.0, 5.0, 3.0, 1.0) \\ X &= (5.0, 4.0, 3.0, 2.0) \end{aligned}$$

## STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, and ZTPMV

### Output:

X = (5.0, 18.0, 32.0, 41.0)

### Example 6

This example shows the computation  $x \leftarrow A^H x$ . Matrix  $A$  is a complex 4 by 4 upper triangular matrix that is unit triangular, stored in upper-triangular-packed storage mode. Vector  $x$  is a vector of length 4. Matrix  $A$  is:

$$\begin{bmatrix} (1.0, 0.0) & (2.0, 2.0) & (3.0, 3.0) & (2.0, 2.0) \\ . & (1.0, 0.0) & (2.0, 2.0) & (5.0, 5.0) \\ . & . & (1.0, 0.0) & (3.0, 3.0) \\ . & . & . & (1.0, 0.0) \end{bmatrix}$$

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of (1.0, 0.0) for the diagonal elements.

### Call Statement and Input:

```
                UPLO TRANSA DIAG  N  AP  X  INCX
                |   |   |   |   |   |   |
CALL CTPMV( 'U' , 'C' , 'U' , 4 , AP , X , 1 )

AP      = ( . , (2.0, 2.0), . , (3.0, 3.0), (2.0, 2.0), . ,
           (2.0, 2.0), (5.0, 5.0), (3.0, 3.0), . )
X       = ((5.0, 5.0), (4.0, 4.0), (3.0, 3.0), (2.0, 2.0))
```

### Output:

X = ((5.0, 5.0), (24.0, 4.0), (49.0, 3.0), (80.0, 2.0))

## STBMV, DTBMV, CTBMV, and ZTBMV — Matrix-Vector Product for a Triangular Band Matrix, Its Transpose, or Its Conjugate Transpose

### Purpose

STBMV and DTBMV compute one of the following matrix-vector products, using the vector  $x$  and triangular band matrix  $A$  or its transpose:

$$x \leftarrow Ax$$

$$x \leftarrow A^T x$$

CTBMV and ZTBMV compute one of the following matrix-vector products, using the vector  $x$  and triangular band matrix  $A$ , its transpose, or its conjugate transpose:

$$x \leftarrow Ax$$

$$x \leftarrow A^T x$$

$$x \leftarrow A^H x$$

Matrix  $A$  can be either upper or lower triangular and is stored in upper- or lower-triangular-band-packed storage mode, respectively.

Table 77. Data Types

$A, x$	Subprogram
Short-precision real	STBMV
Long-precision real	DTBMV
Short-precision complex	CTBMV
Long-precision complex	ZTBMV

### Syntax

Fortran	CALL STBMV   DTBMV   CTBMV   ZTBMV ( <i>uplo, transa, diag, n, k, a, lda, x, incx</i> )
C and C++	stbmvl   dtbmvl   ctbmvl   ztbmvl ( <i>uplo, transa, diag, n, k, a, lda, x, incx</i> );

### On Entry

*uplo* indicates whether matrix  $A$  is an upper or lower triangular band matrix, where:

If *uplo* = 'U',  $A$  is an upper triangular matrix.

If *uplo* = 'L',  $A$  is a lower triangular matrix.

Specified as: a single character. It must be 'U' or 'L'.

*transa* indicates the form of matrix  $A$  to use in the computation, where:

If *transa* = 'N',  $A$  is used in the computation.

If *transa* = 'T',  $A^T$  is used in the computation.

If *transa* = 'C',  $A^H$  is used in the computation.

Specified as: a single character. It must be 'N', 'T', or 'C'.

*diag* indicates the characteristics of the diagonal of matrix  $A$ , where:

If *diag* = 'U',  $A$  is a unit triangular matrix.

If *diag* = 'N', *A* is not a unit triangular matrix.  
 Specified as: a single character. It must be 'U' or 'N'.

*n* is the order of triangular band matrix *A*. Specified as: a fullword integer;  $n \geq 0$ .

*k* is the upper or lower band width *k* of the matrix *A*.  
 Specified as: a fullword integer;  $k \geq 0$ .

*a* is the upper or lower triangular band matrix *A* of order *n*, stored in upper- or lower-triangular-band-packed storage mode, respectively.

**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix *A* should always be stored in its untransposed form. Specified as: an *lda* by (at least) *n* array, containing numbers of the data type indicated in Table 77 on page 354.

*lda* is the leading dimension of the array specified for *a*.  
 Specified as: a fullword integer;  $lda > 0$  and  $lda \geq k+1$ .

*x* is the vector *x* of length *n*.  
 Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 77 on page 354.

*incx* is the stride for vector *x*.  
 Specified as: a fullword integer;  $incx > 0$  or  $incx < 0$ .

### On Return

*x* is the vector *x* of length *n*, containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 77 on page 354.

### Notes

1. These subroutines accept lowercase letters for the *uplo*, *transa*, and *diag* arguments.
2. For STBMV and DTBMV, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
3. Matrix *A* and vector *x* must have no common elements; otherwise, results are unpredictable.
4. To achieve optimal performance in these subroutines, use  $lda = k+1$ .
5. For unit triangular matrices, the elements of the diagonal are assumed to be 1.0 for real matrices and (1.0, 0.0) for complex matrices. As a result, you do not have to set these values.
6. For both upper and lower triangular band matrices, if you specify  $k \geq n$ , ESSL assumes, **only for purposes of the computation**, that the upper or lower band width of matrix *A* is  $n-1$ ; that is, it processes matrix *A*, of order *n*, as though it is a (nonbanded) triangular matrix. However, ESSL uses the original value for *k* **for the purposes of finding the locations** of element  $a_{11}$  and all other elements in the array specified for *A*, as described in "Triangular Band Matrix" on page 88. For an illustration of this technique, see "Example 4" on page 358.

## STBMV, DTBMV, CTBMV, and ZTBMV

7. For a description of triangular band matrices and how they are stored in upper- and lower-triangular-band-packed storage mode, see “Triangular Band Matrix” on page 88.
8. If you are using a lower triangular band matrix, you may want to use this alternate approach instead of using lower-triangular-band-packed storage mode. Leave matrix  $A$  in full-matrix storage mode when you pass it to ESSL and specify the  $lda$  argument to be  $lda+1$ , which is the leading dimension of matrix  $A$  plus 1. ESSL then processes the matrix elements in the same way as though you had set them up in lower-triangular-band-packed storage mode.

### Function

These subroutines can perform the following matrix-vector product computations, using the triangular band matrix  $A$ , its transpose, or its conjugate transpose, where  $A$  can be either upper or lower triangular:

$$\begin{aligned}x &\leftarrow Ax \\x &\leftarrow A^T x \\x &\leftarrow A^H x \quad (\text{for CTBMV and ZTBMV only})\end{aligned}$$

where:

$x$  is a vector of length  $n$ .

$A$  is an upper or lower triangular band matrix of order  $n$ , stored in upper- or lower-triangular-band-packed storage mode, respectively.

See references [36], [48], and [40]. If  $n$  is 0, no computation is performed.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

1.  $uplo \neq 'L'$  or  $'U'$
2.  $transa \neq 'T', 'N',$  or  $'C'$
3.  $diag \neq 'N'$  or  $'U'$
4.  $n < 0$
5.  $k < 0$
6.  $lda \leq 0$
7.  $lda < k+1$
8.  $incx = 0$

### Examples

#### Example 1

This example shows the computation  $x \leftarrow Ax$ . Matrix  $A$  is a real 7 by 7 upper triangular band matrix with a half band width of 3 that is not unit triangular, stored in upper-triangular-band-packed storage mode. Vector  $x$  is a vector of length 7. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & 2.0 & 2.0 & 2.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 3.0 & 3.0 & 3.0 & 3.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 4.0 & 4.0 & 4.0 & 4.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 5.0 & 5.0 & 5.0 \end{bmatrix}$$

$$\begin{bmatrix} 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 6.0 & 6.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 7.0 \end{bmatrix}$$

**Call Statement and Input:**

```

          UPLO  TRANSA  DIAG  N  K  A  LDA  X  INCX
CALL STBMV( 'U' , 'N' , 'N' , 7 , 3 , A , 5 , X , 1 )
    
```

$$A = \begin{bmatrix} . & . & . & 1.0 & 2.0 & 3.0 & 4.0 \\ . & . & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \\ . & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 \\ . & . & . & . & . & . & . \end{bmatrix}$$

$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0)$$

**Output:**

$$X = (10.0, 28.0, 54.0, 88.0, 90.0, 78.0, 49.0)$$

**Example 2**

This example shows the computation  $x \leftarrow A^T x$ . Matrix  $A$  is a real 7 by 7 lower triangular band matrix with a half band width of 3 that is not unit triangular, stored in lower-triangular-band-packed storage mode. Vector  $x$  is a vector of length 7. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 3.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & 3.0 & 4.0 & 5.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 3.0 & 4.0 & 5.0 & 6.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 4.0 & 5.0 & 6.0 & 7.0 \end{bmatrix}$$

**Call Statement and Input:**

```

          UPLO  TRANSA  DIAG  N  K  A  LDA  X  INCX
CALL STBMV( 'L' , 'T' , 'N' , 7 , 3 , A , 5 , X , 1 )
    
```

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & . \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & . & . \\ 1.0 & 2.0 & 3.0 & 4.0 & . & . & . \\ . & . & . & . & . & . & . \end{bmatrix}$$

$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0)$$

**Output:**

$$X = (10.0, 28.0, 54.0, 88.0, 90.0, 78.0, 49.0)$$

**Example 3**

This example shows the computation  $x \leftarrow A^H x$ . Matrix  $A$  is a complex 7 by 7 upper triangular band matrix with a half band width of 3 that is not unit triangular, stored in upper-triangular-band-packed storage mode. Vector  $x$  is a vector of length 7. Matrix  $A$  is:

## STBMV, DTBMV, CTBMV, and ZTBMV

$$\begin{bmatrix} (1.0, 1.0) & (1.0, 1.0) & (1.0, 1.0) & (1.0, 1.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) \\ (0.0, 0.0) & (2.0, 2.0) & (2.0, 2.0) & (2.0, 2.0) & (2.0, 2.0) & (0.0, 0.0) & (0.0, 0.0) \\ (0.0, 0.0) & (0.0, 0.0) & (3.0, 3.0) & (3.0, 3.0) & (3.0, 3.0) & (3.0, 3.0) & (0.0, 0.0) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (4.0, 4.0) & (4.0, 4.0) & (4.0, 4.0) & (4.0, 4.0) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (5.0, 5.0) & (5.0, 5.0) & (5.0, 5.0) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (6.0, 6.0) & (6.0, 6.0) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (7.0, 7.0) \end{bmatrix}$$

### Call Statement and Input:

```

          UPLO  TRANSA  DIAG  N  K  A  LDA  X  INCX
CALL CTBMV( 'U' , 'C' , 'N' , 7 , 3 , A , 5 , X , 1 )

```

$$A = \begin{bmatrix} . & . & . & (1.0, 1.0) & (2.0, 2.0) & (3.0, 3.0) & (4.0, 4.0) \\ . & . & (1.0, 1.0) & (2.0, 2.0) & (3.0, 3.0) & (4.0, 4.0) & (5.0, 5.0) \\ . & (1.0, 1.0) & (2.0, 2.0) & (3.0, 3.0) & (4.0, 4.0) & (5.0, 5.0) & (6.0, 6.0) \\ (1.0, 1.0) & (2.0, 2.0) & (3.0, 3.0) & (4.0, 4.0) & (5.0, 5.0) & (6.0, 6.0) & (7.0, 7.0) \\ . & . & . & . & . & . & . \end{bmatrix}$$

$$X = ((1.0, 2.0), (2.0, 4.0), (3.0, 6.0), (4.0, 8.0), (5.0, 10.0), (6.0, 12.0), (7.0, 14.0))$$

### Output:

$$X = ((1.0, 2.0), (7.0, 9.0), (24.0, 23.0), (58.0, 46.0), (112.0, 79.0), (186.0, 122.0), (280.0, 175.0))$$

### Example 4

This example shows the computation  $x \leftarrow A^T x$ , where  $k > n$ . Matrix  $A$  is a real 4 by 4 upper triangular band matrix with a half band width of 5 that is not unit triangular, stored in upper-triangular-band-packed storage mode. Vector  $x$  is a vector of length 4. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 \\ . & 2.0 & 2.0 & 2.0 \\ . & . & 3.0 & 3.0 \\ . & . & . & 4.0 \end{bmatrix}$$

### Call Statement and Input:

```

          UPLO  TRANSA  DIAG  N  K  A  LDA  X  INCX
CALL STBMV( 'U' , 'T' , 'N' , 4 , 5 , A , 6 , X , 1 )

```

$$A = \begin{bmatrix} . & . & . & . \\ . & . & . & 1.0 \\ . & . & 1.0 & 2.0 \\ . & 1.0 & 2.0 & 3.0 \\ 1.0 & 2.0 & 3.0 & 4.0 \end{bmatrix}$$

$$X = (1.0, 2.0, 3.0, 4.0)$$

### Output:

$$X = (1.0, 5.0, 14.0, 30.0)$$



---

## Sparse Matrix-Vector Subprograms

This section contains the sparse matrix-vector subprogram descriptions.

## DSMMX — Matrix-Vector Product for a Sparse Matrix in Compressed-Matrix Storage Mode

### Purpose

This subprogram computes the matrix-vector product for sparse matrix  $A$ , stored in compressed-matrix storage mode, using the matrix and vectors  $x$  and  $y$ :

$$y \leftarrow Ax$$

where  $A$ ,  $x$ , and  $y$  contain long-precision real numbers. You can use DSMTM to transpose matrix  $A$  before calling this subroutine. The resulting computation performed by this subroutine is then  $y \leftarrow A^T x$ .

### Syntax

Fortran	CALL DSMMX ( <i>m</i> , <i>nz</i> , <i>ac</i> , <i>ka</i> , <i>lda</i> , <i>x</i> , <i>y</i> )
C and C++	dsmmx ( <i>m</i> , <i>nz</i> , <i>ac</i> , <i>ka</i> , <i>lda</i> , <i>x</i> , <i>y</i> );

### On Entry

<i>m</i>	is the number of rows in sparse matrix $A$ and the number of elements in vector $y$ . Specified as: a fullword integer; $m \geq 0$ .
<i>nz</i>	is the maximum number of nonzero elements in each row of sparse matrix $A$ . Specified as: a fullword integer; $nz \geq 0$ .
<i>ac</i>	is the $m$ by $n$ sparse matrix $A$ , stored in compressed-matrix storage mode in an array, referred to as AC. Specified as: an <i>lda</i> by (at least) <i>nz</i> array, containing long-precision real numbers.
<i>ka</i>	is the array, referred to as KA, containing the column numbers of the matrix $A$ elements stored in the corresponding positions in array AC. Specified as: an <i>lda</i> by (at least) <i>nz</i> array, containing fullword integers, where $1 \leq$ (elements of KA) $\leq n$ .
<i>lda</i>	is the size of the leading dimension of the arrays specified for <i>ac</i> and <i>ka</i> . Specified as: a fullword integer; $lda > 0$ and $lda \geq m$ .
<i>x</i>	is the vector $x$ of length $n$ . Specified as: a one-dimensional array of (at least) length $n$ , containing long-precision real numbers.
<i>y</i>	See "On Return."

### On Return

<i>y</i>	is the vector $y$ of length $m$ , containing the result of the computation. Returned as: a one-dimensional array of (at least) length $m$ , containing long-precision real numbers.
----------	---

### Notes

1. Matrix  $A$  must have no common elements with vectors  $x$  and  $y$ ; otherwise, results are unpredictable.
2. For the KA array, where there are no corresponding nonzero elements in AC, you must still fill in a number between 1 and  $n$ . See the "Example" on page 362.
3. For a description of how sparse matrices are stored in compressed-matrix storage mode, see "Compressed-Matrix Storage Mode" on page 95.

4. If your sparse matrix is stored by rows, as defined in “Storage-by-Rows” on page 100, you should first use the DSRSM utility subroutine, described in “DSRSM — Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode” on page 1026, to convert your sparse matrix to compressed-matrix storage mode.

## Function

The matrix-vector product is computed for a sparse matrix, stored in compressed matrix mode:

$$y \leftarrow Ax$$

where:

$A$  is an  $m$  by  $n$  sparse matrix, stored in compressed-matrix storage mode in arrays AC and KA.

$x$  is a vector of length  $n$ .

$y$  is a vector of length  $m$ .

It is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_m \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

See reference [76]. If  $m$  is 0, no computation is performed; if  $nz$  is 0, output vector  $y$  is set to zero, because matrix  $A$  contains all zeros.

If your program uses a sparse matrix stored by rows and you want to use this subroutine, you should first convert your sparse matrix to compressed-matrix storage mode by using the DSRSM utility subroutine described in “DSRSM — Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode” on page 1026.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $m < 0$
2.  $lda \leq 0$
3.  $m > lda$
4.  $nz < 0$

## Examples

### Example

This example shows the matrix-vector product computed for the following sparse matrix  $A$ , which is stored in compressed-matrix storage mode in arrays AC and KA. Matrix  $A$  is:

$$\begin{bmatrix} 4.0 & 0.0 & 7.0 & 0.0 & 0.0 & 0.0 \\ 3.0 & 4.0 & 0.0 & 2.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & 4.0 & 0.0 & 4.0 & 0.0 \\ 0.0 & 0.0 & 7.0 & 4.0 & 0.0 & 1.0 \\ 1.0 & 0.0 & 0.0 & 3.0 & 4.0 & 0.0 \\ 1.0 & 1.0 & 0.0 & 0.0 & 3.0 & 4.0 \end{bmatrix}$$

### Call Statement and Input:

```

           M  NZ  AC  KA  LDA  X  Y
           |  |  |  |  |  |  |
CALL DSMMX( 6 , 4 , AC , KA , 6 , X , Y )

```

$$AC = \begin{bmatrix} 4.0 & 7.0 & 0.0 & 0.0 \\ 4.0 & 3.0 & 2.0 & 0.0 \\ 4.0 & 2.0 & 4.0 & 0.0 \\ 4.0 & 7.0 & 1.0 & 0.0 \\ 4.0 & 1.0 & 3.0 & 0.0 \\ 4.0 & 1.0 & 1.0 & 3.0 \end{bmatrix}$$

$$KA = \begin{bmatrix} 1 & 3 & 1 & 1 \\ 2 & 1 & 4 & 1 \\ 3 & 2 & 5 & 1 \\ 4 & 3 & 6 & 1 \\ 5 & 1 & 4 & 1 \\ 6 & 1 & 2 & 5 \end{bmatrix}$$

$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0)$$

### Output:

$$Y = (25.0, 19.0, 36.0, 43.0, 33.0, 42.0)$$

## DSMTM — Transpose a Sparse Matrix in Compressed-Matrix Storage Mode

### Purpose

This subprogram transposes sparse matrix  $A$ , stored in compressed-matrix storage mode, where  $A$  contains long-precision real numbers.

### Syntax

Fortran	CALL DSMTM ( $m, nz, ac, ka, lda, n, nt, at, kt, ldt, aux, nauX$ )
C and C++	dsmtm ( $m, nz, ac, ka, lda, n, nt, at, kt, ldt, aux, nauX$ );

### On Entry

$m$	is the number of rows in sparse matrix $A$ . Specified as: a fullword integer; $m \geq 0$ .
$nz$	is the maximum number of nonzero elements in each row of sparse matrix $A$ . Specified as: a fullword integer; $nz \geq 0$ .
$ac$	is the $m$ by $n$ sparse matrix $A$ , stored in compressed-matrix storage mode in an array, referred to as AC. Specified as: an $lda$ by (at least) $nz$ array, containing long-precision real numbers.
$ka$	is the array, referred to as KA, containing the column numbers of the matrix $A$ elements stored in the corresponding positions in array AC. Specified as: an $lda$ by (at least) $nz$ array, containing fullword integers, where $1 \leq$ (elements of KA) $\leq n$ .
$lda$	is the size of the leading dimension of the arrays specified for $ac$ and $ka$ . Specified as: a fullword integer; $lda > 0$ and $lda \geq m$ .
$n$	is the number of columns in sparse matrix $A$ . Specified as: a fullword integer; $0 \leq n \leq ldt$ and $n \geq$ (maximum column index in KA).
$nt$	is the number of columns in output arrays AT and KT that are available for use. Specified as: a fullword integer; $nt > 0$ .
$at$	See "On Return" on page 364.
$kt$	See "On Return" on page 364.
$ldt$	is the size of the leading dimension of the arrays specified for $at$ and $kt$ . Specified as: a fullword integer; $ldt > 0$ and $ldt \geq n$ .
$aux$	has the following meaning: If $nauX = 0$ and error 2015 is unrecoverable, $aux$ is ignored. Otherwise, it is a storage work area used by this subroutine. Its size is specified by $nauX$ . Specified as: an area of storage, containing long-precision real numbers. They can have any value.
$nauX$	is the size of the work area specified by $aux$ —that is, the number of elements in $aux$ . Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, DSMTM dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \geq n$ .

### On Return

$n$	is the number of rows in the transposed matrix $A^T$ . Returned as: a fullword integer; $n =$ (maximum column index in KA).
$nt$	is the maximum number of nonzero elements, $nt$ , in each row of the transposed matrix $A^T$ . Returned as: a fullword integer; $nt \leq m$ .
$at$	is the $n$ by (at least) $m$ sparse matrix transpose $A^T$ , stored in compressed-matrix storage mode in an array, referred to as AT. Returned as: an $ldt$ by (at least) $nt$ array, containing long-precision real numbers.
$kt$	is the array, referred to as KT, containing the column numbers of the transposed matrix $A^T$ elements, stored in the corresponding positions in array AT. Returned as: an $ldt$ by (at least) $nt$ array, containing fullword integers, where $1 \leq$ (elements of KT) $\leq m$ .

### Notes

1. In your C program, arguments  $n$  and  $nt$  must be passed by reference.
2. The value specified for input argument  $nt$  should be greater than or equal to the number of nonzero elements you estimate to be in each row of the transposed sparse matrix  $A^T$ . The output value is less than or equal to the input value you specify.
3. For the KA array, where there are no corresponding nonzero elements in AC, you must still fill in a number between 1 and  $n$ . See the "Example" on page 365.
4. For a description of how sparse matrices are stored in compressed-matrix storage mode, see "Compressed-Matrix Storage Mode" on page 95.
5. If your sparse matrix is stored by rows, as defined in "Storage-by-Rows" on page 100, you should first use the DSRSM utility subroutine, described in "DSRSM — Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode" on page 1026, to convert your sparse matrix to compressed-matrix storage mode.
6. You have the option of having the minimum required value for  $naux$  dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

### Function

A sparse matrix  $A$ , stored in arrays AC and KA in compressed-matrix storage mode, is transposed, forming  $A^T$ , and is stored in arrays AT and KT in compressed-matrix storage mode. See reference [76]. This subroutine is provided for when you want to do a matrix-vector product using a transposed matrix,  $A^T$ . First, you transpose a matrix,  $A$ , using this subroutine, then you call DSMMX with the transposed matrix  $A^T$ . This results in the following computation being performed:  $y \leftarrow A^T x$ .

If your program uses a sparse matrix stored by rows and you want to use this subroutine, you should first convert your sparse matrix to compressed-matrix storage mode by using the DSRSM utility subroutine described in "DSRSM — Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode" on page 1026.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $m, n < 0$
2.  $lda, ldt < 1$
3.  $lda < m$
4.  $ldt < n$
5.  $nz < 0$
6.  $n$  is less than the maximum column index in KA.
7.  $nt$  or  $ldt$  are too small.
8. When the following two errors occur, arrays AT, KT, and AUX are overwritten:

$$naux < n$$

$$nt \leq 0$$

9. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example

This example shows how to transpose the following 5 by 4 sparse matrix  $A$ , which is stored in compressed-matrix storage mode in arrays AC and KA. Matrix  $A$  is:

$$\begin{bmatrix} 11.0 & 0.0 & 0.0 & 0.0 \\ 21.0 & 0.0 & 23.0 & 0.0 \\ 0.0 & 0.0 & 33.0 & 34.0 \\ 0.0 & 42.0 & 0.0 & 44.0 \\ 51.0 & 0.0 & 53.0 & 0.0 \end{bmatrix}$$

The resulting 4 by 5 matrix transpose  $A^T$ , stored in compressed-matrix storage mode in arrays AT and KT, is as follows. Matrix  $A^T$  is:

$$\begin{bmatrix} 11.0 & 21.0 & 0.0 & 0.0 & 51.0 \\ 0.0 & 0.0 & 0.0 & 42.0 & 0.0 \\ 0.0 & 23.0 & 33.0 & 0.0 & 53.0 \\ 0.0 & 0.0 & 34.0 & 44.0 & 0.0 \end{bmatrix}$$

As shown here, the value of  $N$  is larger than the actual number of columns in the matrix  $A$ . On output, the exact number of rows in the transposed matrix is returned in the output argument  $N$ .

On output, row 6 of AT and KT is not accessed or modified by the subroutine. Column 4 and row 5 are accessed and modified. They are of no use in further computations and will not be used, because  $NT = 3$  and  $M = 4$ .

### Call Statement and Input:

```

          M  NZ  AC  KA  LDA  N  NT  AT  KT  LDT  AUX  NAUX
          |  |  |  |  |  |  |  |  |  |  |  |
CALL DSMTM( 5 , 2 , AC , KA , 5 , 5 , 4 , AT , KT , 6 , AUX , 5 )

```

## DSMTM

$$AC = \begin{bmatrix} 11.0 & 0.0 \\ 21.0 & 23.0 \\ 33.0 & 34.0 \\ 42.0 & 44.0 \\ 51.0 & 53.0 \end{bmatrix}$$

$$KA = \begin{bmatrix} 1 & 1 \\ 1 & 3 \\ 3 & 4 \\ 2 & 4 \\ 1 & 3 \end{bmatrix}$$

### Output:

$$\begin{aligned} N &= 4 \\ NT &= 3 \end{aligned}$$

$$AT = \begin{bmatrix} 11.0 & 21.0 & 51.0 & 0.0 \\ 42.0 & 0.0 & 0.0 & 0.0 \\ 33.0 & 23.0 & 53.0 & 0.0 \\ 34.0 & 44.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$KT = \begin{bmatrix} 1 & 2 & 5 & 1 \\ 4 & 1 & 1 & 1 \\ 3 & 2 & 5 & 1 \\ 3 & 4 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$



## DSDMX — Matrix-Vector Product for a Sparse Matrix or Its Transpose in Compressed-Diagonal Storage Mode

### Purpose

This subprogram computes the matrix-vector product for square sparse matrix  $A$ , stored in compressed-diagonal storage mode, using either the matrix or its transpose, and vectors  $x$  and  $y$ :

$$\begin{aligned} y &\leftarrow Ax \\ y &\leftarrow A^T x \end{aligned}$$

where  $A$ ,  $x$ , and  $y$  contain long-precision real numbers.

### Syntax

Fortran	CALL DSDMX ( <i>iopt</i> , <i>n</i> , <i>nd</i> , <i>ad</i> , <i>lda</i> , <i>trans</i> , <i>la</i> , <i>x</i> , <i>y</i> )
C and C++	dsdmx ( <i>iopt</i> , <i>n</i> , <i>nd</i> , <i>ad</i> , <i>lda</i> , <i>trans</i> , <i>la</i> , <i>x</i> , <i>y</i> );

### On Entry

<i>iopt</i>	<p>indicates the storage variation used for sparse matrix <math>A</math>, stored in compressed-diagonal storage mode, where:</p> <p>If <math>iopt = 0</math>, matrix <math>A</math> is a general sparse matrix, where all the nonzero diagonals in matrix <math>A</math> are used to set up the storage arrays.</p> <p>If <math>iopt = 1</math>, matrix <math>A</math> is a symmetric sparse matrix, where only the nonzero main diagonal and one of each of the unique nonzero diagonals are used to set up the storage arrays.</p> <p>Specified as: a fullword integer; <math>iopt = 0</math> or 1.</p>
<i>n</i>	<p>is the order of sparse matrix <math>A</math> and the number of elements in vectors <math>x</math> and <math>y</math>. Specified as: a fullword integer; <math>n \geq 0</math>.</p>
<i>nd</i>	<p>is the number of diagonals stored in the columns of array AD, as well as the number of columns in AD and the number of elements in array LA. Specified as: a fullword integer; <math>nd \geq 0</math>.</p>
<i>ad</i>	<p>is the sparse matrix <math>A</math> of order <math>n</math>, stored in compressed diagonal storage in an array, referred to as AD. The <i>iopt</i> argument indicates the storage variation used for storing matrix <math>A</math>. The <i>trans</i> argument indicates the following:</p> <p>If <math>trans = 'N'</math>, <math>A</math> is used in the computation.</p> <p>If <math>trans = 'T'</math>, <math>A^T</math> is used in the computation.</p> <p><b>Note:</b> No data should be moved to form <math>A^T</math>; that is, the matrix <math>A</math> should always be stored in its untransposed form.</p> <p>Specified as: an <i>lda</i> by (at least) <i>nd</i> array, containing long-precision real numbers; <math>lda \geq n</math>.</p>
<i>lda</i>	<p>is the size of the leading dimension of the array specified for <i>ad</i>. Specified as: a fullword integer; <math>lda &gt; 0</math> and <math>lda \geq n</math>.</p>
<i>trans</i>	<p>indicates the form of matrix <math>A</math> to use in the computation, where:</p>

If  $trans = 'N'$ ,  $A$  is used in the computation.

If  $trans = 'T'$ ,  $A^T$  is used in the computation.

Specified as: a single character;  $trans = 'N'$  or  $'T'$ .

$la$  is the array, referred to as  $LA$ , containing the diagonal numbers  $k$  for the diagonals stored in each corresponding column in array  $AD$ . (For an explanation of how diagonal numbers are assigned, see “Compressed-Diagonal Storage Mode” on page 96.)

Specified as: a one-dimensional array of (at least) length  $nd$ , containing fullword integers;  $1-n \leq LA(i) \leq n-1$ .

$x$  is the vector  $x$  of length  $n$ . Specified as: a one-dimensional array, containing long-precision real numbers.

$y$  See “On Return.”

### On Return

$y$  is the vector  $y$  of length  $n$ , containing the result of the computation. Returned as: a one-dimensional array, containing long-precision real numbers.

## Notes

1. All subroutines accept lowercase letters for the  $trans$  argument.
2. Matrix  $A$  must have no common elements with vectors  $x$  and  $y$ ; otherwise, results are unpredictable.
3. For a description of how sparse matrices are stored in compressed-diagonal storage mode, see “Compressed-Diagonal Storage Mode” on page 96.

## Function

The matrix-vector product of a square sparse matrix or its transpose, is computed for a matrix stored in compressed-diagonal storage mode:

$$\begin{aligned} y &\leftarrow Ax \\ y &\leftarrow A^T x \end{aligned}$$

where:

$A$  is a sparse matrix of order  $n$ , stored in compressed-diagonal storage mode in  $AD$  and  $LA$ , using the storage variation for either general or symmetric sparse matrices, as indicated by the  $iopt$  argument.

$x$  and  $y$  are vectors of length  $n$ .

It is expressed as follows for  $y \leftarrow Ax$ :

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

It is expressed as follows for  $y \leftarrow A^T x$ :

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{n1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{1n} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

If  $n$  is 0, no computation is performed; if  $nd$  is 0, output vector  $y$  is set to zero, because matrix  $A$  contains all zeros.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $iopt \neq 0$  or 1
2.  $n < 0$
3.  $lda \leq 0$
4.  $n > lda$
5.  $trans \neq 'N'$  or  $'T'$
6.  $nd < 0$
7.  $LA(j) \leq -n$  or  $LA(j) \geq n$ , for any  $j = 1, n$

## Examples

### Example 1

This example shows the matrix-vector product using  $trans = 'N'$ , which is computed for the following sparse matrix  $A$  of order 6. The matrix is stored in compressed-matrix storage mode in arrays AD and LA using the storage variation for general sparse matrices, storing all nonzero diagonals. Matrix  $A$  is:

$$\begin{bmatrix} 4.0 & 0.0 & 7.0 & 0.0 & 0.0 & 0.0 \\ 3.0 & 4.0 & 0.0 & 2.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & 4.0 & 0.0 & 4.0 & 0.0 \\ 0.0 & 0.0 & 7.0 & 4.0 & 0.0 & 1.0 \\ 1.0 & 0.0 & 0.0 & 3.0 & 4.0 & 0.0 \\ 1.0 & 1.0 & 0.0 & 0.0 & 3.0 & 4.0 \end{bmatrix}$$

### Call Statement and Input:

```

          IOPT  N  ND  AD  LDA  TRANS  LA  X  Y
          |    |  |  |  |    |    |  |  |
CALL DSDMX( 0 , 6 , 5 , AD , 6 , 'N' , LA , X , Y )

```

## DSDMX

$$AD = \begin{bmatrix} 4.0 & 0.0 & 0.0 & 0.0 & 7.0 \\ 4.0 & 0.0 & 0.0 & 3.0 & 2.0 \\ 4.0 & 0.0 & 0.0 & 2.0 & 4.0 \\ 4.0 & 0.0 & 0.0 & 7.0 & 1.0 \\ 4.0 & 0.0 & 1.0 & 3.0 & 0.0 \\ 4.0 & 1.0 & 1.0 & 3.0 & 0.0 \end{bmatrix}$$

$$LA = (0, -5, -4, -1, 2)$$
$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0)$$

### Output:

$$Y = (25.0, 19.0, 36.0, 43.0, 33.0, 42.0)$$

### Example 2

This example shows the matrix-vector product using *trans* = 'N', which is computed for the following sparse matrix *A* of order 6. The matrix is stored in compressed-matrix storage mode in arrays AD and LA using the storage variation for symmetric sparse matrices, storing the nonzero main diagonal and one of each of the unique nonzero diagonals. Matrix *A* is:

$$\begin{bmatrix} 11.0 & 0.0 & 13.0 & 0.0 & 15.0 & 0.0 \\ 0.0 & 22.0 & 0.0 & 24.0 & 0.0 & 26.0 \\ 13.0 & 0.0 & 33.0 & 0.0 & 35.0 & 0.0 \\ 0.0 & 24.0 & 0.0 & 44.0 & 0.0 & 46.0 \\ 15.0 & 0.0 & 35.0 & 0.0 & 55.0 & 0.0 \\ 0.0 & 26.0 & 0.0 & 46.0 & 0.0 & 66.0 \end{bmatrix}$$

### Call Statement and Input:

```
          IOPT  N   ND  AD  LDA TRANS  LA  X  Y
CALL DSDMX( 1 , 6 , 3 , AD , 6 , 'N' , LA , X , Y )
```

$$AD = \begin{bmatrix} 11.0 & 13.0 & 0.0 \\ 22.0 & 24.0 & 0.0 \\ 33.0 & 35.0 & 0.0 \\ 44.0 & 46.0 & 0.0 \\ 55.0 & 0.0 & 15.0 \\ 66.0 & 0.0 & 26.0 \end{bmatrix}$$

$$LA = (0, 2, -4)$$
$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0)$$

### Output:

$$Y = (125.0, 296.0, 287.0, 500.0, 395.0, 632.0)$$

### Example 3

This example is the same as Example 1 except that it shows the matrix-vector product for the transpose of a matrix, using *trans* = 'T'. It is computed using the transpose of the following sparse matrix *A* of order 6, which is stored in compressed-matrix storage mode in arrays AD and LA, using the storage variation for general sparse matrices, storing all nonzero diagonals. It uses the same matrix *A* as in Example 1.

### Call Statement and Input:

```
          IOPT  N   ND  AD  LDA TRANS  LA  X  Y
CALL DSDMX( 0 , 6 , 5 , AD , 6 , 'T' , LA , X , Y )
```

AD       =(same as input AD in Example 1)  
LA       =(same as input LA in Example 1)  
X        =(same as input X in Example 1)

**Output:**

Y        = (21.0, 20.0, 47.0, 35.0, 50.0, 28.0)



## Chapter 9. Matrix Operations

The matrix operation subroutines are described in this chapter.

### Overview of the Matrix Operation Subroutines

Some of the matrix operation subroutines were designed in accordance with the Level 3 BLAS de facto standard. If these subroutines do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subroutines, the updates could require modifications of the calling application program. For details on the Level 3 BLAS, see reference [34]. The matrix operation subroutines also include the commonly used matrix operations: addition, subtraction, multiplication, and transposition (Table 78).

Table 78. List of Matrix Operation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Matrix Addition for General Matrices or Their Transposes	SGEADD CGEADD	DGEADD ZGEADD	377
Matrix Subtraction for General Matrices or Their Transposes	SGESUB CGESUB	DGESUB ZGESUB	383
Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes	SGEMUL CGEMUL	DGEMUL ZGEMUL DGEMLP <sup>§</sup>	389
Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes Using Winograd's Variation of Strassen's Algorithm	SGEMMS CGEMMS	DGEMMS ZGEMMS	398
Combined Matrix Multiplication and Addition for General Matrices, Their Transposes, or Conjugate Transposes	SGEMM* CGEMM*	DGEMM* ZGEMM*	404
Matrix-Matrix Product Where One Matrix is Real or Complex Symmetric or Complex Hermitian	SSYMM* CSYMM* CHEMM*	DSYMM* ZSYMM* ZHEMM*	412
Triangular Matrix-Matrix Product	STRMM* CTRMM*	DTRMM* ZTRMM*	419
Rank-K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYRK* CSYRK* CHERK*	DSYRK* ZSYRK* ZHERK*	426
Rank-2K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYR2K* CSYR2K* CHER2K*	DSYR2K* ZSYR2K* ZHER2K*	432
General Matrix Transpose (In-Place)	SGETMI CGETMI	DGETMI ZGETMI	439
General Matrix Transpose (Out-of-Place)	SGETMO CGETMO	DGETMO ZGETMO	442
* Level 3 BLAS			
<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.			

---

## Use Considerations

This section describes some key points about using the matrix operations subroutines.

### Specifying Normal, Transposed, or Conjugate Transposed Input Matrices

On each invocation, the matrix operation subroutines can perform one of several possible computations, using different forms of the input matrices  $A$  and  $B$ . For the real and complex versions of the subroutines, there are four and nine combinations, respectively, depending on the characters specified for the *transa* and *transb* arguments:

'N' Normal form  
'T' Transposed form  
'C' Conjugate transposed form

The four and nine possible combinations are defined as follows:

Real Combinations	Complex Combinations
$AB$	$AB$
$A^T B$	$A^T B$
	$A^H B$
$AB^T$	$AB^T$
$A^T B^T$	$A^T B^T$
	$A^H B^T$
	$AB^H$
	$A^T B^H$
	$A^H B^H$

### Transposing or Conjugate Transposing:

This section describes some key points about using transposed and conjugate transposed matrices.

#### On Input

In every case, the input arrays for the matrix, its transpose, or its conjugate transpose should be stored in the original untransposed form. You then specify the desired form of the matrix to be used in the computation in the *transa* or *transb* arguments. For a description of matrix transpose and matrix conjugate transpose, see "Matrices" on page 65.

#### On Output

If you want to compute the transpose or the conjugate transpose of a matrix operation—that is, the output stored in matrix  $C$ —you should use the matrix identities described in Special Usage for each subroutine description. Examples are provided in the subroutine descriptions to show the use of these matrix identities. This accomplishes the transpose or conjugate transpose as part of the multiply operation.



---

## Performance and Accuracy Considerations

This section describes some key points about performance and accuracy in the matrix operations subroutines.

### In General

1. The matrix operation subroutines use algorithms that are tuned specifically to the workstation processors they run on. The techniques involve using any one of several computational methods, based on certain operation counts and sizes of data.
2. The short-precision multiplication subroutines provide increased accuracy by partially accumulating results in long precision.
3. Strassen's method is not stable for certain row or column scalings of the input matrices  $A$  and  $B$ . Therefore, for matrices  $A$  and  $B$  with divergent exponent values, Strassen's method may give inaccurate results. For these cases, you should use the `_GEMUL` or `_GEMM` subroutines.
4. There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 48.

### For Large Matrices

If you are using large square matrices in your matrix multiplication operations, you get better performance by using `SGEMMS`, `DGEMMS`, `CGEMMS`, and `ZGEMMS`. These subroutines use Winograd's variation of Strassen's algorithm for both real and complex matrices.

### For Combined Operations

If you want to perform a combined matrix multiplication and addition with scaling, `SGEMM`, `DGEMM`, `CGEMM`, and `ZGEMM` provide better performance than if you perform the parts of the computation separately in your program. See references [34] and [37].

## **Matrix Operation Subroutines**

This section contains the matrix operation subroutine descriptions.

## SGEADD, DGEADD, CGEADD, and ZGEADD — Matrix Addition for General Matrices or Their Transposes

### Purpose

These subroutines can perform any one of the following matrix additions, using matrices  $A$  and  $B$  or their transposes, and matrix  $C$ :

$$C \leftarrow A + B$$

$$C \leftarrow A^T + B$$

$$C \leftarrow A + B^T$$

$$C \leftarrow A^T + B^T$$

Table 79. Data Types

$A, B, C$	Subroutine
Short-precision real	SGEADD
Long-precision real	DGEADD
Short-precision complex	CGEADD
Long-precision complex	ZGEADD

### Syntax

<b>Fortran</b>	CALL SGEADD   DGEADD   CGEADD   ZGEADD ( $a, lda, transa, b, ldb, transb, c, ldc, m, n$ )
<b>C and C++</b>	sgeadd   dgeadd   cgeadd   zgeadd ( $a, lda, transa, b, ldb, transb, c, ldc, m, n$ );

### On Entry

$a$  is the matrix  $A$ , where:

If  $transa = 'N'$ ,  $A$  is used in the computation, and  $A$  has  $m$  rows and  $n$  columns.

If  $transa = 'T'$ ,  $A^T$  is used in the computation, and  $A$  has  $n$  rows and  $m$  columns.

**Note:** No data should be moved to form  $A^T$ ; that is, the matrix  $A$  should always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 79, where:

If  $transa = 'N'$ , its size must be  $lda$  by (at least)  $n$ .

If  $transa = 'T'$ , its size must be  $lda$  by (at least)  $m$ .

$lda$  is the leading dimension of the array specified for  $a$ .

Specified as: a fullword integer;  $lda > 0$  and:

If  $transa = 'N'$ ,  $lda \geq m$ .

If  $transa = 'T'$ ,  $lda \geq n$ .

$transa$  indicates the form of matrix  $A$  to use in the computation, where:

If  $transa = 'N'$ ,  $A$  is used in the computation.

## SGEADD, DGEADD, CGEADD, and ZGEADD

	<p>If <i>transa</i> = 'T', <math>A^T</math> is used in the computation. Specified as: a single character; <i>transa</i> = 'N' or 'T'.</p>
<i>b</i>	<p>is the matrix <i>B</i>, where: If <i>transb</i> = 'N', <i>B</i> is used in the computation, and <i>B</i> has <i>m</i> rows and <i>n</i> columns. If <i>transb</i> = 'T', <math>B^T</math> is used in the computation, and <i>B</i> has <i>n</i> rows and <i>m</i> columns.</p> <p><b>Note:</b> No data should be moved to form <math>B^T</math>; that is, the matrix <i>B</i> should always be stored in its untransposed form.</p> <p>Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 79 on page 377, where: If <i>transb</i> = 'N', its size must be <i>ldb</i> by (at least) <i>n</i>. If <i>transb</i> = 'T', its size must be <i>ldb</i> by (at least) <i>m</i>.</p>
<i>ldb</i>	<p>is the leading dimension of the array specified for <i>b</i>. Specified as: a fullword integer; <i>ldb</i> &gt; 0 and: If <i>transb</i> = 'N', <i>ldb</i> ≥ <i>m</i>. If <i>transb</i> = 'T', <i>ldb</i> ≥ <i>n</i>.</p>
<i>transb</i>	<p>indicates the form of matrix <i>B</i> to use in the computation, where: If <i>transb</i> = 'N', <i>B</i> is used in the computation. If <i>transb</i> = 'T', <math>B^T</math> is used in the computation. Specified as: a single character; <i>transb</i> = 'N' or 'T'.</p>
<i>c</i>	<p>See "On Return."</p>
<i>ldc</i>	<p>is the leading dimension of the array specified for <i>c</i>. Specified as: a fullword integer; <i>ldc</i> &gt; 0 and <i>ldc</i> ≥ <i>m</i>.</p>
<i>m</i>	<p>is the number of rows in matrix <i>C</i>. Specified as: a fullword integer; <math>0 \leq m \leq ldc</math>.</p>
<i>n</i>	<p>is the number of columns in matrix <i>C</i>. Specified as: a fullword integer; <math>0 \leq n</math>.</p>

### On Return

<i>c</i>	<p>is the <i>m</i> by <i>n</i> matrix <i>C</i>, containing the results of the computation. Returned as: an <i>ldc</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 79 on page 377.</p>
----------	--

## Notes

1. All subroutines accept lowercase letters for the *transa* and *transb* arguments.
2. Matrix *C* must have no common elements with matrices *A* or *B*. However, *C* may (exactly) coincide with *A* if *transa* = 'N', and *C* may (exactly) coincide with *B* if *transb* = 'N'. Otherwise, results are unpredictable. See "Concepts" on page 59.

## Function

The matrix sum is expressed as follows, where  $a_{ij}$ ,  $b_{ij}$ , and  $c_{ij}$  are elements of matrices  $A$ ,  $B$ , and  $C$ , respectively:

$$\begin{aligned} c_{ij} &= a_{ij} + b_{ij} && \text{for } C \leftarrow A + B \\ c_{ij} &= a_{ij} + b_{ji} && \text{for } C \leftarrow A + B^T \\ c_{ij} &= a_{ji} + b_{ij} && \text{for } C \leftarrow A^T + B \\ c_{ij} &= a_{ji} + b_{ji} && \text{for } C \leftarrow A^T + B^T \end{aligned}$$

for  $i = 1, m$  and  $j = 1, n$

If  $m$  or  $n$  is 0, no computation is performed.

## Special Usage

You can compute the transpose  $C^T$  of each of the four computations listed under "Function" by using the following matrix identities:

$$\begin{aligned} (A+B)^T &= A^T + B^T \\ (A+B^T)^T &= A^T + B \\ (A^T+B)^T &= A + B^T \\ (A^T+B^T)^T &= A + B \end{aligned}$$

Be careful that your output array receiving  $C^T$  has dimensions large enough to hold the transposed matrix. See "Example 4" on page 381.

## Error conditions

### Input-Argument Errors

1.  $lda, ldb, ldc \leq 0$
2.  $m, n < 0$
3.  $m > ldc$
4.  $transa, transb \neq 'N'$  or  $'T'$
5.  $transa = 'N'$  and  $m > lda$
6.  $transa = 'T'$  and  $n > lda$
7.  $transb = 'N'$  and  $m > ldb$
8.  $transb = 'T'$  and  $n > ldb$

## Examples

### Example 1

This example shows the computation  $C \leftarrow A + B$ , where  $A$  and  $C$  are contained in larger arrays  $A$  and  $C$ , respectively, and  $B$  is the same size as array  $B$ , in which it is contained.

#### Call Statement and Input:

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
CALL SGEADD( A , 6 , 'N' , B , 4 , 'N' , C , 5 , 4 , 3 )
    
```

$$A = \begin{bmatrix} 110000.0 & 120000.0 & 130000.0 \\ 210000.0 & 220000.0 & 230000.0 \\ 310000.0 & 320000.0 & 330000.0 \\ 410000.0 & 420000.0 & 430000.0 \\ \vdots & \vdots & \vdots \end{bmatrix}$$

## SGEADD, DGEADD, CGEADD, and ZGEADD

$$B = \begin{bmatrix} 11.0 & 12.0 & 13.0 \\ 21.0 & 22.0 & 23.0 \\ 31.0 & 32.0 & 33.0 \\ 41.0 & 42.0 & 43.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 110011.0 & 120012.0 & 130013.0 \\ 210021.0 & 220022.0 & 230023.0 \\ 310031.0 & 320032.0 & 330033.0 \\ 410041.0 & 420042.0 & 430043.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 2

This example shows the computation  $C \leftarrow A^T + B$ , where  $A$ ,  $B$ , and  $C$  are the same size as arrays  $A$ ,  $B$ , and  $C$ , in which they are contained.

**Call Statement and Input:**

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
          |  |    |      |  |  |      |  |  |  |  |
CALL SGEADD( A , 3 , 'T' , B , 4 , 'N' , C , 4 , 4 , 3 )

```

$$A = \begin{bmatrix} 110000.0 & 120000.0 & 130000.0 & 140000.0 \\ 210000.0 & 220000.0 & 230000.0 & 240000.0 \\ 310000.0 & 320000.0 & 330000.0 & 340000.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 11.0 & 12.0 & 13.0 \\ 21.0 & 22.0 & 23.0 \\ 31.0 & 32.0 & 33.0 \\ 41.0 & 42.0 & 43.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 110011.0 & 210012.0 & 310013.0 \\ 120021.0 & 220022.0 & 320023.0 \\ 130031.0 & 230032.0 & 330033.0 \\ 140041.0 & 240042.0 & 340043.0 \end{bmatrix}$$

### Example 3

This example shows computation  $C \leftarrow A + B^T$ , where  $A$  is contained in a larger array  $A$ , and  $B$  and  $C$  are the same size as arrays  $B$  and  $C$ , in which they are contained.

**Call Statement and Input:**

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
          |  |    |      |  |  |      |  |  |  |  |
CALL SGEADD( A , 5 , 'N' , B , 3 , 'T' , C , 4 , 4 , 3 )

```

$$A = \begin{bmatrix} 110000.0 & 120000.0 & 130000.0 \\ 210000.0 & 220000.0 & 230000.0 \\ 310000.0 & 320000.0 & 330000.0 \\ 410000.0 & 420000.0 & 430000.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 11.0 & 12.0 & 13.0 & 14.0 \\ 21.0 & 22.0 & 23.0 & 24.0 \\ 31.0 & 32.0 & 33.0 & 34.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 110011.0 & 120021.0 & 130031.0 \\ 210012.0 & 220022.0 & 230032.0 \\ 310013.0 & 320023.0 & 330033.0 \\ 410014.0 & 420024.0 & 430034.0 \end{bmatrix}$$

### Example 4

This example shows how to produce the transpose of the result of the computation performed in “Example 3” on page 380,  $C \leftarrow A + B^T$ , which uses the calling sequence:

```
CALL SGEADD( A , 5 , 'N' , B , 3 , 'T' , C , 4 , 4 , 3 )
```

You instead code a calling sequence for  $C^T \leftarrow A^T + B$ , as shown below, where the resulting matrix  $C^T$  in the output array CT is the transpose of the matrix in the output array C in Example 3. Note that the array CT has dimensions large enough to receive the transposed matrix. For a description of all the matrix identities, see “Special Usage” on page 379.

**Call Statement and Input:**

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
          |  |    |      |  |  |      |  |  |  |  |
CALL SGEADD( A , 5 , 'T' , B , 3 , 'N' , CT , 4 , 3 , 4 )

```

$$A = \begin{bmatrix} 110000.0 & 120000.0 & 130000.0 \\ 210000.0 & 220000.0 & 230000.0 \\ 310000.0 & 320000.0 & 330000.0 \\ 410000.0 & 420000.0 & 430000.0 \\ . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} 11.0 & 12.0 & 13.0 & 14.0 \\ 21.0 & 22.0 & 23.0 & 24.0 \\ 31.0 & 32.0 & 33.0 & 34.0 \end{bmatrix}$$

**Output:**

$$CT = \begin{bmatrix} 110011.0 & 210012.0 & 310013.0 & 410014.0 \\ 120021.0 & 220022.0 & 320023.0 & 420024.0 \\ 130031.0 & 230032.0 & 330033.0 & 430034.0 \\ . & . & . & . \end{bmatrix}$$

### Example 5

This example shows the computation  $C \leftarrow A^T + B^T$ , where  $A$ ,  $B$ , and  $C$  are the same size as the arrays  $A$ ,  $B$ , and  $C$ , in which they are contained.

**Call Statement and Input:**

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
          |  |    |      |  |  |      |  |  |  |  |
CALL SGEADD( A , 3 , 'T' , B , 3 , 'T' , C , 4 , 4 , 3 )

```

## SGEADD, DGEADD, CGEADD, and ZGEADD

$$A = \begin{bmatrix} 110000.0 & 120000.0 & 130000.0 & 140000.0 \\ 210000.0 & 220000.0 & 230000.0 & 240000.0 \\ 310000.0 & 320000.0 & 330000.0 & 340000.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 11.0 & 12.0 & 13.0 & 14.0 \\ 21.0 & 22.0 & 23.0 & 24.0 \\ 31.0 & 32.0 & 33.0 & 34.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 110011.0 & 210021.0 & 310031.0 \\ 120012.0 & 220022.0 & 320032.0 \\ 130013.0 & 230023.0 & 330033.0 \\ 140014.0 & 240024.0 & 340034.0 \end{bmatrix}$$

### Example 6

This example shows the computation  $C \leftarrow A+B$ , where  $A$ ,  $B$ , and  $C$  are contained in larger arrays  $A$ ,  $B$ , and  $C$ , respectively, and the arrays contain complex data.

**Call Statement and Input:**

```

          A  LDA TRANSA  B  LDB TRANSB  C  LDC  M  N
CALL CGEADD( A , 6 , 'N' , B , 5 , 'N' , C , 5 , 4 , 3 )

```

$$A = \begin{bmatrix} (1.0, 5.0) & (9.0, 2.0) & (1.0, 9.0) \\ (2.0, 4.0) & (8.0, 3.0) & (1.0, 8.0) \\ (3.0, 3.0) & (7.0, 5.0) & (1.0, 7.0) \\ (6.0, 6.0) & (3.0, 6.0) & (1.0, 4.0) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} (1.0, 8.0) & (2.0, 7.0) & (3.0, 2.0) \\ (4.0, 4.0) & (6.0, 8.0) & (6.0, 3.0) \\ (6.0, 2.0) & (4.0, 5.0) & (4.0, 5.0) \\ (7.0, 2.0) & (6.0, 4.0) & (1.0, 6.0) \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} (2.0, 13.0) & (11.0, 9.0) & (4.0, 11.0) \\ (6.0, 8.0) & (14.0, 11.0) & (7.0, 11.0) \\ (9.0, 5.0) & (11.0, 10.0) & (5.0, 12.0) \\ (13.0, 8.0) & (9.0, 10.0) & (2.0, 10.0) \\ \cdot & \cdot & \cdot \end{bmatrix}$$



## SGESUB, DGESUB, CGESUB, and ZGESUB — Matrix Subtraction for General Matrices or Their Transposes

### Purpose

These subroutines can perform any one of the following matrix subtractions, using matrices  $A$  and  $B$  or their transposes, and matrix  $C$ :

$$C \leftarrow A - B$$

$$C \leftarrow A^T - B$$

$$C \leftarrow A - B^T$$

$$C \leftarrow A^T - B^T$$

Table 80. Data Types

$A, B, C$	Subroutine
Short-precision real	SGESUB
Long-precision real	DGESUB
Short-precision complex	CGESUB
Long-precision complex	ZGESUB

### Syntax

<b>Fortran</b>	CALL SGESUB   DGESUB   CGESUB   ZGESUB ( $a, lda, transa, b, ldb, transb, c, ldc, m, n$ )
<b>C and C++</b>	sgesub   dgesub   cgesub   zgesub ( $a, lda, transa, b, ldb, transb, c, ldc, m, n$ );

### On Entry

$a$  is the matrix  $A$ , where:

If  $transa = 'N'$ ,  $A$  is used in the computation, and  $A$  has  $m$  rows and  $n$  columns.

If  $transa = 'T'$ ,  $A^T$  is used in the computation, and  $A$  has  $n$  rows and  $m$  columns.

**Note:** No data should be moved to form  $A^T$ ; that is, the matrix  $A$  should always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 80, where:

If  $transa = 'N'$ , its size must be  $lda$  by (at least)  $n$ .

If  $transa = 'T'$ , its size must be  $lda$  by (at least)  $m$ .

$lda$  is the leading dimension of the array specified for  $a$ .

Specified as: a fullword integer;  $lda > 0$  and:

If  $transa = 'N'$ ,  $lda \geq m$ .

If  $transa = 'T'$ ,  $lda \geq n$ .

$transa$  indicates the form of matrix  $A$  to use in the computation, where:

If  $transa = 'N'$ ,  $A$  is used in the computation.

## SGESUB, DGESUB, CGESUB, and ZGESUB

	<p>If <i>transa</i> = 'T', <math>A^T</math> is used in the computation. Specified as: a single character; <i>transa</i> = 'N' or 'T'.</p>
<i>b</i>	<p>is the matrix <i>B</i>, where: If <i>transb</i> = 'N', <i>B</i> is used in the computation, and <i>B</i> has <i>m</i> rows and <i>n</i> columns. If <i>transb</i> = 'T', <math>B^T</math> is used in the computation, and <i>B</i> has <i>n</i> rows and <i>m</i> columns.</p> <p><b>Note:</b> No data should be moved to form <math>B^T</math>; that is, the matrix <i>B</i> should always be stored in its untransposed form.</p> <p>Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 79 on page 377, where: If <i>transb</i> = 'N', its size must be <i>ldb</i> by (at least) <i>n</i>. If <i>transb</i> = 'T', its size must be <i>ldb</i> by (at least) <i>m</i>.</p>
<i>ldb</i>	<p>is the leading dimension of the array specified for <i>b</i>. Specified as: a fullword integer; <i>ldb</i> &gt; 0 and: If <i>transb</i> = 'N', <i>ldb</i> ≥ <i>m</i>. If <i>transb</i> = 'T', <i>ldb</i> ≥ <i>n</i>.</p>
<i>transb</i>	<p>indicates the form of matrix <i>B</i> to use in the computation, where: If <i>transb</i> = 'N', <i>B</i> is used in the computation. If <i>transb</i> = 'T', <math>B^T</math> is used in the computation. Specified as: a single character; <i>transb</i> = 'N' or 'T'.</p>
<i>c</i>	<p>See "On Return."</p>
<i>ldc</i>	<p>is the leading dimension of the array specified for <i>c</i>. Specified as: a fullword integer; <i>ldc</i> &gt; 0 and <i>ldc</i> ≥ <i>m</i>.</p>
<i>m</i>	<p>is the number of rows in matrix <i>C</i>. Specified as: a fullword integer; <math>0 \leq m \leq ldc</math>.</p>
<i>n</i>	<p>is the number of columns in matrix <i>C</i>. Specified as: a fullword integer; <math>0 \leq n</math>.</p>

### On Return

<i>c</i>	<p>is the <i>m</i> by <i>n</i> matrix <i>C</i>, containing the results of the computation. Returned as: an <i>ldc</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 80 on page 383.</p>
----------	--

## Notes

1. All subroutines accept lowercase letters for the *transa* and *transb* arguments.
2. Matrix *C* must have no common elements with matrices *A* or *B*. However, *C* may (exactly) coincide with *A* if *transa* = 'N', and *C* may (exactly) coincide with *B* if *transb* = 'N'. Otherwise, results are unpredictable. See "Concepts" on page 59.

## Function

The matrix subtraction is expressed as follows, where  $a_{ij}$ ,  $b_{ij}$ , and  $c_{ij}$  are elements of matrices  $A$ ,  $B$ , and  $C$ , respectively:

$$\begin{aligned} c_{ij} &= a_{ij} - b_{ij} && \text{for } C \leftarrow A - B \\ c_{ij} &= a_{ij} - b_{ji} && \text{for } C \leftarrow A - B^T \\ c_{ij} &= a_{ji} - b_{ij} && \text{for } C \leftarrow A^T - B \\ c_{ij} &= a_{ji} - b_{ji} && \text{for } C \leftarrow A^T - B^T \end{aligned}$$

for  $i = 1, m$  and  $j = 1, n$

If  $m$  or  $n$  is 0, no computation is performed.

## Special Usage

You can compute the transpose  $C^T$  of each of the four computations listed under "Function" by using the following matrix identities:

$$\begin{aligned} (A - B)^T &= A^T - B^T \\ (A - B^T)^T &= A^T - B \\ (A^T - B)^T &= A - B^T \\ (A^T - B^T)^T &= A - B \end{aligned}$$

Be careful that your output array receiving  $C^T$  has dimensions large enough to hold the transposed matrix. See "Example 5" on page 387.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $lda, ldb, ldc \leq 0$
2.  $m, n < 0$
3.  $m > ldc$
4.  $transa, transb \neq 'N'$  or  $'T'$
5.  $transa = 'N'$  and  $m > lda$
6.  $transa = 'T'$  and  $n > lda$
7.  $transb = 'N'$  and  $m > ldb$
8.  $transb = 'T'$  and  $n > ldb$

## Examples

### Example 1

This example shows the computation  $C \leftarrow A - B$ , where  $A$  and  $C$  are contained in larger arrays  $A$  and  $C$ , respectively, and  $B$  is the same size as array  $B$ , in which it is contained.

#### Call Statement and Input:

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
          |  |  |  |  |  |  |  |  |  |
CALL SGESUB( A , 6 , 'N' , B , 4 , 'N' , C , 5 , 4 , 3 )
    
```

$$A = \begin{bmatrix} 110000.0 & 120000.0 & 130000.0 \\ 210000.0 & 220000.0 & 230000.0 \\ 310000.0 & 320000.0 & 330000.0 \end{bmatrix}$$

## SGESUB, DGESUB, CGESUB, and ZGESUB

$$\begin{bmatrix} 410000.0 & 420000.0 & 430000.0 \\ \vdots & \vdots & \vdots \end{bmatrix}$$

$$B = \begin{bmatrix} -11.0 & -12.0 & -13.0 \\ -21.0 & -22.0 & -23.0 \\ -31.0 & -32.0 & -33.0 \\ -41.0 & -42.0 & -43.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 110011.0 & 120012.0 & 130013.0 \\ 210021.0 & 220022.0 & 230023.0 \\ 310031.0 & 320032.0 & 330033.0 \\ 410041.0 & 420042.0 & 430043.0 \\ \vdots & \vdots & \vdots \end{bmatrix}$$

### Example 2

This example shows the computation  $C \leftarrow A^T - B$ , where  $A$ ,  $B$ , and  $C$  are the same size as arrays  $A$ ,  $B$ , and  $C$ , in which they are contained.

**Call Statement and Input:**

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
CALL SGESUB( A , 3 , 'T' , B , 4 , 'N' , C , 4 , 4 , 3 )

```

$$A = \begin{bmatrix} 110000.0 & 120000.0 & 130000.0 & 140000.0 \\ 210000.0 & 220000.0 & 230000.0 & 240000.0 \\ 310000.0 & 320000.0 & 330000.0 & 340000.0 \end{bmatrix}$$

$$B = \begin{bmatrix} -11.0 & -12.0 & -13.0 \\ -21.0 & -22.0 & -23.0 \\ -31.0 & -32.0 & -33.0 \\ -41.0 & -42.0 & -43.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 110011.0 & 210012.0 & 310013.0 \\ 120021.0 & 220022.0 & 320023.0 \\ 130031.0 & 230032.0 & 330033.0 \\ 140041.0 & 240042.0 & 340043.0 \end{bmatrix}$$

### Example 3

This example shows computation  $C \leftarrow A - B^T$ , where  $A$  is contained in a larger array  $A$ , and  $B$  and  $C$  are the same size as arrays  $B$  and  $C$ , in which they are contained.

**Call Statement and Input:**

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
CALL SGESUB( A , 5 , 'N' , B , 3 , 'T' , C , 4 , 4 , 3 )

```

$$\begin{bmatrix} 110000.0 & 120000.0 & 130000.0 \\ 210000.0 & 220000.0 & 230000.0 \end{bmatrix}$$

$$A = \begin{bmatrix} 310000.0 & 320000.0 & 330000.0 \\ 410000.0 & 420000.0 & 430000.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} -11.0 & -12.0 & -13.0 & -14.0 \\ -21.0 & -22.0 & -23.0 & -24.0 \\ -31.0 & -32.0 & -33.0 & -34.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 110011.0 & 120021.0 & 130031.0 \\ 210012.0 & 220022.0 & 230032.0 \\ 310013.0 & 320023.0 & 330033.0 \\ 410014.0 & 420024.0 & 430034.0 \end{bmatrix}$$

### Example 4

This example shows the computation  $C \leftarrow A^T - B^T$ , where  $A$ ,  $B$ , and  $C$  are the same size as the arrays  $A$ ,  $B$ , and  $C$ , in which they are contained.

**Call Statement and Input:**

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
          |  |    |      |  |  |      |  |  |  |  |
CALL SGESUB( A , 3 , 'T' , B , 3 , 'T' , C , 4 , 4 , 3 )

```

$$A = \begin{bmatrix} 110000.0 & 120000.0 & 130000.0 & 140000.0 \\ 210000.0 & 220000.0 & 230000.0 & 240000.0 \\ 310000.0 & 320000.0 & 330000.0 & 340000.0 \end{bmatrix}$$

$$B = \begin{bmatrix} -11.0 & -12.0 & -13.0 & -14.0 \\ -21.0 & -22.0 & -23.0 & -24.0 \\ -31.0 & -32.0 & -33.0 & -34.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 110011.0 & 210021.0 & 310031.0 \\ 120012.0 & 220022.0 & 320032.0 \\ 130013.0 & 230023.0 & 330033.0 \\ 140014.0 & 240024.0 & 340034.0 \end{bmatrix}$$

### Example 5

This example shows how to produce the transpose of the result of the computation performed in “Example 4,”  $C \leftarrow A^T - B^T$ , which uses the calling sequence:

```
CALL SGESUB( A , 3 , 'T' , B , 3 , 'T' , C , 4 , 4 , 3 )
```

You instead code a calling sequence for  $C^T \leftarrow A - B$ , as shown below, where the resulting matrix  $C^T$  in the output array  $CT$  is the transpose of the matrix in the output array  $C$  in Example 4. Note that the array  $CT$  has dimensions large enough to receive the transposed matrix. For a description of all the matrix identities, see “Special Usage” on page 385.

**Call Statement and Input:**

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
          |  |    |      |  |  |      |  |  |  |  |
CALL SGESUB( A , 3 , 'N' , B , 3 , 'N' , CT , 3 , 3 , 4 )

```

## SGESUB, DGESUB, CGESUB, and ZGESUB

$$A = \begin{bmatrix} 110000.0 & 120000.0 & 130000.0 & 140000.0 \\ 210000.0 & 220000.0 & 230000.0 & 240000.0 \\ 310000.0 & 320000.0 & 330000.0 & 340000.0 \end{bmatrix}$$

$$B = \begin{bmatrix} -11.0 & -12.0 & -13.0 & -14.0 \\ -21.0 & -22.0 & -23.0 & -24.0 \\ -31.0 & -32.0 & -33.0 & -34.0 \end{bmatrix}$$

**Output:**

$$CT = \begin{bmatrix} 110011.0 & 120012.0 & 130013.0 & 140014.0 \\ 210021.0 & 220022.0 & 230023.0 & 240024.0 \\ 310031.0 & 320032.0 & 330033.0 & 340034.0 \end{bmatrix}$$

### Example 6

This example shows the computation  $C \leftarrow A - B$ , where  $A$ ,  $B$ , and  $C$  are contained in larger arrays  $A$ ,  $B$ , and  $C$ , respectively, and the arrays contain complex data.

**Call Statement and Input:**

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  M  N
          |  |    |      |  |  |    |  |  |  |  |
CALL CGESUB( A , 6 , 'N' , B , 5 , 'N' , C , 5 , 4 , 3 )

```

$$A = \begin{bmatrix} (1.0, 5.0) & (9.0, 2.0) & (1.0, 9.0) \\ (2.0, 4.0) & (8.0, 3.0) & (1.0, 8.0) \\ (3.0, 3.0) & (7.0, 5.0) & (1.0, 7.0) \\ (6.0, 6.0) & (3.0, 6.0) & (1.0, 4.0) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} (1.0, 8.0) & (2.0, 7.0) & (3.0, 2.0) \\ (4.0, 4.0) & (6.0, 8.0) & (6.0, 3.0) \\ (6.0, 2.0) & (4.0, 5.0) & (4.0, 5.0) \\ (7.0, 2.0) & (6.0, 4.0) & (1.0, 6.0) \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} (0.0, -3.0) & (7.0, -5.0) & (-2.0, 7.0) \\ (-2.0, 0.0) & (2.0, -5.0) & (-5.0, 5.0) \\ (-3.0, 1.0) & (3.0, 0.0) & (-3.0, 2.0) \\ (-1.0, 4.0) & (-3.0, 2.0) & (0.0, -2.0) \\ \cdot & \cdot & \cdot \end{bmatrix}$$

## SGEMUL, DGEMUL, CGEMUL, and ZGEMUL — Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes

### Purpose

SGEMUL and DGEMUL can perform any one of the following matrix multiplications, using matrices  $A$  and  $B$  or their transposes, and matrix  $C$ :

$$\begin{array}{ll} C \leftarrow AB & C \leftarrow AB^T \\ C \leftarrow A^T B & C \leftarrow A^T B^T \end{array}$$

CGEMUL and ZGEMUL can perform any one of the following matrix multiplications, using matrices  $A$  and  $B$ , their transposes or their conjugate transposes, and matrix  $C$ :

$$\begin{array}{lll} C \leftarrow AB & C \leftarrow AB^T & C \leftarrow AB^H \\ C \leftarrow A^T B & C \leftarrow A^T B^T & C \leftarrow A^T B^H \\ C \leftarrow A^H B & C \leftarrow A^H B^T & C \leftarrow A^H B^H \end{array}$$

Table 81. Data Types

$A, B, C$	Subroutine
Short-precision real	SGEMUL
Long-precision real	DGEMUL
Short-precision complex	CGEMUL
Long-precision complex	ZGEMUL

### Syntax

<b>Fortran</b>	CALL SGEMUL   DGEMUL   CGEMUL   ZGEMUL ( $a, lda, transa, b, ldb, transb, c, ldc, l, m, n$ )
<b>C and C++</b>	sgemul   dgemul   cgemul   zgemul ( $a, lda, transa, b, ldb, transb, c, ldc, l, m, n$ );

### On Entry

$a$

is the matrix  $A$ , where:

If  $transa = 'N'$ ,  $A$  is used in the computation, and  $A$  has  $l$  rows and  $m$  columns.

If  $transa = 'T'$ ,  $A^T$  is used in the computation, and  $A$  has  $m$  rows and  $l$  columns.

If  $transa = 'C'$ ,  $A^H$  is used in the computation, and  $A$  has  $m$  rows and  $l$  columns.

**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix  $A$  should always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 81, where:

If  $transa = 'N'$ , its size must be  $lda$  by (at least)  $m$ .

If  $transa = 'T'$  or  $'C'$ , its size must be  $lda$  by (at least)  $l$ .

## SGEMUL, DGEMUL, CGEMUL, and ZGEMUL

<i>lda</i>	<p>is the leading dimension of the array specified for <i>a</i>. Specified as: a fullword integer; <math>lda &gt; 0</math> and: If <i>transa</i> = 'N', <math>lda \geq l</math>. If <i>transa</i> = 'T' or 'C', <math>lda \geq m</math>.</p>
<i>transa</i>	<p>indicates the form of matrix <i>A</i> to use in the computation, where: If <i>transa</i> = 'N', <i>A</i> is used in the computation. If <i>transa</i> = 'T', <math>A^T</math> is used in the computation. If <i>transa</i> = 'C', <math>A^H</math> is used in the computation. Specified as: a single character; <i>transa</i> = 'N' or 'T' for SGEMUL and DGEMUL; <i>transa</i> = 'N', 'T', or 'C' for CGEMUL and ZGEMUL.</p>
<i>b</i>	<p>is the matrix <i>B</i>, where: If <i>transb</i> = 'N', <i>B</i> is used in the computation, and <i>B</i> has <i>m</i> rows and <i>n</i> columns. If <i>transb</i> = 'T', <math>B^T</math> is used in the computation, and <i>B</i> has <i>n</i> rows and <i>m</i> columns. If <i>transb</i> = 'C', <math>B^H</math> is used in the computation, and <i>B</i> has <i>n</i> rows and <i>m</i> columns.  <b>Note:</b> No data should be moved to form <math>B^T</math> or <math>B^H</math>; that is, the matrix <i>B</i> should always be stored in its untransposed form.  Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 81 on page 389, where: If <i>transb</i> = 'N', its size must be <i>ldb</i> by (at least) <i>n</i>. If <i>transb</i> = 'T' or 'C', its size must be <i>ldb</i> by (at least) <i>m</i>.</p>
<i>ldb</i>	<p>is the leading dimension of the array specified for <i>b</i>. Specified as: a fullword integer; <math>ldb &gt; 0</math> and: If <i>transb</i> = 'N', <math>ldb \geq m</math>. If <i>transb</i> = 'T' or 'C', <math>ldb \geq n</math>.</p>
<i>transb</i>	<p>indicates the form of matrix <i>B</i> to use in the computation, where: If <i>transb</i> = 'N', <i>B</i> is used in the computation. If <i>transb</i> = 'T', <math>B^T</math> is used in the computation. If <i>transb</i> = 'C', <math>B^H</math> is used in the computation. Specified as: a single character; <i>transb</i> = 'N' or 'T' for SGEMUL and DGEMUL; <i>transb</i> = 'N', 'T', or 'C' for CGEMUL and ZGEMUL.</p>
<i>c</i>	<p>See "On Return" on page 391.</p>
<i>ldc</i>	<p>is the leading dimension of the array specified for <i>c</i>. Specified as: a fullword integer; <math>ldc &gt; 0</math> and <math>ldc \geq l</math>.</p>
<i>l</i>	<p>is the number of rows in matrix <i>C</i>. Specified as: a fullword integer; <math>0 \leq l \leq ldc</math>.</p>



*m* has the following meaning, where:  
 If *transa* = 'N', it is the number of columns in matrix *A*.  
 If *transa* = 'T' or 'C', it is the number of rows in matrix *A*.  
 In addition:  
 If *transb* = 'N', it is the number of rows in matrix *B*.  
 If *transb* = 'T' or 'C', it is the number of columns in matrix *B*.  
 Specified as: a fullword integer;  $m \geq 0$ .

*n* is the number of columns in matrix *C*.  
 Specified as: a fullword integer;  $n \geq 0$ .

**On Return**

*c* is the *l* by *n* matrix *C*, containing the results of the computation.  
 Returned as: an *ldc* by (at least) *n* numbers of the data type indicated in Table 81 on page 389.

**Notes**

1. All subroutines accept lowercase letters for the *transa* and *transb* arguments.
2. Matrix *C* must have no common elements with matrices *A* or *B*; otherwise, results are unpredictable. See "Concepts" on page 59.

**Function**

The matrix multiplication is expressed as follows, where  $a_{ik}$ ,  $b_{kj}$ , and  $c_{ij}$  are elements of matrices *A*, *B*, and *C*, respectively:

$$c_{ij} = \sum_{k=1}^m a_{ik} b_{kj} \quad \text{for } C \leftarrow A B$$

$$c_{ij} = \sum_{k=1}^m a_{ki} b_{kj} \quad \text{for } C \leftarrow A^T B$$

$$c_{ij} = \sum_{k=1}^m \bar{a}_{ki} b_{kj} \quad \text{for } C \leftarrow A^H B$$

$$c_{ij} = \sum_{k=1}^m a_{ik} \bar{b}_{jk} \quad \text{for } C \leftarrow A B^T$$

$$c_{ij} = \sum_{k=1}^m a_{ki} \bar{b}_{jk} \quad \text{for } C \leftarrow A^T B^T$$

$$c_{ij} = \sum_{k=1}^m \bar{a}_{ki} \bar{b}_{jk} \quad \text{for } C \leftarrow A^H B^T$$

$$c_{ij} = \sum_{k=1}^m a_{ik} \bar{b}_{jk} \quad \text{for } C \leftarrow A B^H$$

$$c_{ij} = \sum_{k=1}^m a_{ki} \bar{b}_{jk} \quad \text{for } C \leftarrow A^T B^H$$

$$c_{ij} = \sum_{k=1}^m \bar{a}_{ki} \bar{b}_{jk} \quad \text{for } C \leftarrow A^H B^H$$

for  $i = 1, l$  and  $j = 1, n$

See reference [40]. If  $l$  or  $n$  is 0, no computation is performed. If  $l$  and  $n$  are greater than 0, and  $m$  is 0, an  $l$  by  $n$  matrix of zeros is returned.

## Special Usage

### Equivalence Rules

By using the following equivalence rules, you can compute the transpose  $C^T$  or the conjugate transpose  $C^H$  of some of the computations performed by these subroutines:

#### Transpose

$$(AB)^T = B^T A^T$$

$$(A^T B)^T = B^T A$$

$$(AB^T)^T = B A^T$$

$$(A^T B^T)^T = B A$$

#### Conjugate Transpose

$$(AB)^H = B^H A^H$$

$$(A^H B)^H = B^H A$$

$$(AB^H)^H = B A^H$$

$$(A^H B^H)^H = B A$$

When coding the calling sequences for these cases, be careful to code your matrix arguments and dimension arguments in the order indicated by the rule. Also, be careful that your output array, receiving  $C^T$  or  $C^H$ , has dimensions large enough to hold the resulting transposed or conjugate transposed matrix. See “Example 2” on page 394 and “Example 4” on page 395.

## Error conditions

### Resource Errors

Unable to allocate internal work area (CGEMUL and ZGEMUL only).

### Computational Errors

None

### Input-Argument Errors

1.  $lda, ldb, ldc \leq 0$
2.  $l, m, n < 0$
3.  $l > ldc$
4.  $transa, transb \neq 'N'$  or  $'T'$  for SGEMUL and DGEMUL
5.  $transa, transb \neq 'N', 'T',$  or  $'C'$  for CGEMUL and ZGEMUL
6.  $transa = 'N'$  and  $l > lda$
7.  $transa = 'T'$  or  $'C'$  and  $m > lda$
8.  $transb = 'N'$  and  $m > ldb$
9.  $transb = 'T'$  or  $'C'$  and  $n > ldb$

## Examples

### Example 1

This example shows the computation  $C \leftarrow AB$ , where  $A$ ,  $B$ , and  $C$  are contained in larger arrays  $A$ ,  $B$ , and  $C$ , respectively.

#### Call Statement and Input:

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  L  M  N
          |  |  |  |  |  |  |  |  |  |  |
CALL SGEMUL( A , 8 , 'N' , B , 6 , 'N' , C , 7 , 6 , 5 , 4 )
    
```

$$A = \begin{bmatrix} 1.0 & 2.0 & -1.0 & -1.0 & 4.0 \\ 2.0 & 0.0 & 1.0 & 1.0 & -1.0 \\ 1.0 & -1.0 & -1.0 & 1.0 & 2.0 \\ -3.0 & 2.0 & 2.0 & 2.0 & 0.0 \\ 4.0 & 0.0 & -2.0 & 1.0 & -1.0 \\ -1.0 & -1.0 & 1.0 & -3.0 & 2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -1.0 & 0.0 & 2.0 \\ 2.0 & 2.0 & -1.0 & -2.0 \\ 1.0 & 0.0 & -1.0 & 1.0 \\ -3.0 & -1.0 & 1.0 & -1.0 \\ 4.0 & 2.0 & -1.0 & 1.0 \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

#### Output:

$$C = \begin{bmatrix} 23.0 & 12.0 & -6.0 & 2.0 \\ -4.0 & -5.0 & 1.0 & 3.0 \\ 3.0 & 0.0 & 1.0 & 4.0 \\ -3.0 & 5.0 & -2.0 & -10.0 \\ -5.0 & -7.0 & 4.0 & 4.0 \\ 15.0 & 6.0 & -5.0 & 6.0 \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

## SGEMUL, DGEMUL, CGEMUL, and ZGEMUL

### Example 2

This example shows how to produce the transpose of the result of the computation performed in “Example 1” on page 393,  $C \leftarrow AB$ , which uses the calling sequence:

```
CALL SGEMUL (A,8,'N',B,6,'N',C,7,6,5,4)
```

You instead code a calling sequence for  $C^T \leftarrow B^T A^T$ , as shown below, where the resulting matrix  $C^T$  in the output array CT is the transpose of the matrix in the output array C in Example 1. Note that the array CT has dimensions large enough to receive the transposed matrix. For a description of all the matrix identities, see “Special Usage” on page 392.

#### Call Statement and Input:

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  L  M  N
CALL SGEMUL( B , 6 , 'T' , A , 8 , 'T' , CT , 5 , 4 , 5 , 6 )

```

$$B = \begin{bmatrix} 1.0 & -1.0 & 0.0 & 2.0 \\ 2.0 & 2.0 & -1.0 & -2.0 \\ 1.0 & 0.0 & -1.0 & 1.0 \\ -3.0 & -1.0 & 1.0 & -1.0 \\ 4.0 & 2.0 & -1.0 & 1.0 \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$A = \begin{bmatrix} 1.0 & 2.0 & -1.0 & -1.0 & 4.0 \\ 2.0 & 0.0 & 1.0 & 1.0 & -1.0 \\ 1.0 & -1.0 & -1.0 & 1.0 & 2.0 \\ -3.0 & 2.0 & 2.0 & 2.0 & 0.0 \\ 4.0 & 0.0 & -2.0 & 1.0 & -1.0 \\ -1.0 & -1.0 & 1.0 & -3.0 & 2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

#### Output:

$$CT = \begin{bmatrix} 23.0 & -4.0 & 3.0 & -3.0 & -5.0 & 15.0 \\ 12.0 & -5.0 & 0.0 & 5.0 & -7.0 & 6.0 \\ -6.0 & 1.0 & 1.0 & -2.0 & 4.0 & -5.0 \\ 2.0 & 3.0 & 4.0 & -10.0 & 4.0 & 6.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 3

This example shows the computation  $C \leftarrow A^T B$ , where  $A$  and  $C$  are contained in larger arrays  $A$  and  $C$ , respectively, and  $B$  is the same size as the

#### Call Statement and Input:

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  L  M  N
CALL SGEMUL( A , 4 , 'T' , B , 3 , 'N' , C , 5 , 3 , 3 , 6 )

```

$$A = \begin{bmatrix} 1.0 & -3.0 & 2.0 \\ 2.0 & 4.0 & 0.0 \\ 1.0 & -1.0 & -1.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 & 2.0 & 2.0 & -1.0 & 2.0 \\ 2.0 & 4.0 & 0.0 & 0.0 & 1.0 & -2.0 \\ 1.0 & -1.0 & -1.0 & -1.0 & -1.0 & 1.0 \end{bmatrix}$$

Output:

$$C = \begin{bmatrix} 6.0 & 4.0 & 1.0 & 1.0 & 0.0 & -1.0 \\ 4.0 & 26.0 & -5.0 & -5.0 & 8.0 & -15.0 \\ 1.0 & -5.0 & 5.0 & 5.0 & -1.0 & 3.0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

### Example 4

This example shows how to produce the transpose of the result of the computation performed in “Example 3” on page 394,  $C \leftarrow A^T B$ , which uses the calling sequence:

```
CALL SGEMUL (A,4,'T',B,3,'N',C,5,3,3,6)
```

You instead code the calling sequence for  $C^T \leftarrow B^T A$ , as shown below, where the resulting matrix  $C^T$  in the output array CT is the transpose of the matrix in the output array C in Example 3. Note that the array CT has dimensions large enough to receive the transposed matrix. For a description of all the matrix identities, see “Special Usage” on page 392.

Call Statement and Input:

```
CALL SGEMUL( B , 3 , 'T' , A , 4 , 'N' , CT , 8 , 6 , 3 , 3 )
```

$$B = \begin{bmatrix} 1.0 & -3.0 & 2.0 & 2.0 & -1.0 & 2.0 \\ 2.0 & 4.0 & 0.0 & 0.0 & 1.0 & -2.0 \\ 1.0 & -1.0 & -1.0 & -1.0 & -1.0 & 1.0 \end{bmatrix}$$

$$A = \begin{bmatrix} 1.0 & -3.0 & 2.0 \\ 2.0 & 4.0 & 0.0 \\ 1.0 & -1.0 & -1.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

Output:

$$CT = \begin{bmatrix} 6.0 & 4.0 & 1.0 \\ 4.0 & 26.0 & -5.0 \\ 1.0 & -5.0 & 5.0 \\ 1.0 & -5.0 & 5.0 \\ 0.0 & 8.0 & -1.0 \\ -1.0 & -15.0 & 3.0 \\ \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \end{bmatrix}$$

### Example 5

This example shows the computation  $C \leftarrow AB^T$ , where  $A$  and  $C$  are contained in larger arrays A and C, respectively, and  $B$  is the same size as the array B in which it is contained.

Call Statement and Input:

## SGEMUL, DGEMUL, CGEMUL, and ZGEMUL

```

          A  LDA TRANSA  B  LDB TRANSB  C  LDC  L  M  N
CALL SGEMUL( A , 4 , 'N' , B , 3 , 'T' , C , 5 , 3 , 2 , 3 )

```

$$A = \begin{bmatrix} 1.0 & -3.0 \\ 2.0 & 4.0 \\ 1.0 & -1.0 \\ \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 \\ 2.0 & 4.0 \\ 1.0 & -1.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 10.0 & -10.0 & 4.0 \\ -10.0 & 20.0 & -2.0 \\ 4.0 & -2.0 & 2.0 \\ \vdots & \vdots & \vdots \end{bmatrix}$$

### Example 6

This example shows the computation  $C \leftarrow A^T B^T$ , where  $A$ ,  $B$ , and  $C$  are the same size as the arrays  $A$ ,  $B$ , and  $C$  in which they are contained. (Based on the dimensions of the matrices,  $A$  is actually a column vector, and  $C$  is actually a row vector.)

**Call Statement and Input:**

```

          A  LDA TRANSA  B  LDB TRANSB  C  LDC  L  M  N
CALL SGEMUL( A , 3 , 'T' , B , 3 , 'T' , C , 1 , 1 , 3 , 3 )

```

$$A = \begin{bmatrix} 1.0 \\ 2.0 \\ 1.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 & 2.0 \\ 2.0 & 4.0 & 0.0 \\ 1.0 & -1.0 & -1.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} -3.0 & 10.0 & -2.0 \end{bmatrix}$$

### Example 7

This example shows the computation  $C \leftarrow A^T B$  using complex data, where  $A$ ,  $B$ , and  $C$  are contained in larger arrays  $A$ ,  $B$ , and  $C$ , respectively.

**Call Statement and Input:**

```

          A  LDA TRANSA  B  LDB TRANSB  C  LDC  L  M  N
CALL CGEMUL( A , 6 , 'T' , B , 7 , 'N' , C , 3 , 2 , 3 , 3 )

```

$$A = \begin{bmatrix} (1.0, 2.0) & (3.0, 4.0) \\ (4.0, 6.0) & (7.0, 1.0) \\ (6.0, 3.0) & (2.0, 5.0) \end{bmatrix}$$

$$\begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} (1.0, 9.0) & (2.0, 6.0) & (5.0, 6.0) \\ (2.0, 5.0) & (6.0, 2.0) & (6.0, 4.0) \\ (2.0, 6.0) & (5.0, 4.0) & (2.0, 6.0) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

Output:

$$C = \begin{bmatrix} (-45.0, 85.0) & (20.0, 93.0) & (-13.0, 110.0) \\ (-50.0, 90.0) & (12.0, 79.0) & (3.0, 94.0) \\ \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 8

This example shows the computation  $C \leftarrow AB^H$  using complex data, where  $A$  and  $C$  are contained in larger arrays  $A$  and  $C$ , respectively, and  $B$  is the same size as the array  $B$  in which it is contained.

Call Statement and Input:

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  L  M  N
CALL CGEMUL( A , 4 , 'N' , B , 3 , 'C' , C , 4 , 3 , 2 , 3 )

```

$$A = \begin{bmatrix} (1.0, 2.0) & (-3.0, 2.0) \\ (2.0, 6.0) & (4.0, 5.0) \\ (1.0, 2.0) & (-1.0, 8.0) \\ \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} (1.0, 3.0) & (-3.0, 2.0) \\ (2.0, 5.0) & (4.0, 6.0) \\ (1.0, 1.0) & (-1.0, 9.0) \end{bmatrix}$$

Output:

$$C = \begin{bmatrix} (20.0, -1.0) & (12.0, 25.0) & (24.0, 26.0) \\ (18.0, -23.0) & (80.0, -2.0) & (49.0, -37.0) \\ (26.0, -23.0) & (56.0, 37.0) & (76.0, 2.0) \\ \cdot & \cdot & \cdot \end{bmatrix}$$

## SGEMMS, DGEMMS, CGEMMS, and ZGEMMS — Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes Using Winograd’s Variation of Strassen’s Algorithm

### Purpose

These subroutines use Winograd’s variation of the Strassen’s algorithm to perform the matrix multiplication for both real and complex matrices. SGEMMS and DGEMMS can perform any one of the following matrix multiplications, using matrices  $A$  and  $B$  or their transposes, and matrix  $C$ :

$$\begin{array}{ll} C \leftarrow AB & C \leftarrow AB^T \\ C \leftarrow A^T B & C \leftarrow A^T B^T \end{array}$$

CGEMMS and ZGEMMS can perform any one of the following matrix multiplications, using matrices  $A$  and  $B$ , their transposes or their conjugate transposes, and matrix  $C$ :

$$\begin{array}{lll} C \leftarrow AB & C \leftarrow AB^T & C \leftarrow AB^H \\ C \leftarrow A^T B & C \leftarrow A^T B^T & C \leftarrow A^T B^H \\ C \leftarrow A^H B & C \leftarrow A^H B^T & C \leftarrow A^H B^H \end{array}$$

Table 82. Data Types

$A, B, C$	$aux$	Subroutine
Short-precision real	Short-precision real	SGEMMS
Long-precision real	Long-precision real	DGEMMS
Short-precision complex	Short-precision real	CGEMMS
Long-precision complex	Long-precision real	ZGEMMS

### Syntax

<b>Fortran</b>	CALL SGEMMS   DGEMMS   CGEMMS   ZGEMMS ( $a, lda, transa, b, ldb, transb, c, ldc, l, m, n, aux, naux$ )
<b>C and C++</b>	sgemms   dgemms   cgemms   zgemms ( $a, lda, transa, b, ldb, transb, c, ldc, l, m, n, aux, naux$ );

### On Entry

$a$  is the matrix  $A$ , where:

If  $transa = 'N'$ ,  $A$  is used in the computation, and  $A$  has  $l$  rows and  $m$  columns.

If  $transa = 'T'$ ,  $A^T$  is used in the computation, and  $A$  has  $m$  rows and  $l$  columns.

If  $transa = 'C'$ ,  $A^H$  is used in the computation, and  $A$  has  $m$  rows and  $l$  columns.

**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix  $A$  should always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 82, where:



## SGEMMS, DGEMMS, CGEMMS, and ZGEMMS

	<p>If <i>transa</i> = 'N', its size must be <i>lda</i> by (at least) <i>m</i>.</p> <p>If <i>transa</i> = 'T' or 'C', its size must be <i>lda</i> by (at least) <i>l</i>.</p>
<i>lda</i>	<p>is the leading dimension of the array specified for <i>a</i>.</p> <p>Specified as: a fullword integer; <i>lda</i> &gt; 0 and:</p> <p>If <i>transa</i> = 'N', <i>lda</i> ≥ <i>l</i>.</p> <p>If <i>transa</i> = 'T' or 'C', <i>lda</i> ≥ <i>m</i>.</p>
<i>transa</i>	<p>indicates the form of matrix <i>A</i> to use in the computation, where:</p> <p>If <i>transa</i> = 'N', <i>A</i> is used in the computation.</p> <p>If <i>transa</i> = 'T', <math>A^T</math> is used in the computation.</p> <p>If <i>transa</i> = 'C', <math>A^H</math> is used in the computation.</p> <p>Specified as: a single character; <i>transa</i> = 'N' or 'T' for SGEMMS and DGEMMS; <i>transa</i> = 'N', 'T', or 'C' for CGEMMS and ZGEMMS.</p>
<i>b</i>	<p>is the matrix <i>B</i>, where:</p> <p>If <i>transb</i> = 'N', <i>B</i> is used in the computation, and <i>B</i> has <i>m</i> rows and <i>n</i> columns.</p> <p>If <i>transb</i> = 'T', <math>B^T</math> is used in the computation, and <i>B</i> has <i>n</i> rows and <i>m</i> columns.</p> <p>If <i>transb</i> = 'C', <math>B^H</math> is used in the computation, and <i>B</i> has <i>n</i> rows and <i>m</i> columns.</p> <p><b>Note:</b> No data should be moved to form <math>B^T</math> or <math>B^H</math>; that is, the matrix <i>B</i> should always be stored in its untransposed form.</p> <p>Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 82 on page 398, where:</p> <p>If <i>transb</i> = 'N', its size must be <i>ldb</i> by (at least) <i>n</i>.</p> <p>If <i>transb</i> = 'T' or 'C', its size must be <i>ldb</i> by (at least) <i>m</i>.</p>
<i>ldb</i>	<p>is the leading dimension of the array specified for <i>b</i>.</p> <p>Specified as: a fullword integer; <i>ldb</i> &gt; 0 and:</p> <p>If <i>transb</i> = 'N', <i>ldb</i> ≥ <i>m</i>.</p> <p>If <i>transb</i> = 'T' or 'C', <i>ldb</i> ≥ <i>n</i>.</p>
<i>transb</i>	<p>indicates the form of matrix <i>B</i> to use in the computation, where:</p> <p>If <i>transb</i> = 'N', <i>B</i> is used in the computation.</p> <p>If <i>transb</i> = 'T', <math>B^T</math> is used in the computation.</p> <p>If <i>transb</i> = 'C', <math>B^H</math> is used in the computation.</p> <p>Specified as: a single character; <i>transb</i> = 'N' or 'T' for SGEMMS and DGEMMS; <i>transb</i> = 'N', 'T', or 'C' for CGEMMS and ZGEMMS.</p>
<i>c</i>	<p>See "On Return" on page 401.</p>
<i>ldc</i>	<p>is the leading dimension of the array specified for <i>c</i>.</p>

## SGEMMS, DGEMMS, CGEMMS, and ZGEMMS

	Specified as: a fullword integer; $ldc > 0$ and $ldc \geq l$ .
<i>l</i>	is the number of rows in matrix <i>C</i> .
	Specified as: a fullword integer; $0 \leq l \leq ldc$ .
<i>m</i>	has the following meaning, where: If <i>transa</i> = 'N', it is the number of columns in matrix <i>A</i> . If <i>transa</i> = 'T' or 'C', it is the number of rows in matrix <i>A</i> . In addition: If <i>transb</i> = 'N', it is the number of rows in matrix <i>B</i> . If <i>transb</i> = 'T' or 'C', it is the number of columns in matrix <i>B</i> . Specified as: a fullword integer; $m \geq 0$ .
<i>n</i>	is the number of columns in matrix <i>C</i> . Specified as: a fullword integer; $n \geq 0$ .
<i>aux</i>	has the following meaning: If <i>naux</i> = 0 and error 2015 is unrecoverable, <i>aux</i> is ignored. Otherwise, is the storage work area used by this subroutine. Its size is specified by <i>naux</i> . Specified as: an area of storage containing numbers of the data type indicated in Table 82 on page 398.
<i>naux</i>	is the size of the work area specified by <i>aux</i> —that is, the number of elements in <i>aux</i> . Specified as: a fullword integer, where: If <i>naux</i> = 0 and error 2015 is unrecoverable, SGEMMS, DGEMMS, CGEMMS, and ZGEMMS dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program. Otherwise, When this subroutine uses Strassen's algorithm: <ul style="list-style-type: none"><li>• For SGEMMS and DGEMMS: Use <math>naux = \max[(n)(l), 0.7m(l+n)]</math>.</li><li>• For CGEMMS and ZGEMMS: Use <math>naux = \max[(n)(l), 0.7m(l+n)] + nb1 + nb2</math>, where: If <math>l \geq n</math>, then <math>nb1 \geq (l)(n+20)</math> and <math>nb2 \geq \max[(n)(l), (m)(n+20)]</math>. If <math>l &lt; n</math>, then <math>nb1 \geq (m)(n+20)</math> and <math>nb2 \geq \max[(n)(l), (l)(m+20)]</math>.</li></ul> When this subroutine uses the direct method (_GEMUL), use $naux \geq 0$ .

### Notes:

1. In most cases, these formulas provide an overestimate.
2. For an explanation of when this subroutine uses the direct method versus Strassen's algorithm, see "Notes" on page 401.

## On Return

$c$  is the  $l$  by  $n$  matrix  $C$ , containing the results of the computation. Returned as: an  $ldc$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 82 on page 398.

## Notes

1. There are two instances when these subroutines use the direct method (`_GEMUL`), rather than using Strassen's algorithm:
  - When either or both of the input matrices are small
  - For CGEMMS and ZGEMMS, when input matrices  $A$  and  $B$  overlap
 In these instances when the direct method is used, the subroutine does not use auxiliary storage, and you can specify `naux = 0`.
2. For CGEMMS and ZGEMMS, one of the input matrices,  $A$  or  $B$ , is rearranged during the computation and restored to its original form on return. Keep this in mind when diagnosing an abnormal termination.
3. All subroutines accept lowercase letters for the `transa` and `transb` arguments.
4. Matrix  $C$  must have no common elements with matrices  $A$  or  $B$ ; otherwise, results are unpredictable. See "Concepts" on page 59.
5. You have the option of having the minimum required value for `naux` dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

## Function

The matrix multiplications performed by these subroutines are functionally equivalent to those performed by `SGEMUL`, `DGEMUL`, `CGEMUL`, and `ZGEMUL`. For details on the computations performed, see "Function" on page 391.

SGEMMS, DGEMMS, CGEMMS, and ZGEMMS use Winograd's variation of the Strassen's algorithm with minor changes for tuning purposes. (See pages 45 and 46 in reference [13].) The subroutines compute matrix multiplication for both real and complex matrices of large sizes. Complex matrix multiplication uses a special technique, using three real matrix multiplications and five real matrix additions. Each of these three resulting matrix multiplications then uses Strassen's algorithm.

### Strassen's Algorithm

The steps of Strassen's algorithm can be repeated up to four times by these subroutines, with each step reducing the dimensions of the matrix by a factor of two. The number of steps used by this subroutine depends on the size of the input matrices. Each step reduces the number of operations by about 10% from the normal matrix multiplication. On the other hand, if the matrix is small, a normal matrix multiplication is performed without using the Strassen's algorithm, and no improvement is gained. For details about small matrices, see "Notes."

### Complex Matrix Multiplication

The complex multiplication is performed by forming the real and imaginary parts of the input matrices. These subroutines uses three real matrix multiplications and five real matrix additions, instead of the normal four real matrix multiplications and two real matrix additions. Using only three real matrix multiplications allows the subroutine to achieve up to a 25% reduction in matrix operations, which can result in a significant savings in computing time for large matrices.

### Accuracy Considerations

Strassen’s method is not stable for certain row or column scalings of the input matrices *A* and *B*. Therefore, for matrices *A* and *B* with divergent exponent values Strassen’s method may give inaccurate results. For these cases, you should use the `_GEMUL` or `_GEMM` subroutines.

### Special Usage

The equivalence rules, defined for matrix multiplication of *A* and *B* in “Special Usage” on page 392, also apply to these subroutines. You should use the equivalence rules when you want to transpose or conjugate transpose the result of the multiplication computation. When coding the calling sequences for these cases, be careful to code your matrix arguments and dimension arguments in the order indicated by the rule. Also, be careful that your output array, receiving  $C^T$  or  $C^H$ , has dimensions large enough to hold the resulting transposed or conjugate transposed matrix. See “Example 2” on page 394 and “Example 4” on page 395.

### Error conditions

#### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

#### Computational Errors

None

#### Input-Argument Errors

1.  $lda, ldb, ldc \leq 0$
2.  $l, m, n < 0$
3.  $l > ldc$
4.  $transa, transb \neq 'N'$  or  $'T'$  for SGEMMS and DGEMMS
5.  $transa, transb \neq 'N', 'T',$  or  $'C'$  for CGEMMS and ZGEMMS
6.  $transa = 'N'$  and  $l > lda$
7.  $transa = 'T'$  or  $'C'$  and  $m > lda$
8.  $transb = 'N'$  and  $m > ldb$
9.  $transb = 'T'$  or  $'C'$  and  $n > ldb$
10. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

### Examples

#### Example 1

This example shows the computation  $C \leftarrow AB$ , where *A*, *B*, and *C* are contained in larger arrays *A*, *B*, and *C*, respectively. It shows how to code the calling sequence for SGEMMS, but does not use the Strassen algorithm for doing the computation. The calling sequence is shown below. The input and output, other than auxiliary storage, is the same as in “Example 1” on page 393 for SGEMUL.

#### Call Statement and Input:

```

          A  LDA TRANSA  B  LDB TRANSB  C  LDC  L  M  N  AUX  NAUX
CALL SGEMMS( A , 8 , 'N' , B , 6 , 'N' , C , 7 , 6 , 5 , 4 , AUX , 0 )

```

#### Example 2

This example shows the computation  $C \leftarrow AB^H$ , where *A* and *C* are contained in larger arrays *A* and *C*, respectively, and *B* is the same size as the array *B* in which it

## SGEMMS, DGEMMS, CGEMMS, and ZGEMMS

is contained. The arrays contain complex data. This example shows how to code the calling sequence for CGEMMS, but does not use the Strassen algorithm for doing the computation. The calling sequence is shown below. The input and output, other than auxiliary storage, is the same as in "Example 8" on page 397 for CGEMUL.

### Call Statement and Input:

```

          A  LDA  TRANSA  B  LDB  TRANSB  C  LDC  L  M  N  AUX  NAUX
          |  |  |  |  |  |  |  |  |  |  |  |  |
CALL CGEMMS( A , 4 , 'N' , B , 3 , 'C' , C , 4 , 3 , 2 , 3 , AUX , 0 )
```

## SGEMM, DGEMM, CGEMM, and ZGEMM — Combined Matrix Multiplication and Addition for General Matrices, Their Transposes, or Conjugate Transposes

### Purpose

SGEMM and DGEMM can perform any one of the following combined matrix computations, using scalars  $\alpha$  and  $\beta$ , matrices  $A$  and  $B$  or their transposes, and matrix  $C$ :

$$\begin{array}{ll} C \leftarrow \alpha AB + \beta C & C \leftarrow \alpha AB^T + \beta C \\ C \leftarrow \alpha A^T B + \beta C & C \leftarrow \alpha A^T B^T + \beta C \end{array}$$

CGEMM and ZGEMM can perform any one of the following combined matrix computations, using scalars  $\alpha$  and  $\beta$ , matrices  $A$  and  $B$ , their transposes or their conjugate transposes, and matrix  $C$ :

$$\begin{array}{lll} C \leftarrow \alpha AB + \beta C & C \leftarrow \alpha AB^T + \beta C & C \leftarrow \alpha AB^H + \beta C \\ C \leftarrow \alpha A^T B + \beta C & C \leftarrow \alpha A^T B^T + \beta C & C \leftarrow \alpha A^T B^H + \beta C \\ C \leftarrow \alpha A^H B + \beta C & C \leftarrow \alpha A^H B^T + \beta C & C \leftarrow \alpha A^H B^H + \beta C \end{array}$$

Table 83. Data Types

$A, B, C, \alpha, \beta$	Subroutine
Short-precision real	SGEMM
Long-precision real	DGEMM
Short-precision complex	CGEMM
Long-precision complex	ZGEMM

### Syntax

Fortran	CALL SGEMM   DGEMM   CGEMM   ZGEMM ( <i>transa</i> , <i>transb</i> , <i>l</i> , <i>n</i> , <i>m</i> , <i>alpha</i> , <i>a</i> , <i>lda</i> , <i>b</i> , <i>ldb</i> , <i>beta</i> , <i>c</i> , <i>ldc</i> )
C and C++	sgemm   dgemm   cgemm   zgemm ( <i>transa</i> , <i>transb</i> , <i>l</i> , <i>n</i> , <i>m</i> , <i>alpha</i> , <i>a</i> , <i>lda</i> , <i>b</i> , <i>ldb</i> , <i>beta</i> , <i>c</i> , <i>ldc</i> );

### On Entry

*transa* indicates the form of matrix  $A$  to use in the computation, where:

- If *transa* = 'N',  $A$  is used in the computation.
- If *transa* = 'T',  $A^T$  is used in the computation.
- If *transa* = 'C',  $A^H$  is used in the computation.

Specified as: a single character; *transa* = 'N', 'T', or 'C'.

*transb* indicates the form of matrix  $B$  to use in the computation, where:

- If *transb* = 'N',  $B$  is used in the computation.
- If *transb* = 'T',  $B^T$  is used in the computation.
- If *transb* = 'C',  $B^H$  is used in the computation.

Specified as: a single character; *transb* = 'N', 'T', or 'C'.

*l* is the number of rows in matrix *C*.  
Specified as: a fullword integer;  $0 \leq l \leq ldc$ .

*n* is the number of columns in matrix *C*.  
Specified as: a fullword integer;  $n \geq 0$ .

*m* has the following meaning, where:  
If *transa* = 'N', it is the number of columns in matrix *A*.  
If *transa* = 'T' or 'C', it is the number of rows in matrix *A*.  
In addition:  
If *transb* = 'N', it is the number of rows in matrix *B*.  
If *transb* = 'T' or 'C', it is the number of columns in matrix *B*.  
Specified as: a fullword integer;  $m \geq 0$ .

*alpha* is the scalar  $\alpha$ .  
Specified as: a number of the data type indicated in Table 83 on page 404.

*a* is the matrix *A*, where:  
If *transa* = 'N', *A* is used in the computation, and *A* has *l* rows and *m* columns.  
If *transa* = 'T',  $A^T$  is used in the computation, and *A* has *m* rows and *l* columns.  
If *transa* = 'C',  $A^H$  is used in the computation, and *A* has *m* rows and *l* columns.  
**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix *A* should always be stored in its untransposed form.  
Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 83 on page 404, where:  
If *transa* = 'N', its size must be *lda* by (at least) *m*.  
If *transa* = 'T' or 'C', its size must be *lda* by (at least) *l*.

*lda* is the leading dimension of the array specified for *a*.  
Specified as: a fullword integer;  $lda > 0$  and:  
If *transa* = 'N',  $lda \geq l$ .  
If *transa* = 'T' or 'C',  $lda \geq m$ .

*b* is the matrix *B*, where:  
If *transb* = 'N', *B* is used in the computation, and *B* has *m* rows and *n* columns.  
If *transb* = 'T',  $B^T$  is used in the computation, and *B* has *n* rows and *m* columns.  
If *transb* = 'C',  $B^H$  is used in the computation, and *B* has *n* rows and *m* columns.

## SGEMM, DGEMM, CGEMM, and ZGEMM

**Note:** No data should be moved to form  $B^T$  or  $B^H$ ; that is, the matrix  $B$  should always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 83 on page 404, where:

If  $transb = 'N'$ , its size must be  $ldb$  by (at least)  $n$ .

If  $transb = 'T'$  or  $'C'$ , its size must be  $ldb$  by (at least)  $m$ .

$ldb$

is the leading dimension of the array specified for  $b$ .

Specified as: a fullword integer;  $ldb > 0$  and:

If  $transb = 'N'$ ,  $ldb \geq m$ .

If  $transb = 'T'$  or  $'C'$ ,  $ldb \geq n$ .

$beta$

is the scalar  $\beta$ .

Specified as: a number of the data type indicated in Table 83 on page 404.

$c$

is the  $l$  by  $n$  matrix  $C$ .

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 83 on page 404.

$ldc$

is the leading dimension of the array specified for  $c$ .

Specified as: a fullword integer;  $ldc > 0$  and  $ldc \geq l$ .

### On Return

$c$

is the  $l$  by  $n$  matrix  $C$ , containing the results of the computation.

Returned as: an  $ldc$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 83 on page 404.

### Notes

1. All subroutines accept lowercase letters for the  $transa$  and  $transb$  arguments.
2. For SGEMM and DGEMM, if you specify 'C' for the  $transa$  or  $transb$  argument, it is interpreted as though you specified 'T'.
3. Matrix  $C$  must have no common elements with matrices  $A$  or  $B$ ; otherwise, results are unpredictable. See "Concepts" on page 59.

### Function

The combined matrix addition and multiplication is expressed as follows, where  $a_{ik}$ ,  $b_{kj}$ , and  $c_{ij}$  are elements of matrices  $A$ ,  $B$ , and  $C$ , respectively:



$$c_{ij} = \left( \alpha \sum_{k=1}^m a_{ik} b_{kj} \right) + \beta c_{ij} \quad \text{for } C \leftarrow \alpha A B + \beta C$$

$$c_{ij} = \left( \alpha \sum_{k=1}^m a_{ki} b_{kj} \right) + \beta c_{ij} \quad \text{for } C \leftarrow \alpha A^T B + \beta C$$

$$c_{ij} = \left( \alpha \sum_{k=1}^m \bar{a}_{ki} b_{kj} \right) + \beta c_{ij} \quad \text{for } C \leftarrow \alpha A^H B + \beta C$$

$$c_{ij} = \left( \alpha \sum_{k=1}^m a_{ik} b_{jk} \right) + \beta c_{ij} \quad \text{for } C \leftarrow \alpha A B^T + \beta C$$

$$c_{ij} = \left( \alpha \sum_{k=1}^m a_{ki} b_{jk} \right) + \beta c_{ij} \quad \text{for } C \leftarrow \alpha A^T B^T + \beta C$$

$$c_{ij} = \left( \alpha \sum_{k=1}^m \bar{a}_{ki} b_{jk} \right) + \beta c_{ij} \quad \text{for } C \leftarrow \alpha A^H B^T + \beta C$$

$$c_{ij} = \left( \alpha \sum_{k=1}^m a_{ik} \bar{b}_{jk} \right) + \beta c_{ij} \quad \text{for } C \leftarrow \alpha A B^H + \beta C$$

$$c_{ij} = \left( \alpha \sum_{k=1}^m a_{ki} \bar{b}_{jk} \right) + \beta c_{ij} \quad \text{for } C \leftarrow \alpha A^T B^H + \beta C$$

$$c_{ij} = \left( \alpha \sum_{k=1}^m \bar{a}_{ki} \bar{b}_{jk} \right) + \beta c_{ij} \quad \text{for } C \leftarrow \alpha A^H B^H + \beta C$$

for  $i = 1, l$  and  $j = 1, n$

See references [34] and [40]. In the following three cases, no computation is performed:

- $l$  is 0.
- $n$  is 0.
- $\beta$  is 1 and  $\alpha$  is 0.

Assuming the above conditions do not exist, if  $\beta \neq 1$  and  $m$  is 0, then  $\beta C$  is returned.

## Special Usage

### Equivalence Rules

The equivalence rules, defined for matrix multiplication of  $A$  and  $B$  in “Special Usage” on page 392, also apply to the matrix multiplication part of the computation performed by this subroutine. You should use the equivalent rules when you want to transpose or conjugate transpose the multiplication part of the computation. When coding the calling sequences for these cases, be careful to code your matrix arguments and dimension arguments in the order indicated by the rule. Also, be careful that your input and output array  $C$  has dimensions large enough to hold the resulting matrix. See “Example 4” on page 410.

## Error conditions

### Resource Errors

Unable to allocate internal work area (CGEMM and ZGEMM only).

### Computational Errors

None

### Input-Argument Errors

1.  $lda, ldb, ldc \leq 0$
2.  $l, m, n < 0$
3.  $l > ldc$
4.  $transa, transb \neq 'N', 'T', \text{ or } 'C'$
5.  $transa = 'N'$  and  $l > lda$
6.  $transa = 'T'$  or  $'C'$  and  $m > lda$
7.  $transb = 'N'$  and  $m > ldb$
8.  $transb = 'T'$  or  $'C'$  and  $n > ldb$

## Examples

### Example 1

This example shows the computation  $C \leftarrow \alpha AB + \beta C$ , where  $A$ ,  $B$ , and  $C$  are contained in larger arrays  $A$ ,  $B$ , and  $C$ , respectively.

#### Call Statement and Input:

```

          TRANSA  TRANSB  L   N   M  ALPHA  A  LDA  B  LDB  BETA  C  LDC
          |         |         |   |   |   |   |   |   |   |   |   |   |
CALL SGEMM( 'N' , 'N' , 6 , 4 , 5 , 1.0 , A , 8 , B , 6 , 2.0 , C , 7 )
    
```

$$A = \begin{bmatrix} 1.0 & 2.0 & -1.0 & -1.0 & 4.0 \\ 2.0 & 0.0 & 1.0 & 1.0 & -1.0 \\ 1.0 & -1.0 & -1.0 & 1.0 & 2.0 \\ -3.0 & 2.0 & 2.0 & 2.0 & 0.0 \\ 4.0 & 0.0 & -2.0 & 1.0 & -1.0 \\ -1.0 & -1.0 & 1.0 & -3.0 & 2.0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -1.0 & 0.0 & 2.0 \\ 2.0 & 2.0 & -1.0 & -2.0 \\ 1.0 & 0.0 & -1.0 & 1.0 \\ -3.0 & -1.0 & 1.0 & -1.0 \\ 4.0 & 2.0 & -1.0 & 1.0 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

$$C = \begin{bmatrix} 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 & 0.5 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

#### Output:

$$\begin{bmatrix} 24.0 & 13.0 & -5.0 & 3.0 \\ -3.0 & -4.0 & 2.0 & 4.0 \end{bmatrix}$$

$$C = \begin{bmatrix} 4.0 & 1.0 & 2.0 & 5.0 \\ -2.0 & 6.0 & -1.0 & -9.0 \\ -4.0 & -6.0 & 5.0 & 5.0 \\ 16.0 & 7.0 & -4.0 & 7.0 \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 2

This example shows the computation  $C \leftarrow \alpha AB^T + \beta C$ , where  $A$  and  $C$  are contained in larger arrays  $A$  and  $C$ , respectively, and  $B$  is the same size as array  $B$  in which it is contained.

#### Call Statement and Input:

```

          TRANSA  TRANSB  L  N  M  ALPHA  A  LDA  B  LDB  BETA  C  LDC
CALL SGEMM( 'N' , 'T' , 3 , 3 , 2 , 1.0 , A , 4 , B , 3 , 2.0 , C , 5 )

```

$$A = \begin{bmatrix} 1.0 & -3.0 \\ 2.0 & 4.0 \\ 1.0 & -1.0 \\ \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 \\ 2.0 & 4.0 \\ 1.0 & -1.0 \end{bmatrix}$$

$$C = \begin{bmatrix} 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

#### Output:

$$C = \begin{bmatrix} 11.0 & -9.0 & 5.0 \\ -9.0 & 21.0 & -1.0 \\ 5.0 & -1.0 & 3.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 3

This example shows the computation  $C \leftarrow \alpha AB + \beta C$  using complex data, where  $A$ ,  $B$ , and  $C$  are contained in larger arrays,  $A$ ,  $B$ , and  $C$ , respectively.

#### Call Statement and Input:

```

          TRANSA  TRANSB  L  N  M  ALPHA  A  LDA  B  LDB  BETA  C  LDC
CALL CGEMM( 'N' , 'N' , 6 , 2 , 3 , ALPHA , A , 8 , B , 4 , BETA , C , 8 )
ALPHA = (1.0, 0.0)
BETA  = (2.0, 0.0)

```

$$A = \begin{bmatrix} (1.0, 5.0) & (9.0, 2.0) & (1.0, 9.0) \\ (2.0, 4.0) & (8.0, 3.0) & (1.0, 8.0) \\ (3.0, 3.0) & (7.0, 5.0) & (1.0, 7.0) \\ (4.0, 2.0) & (4.0, 7.0) & (1.0, 5.0) \\ (5.0, 1.0) & (5.0, 1.0) & (1.0, 6.0) \\ (6.0, 6.0) & (3.0, 6.0) & (1.0, 4.0) \end{bmatrix}$$

## SGEMM, DGEMM, CGEMM, and ZGEMM

$$\begin{aligned}
 & \left[ \begin{array}{ccc} \vdots & \vdots & \vdots \end{array} \right] \\
 B &= \begin{bmatrix} (1.0, 8.0) & (2.0, 7.0) \\ (4.0, 4.0) & (6.0, 8.0) \\ (6.0, 2.0) & (4.0, 5.0) \\ \cdot & \cdot \end{bmatrix} \\
 C &= \begin{bmatrix} (0.5, 0.0) & (0.5, 0.0) \\ (0.5, 0.0) & (0.5, 0.0) \\ (0.5, 0.0) & (0.5, 0.0) \\ (0.5, 0.0) & (0.5, 0.0) \\ (0.5, 0.0) & (0.5, 0.0) \\ (0.5, 0.0) & (0.5, 0.0) \\ \vdots & \vdots \\ \cdot & \cdot \end{bmatrix}
 \end{aligned}$$

**Output:**

$$C = \begin{bmatrix} (-22.0, 113.0) & (-35.0, 142.0) \\ (-19.0, 114.0) & (-35.0, 141.0) \\ (-20.0, 119.0) & (-43.0, 146.0) \\ (-27.0, 110.0) & (-58.0, 131.0) \\ (8.0, 103.0) & (0.0, 112.0) \\ (-55.0, 116.0) & (-75.0, 135.0) \\ \vdots & \vdots \\ \cdot & \cdot \end{bmatrix}$$

### Example 4

This example shows how to obtain the conjugate transpose of  $AB^H$ .

$$(AB^H)^H = \overline{BA^T} = BA^H$$

This shows the conjugate transpose of the computation performed in “Example 8” on page 397 for CGEMUL, which uses the following calling sequence:

```
CALL CGEMUL( A , 4 , 'N' , B , 3 , 'C' , C , 4 , 3 , 2 , 3 )
```

You instead code the calling sequence for  $C \leftarrow \beta C + \alpha BA^H$ , where  $\beta = 0$ ,  $\alpha = 1$ , and the array  $C$  has the correct dimensions to receive the transposed matrix. Because  $\beta$  is zero,  $\beta C = 0$ . For a description of all the matrix identities, see “Special Usage” on page 392.

**Call Statement and Input:**

```

          TRANSA  TRANSB  L  N  M  ALPHA  A  LDA  B  LDB  BETA  C  LDC
          |         |         |  |  |  |         |  |  |  |         |  |
CALL CGEMM( 'N' , 'C' , 3 , 3 , 2 , ALPHA , B , 3 , A , 3 , BETA , C , 4 )
ALPHA    = (1.0, 0.0)
BETA     = (0.0, 0.0)

```

$$B = \begin{bmatrix} (1.0, 3.0) & (-3.0, 2.0) \\ (2.0, 5.0) & (4.0, 6.0) \\ (1.0, 1.0) & (-1.0, 9.0) \end{bmatrix}$$

$$A = \begin{bmatrix} (1.0, 2.0) & (-3.0, 2.0) \\ (2.0, 6.0) & (4.0, 5.0) \\ (1.0, 2.0) & (-1.0, 8.0) \\ \cdot & \cdot \end{bmatrix}$$

C = (not relevant)

**Output:**

$$C = \begin{bmatrix} (20.0, 1.0) & (18.0, 23.0) & (26.0, 23.0) \\ (12.0, -25.0) & (80.0, 2.0) & (56.0, -37.0) \\ (24.0, -26.0) & (49.0, 37.0) & (76.0, -2.0) \\ \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 5

This example shows the computation  $C \leftarrow \alpha A^T B^H + \beta C$  using complex data, where  $A$ ,  $B$ , and  $C$  are the same size as the arrays  $A$ ,  $B$ , and  $C$ , in which they are contained. Because  $\beta$  is zero,  $\beta C = 0$ . (Based on the dimensions of the matrices,  $A$  is actually a column vector, and  $C$  is actually a row vector.)

**Call Statement and Input:**

```

          TRANSA TRANSB  L  N  M  ALPHA  A  LDA  B  LDB  BETA  C  LDC
          |         |    |  |  |  |     |  |   |  |   |   |   |
CALL CGEMM( 'T' , 'C' , 1 , 3 , 3 , ALPHA , A , 3 , B , 3 , BETA , C , 1 )
ALPHA    = (1.0, 1.0)
BETA     = (0.0, 0.0)

```

$$A = \begin{bmatrix} (1.0, 2.0) \\ (2.0, 5.0) \\ (1.0, 6.0) \end{bmatrix}$$

$$B = \begin{bmatrix} (1.0, 6.0) & (-3.0, 4.0) & (2.0, 6.0) \\ (2.0, 3.0) & (4.0, 6.0) & (0.0, 3.0) \\ (1.0, 3.0) & (-1.0, 6.0) & (-1.0, 9.0) \end{bmatrix}$$

C = (not relevant)

**Output:**

$$C = \begin{bmatrix} (86.0, 44.0) & (58.0, 70.0) & (121.0, 55.0) \end{bmatrix}$$

## SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, and ZHEMM — Matrix-Matrix Product Where One Matrix is Real or Complex Symmetric or Complex Hermitian

### Purpose

These subroutines compute one of the following matrix-matrix products, using the scalars  $\alpha$  and  $\beta$  and matrices  $A$ ,  $B$ , and  $C$ :

1.  $C \leftarrow \alpha AB + \beta C$
2.  $C \leftarrow \alpha BA + \beta C$

where matrix  $A$  is stored in either upper or lower storage mode, and:

- For SSYMM and DSYMM, matrix  $A$  is real symmetric.
- For CSYMM and ZSYMM, matrix  $A$  is complex symmetric.
- For CHEMM and ZHEMM, matrix  $A$  is complex Hermitian.

Table 84. Data Types

$\alpha$ , $A$ , $B$ , $\beta$ , $C$	Subprogram
Short-precision real	SSYMM
Long-precision real	DSYMM
Short-precision complex	CSYMM and CHEMM
Long-precision complex	ZSYMM and ZHEMM

### Syntax

<b>Fortran</b>	CALL SSYMM   DSYMM   CSYMM   ZSYMM   CHEMM   ZHEMM ( <i>side, uplo, m, n, alpha, a, lda, b, ldb, beta, c, ldc</i> )
<b>C and C++</b>	ssymm   dsymm   csymm   zsyymm   chemm   zhemm ( <i>side, uplo, m, n, alpha, a, lda, b, ldb, beta, c, ldc</i> );

### On Entry

*side* indicates whether matrix  $A$  is located to the left or right of rectangular matrix  $B$  in the equation used for this computation, where:

If *side* = 'L',  $A$  is to the left of  $B$ , resulting in equation 1.

If *side* = 'R',  $A$  is to the right of  $B$ , resulting in equation 2.

Specified as: a single character. It must be 'L' or 'R'.

*uplo* indicates the storage mode used for matrix  $A$ , where:

If *uplo* = 'U',  $A$  is stored in upper storage mode.

If *uplo* = 'L',  $A$  is stored in lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

*m* is the number of rows in rectangular matrices  $B$  and  $C$ , and:

If *side* = 'L',  $m$  is the order of matrix  $A$ .

Specified as: a fullword integer;  $0 \leq m \leq ldb$ ,  $m \leq ldc$ , and:

If *side* = 'L',  $m \leq lda$ .

## SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, and ZHEMM

- n* is the number of columns in rectangular matrices *B* and *C*, and:  
If *side* = 'R', *n* is the order of matrix *A*.  
Specified as: a fullword integer;  $n \geq 0$  and:  
If *side* = 'R',  $n \leq lda$ .
- alpha* is the scalar  $\alpha$ .  
Specified as: a number of the data type indicated in Table 84 on page 412.
- a* is the real symmetric, complex symmetric, or complex Hermitian matrix *A*, where:  
If *side* = 'L', *A* is order *m*.  
If *side* = 'R', *A* is order *n*.  
and where it is stored as follows:  
If *uplo* = 'U', *A* is stored in upper storage mode.  
If *uplo* = 'L', *A* is stored in lower storage mode.  
Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 84 on page 412, where:  
If *side* = 'L', its size must be *lda* by (at least) *m*.  
If *side* = 'R', its size must be *lda* by (at least) *n*.
- lda* is the leading dimension of the array specified for *a*.  
Specified as: a fullword integer;  $lda > 0$  and:  
If *side* = 'L',  $lda \geq m$ .  
If *side* = 'R',  $lda \geq n$ .
- b* is the *m* by *n* rectangular matrix *B*.  
Specified as: an *ldb* by (at least) *n* array, containing numbers of the data type indicated in Table 84 on page 412.
- ldb* is the leading dimension of the array specified for *b*.  
Specified as: a fullword integer;  $ldb > 0$  and  $ldb \geq m$ .
- beta* is the scalar  $\beta$ .  
Specified as: a number of the data type indicated in Table 84 on page 412.
- c* is the *m* by *n* rectangular matrix *C*.  
Specified as: an *ldc* by (at least) *n* array, containing numbers of the data type indicated in Table 84 on page 412.
- ldc* is the leading dimension of the array specified for *c*.  
Specified as: a fullword integer;  $ldc > 0$  and  $ldc \geq m$ .

### On Return

- c* is the *m* by *n* matrix *C*, containing the results of the computation.  
Returned as: an *ldc* by (at least) *n* array, containing numbers of the data type indicated in Table 84 on page 412.

## Notes

1. These subroutines accept lowercase letters for the *side* and *uplo* arguments.
2. Matrices *A*, *B*, and *C* must have no common elements; otherwise, results are unpredictable.
3. If matrix *A* is upper triangular (*uplo* = 'U'), these subroutines use only the data in the upper triangular portion of the array. If matrix *A* is lower triangular, (*uplo* = 'L'), these subroutines use only the data in the lower triangular portion of the array. In each case, the other portion of the array is altered during the computation, but restored before exit.
4. The imaginary parts of the diagonal elements of a complex Hermitian matrix *A* are assumed to be zero, so you do not have to set these values.
5. For a description of how symmetric matrices are stored in upper and lower storage mode, see "Symmetric Matrix" on page 69. For a description of how complex Hermitian matrices are stored in upper and lower storage mode, see "Complex Hermitian Matrix" on page 73.

## Function

These subroutines can perform the following matrix-matrix product computations using matrix *A*, which is real symmetric for SSYMM and DSYMM, complex symmetric for CSYMM and ZSYMM, and complex Hermitian for CHEMM and ZHEMM:

1.  $C \leftarrow \alpha AB + \beta C$
2.  $C \leftarrow \alpha BA + \beta C$

where:

$\alpha$  and  $\beta$  are scalars.

*A* is a matrix of the type indicated above, stored in upper or lower storage mode. It is order *m* for equation 1 and order *n* for equation 2.

*B* and *C* are *m* by *n* rectangular matrices.

See references [34] and [40]. In the following two cases, no computation is performed:

- *n* or *m* is 0.
- $\beta$  is one and  $\alpha$  is zero.

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

None

### Input-Argument Errors

1.  $m < 0$
2.  $m > ldb$
3.  $m > ldc$
4.  $n < 0$
5.  $lda, ldb, ldc \leq 0$
6. *side*  $\neq$  'L' or 'R'
7. *uplo*  $\neq$  'L' or 'U'
8. *side* = 'L' and  $m > lda$
9. *side* = 'R' and  $n > lda$



## Examples

### Example 1

This example shows the computation  $C \leftarrow \alpha AB + \beta C$ , where  $A$  is a real symmetric matrix of order 5, stored in upper storage mode, and  $B$  and  $C$  are 5 by 4 rectangular matrices.

#### Call Statement and Input:

```

          SIDE UPLO M  N  ALPHA  A  LDA  B  LDB  BETA  C  LDC
          |   |   |   |   |   |   |   |   |   |   |
CALL SSYMM( 'L' , 'U' , 5 , 4 , 2.0 , A , 8 , B , 6 , 1.0 , C , 5 )
    
```

$$A = \begin{bmatrix} 1.0 & 2.0 & -1.0 & -1.0 & 4.0 \\ . & 0.0 & 1.0 & 1.0 & -1.0 \\ . & . & -1.0 & 1.0 & 2.0 \\ . & . & . & 2.0 & 0.0 \\ . & . & . & . & -1.0 \\ . & . & . & . & . \\ . & . & . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -1.0 & 0.0 & 2.0 \\ 2.0 & 2.0 & -1.0 & -2.0 \\ 1.0 & 0.0 & -1.0 & 1.0 \\ -3.0 & -1.0 & 1.0 & -1.0 \\ 4.0 & 2.0 & -1.0 & 1.0 \\ . & . & . & . \end{bmatrix}$$

$$C = \begin{bmatrix} 23.0 & 12.0 & -6.0 & 2.0 \\ -4.0 & -5.0 & 1.0 & 3.0 \\ 5.0 & 6.0 & -1.0 & -4.0 \\ -4.0 & 1.0 & 0.0 & -5.0 \\ 8.0 & -4.0 & -2.0 & 13.0 \end{bmatrix}$$

#### Output:

$$C = \begin{bmatrix} 69.0 & 36.0 & -18.0 & 6.0 \\ -12.0 & -15.0 & 3.0 & 9.0 \\ 15.0 & 18.0 & -3.0 & -12.0 \\ -12.0 & 3.0 & 0.0 & -15.0 \\ 8.0 & -20.0 & -2.0 & 35.0 \end{bmatrix}$$

### Example 2

This example shows the computation  $C \leftarrow \alpha AB + \beta C$ , where  $A$  is a real symmetric matrix of order 3, stored in lower storage mode, and  $B$  and  $C$  are 3 by 6 rectangular matrices.

#### Call Statement and Input:

```

          SIDE UPLO M  N  ALPHA  A  LDA  B  LDB  BETA  C  LDC
          |   |   |   |   |   |   |   |   |   |   |
CALL SSYMM( 'L' , 'L' , 3 , 6 , 2.0 , A , 4 , B , 3 , 2.0 , C , 5 )
    
```

$$A = \begin{bmatrix} 1.0 & . & . \\ 2.0 & 4.0 & . \\ 1.0 & -1.0 & -1.0 \\ . & . & . \end{bmatrix}$$

## SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, and ZHEMM

$$B = \begin{bmatrix} 1.0 & -3.0 & 2.0 & 2.0 & -1.0 & 2.0 \\ 2.0 & 4.0 & 0.0 & 0.0 & 1.0 & -2.0 \\ 1.0 & -1.0 & -1.0 & -1.0 & -1.0 & 1.0 \end{bmatrix}$$

$$C = \begin{bmatrix} 6.0 & 4.0 & 1.0 & 1.0 & 0.0 & -1.0 \\ 9.0 & 11.0 & 5.0 & 5.0 & 3.0 & -5.0 \\ -2.0 & -6.0 & 3.0 & 3.0 & -1.0 & 32.0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 24.0 & 16.0 & 4.0 & 4.0 & 0.0 & -4.0 \\ 36.0 & 44.0 & 20.0 & 20.0 & 12.0 & -20.0 \\ -8.0 & -24.0 & 12.0 & 12.0 & -4.0 & 12.0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

### Example 3

This example shows the computation  $C \leftarrow \alpha BA + \beta C$ , where  $A$  is a real symmetric matrix of order 3, stored in upper storage mode, and  $B$  and  $C$  are 2 by 3 rectangular matrices.

**Call Statement and Input:**

```

          SIDE UPLO M  N  ALPHA  A  LDA  B  LDB  BETA  C  LDC
          |   |   |   |   |   |   |   |   |   |   |
CALL SSYMM( 'R' , 'U' , 2 , 3 , 2.0 , A , 4 , B , 3 , 1.0 , C , 5 )

```

$$A = \begin{bmatrix} 1.0 & -3.0 & 1.0 \\ . & 4.0 & -1.0 \\ . & . & 2.0 \\ . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 & 3.0 \\ 2.0 & 4.0 & -1.0 \\ . & . & . \end{bmatrix}$$

$$C = \begin{bmatrix} 13.0 & -18.0 & 10.0 \\ -11.0 & 11.0 & -4.0 \\ . & . & . \\ \vdots & \vdots & \vdots \\ . & . & . \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 39.0 & -54.0 & 30.0 \\ -33.0 & 33.0 & -12.0 \\ . & . & . \\ \vdots & \vdots & \vdots \\ . & . & . \end{bmatrix}$$

### Example 4

This example shows the computation  $C \leftarrow \alpha BA + \beta C$ , where  $A$  is a real symmetric matrix of order 3, stored in lower storage mode, and  $B$  and  $C$  are 3 by 3 square matrices.

#### Call Statement and Input:

```

          SIDE UPLO M  N  ALPHA  A  LDA  B  LDB  BETA  C  LDC
          |   |   |   |   |   |   |   |   |   |   |
CALL SSYMM( 'R' , 'L' , 3 , 3 , -1.0 , A , 3 , B , 3 , 1.0 , C , 3 )
    
```

$$A = \begin{bmatrix} 1.0 & . & . \\ 2.0 & 10.0 & . \\ 1.0 & 11.0 & 4.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 & 2.0 \\ 2.0 & 4.0 & 0.0 \\ 1.0 & -1.0 & -1.0 \end{bmatrix}$$

$$C = \begin{bmatrix} 1.0 & 5.0 & -9.0 \\ -3.0 & 10.0 & -2.0 \\ -2.0 & 8.0 & 0.0 \end{bmatrix}$$

#### Output:

$$C = \begin{bmatrix} 4.0 & 11.0 & 15.0 \\ -13.0 & -34.0 & -48.0 \\ 0.0 & 27.0 & 14.0 \end{bmatrix}$$

### Example 5

This example shows the computation  $C \leftarrow \alpha BA + \beta C$ , where  $A$  is a complex symmetric matrix of order 3, stored in upper storage mode, and  $B$  and  $C$  are 2 by 3 rectangular matrices.

#### Call Statement and Input:

```

          SIDE UPLO M  N  ALPHA  A  LDA  B  LDB  BETA  C  LDC
          |   |   |   |   |   |   |   |   |   |   |
CALL CSYMM( 'R' , 'U' , 2 , 3 , ALPHA , A , 4 , B , 3 , BETA , C , 5 )
    
```

$$\text{ALPHA} = (2.0, 3.0)$$

$$\text{BETA} = (1.0, 6.0)$$

$$A = \begin{bmatrix} (1.0, 5.0) & (-3.0, 2.0) & (1.0, 6.0) \\ . & (4.0, 5.0) & (-1.0, 4.0) \\ . & . & (2.0, 5.0) \\ . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} (1.0, 1.0) & (-3.0, 2.0) & (3.0, 3.0) \\ (2.0, 6.0) & (4.0, 5.0) & (-1.0, 4.0) \\ . & . & . \end{bmatrix}$$

$$C = \begin{bmatrix} (13.0, 6.0) & (-18.0, 6.0) & (10.0, 7.0) \\ (-11.0, 8.0) & (11.0, 1.0) & (-4.0, 2.0) \\ . & . & . \end{bmatrix}$$

## SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, and ZHEMM

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} (-96.0, 72.0) & (-141.0, -226.0) & (-112.0, 38.0) \\ (-230.0, -269.0) & (-133.0, -23.0) & (-272.0, -198.0) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 6

This example shows the computation  $C \leftarrow \alpha BA + \beta C$ , where  $A$  is a complex Hermitian matrix of order 3, stored in lower storage mode, and  $B$  and  $C$  are 3 by 3 square matrices.

**Note:** The imaginary parts of the diagonal elements of a complex Hermitian matrix are assumed to be zero, so you do not have to set these values.

**Call Statement and Input:**

```

          SIDE  UPLO  M  N  ALPHA  A  LDA  B  LDB  BETA  C  LDC
CALL CHEMM( 'R' , 'L' , 2 , 3 , ALPHA , A , 4 , B , 3 , BETA , C , 5 )

```

ALPHA = (2.0, 3.0)

BETA = (1.0, 6.0)

$$A = \begin{bmatrix} (1.0, \cdot) & \cdot & \cdot \\ (3.0, 2.0) & (4.0, \cdot) & \cdot \\ (-1.0, 6.0) & (1.0, 4.0) & (2.0, \cdot) \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} (1.0, 1.0) & (-3.0, 2.0) & (3.0, 3.0) \\ (2.0, 6.0) & (4.0, 5.0) & (-1.0, 4.0) \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$C = \begin{bmatrix} (13.0, 6.0) & (-18.0, 6.0) & (10.0, 7.0) \\ (-11.0, 8.0) & (11.0, 1.0) & (-4.0, 2.0) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} (-137.0, 17.0) & (-158.0, -102.0) & (-39.0, 141.0) \\ (-154.0, -77.0) & (-63.0, 186.0) & (159.0, 104.0) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

## STRMM, DTRMM, CTRMM, and ZTRMM — Triangular Matrix-Matrix Product

### Purpose

STRMM and DTRMM compute one of the following matrix-matrix products, using the scalar  $\alpha$ , rectangular matrix  $B$ , and triangular matrix  $A$  or its transpose:

1.  $B \leftarrow \alpha AB$
2.  $B \leftarrow \alpha A^T B$
3.  $B \leftarrow \alpha BA$
4.  $B \leftarrow \alpha BA^T$

CTRMM and ZTRMM compute one of the following matrix-matrix products, using the scalar  $\alpha$ , rectangular matrix  $B$ , and triangular matrix  $A$ , its transpose, or its conjugate transpose:

1.  $B \leftarrow \alpha AB$
2.  $B \leftarrow \alpha A^T B$
3.  $B \leftarrow \alpha BA$
4.  $B \leftarrow \alpha BA^T$
5.  $B \leftarrow \alpha A^H B$
6.  $B \leftarrow \alpha BA^H$

Table 85. Data Types

$A, B, \alpha$	Subroutine
Short-precision real	STRMM
Long-precision real	DTRMM
Short-precision complex	CTRMM
Long-precision complex	ZTRMM

### Syntax

<b>Fortran</b>	CALL STRMM   DTRMM   CTRMM   ZTRMM ( <i>side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb</i> )
<b>C and C++</b>	strmm   dtrmm   ctrmm   ztrmm ( <i>side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb</i> );

### On Entry

- side* indicates whether the triangular matrix  $A$  is located to the left or right of rectangular matrix  $B$  in the equation used for this computation, where:
- If *side* = 'L',  $A$  is to the left of  $B$  in the equation, resulting in either equation 1, 2, or 5.
- If *side* = 'R',  $A$  is to the right of  $B$  in the equation, resulting in either equation 3, 4, or 6.
- Specified as: a single character. It must be 'L' or 'R'.
- uplo* indicates whether matrix  $A$  is an upper or lower triangular matrix, where:
- If *uplo* = 'U',  $A$  is an upper triangular matrix.
- If *uplo* = 'L',  $A$  is a lower triangular matrix.
- Specified as: a single character. It must be 'U' or 'L'.
- transa* indicates the form of matrix  $A$  to use in the computation, where:

## STRMM, DTRMM, CTRMM, and ZTRMM

	<p>If <i>transa</i> = 'N', <i>A</i> is used in the computation, resulting in either equation 1 or 3.</p> <p>If <i>transa</i> = 'T', <math>A^T</math> is used in the computation, resulting in either equation 2 or 4.</p> <p>If <i>transa</i> = 'C', <math>A^H</math> is used in the computation, resulting in either equation 5 or 6.</p> <p>Specified as: a single character. It must be 'N', 'T', or 'C'.</p>
<i>diag</i>	<p>indicates the characteristics of the diagonal of matrix <i>A</i>, where:</p> <p>If <i>diag</i> = 'U', <i>A</i> is a unit triangular matrix.</p> <p>If <i>diag</i> = 'N', <i>A</i> is not a unit triangular matrix.</p> <p>Specified as: a single character. It must be 'U' or 'N'.</p>
<i>m</i>	<p>is the number of rows in rectangular matrix <i>B</i>, and:</p> <p>If <i>side</i> = 'L', <i>m</i> is the order of triangular matrix <i>A</i>.</p> <p>Specified as: a fullword integer, where:</p> <p>If <i>side</i> = 'L', <math>0 \leq m \leq lda</math> and <math>m \leq ldb</math>.</p> <p>If <i>side</i> = 'R', <math>0 \leq m \leq ldb</math>.</p>
<i>n</i>	<p>is the number of columns in rectangular matrix <i>B</i>, and:</p> <p>If <i>side</i> = 'R', <i>n</i> is the order of triangular matrix <i>A</i>.</p> <p>Specified as: a fullword integer; <math>n \geq 0</math> and:</p> <p>If <i>side</i> = 'R', <math>n \leq lda</math>.</p>
<i>alpha</i>	<p>is the scalar <math>\alpha</math>.</p> <p>Specified as: a number of the data type indicated in Table 85 on page 419.</p>
<i>a</i>	<p>is the triangular matrix <i>A</i>, of which only the upper or lower triangular portion is used, where:</p> <p>If <i>side</i> = 'L', <i>A</i> is order <i>m</i>.</p> <p>If <i>side</i> = 'R', <i>A</i> is order <i>n</i>.</p> <p><b>Note:</b> No data should be moved to form <math>A^T</math> or <math>A^H</math>; that is, the matrix <i>A</i> should always be stored in its untransposed form.</p>
	<p>Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 85 on page 419, where:</p> <p>If <i>side</i> = 'L', its size must be <i>lda</i> by (at least) <i>m</i>.</p> <p>If <i>side</i> = 'R', its size must be <i>lda</i> by (at least) <i>n</i>.</p>
<i>lda</i>	<p>is the leading dimension of the array specified for <i>a</i>.</p> <p>Specified as: a fullword integer; <math>lda &gt; 0</math> and:</p> <p>If <i>side</i> = 'L', <math>lda \geq m</math>.</p> <p>If <i>side</i> = 'R', <math>lda \geq n</math>.</p>
<i>b</i>	<p>is the <i>m</i> by <i>n</i> rectangular matrix <i>B</i>.</p>

Specified as: an  $ldb$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 85 on page 419.

$ldb$  is the leading dimension of the array specified for  $b$ .  
Specified as: a fullword integer;  $ldb > 0$  and  $ldb \geq m$ .

### On Return

$b$  is the  $m$  by  $n$  matrix  $B$ , containing the results of the computation. Returned as: an  $ldb$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 85 on page 419.

### Notes

1. These subroutines accept lowercase letters for the *side*, *uplo*, *transa*, and *diag* arguments.
2. For STRMM and DTRMM, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
3. Matrices  $A$  and  $B$  must have no common elements; otherwise, results are unpredictable.
4. ESSL assumes certain values in your array for parts of a triangular matrix. As a result, you do not have to set these values. For unit triangular matrices, the elements of the diagonal are assumed to be 1.0 for real matrices and (1.0, 0.0) for complex matrices. When using upper- or lower-triangular storage, the unreferenced elements in the lower and upper triangular part, respectively, are assumed to be zero.
5. For a description of triangular matrices and how they are stored, see "Triangular Matrix" on page 77.

### Function

These subroutines can perform the following matrix-matrix product computations, using the triangular matrix  $A$ , its transpose, or its conjugate transpose, where  $A$  can be either upper- or lower-triangular:

1.  $B \leftarrow \alpha AB$
2.  $B \leftarrow \alpha A^T B$
3.  $B \leftarrow \alpha A^H B$  (for CTRMM and ZTRMM only)

where:

$\alpha$  is a scalar.

$A$  is a triangular matrix of order  $m$ .

$B$  is an  $m$  by  $n$  rectangular matrix.

4.  $B \leftarrow \alpha BA$
5.  $B \leftarrow \alpha BA^T$
6.  $B \leftarrow \alpha BA^H$  (for CTRMM and ZTRMM only)

where:

$\alpha$  is a scalar.

$A$  is a triangular matrix of order  $n$ .

$B$  is an  $m$  by  $n$  rectangular matrix.

See references [34] and [40]. If  $n$  or  $m$  is 0, no computation is performed.

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

None

### Input-Argument Errors

1.  $m < 0$
2.  $n < 0$
3.  $lda, ldb \leq 0$
4.  $side \neq 'L'$  or  $'R'$
5.  $uplo \neq 'L'$  or  $'U'$
6.  $transa \neq 'T', 'N',$  or  $'C'$
7.  $diag \neq 'N'$  or  $'U'$
8.  $side = 'L'$  and  $m > lda$
9.  $m > ldb$
10.  $side = 'R'$  and  $n > lda$

## Examples

### Example 1

This example shows the computation  $B \leftarrow \alpha AB$ , where  $A$  is a 5 by 5 upper triangular matrix that is not unit triangular, and  $B$  is a 5 by 3 rectangular matrix.

#### Call Statement and Input:

```

          SIDE  UPLO  TRANSA  DIAG  M  N  ALPHA  A  LDA  B  LDB
CALL STRMM( 'L' , 'U' , 'N' , 'N' , 5 , 3 , 1.0 , A , 7 , B , 6 )

```

$$A = \begin{bmatrix} 3.0 & -1.0 & 2.0 & 2.0 & 1.0 \\ . & -2.0 & 4.0 & -1.0 & 3.0 \\ . & . & -3.0 & 0.0 & 2.0 \\ . & . & . & 4.0 & -2.0 \\ . & . & . & . & 1.0 \\ . & . & . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} 2.0 & 3.0 & 1.0 \\ 5.0 & 5.0 & 4.0 \\ 0.0 & 1.0 & 2.0 \\ 3.0 & 1.0 & -3.0 \\ -1.0 & 2.0 & 1.0 \\ . & . & . \end{bmatrix}$$

#### Output:

$$B = \begin{bmatrix} 6.0 & 10.0 & -2.0 \\ -16.0 & -1.0 & 6.0 \\ -2.0 & 1.0 & -4.0 \\ 14.0 & 0.0 & -14.0 \\ -1.0 & 2.0 & 1.0 \\ . & . & . \end{bmatrix}$$



**Example 2**

This example shows the computation  $B \leftarrow \alpha A^T B$ , where  $A$  is a 5 by 5 upper triangular matrix that is not unit triangular, and  $B$  is a 5 by 4 rectangular matrix.

**Call Statement and Input:**

```

          SIDE UPLO TRANSA DIAG M N ALPHA A LDA B LDB
CALL STRMM( 'L' , 'U' , 'T' , 'N' , 5 , 4 , 1.0 , A , 7 , B , 6 )

```

$$A = \begin{bmatrix} -1.0 & -4.0 & -2.0 & 2.0 & 3.0 \\ . & -2.0 & 2.0 & 2.0 & 2.0 \\ . & . & -3.0 & -1.0 & 4.0 \\ . & . & . & 1.0 & 0.0 \\ . & . & . & . & -2.0 \\ . & . & . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 4.0 \\ 3.0 & 3.0 & -1.0 & 2.0 \\ -2.0 & -1.0 & 0.0 & 1.0 \\ 4.0 & 4.0 & -3.0 & -3.0 \\ 2.0 & 2.0 & 2.0 & 2.0 \\ . & . & . & . \end{bmatrix}$$

**Output:**

$$B = \begin{bmatrix} -1.0 & -2.0 & -3.0 & -4.0 \\ 2.0 & -2.0 & -14.0 & -12.0 \\ 10.0 & 5.0 & -8.0 & -7.0 \\ 14.0 & 15.0 & 1.0 & 8.0 \\ -3.0 & 4.0 & 3.0 & 16.0 \\ . & . & . & . \end{bmatrix}$$

**Example 3**

This example shows the computation  $B \leftarrow \alpha B A$ , where  $A$  is a 5 by 5 lower triangular matrix that is not unit triangular, and  $B$  is a 3 by 5 rectangular matrix.

**Call Statement and Input:**

```

          SIDE UPLO TRANSA DIAG M N ALPHA A LDA B LDB
CALL STRMM( 'R' , 'L' , 'N' , 'N' , 3 , 5 , 1.0 , A , 7 , B , 4 )

```

$$A = \begin{bmatrix} 2.0 & . & . & . & . \\ 2.0 & 3.0 & . & . & . \\ 2.0 & 1.0 & 1.0 & . & . \\ 0.0 & 3.0 & 0.0 & -2.0 & . \\ 2.0 & 4.0 & -1.0 & 2.0 & -1.0 \\ . & . & . & . & . \\ . & . & . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} 3.0 & 4.0 & -1.0 & -1.0 & -1.0 \\ 2.0 & 1.0 & -1.0 & 0.0 & 3.0 \\ -2.0 & -1.0 & -3.0 & 0.0 & 2.0 \\ . & . & . & . & . \end{bmatrix}$$

**Output:**

## STRMM, DTRMM, CTRMM, and ZTRMM

$$B = \begin{bmatrix} 10.0 & 4.0 & 0.0 & 0.0 & 1.0 \\ 10.0 & 14.0 & -4.0 & 6.0 & -3.0 \\ -8.0 & 2.0 & -5.0 & 4.0 & -2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 4

This example shows the computation  $B \leftarrow \alpha BA$ , where  $A$  is a 6 by 6 upper triangular matrix that is unit triangular, and  $B$  is a 1 by 6 rectangular matrix.

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

#### Call Statement and Input:

```

                SIDE  UPLO  TRANSA  DIAG  M  N  ALPHA  A  LDA  B  LDB
CALL STRMM( 'R' , 'U' , 'N' , 'U' , 1 , 6 , 1.0 , A , 7 , B , 2 )

```

$$A = \begin{bmatrix} \cdot & 2.0 & -3.0 & 1.0 & 2.0 & 4.0 \\ \cdot & \cdot & 0.0 & 1.0 & 1.0 & -2.0 \\ \cdot & \cdot & \cdot & 4.0 & -1.0 & 1.0 \\ \cdot & \cdot & \cdot & \cdot & 0.0 & -1.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & 2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & 2.0 & 1.0 & 3.0 & -1.0 & -2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

#### Output:

$$B = \begin{bmatrix} 1.0 & 4.0 & -2.0 & 10.0 & 2.0 & -6.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 5

This example shows the computation  $B \leftarrow \alpha A^H B$ , where  $A$  is a 5 by 5 upper triangular matrix that is not unit triangular, and  $B$  is a 5 by 1 rectangular matrix.

#### Call Statement and Input:

```

                SIDE  UPLO  TRANSA  DIAG  M  N  ALPHA  A  LDA  B  LDB
CALL CTRMM( 'L' , 'U' , 'C' , 'N' , 5 , 1 , ALPHA , A , 6 , B , 6 )

```

ALPHA = (1.0, 0.0)

$$A = \begin{bmatrix} (-4.0, 1.0) & (4.0, -3.0) & (-1.0, 3.0) & (0.0, 0.0) & (-1.0, 0.0) \\ \cdot & (-2.0, 0.0) & (-3.0, -1.0) & (-2.0, -1.0) & (4.0, 3.0) \\ \cdot & \cdot & (-5.0, 3.0) & (-3.0, -3.0) & (-5.0, -5.0) \\ \cdot & \cdot & \cdot & (4.0, -4.0) & (2.0, 0.0) \\ \cdot & \cdot & \cdot & \cdot & (2.0, -1.0) \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} (3.0, 4.0) \\ (-4.0, 2.0) \\ (-5.0, 0.0) \end{bmatrix}$$

$$\begin{bmatrix} (1.0, 3.0) \\ (3.0, 1.0) \\ . \end{bmatrix}$$

**Output:**

$$B = \begin{bmatrix} (-8.0, -19.0) \\ (8.0, 21.0) \\ (44.0, -8.0) \\ (13.0, -7.0) \\ (19.0, 2.0) \\ . \end{bmatrix}$$

## SSYRK, DSYRK, CSYRK, ZSYRK, CHERK, and ZHERK — Rank-K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix

### Purpose

These subroutines compute one of the following rank-k updates, where matrix  $C$  is stored in either upper or lower storage mode. SSYRK, DSYRK, CSYRK, and ZSYRK use the scalars  $\alpha$  and  $\beta$ , real or complex matrix  $A$  or its transpose, and real or complex symmetric matrix  $C$  to compute:

1.  $C \leftarrow \alpha AA^T + \beta C$
2.  $C \leftarrow \alpha A^T A + \beta C$

CHERK and ZHERK use the scalars  $\alpha$  and  $\beta$ , complex matrix  $A$  or its complex conjugate transpose, and complex Hermitian matrix  $C$  to compute:

1.  $C \leftarrow \alpha AA^H + \beta C$
2.  $C \leftarrow \alpha A^H A + \beta C$

Table 86. Data Types

$A, C$	$\alpha, \beta$	Subprogram
Short-precision real	Short-precision real	SSYRK
Long-precision real	Long-precision real	DSYRK
Short-precision complex	Short-precision complex	CSYRK
Long-precision complex	Long-precision complex	ZSYRK
Short-precision complex	Short-precision real	CHERK
Long-precision complex	Long-precision real	ZHERK

### Syntax

<b>Fortran</b>	CALL SSYRK   DSYRK   CSYRK   ZSYRK   CHERK   ZHERK ( <i>uplo, trans, n, k, alpha, a, lda, beta, c, ldc</i> )
<b>C and C++</b>	ssyrk   dsyrk   csyrk   zsyrk   cherk   zherk ( <i>uplo, trans, n, k, alpha, a, lda, beta, c, ldc</i> );

### On Entry

*uplo* indicates the storage mode used for matrix  $C$ , where:

If *uplo* = 'U',  $C$  is stored in upper storage mode.

If *uplo* = 'L',  $C$  is stored in lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

*trans* indicates the form of matrix  $A$  to use in the computation, where:

If *trans* = 'N',  $A$  is used, resulting in equation 1 or 3.

If *trans* = 'T',  $A^T$  is used, resulting in equation 2.

If *trans* = 'C',  $A^H$  is used, resulting in equation 4.

Specified as: a single character, where:

For SSYRK and DSYRK, it must be 'N', 'T', or 'C'.

For CSYRK and ZSYRK, it must be 'N' or 'T'.

## SSYRK, DSYRK, CSYRK, ZSYRK, CHERK, and ZHERK

For CHERK and ZHERK, it must be 'N' or 'C'.

<i>n</i>	is the order of matrix <i>C</i> . Specified as: a fullword integer; $0 \leq n \leq ldc$ and: If <i>trans</i> = 'N', then $n \leq lda$ .
<i>k</i>	has the following meaning, where: If <i>trans</i> = 'N', it is the number of columns in matrix <i>A</i> . If <i>trans</i> = 'T' or 'C', it is the number of rows in matrix <i>A</i> . Specified as: a fullword integer; $k \geq 0$ and: If <i>trans</i> = 'T' or 'C', then $k \leq lda$ .
<i>alpha</i>	is the scalar $\alpha$ . Specified as: a number of the data type indicated in Table 86 on page 426.
<i>a</i>	is the rectangular matrix <i>A</i> , where: If <i>trans</i> = 'N', <i>A</i> is <i>n</i> by <i>k</i> . If <i>trans</i> = 'T' or 'C', <i>A</i> is <i>k</i> by <i>n</i> .  <b>Note:</b> No data should be moved to form $A^T$ or $A^H$ ; that is, the matrix <i>A</i> should always be stored in its untransposed form.  Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 86 on page 426, where:  If <i>trans</i> = 'N', its size must be <i>lda</i> by (at least) <i>k</i> .  If <i>trans</i> = 'T' or 'C', its size must be <i>lda</i> by (at least) <i>n</i> .
<i>lda</i>	is the leading dimension of the array specified for <i>a</i> . Specified as: a fullword integer; $lda > 0$ and: If <i>trans</i> = 'N', $lda \geq n$ . If <i>trans</i> = 'T' or 'C', $lda \geq k$ .
<i>beta</i>	is the scalar $\beta$ . Specified as: a number of the data type indicated in Table 86 on page 426.
<i>c</i>	is matrix <i>C</i> of order <i>n</i> , which is real symmetric, complex symmetric, or complex Hermitian, where: If <i>uplo</i> = 'U', <i>C</i> is stored in upper storage mode. If <i>uplo</i> = 'L', <i>C</i> is stored in lower storage mode. Specified as: an <i>ldc</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 86 on page 426.
<i>ldc</i>	is the leading dimension of the array specified for <i>c</i> . Specified as: a fullword integer; $ldc > 0$ and $ldc \geq n$ .

## On Return

*c* is matrix *C* of order *n*, which is real symmetric, complex symmetric, or complex Hermitian, containing the results of the computation, where:

If *uplo* = 'U', *C* is stored in upper storage mode.

If *uplo* = 'L', *C* is stored in lower storage mode.

Returned as: an *ldc* by (at least) *n* array, containing numbers of the data type indicated in Table 86 on page 426.

## Notes

1. These subroutines accept lowercase letters for the *uplo* and *trans* arguments.
2. For SSYRK and DSYRK, if you specify 'C' for the *trans* argument, it is interpreted as though you specified 'T'.
3. Matrices *A* and *C* must have no common elements; otherwise, results are unpredictable.
4. The imaginary parts of the diagonal elements of a complex Hermitian matrix *C* are assumed to be zero, so you do not have to set these values. On output, they are set to zero, except when  $\beta$  is one and  $\alpha$  or *k* is zero, in which case no computation is performed.
5. For a description of how symmetric matrices are stored in upper and lower storage mode, see "Symmetric Matrix" on page 69. For a description of how complex Hermitian matrices are stored in upper and lower storage mode, see "Complex Hermitian Matrix" on page 73.

## Function

These subroutines can perform the following rank-*k* updates. For SSYRK and DSYRK, matrix *C* is real symmetric. For CSYRK and ZSYRK, matrix *C* is complex symmetric. They perform:

1.  $C \leftarrow \alpha AA^T + \beta C$
2.  $C \leftarrow \alpha A^T A + \beta C$

For CHERK and ZHERK, matrix *C* is complex Hermitian. They perform:

1.  $C \leftarrow \alpha AA^H + \beta C$
2.  $C \leftarrow \alpha A^H A + \beta C$

where:

$\alpha$  and  $\beta$  are scalars.

*A* is a rectangular matrix, which is *n* by *k* for equations 1 and 3, and is *k* by *n* for equations 2 and 4.

*C* is a matrix of order *n* of the type indicated above, stored in upper or lower storage mode.

See references [34] and [40]. In the following two cases, no computation is performed:

- *n* is 0.
- $\beta$  is one, and  $\alpha$  is zero or *k* is zero.

## SSYRK, DSYRK, CSYRK, ZSYRK, CHERK, and ZHERK

Assuming the above conditions do not exist, if  $\beta$  is not one, and  $\alpha$  is zero or  $k$  is zero, then  $\beta C$  is returned.

### Error conditions

#### Resource Errors

Unable to allocate internal work area.

#### Computational Errors

None

#### Input-Argument Errors

1.  $lda, ldc \leq 0$
2.  $ldc < n$
3.  $k, n < 0$
4.  $uplo \neq 'U'$  or  $'L'$
5.  $trans \neq 'N', 'T',$  or  $'C'$  for SSYRK and DSYRK
6.  $trans \neq 'N'$  or  $'T'$  for CSYRK and ZSYRK
7.  $trans \neq 'N'$  or  $'C'$  for CHERK and ZHERK
8.  $trans = 'N'$  and  $lda < n$
9.  $trans = 'T'$  or  $'C'$  and  $lda < k$

### Examples

#### Example 1

This example shows the computation  $C \leftarrow \alpha AA^T + \beta C$ , where  $A$  is an 8 by 2 real rectangular matrix, and  $C$  is a real symmetric matrix of order 8, stored in upper storage mode.

#### Call Statement and Input:

```

          UPLO TRANS  N  K  ALPHA  A  LDA  BETA  C  LDC
CALL SSYRK( 'U' , 'N' ,  8 , 2 ,  1.0 , A , 9 , 1.0 , C , 10 )

```

$$A = \begin{bmatrix} 0.0 & 8.0 \\ 1.0 & 9.0 \\ 2.0 & 10.0 \\ 3.0 & 11.0 \\ 4.0 & 12.0 \\ 5.0 & 13.0 \\ 6.0 & 14.0 \\ 7.0 & 15.0 \\ \cdot & \cdot \end{bmatrix}$$

$$C = \begin{bmatrix} 0.0 & 1.0 & 3.0 & 6.0 & 10.0 & 15.0 & 21.0 & 28.0 \\ \cdot & 2.0 & 4.0 & 7.0 & 11.0 & 16.0 & 22.0 & 29.0 \\ \cdot & \cdot & 5.0 & 8.0 & 12.0 & 17.0 & 23.0 & 30.0 \\ \cdot & \cdot & \cdot & 9.0 & 13.0 & 18.0 & 24.0 & 31.0 \\ \cdot & \cdot & \cdot & \cdot & 14.0 & 19.0 & 25.0 & 32.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & 20.0 & 26.0 & 33.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 27.0 & 34.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 35.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

#### Output:

## SSYRK, DSYRK, CSYRK, ZSYRK, CHERK, and ZHERK

$$C = \begin{bmatrix} 64.0 & 73.0 & 83.0 & 94.0 & 106.0 & 119.0 & 133.0 & 148.0 \\ . & 84.0 & 96.0 & 109.0 & 123.0 & 138.0 & 154.0 & 171.0 \\ . & . & 109.0 & 124.0 & 140.0 & 157.0 & 175.0 & 194.0 \\ . & . & . & 139.0 & 157.0 & 176.0 & 196.0 & 217.0 \\ . & . & . & . & 174.0 & 195.0 & 217.0 & 240.0 \\ . & . & . & . & . & 214.0 & 238.0 & 263.0 \\ . & . & . & . & . & . & 259.0 & 286.0 \\ . & . & . & . & . & . & . & 309.0 \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \end{bmatrix}$$

### Example 2

This example shows the computation  $C \leftarrow \alpha A^T A + \beta C$ , where  $A$  is a 3 by 8 real rectangular matrix, and  $C$  is a real symmetric matrix of order 8, stored in lower storage mode.

#### Call Statement and Input:

```

          UPLO TRANS  N  K  ALPHA  A  LDA  BETA  C  LDC
          |   |     |  |  |   |   |   |   |   |
CALL SSYRK( 'L' , 'T' , 8 , 3 , 1.0 , A , 4 , 1.0 , C , 8 )

```

$$A = \begin{bmatrix} 0.0 & 3.0 & 6.0 & 9.0 & 12.0 & 15.0 & 18.0 & 21.0 \\ 1.0 & 4.0 & 7.0 & 10.0 & 13.0 & 16.0 & 19.0 & 22.0 \\ 2.0 & 5.0 & 8.0 & 11.0 & 14.0 & 17.0 & 20.0 & 23.0 \\ . & . & . & . & . & . & . & . \end{bmatrix}$$

$$C = \begin{bmatrix} 0.0 & . & . & . & . & . & . & . \\ 1.0 & 8.0 & . & . & . & . & . & . \\ 2.0 & 9.0 & 15.0 & . & . & . & . & . \\ 3.0 & 10.0 & 16.0 & 21.0 & . & . & . & . \\ 4.0 & 11.0 & 17.0 & 22.0 & 26.0 & . & . & . \\ 5.0 & 12.0 & 18.0 & 23.0 & 27.0 & 30.0 & . & . \\ 6.0 & 13.0 & 19.0 & 24.0 & 28.0 & 31.0 & 33.0 & . \\ 7.0 & 14.0 & 20.0 & 25.0 & 29.0 & 32.0 & 34.0 & 35.0 \end{bmatrix}$$

#### Output:

$$C = \begin{bmatrix} 5.0 & . & . & . & . & . & . & . \\ 15.0 & 58.0 & . & . & . & . & . & . \\ 25.0 & 95.0 & 164.0 & . & . & . & . & . \\ 35.0 & 132.0 & 228.0 & 323.0 & . & . & . & . \\ 45.0 & 169.0 & 292.0 & 414.0 & 535.0 & . & . & . \\ 55.0 & 206.0 & 356.0 & 505.0 & 653.0 & 800.0 & . & . \\ 65.0 & 243.0 & 420.0 & 596.0 & 771.0 & 945.0 & 1118.0 & . \\ 75.0 & 280.0 & 484.0 & 687.0 & 889.0 & 1090.0 & 1290.0 & 1489.0 \end{bmatrix}$$

### Example 3

This example shows the computation  $C \leftarrow \alpha A A^T + \beta C$ , where  $A$  is a 3 by 5 complex rectangular matrix, and  $C$  is a complex symmetric matrix of order 3, stored in upper storage mode.

#### Call Statement and Input:

```

          UPLO TRANS  N  K  ALPHA  A  LDA  BETA  C  LDC
          |   |     |  |  |   |   |   |   |   |
CALL CSYRK( 'U' , 'N' , 3 , 5 , ALPHA , A , 3 , BETA , C , 4 )
ALPHA = (1.0, 1.0)
BETA  = (1.0, 1.0)

```



## SSYRK, DSYRK, CSYRK, ZSYRK, CHERK, and ZHERK

$$A = \begin{bmatrix} (2.0, 0.0) & (3.0, 2.0) & (4.0, 1.0) & (1.0, 7.0) & (0.0, 0.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) & (2.0, 4.0) & (1.0, 2.0) \\ (1.0, 3.0) & (2.0, 1.0) & (6.0, 0.0) & (3.0, 2.0) & (2.0, 2.0) \end{bmatrix}$$

$$C = \begin{bmatrix} (2.0, 1.0) & (1.0, 9.0) & (4.0, 5.0) \\ . & (3.0, 1.0) & (6.0, 7.0) \\ . & . & (8.0, 1.0) \\ . & . & . \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} (-57.0, 13.0) & (-63.0, 79.0) & (-24.0, 70.0) \\ . & (-28.0, 90.0) & (-55.0, 103.0) \\ . & . & (13.0, 75.0) \\ . & . & . \end{bmatrix}$$

### Example 4

This example shows the computation  $C \leftarrow \alpha A^H A + \beta C$ , where  $A$  is a 5 by 3 complex rectangular matrix, and  $C$  is a complex Hermitian matrix of order 3, stored in lower storage mode.

**Note:** The imaginary parts of the diagonal elements of a complex Hermitian matrix are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

**Call Statement and Input:**

```

          UPLO TRANS  N  K  ALPHA  A  LDA  BETA  C  LDC
CALL CHERK( 'L' , 'C' , 3 , 5 , 1.0 , A , 5 , 1.0 , C , 4 )

```

$$A = \begin{bmatrix} (2.0, 0.0) & (3.0, 2.0) & (4.0, 1.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) \\ (1.0, 3.0) & (2.0, 1.0) & (6.0, 0.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) \\ (1.0, 9.0) & (3.0, 0.0) & (6.0, 7.0) \end{bmatrix}$$

$$C = \begin{bmatrix} (6.0, .) & . & . \\ (3.0, 4.0) & (10.0, .) & . \\ (9.0, 1.0) & (12.0, 2.0) & (3.0, .) \\ . & . & . \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} (138.0, 0.0) & . & . \\ (65.0, 80.0) & (165.0, 0.0) & . \\ (134.0, 46.0) & (88.0, -88.0) & (199.0, 0.0) \\ . & . & . \end{bmatrix}$$

## SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, and ZHER2K — Rank-2K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix

### Purpose

These subroutines compute one of the following rank-2k updates, where matrix  $C$  is stored in upper or lower storage mode. SSYR2K, DSYR2K, CSYR2K, and ZSYR2K use the scalars  $\alpha$  and  $\beta$ , real or complex matrices  $A$  and  $B$  or their transposes, and real or complex symmetric matrix  $C$  to compute:

1.  $C \leftarrow \alpha AB^T + \alpha BA^T + \beta C$
2.  $C \leftarrow \alpha A^T B + \alpha B^T A + \beta C$

CHER2K and ZHER2K use the scalars  $\alpha$  and  $\beta$ , complex matrices  $A$  and  $B$  or their complex conjugate transposes, and complex Hermitian matrix  $C$  to compute:

3.  $C \leftarrow \alpha AB^H + \bar{\alpha} BA^H + \beta C$
4.  $C \leftarrow \alpha A^H B + \bar{\alpha} B^H A + \beta C$

Table 87. Data Types

$A, B, C, \alpha$	$\beta$	Subprogram
Short-precision real	Short-precision real	SSYR2K
Long-precision real	Long-precision real	DSYR2K
Short-precision complex	Short-precision complex	CSYR2K
Long-precision complex	Long-precision complex	ZSYR2K
Short-precision complex	Short-precision real	CHER2K
Long-precision complex	Long-precision real	ZHER2K

### Syntax

<b>Fortran</b>	CALL SSYR2K   DSYR2K   CSYR2K   ZSYR2K   CHER2K   ZHER2K ( <i>uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc</i> )
<b>C and C++</b>	ssyr2k   dsyr2k   csyr2k   zsyr2k   cher2k   zher2k ( <i>uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc</i> );

### On Entry

- uplo* indicates the storage mode used for matrix  $C$ , where:
- If *uplo* = 'U',  $C$  is stored in upper storage mode.
  - If *uplo* = 'L',  $C$  is stored in lower storage mode.
- Specified as: a single character. It must be 'U' or 'L'.
- trans* indicates the form of matrices  $A$  and  $B$  to use in the computation, where:
- If *trans* = 'N',  $A$  and  $B$  are used, resulting in equation 1 or 3.
  - If *trans* = 'T',  $A^T$  and  $B^T$  are used, resulting in equation 2.

## SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, and ZHER2K

If  $trans = 'C'$ ,  $A^H$  and  $B^H$  are used, resulting in equation 4.

Specified as: a single character, where:

For SSYR2K and DSYR2K, it must be 'N', 'T', or 'C'.

For CSYR2K and ZSYR2K, it must be 'N' or 'T'.

For CHER2K and ZHER2K, it must be 'N' or 'C'.

$n$  is the order of matrix  $C$ .

Specified as: a fullword integer;  $0 \leq n \leq ldc$  and:

If  $trans = 'N'$ , then  $n \leq lda$  and  $n \leq ldb$ .

$k$  has the following meaning, where:

If  $trans = 'N'$ , it is the number of columns in matrices  $A$  and  $B$ .

If  $trans = 'T'$  or 'C', it is the number of rows in matrices  $A$  and  $B$ .

Specified as: a fullword integer;  $k \geq 0$  and:

If  $trans = 'T'$  or 'C', then  $k \leq lda$  and  $k \leq ldb$ .

$alpha$  is the scalar  $\alpha$ .

Specified as: a number of the data type indicated in Table 87 on page 432.

$a$  is the rectangular matrix  $A$ , where:

If  $trans = 'N'$ ,  $A$  is  $n$  by  $k$ .

If  $trans = 'T'$  or 'C',  $A$  is  $k$  by  $n$ .

**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix  $A$  should always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 87 on page 432, where:

If  $trans = 'N'$ , its size must be  $lda$  by (at least)  $k$ .

If  $trans = 'T'$  or 'C', its size must be  $lda$  by (at least)  $n$ .

$lda$  is the leading dimension of the array specified for  $a$ .

Specified as: a fullword integer;  $lda > 0$  and:

If  $trans = 'N'$ ,  $lda \geq n$ .

If  $trans = 'T'$  or 'C',  $lda \geq k$ .

$b$  is the rectangular matrix  $B$ , where:

If  $trans = 'N'$ ,  $B$  is  $n$  by  $k$ .

If  $trans = 'T'$  or 'C',  $B$  is  $k$  by  $n$ .

**Note:** No data should be moved to form  $B^T$  or  $B^H$ ; that is, the matrix  $B$  should always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 87 on page 432, where:

If  $trans = 'N'$ , its size must be  $ldb$  by (at least)  $k$ .

## SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, and ZHER2K

	If <i>trans</i> = 'T' or 'C', its size must be <i>ldb</i> by (at least) <i>n</i> .
<i>ldb</i>	is the leading dimension of the array specified for <i>b</i> . Specified as: a fullword integer; <i>ldb</i> > 0 and: If <i>trans</i> = 'N', <i>ldb</i> ≥ <i>n</i> . If <i>trans</i> = 'T' or 'C', <i>ldb</i> ≥ <i>k</i> .
<i>beta</i>	is the scalar $\beta$ . Specified as: a number of the data type indicated in Table 87 on page 432.
<i>c</i>	is matrix <i>C</i> of order <i>n</i> , which is real symmetric, complex symmetric, or complex Hermitian, where: If <i>uplo</i> = 'U', <i>C</i> is stored in upper storage mode. If <i>uplo</i> = 'L', <i>C</i> is stored in lower storage mode. Specified as: an <i>ldc</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 87 on page 432.
<i>ldc</i>	is the leading dimension of the array specified for <i>c</i> . Specified as: a fullword integer; <i>ldc</i> > 0 and <i>ldc</i> ≥ <i>n</i> .

### On Return

<i>c</i>	is matrix <i>C</i> of order <i>n</i> , which is real symmetric, complex symmetric, or complex Hermitian, containing the results of the computation, where: If <i>uplo</i> = 'U', <i>C</i> is stored in upper storage mode. If <i>uplo</i> = 'L', <i>C</i> is stored in lower storage mode. Returned as: an <i>ldc</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 87 on page 432.
----------	---

### Notes

1. These subroutines accept lowercase letters for the *uplo* and *trans* arguments.
2. For SSYR2K and DSYR2K, if you specify 'C' for the *trans* argument, it is interpreted as though you specified 'T'.
3. Matrices *A* and *B* must have no common elements with matrix *C*; otherwise, results are unpredictable.
4. The imaginary parts of the diagonal elements of a complex Hermitian matrix *C* are assumed to be zero, so you do not have to set these values. On output, they are set to zero, except when  $\beta$  is one and  $\alpha$  or *k* is zero, in which case no computation is performed.
5. For a description of how symmetric matrices are stored in upper and lower storage mode, see "Symmetric Matrix" on page 69. For a description of how complex Hermitian matrices are stored in upper and lower storage mode, see "Complex Hermitian Matrix" on page 73.

### Function

These subroutines can perform the following rank-2k updates. For SSYR2K and DSYR2K, matrix *C* is real symmetric. For CSYR2K and ZSYR2K, matrix *C* is complex symmetric. They perform:

$$1. \quad C \leftarrow \alpha AB^T + \alpha BA^T + \beta C$$

## SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, and ZHER2K

$$2. C \leftarrow \alpha A^T B + \alpha B^T A + \beta C$$

For CHER2K and ZHER2K, matrix  $C$  is complex Hermitian. They perform:

$$3. C \leftarrow \alpha A B^H + \bar{\alpha} B A^H + \beta C$$

$$4. C \leftarrow \alpha A^H B + \bar{\alpha} B^H A + \beta C$$

where:

$\alpha$  and  $\beta$  are scalars.

$A$  and  $B$  are rectangular matrices, which are  $n$  by  $k$  for equations 1 and 3, and are  $k$  by  $n$  for equations 2 and 4.

$C$  is a matrix of order  $n$  of the type indicated above, stored in upper or lower storage mode.

See references [34], [40], and [75]. In the following two cases, no computation is performed:

- $n$  is 0.
- $\beta$  is one, and  $\alpha$  is zero or  $k$  is zero.

Assuming the above conditions do not exist, if  $\beta$  is not one, and  $\alpha$  is zero or  $k$  is zero, then  $\beta C$  is returned.

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

None

### Input-Argument Errors

1.  $lda, ldb, ldc \leq 0$
2.  $ldc < n$
3.  $k, n < 0$
4.  $uplo \neq 'U'$  or  $'L'$
5.  $trans \neq 'N', 'T',$  or  $'C'$  for SSYR2K and DSYR2K
6.  $trans \neq 'N'$  or  $'T'$  for CSYR2K and ZSYR2K
7.  $trans \neq 'N'$  or  $'C'$  for CHER2K and ZHER2K
8.  $trans = 'N'$  and  $lda < n$
9.  $trans = 'T'$  or  $'C'$  and  $lda < k$
10.  $trans = 'N'$  and  $ldb < n$
11.  $trans = 'T'$  or  $'C'$  and  $ldb < k$

## Examples

### Example 1

This example shows the computation  $C \leftarrow \alpha A B^T + \alpha B A^T + \beta C$ , where  $A$  and  $B$  are 8 by 2 real rectangular matrices, and  $C$  is a real symmetric matrix of order 8, stored in upper storage mode.

## SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, and ZHER2K

### Call Statement and Input:

```

          UPLO TRANS  N  K  ALPHA  A  LDA  B  LDB  BETA  C  LDC
CALL SSYR2K( 'U' , 'N' , 8 , 2 , 1.0 , A , 9 , B , 8 , 1.0 , C , 10 )

```

$$A = \begin{bmatrix} 0.0 & 8.0 \\ 1.0 & 9.0 \\ 2.0 & 10.0 \\ 3.0 & 11.0 \\ 4.0 & 12.0 \\ 5.0 & 13.0 \\ 6.0 & 14.0 \\ 7.0 & 15.0 \\ \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 15.0 & 7.0 \\ 14.0 & 6.0 \\ 13.0 & 5.0 \\ 12.0 & 4.0 \\ 11.0 & 3.0 \\ 10.0 & 2.0 \\ 9.0 & 1.0 \\ 8.0 & 0.0 \end{bmatrix}$$

$$C = \begin{bmatrix} 0.0 & 1.0 & 3.0 & 6.0 & 10.0 & 15.0 & 21.0 & 28.0 \\ \cdot & 2.0 & 4.0 & 7.0 & 11.0 & 16.0 & 22.0 & 29.0 \\ \cdot & \cdot & 5.0 & 8.0 & 12.0 & 17.0 & 23.0 & 30.0 \\ \cdot & \cdot & \cdot & 9.0 & 13.0 & 18.0 & 24.0 & 31.0 \\ \cdot & \cdot & \cdot & \cdot & 14.0 & 19.0 & 25.0 & 32.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & 20.0 & 26.0 & 33.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 27.0 & 34.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 35.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Output:

$$C = \begin{bmatrix} 112.0 & 127.0 & 143.0 & 160.0 & 178.0 & 197.0 & 217.0 & 238.0 \\ \cdot & 138.0 & 150.0 & 163.0 & 177.0 & 192.0 & 208.0 & 225.0 \\ \cdot & \cdot & 157.0 & 166.0 & 176.0 & 187.0 & 199.0 & 212.0 \\ \cdot & \cdot & \cdot & 169.0 & 175.0 & 182.0 & 190.0 & 199.0 \\ \cdot & \cdot & \cdot & \cdot & 174.0 & 177.0 & 181.0 & 186.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & 172.0 & 172.0 & 173.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 163.0 & 160.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 147.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 2

This example shows the computation  $C \leftarrow \alpha A^T B + \alpha B^T A + \beta C$ , where  $A$  and  $B$  are 3 by 8 real rectangular matrices, and  $C$  is a real symmetric matrix of order 8, stored in lower storage mode.

### Call Statement and Input:

```

          UPLO TRANS  N  K  ALPHA  A  LDA  B  LDB  BETA  C  LDC
CALL SSYR2K( 'L' , 'T' , 8 , 3 , 1.0 , A , 4 , B , 5 , 1.0 , C , 8 )

```

## SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, and ZHER2K

$$A = \begin{bmatrix} 0.0 & 3.0 & 6.0 & 9.0 & 12.0 & 15.0 & 18.0 & 21.0 \\ 1.0 & 4.0 & 7.0 & 10.0 & 13.0 & 16.0 & 19.0 & 22.0 \\ 2.0 & 5.0 & 8.0 & 11.0 & 14.0 & 17.0 & 20.0 & 23.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 \\ 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 & 9.0 \\ 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 & 9.0 & 10.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$C = \begin{bmatrix} 0.0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1.0 & 8.0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 2.0 & 9.0 & 15.0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ 3.0 & 10.0 & 16.0 & 21.0 & \cdot & \cdot & \cdot & \cdot \\ 4.0 & 11.0 & 17.0 & 22.0 & 26.0 & \cdot & \cdot & \cdot \\ 5.0 & 12.0 & 18.0 & 23.0 & 27.0 & 30.0 & \cdot & \cdot \\ 6.0 & 13.0 & 19.0 & 24.0 & 28.0 & 31.0 & 33.0 & \cdot \\ 7.0 & 14.0 & 20.0 & 25.0 & 29.0 & 32.0 & 34.0 & 35.0 \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} 16.0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 38.0 & 84.0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 60.0 & 124.0 & 187.0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ 82.0 & 164.0 & 245.0 & 325.0 & \cdot & \cdot & \cdot & \cdot \\ 104.0 & 204.0 & 303.0 & 401.0 & 498.0 & \cdot & \cdot & \cdot \\ 126.0 & 244.0 & 361.0 & 477.0 & 592.0 & 706.0 & \cdot & \cdot \\ 148.0 & 284.0 & 419.0 & 553.0 & 686.0 & 818.0 & 949.0 & \cdot \\ 170.0 & 324.0 & 477.0 & 629.0 & 780.0 & 930.0 & 1079.0 & 1227.0 \end{bmatrix}$$

### Example 3

This example shows the computation  $C \leftarrow \alpha AB^T + \alpha BA^T + \beta C$ , where  $A$  and  $B$  are 3 by 5 complex rectangular matrices, and  $C$  is a complex symmetric matrix of order 3, stored in lower storage mode.

**Call Statement and Input:**

```

          UPLO TRANS  N  K  ALPHA  A  LDA  B  LDB  BETA  C  LDC
CALL CSYR2K( 'L' , 'N' , 3 , 5 , ALPHA , A , 3 , B , 3 , BETA , C , 4 )

```

ALPHA = (1.0, 1.0)

BETA = (1.0, 1.0)

$$A = \begin{bmatrix} (2.0, 5.0) & (3.0, 2.0) & (4.0, 1.0) & (1.0, 7.0) & (0.0, 0.0) \\ (3.0, 3.0) & (8.0, 5.0) & (2.0, 5.0) & (2.0, 4.0) & (1.0, 2.0) \\ (1.0, 3.0) & (2.0, 1.0) & (6.0, 5.0) & (3.0, 2.0) & (2.0, 2.0) \end{bmatrix}$$

$$B = \begin{bmatrix} (1.0, 5.0) & (6.0, 2.0) & (3.0, 1.0) & (2.0, 0.0) & (1.0, 0.0) \\ (2.0, 4.0) & (7.0, 5.0) & (2.0, 5.0) & (2.0, 4.0) & (0.0, 0.0) \\ (3.0, 5.0) & (8.0, 1.0) & (1.0, 5.0) & (1.0, 0.0) & (1.0, 1.0) \end{bmatrix}$$

$$C = \begin{bmatrix} (2.0, 3.0) & \cdot & \cdot \\ (1.0, 9.0) & (3.0, 3.0) & \cdot \end{bmatrix}$$

## SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, and ZHER2K

$$\begin{bmatrix} (4.0, 5.0) & (6.0, 7.0) & (8.0, 3.0) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} (-101.0, 121.0) & \cdot & \cdot \\ (-182.0, 192.0) & (-274.0, 248.0) & \cdot \\ (-98.0, 146.0) & (-163.0, 205.0) & (-151.0, 115.0) \\ \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 4

This example shows the computation:

$$C \leftarrow \alpha A^H B + \bar{\alpha} B^H A + \beta C$$

where  $A$  and  $B$  are 5 by 3 complex rectangular matrices, and  $C$  is a complex Hermitian matrix of order 3, stored in upper storage mode.

**Note:** The imaginary parts of the diagonal elements of a complex Hermitian matrix are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

**Call Statement and Input:**

```

          UPLO TRANS  N  K  ALPHA  A  LDA  B  LDB  BETA  C  LDC
          |   |     |  |  |   |   |   |   |   |   |   |
CALL CHER2K( 'U' , 'C' , 3 , 5 , ALPHA , A , 5 , B , 5 , 1.0 , C , 4 )

```

ALPHA = (1.0, 1.0)

$$A = \begin{bmatrix} (2.0, 0.0) & (3.0, 2.0) & (4.0, 1.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) \\ (1.0, 3.0) & (2.0, 1.0) & (6.0, 0.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) \\ (1.0, 9.0) & (3.0, 0.0) & (6.0, 7.0) \end{bmatrix}$$

$$B = \begin{bmatrix} (4.0, 5.0) & (6.0, 7.0) & (8.0, 0.0) \\ (1.0, 9.0) & (3.0, 0.0) & (6.0, 7.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) \\ (1.0, 3.0) & (2.0, 1.0) & (6.0, 0.0) \\ (2.0, 0.0) & (3.0, 2.0) & (4.0, 1.0) \end{bmatrix}$$

$$C = \begin{bmatrix} (6.0, \cdot) & (3.0, 4.0) & (9.0, 1.0) \\ \cdot & (10.0, \cdot) & (12.0, 2.0) \\ \cdot & \cdot & (3.0, \cdot) \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$C = \begin{bmatrix} (102.0, 0.0) & (56.0, -143.0) & (244.0, -96.0) \\ \cdot & (174.0, 0.0) & (238.0, 78.0) \\ \cdot & \cdot & (363.0, 0.0) \\ \cdot & \cdot & \cdot \end{bmatrix}$$



## SGETMI, DGETMI, CGETMI, and ZGETMI — General Matrix Transpose (In-Place)

### Purpose

These subroutines transpose an  $n$  by  $n$  matrix  $A$  in place—that is, in matrix  $A$ :

$$A \leftarrow A^T$$

Table 88. Data Types

$A$	Subroutine
Short-precision real	SGETMI
Long-precision real	DGETMI
Short-precision complex	CGETMI
Long-precision complex	ZGETMI

### Syntax

Fortran	CALL SGETMI   DGETMI   CGETMI   ZGETMI ( $a, lda, n$ )
C and C++	sgetmi   dgetmi   cgetmi   zgetmi ( $a, lda, n$ );

### On Entry

- $a$  is the matrix  $A$  having  $n$  rows and  $n$  columns.  
Specified as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 88.
- $lda$  is the leading dimension of the array specified for  $a$ .  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .
- $n$  is the number of rows and columns in matrix  $A$ .  
Specified as: a fullword integer;  $n \geq 0$ .

### On Return

- $a$  is the  $n$  by  $n$  matrix  $A^T$ , containing the results of the matrix transpose operation. Returned as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 88.

### Notes

- To achieve optimal performance in these subroutines, specify an even value for  $lda$ . An odd value may degrade performance.
- To achieve optimal performance in CGETMI, align the array specified for  $a$  on a doubleword boundary.

### Function

Matrix  $A$  is transposed in place; that is, the  $n$  rows and  $n$  columns in matrix  $A$  are exchanged. For matrix  $A$  with elements  $a_{ij}$ , where  $i, j = 1, n$ , the in-place transpose is expressed as  $a_{ji} = a_{ij}$  for  $i, j = 1, n$ .

For the following input matrix  $A$ :

## SGETMI, DGETMI, CGETMI, and ZGETMI

$$A = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix}$$

the in-place matrix transpose operation  $A \leftarrow A^T$  is expressed as:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{n1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{1n} & \dots & a_{nn} \end{bmatrix}$$

If  $n$  is 0, no computation is performed.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

1.  $n < 0$  or  $n > lda$
2.  $lda \leq 0$

### Examples

#### Example

This example shows an in-place matrix transpose of matrix  $A$  having 5 rows and 5 columns.

#### Call Statement and Input:

```

          A      LDA  N
          |      |   |
CALL SGETMI( A(2,3) , 10 , 5 )

```

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1.0 & 6.0 & 11.0 & 16.0 & 21.0 \\ \cdot & \cdot & 2.0 & 7.0 & 12.0 & 17.0 & 22.0 \\ \cdot & \cdot & 3.0 & 8.0 & 13.0 & 18.0 & 23.0 \\ \cdot & \cdot & 4.0 & 9.0 & 14.0 & 19.0 & 24.0 \\ \cdot & \cdot & 5.0 & 10.0 & 15.0 & 20.0 & 25.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

#### Output:

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \\ \cdot & \cdot & 6.0 & 7.0 & 8.0 & 9.0 & 10.0 \\ \cdot & \cdot & 11.0 & 12.0 & 13.0 & 14.0 & 15.0 \\ \cdot & \cdot & 16.0 & 17.0 & 18.0 & 19.0 & 20.0 \end{bmatrix}$$

## SGETMI, DGETMI, CGETMI, and ZGETMI

$$\begin{bmatrix} . & . & 21.0 & 22.0 & 23.0 & 24.0 & 25.0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{bmatrix}$$

## SGETMO, DGETMO, CGETMO, and ZGETMO — General Matrix Transpose (Out-of-Place)

### Purpose

These subroutines transpose an  $m$  by  $n$  matrix  $A$  out of place, returning the result in matrix  $B$ :

$$B \leftarrow A^T$$

Table 89. Data Types

$A, B$	Subroutine
Short-precision real	SGETMO
Long-precision real	DGETMO
Short-precision complex	CGETMO
Long-precision complex	ZGETMO

### Syntax

<b>Fortran</b>	CALL SGETMO   DGETMO   CGETMO   ZGETMO ( $a, lda, m, n, b, ldb$ )
<b>C and C++</b>	sgetmo   dgetmo   cgetmo   zgetmo ( $a, lda, m, n, b, ldb$ );

### On Entry

- $a$  is the matrix  $A$  having  $m$  rows and  $n$  columns.  
Specified as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 89.
- $lda$  is the leading dimension of the array specified for  $a$ .  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq m$ .
- $m$  is the number of rows in matrix  $A$  and the number of columns in matrix  $B$ .  
Specified as: a fullword integer;  $m \geq 0$ .
- $n$  is the number of columns in matrix  $A$  and the number of rows in matrix  $B$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $b$  See "On Return."
- $ldb$  is the leading dimension of the array specified for  $b$ .  
Specified as: a fullword integer;  $ldb > 0$  and  $ldb \geq n$ .

### On Return

- $b$  is the matrix  $B$  having  $n$  rows and  $m$  columns, containing the results of the matrix transpose operation,  $A^T$ . Returned as: an  $ldb$  by (at least)  $m$  array, containing numbers of the data type indicated in Table 89.

## Notes

1. The matrix  $B$  must have no common elements with matrix  $A$ ; otherwise, results are unpredictable. See "Concepts" on page 59.
2. To achieve optimal performance in CGETMO, align the arrays specified for  $a$  and  $b$  on doubleword boundaries.

## Function

Matrix  $A$  is transposed out of place; that is, the  $m$  rows and  $n$  columns in matrix  $A$  are stored in  $n$  rows and  $m$  columns of matrix  $B$ . For matrix  $A$  with elements  $a_{ij}$ , where  $i = 1, m$  and  $j = 1, n$ , the out-of-place transpose is expressed as  $b_{ji} = a_{ij}$  for  $i = 1, m$  and  $j = 1, n$ .

For the following input matrix  $A$ :

$$A = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix}$$

the out-of-place matrix transpose operation  $B \leftarrow A^T$  is expressed as:

$$\begin{bmatrix} b_{11} & \dots & b_{1m} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ b_{n1} & \dots & b_{nm} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{m1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{1n} & \dots & a_{mn} \end{bmatrix}$$

If  $m$  or  $n$  is 0, no computation is performed.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $m < 0$  or  $m > lda$
2.  $n < 0$  or  $n > ldb$
3.  $lda \leq 0$
4.  $ldb \leq 0$

## Examples

### Example 1

This example shows an out-of-place matrix transpose of matrix  $A$ , having 5 rows and 4 columns, with the result going into matrix  $B$ .

Call Statement and Input:

```

          A      LDA  M  N      B      LDB
          |      |   |  |   |      |      |
CALL SGETMO( A(2,3) , 10 , 5 , 4 , B(2,2) , 6 )
    
```

## SGETMO, DGETMO, CGETMO, and ZGETMO

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1.0 & 6.0 & 11.0 & 16.0 & \cdot \\ \cdot & \cdot & 2.0 & 7.0 & 12.0 & 17.0 & \cdot \\ \cdot & \cdot & 3.0 & 8.0 & 13.0 & 18.0 & \cdot \\ \cdot & \cdot & 4.0 & 9.0 & 14.0 & 19.0 & \cdot \\ \cdot & \cdot & 5.0 & 10.0 & 15.0 & 20.0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$B = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & \cdot \\ \cdot & 6.0 & 7.0 & 8.0 & 9.0 & 10.0 & \cdot \\ \cdot & 11.0 & 12.0 & 13.0 & 14.0 & 15.0 & \cdot \\ \cdot & 16.0 & 17.0 & 18.0 & 19.0 & 20.0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 2

This example uses the same input matrix *A* as in Example 1 to show that transposes can be achieved in the same array as long as the input and output data do not overlap. On output, the input data is not overwritten in the array.

**Call Statement and Input:**

```

          A   LDA  M  N   B   LDB
          |   |   |  |   |   |
CALL SGETMO( A(2,3) , 10 , 5 , 4 , A(7,1) , 10 )

```

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1.0 & 6.0 & 11.0 & 16.0 & \cdot \\ \cdot & \cdot & 2.0 & 7.0 & 12.0 & 17.0 & \cdot \\ \cdot & \cdot & 3.0 & 8.0 & 13.0 & 18.0 & \cdot \\ \cdot & \cdot & 4.0 & 9.0 & 14.0 & 19.0 & \cdot \\ \cdot & \cdot & 5.0 & 10.0 & 15.0 & 20.0 & \cdot \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & \cdot & \cdot \\ 6.0 & 7.0 & 8.0 & 9.0 & 10.0 & \cdot & \cdot \\ 11.0 & 12.0 & 13.0 & 14.0 & 15.0 & \cdot & \cdot \\ 16.0 & 17.0 & 18.0 & 19.0 & 20.0 & \cdot & \cdot \end{bmatrix}$$

---

## Chapter 10. Linear Algebraic Equations

The linear algebraic equation subroutines, provided in four areas, are described in this chapter.

---

### Overview of the Linear Algebraic Equation Subroutines

This section describes the subroutines in each of the four linear algebraic equation areas:

- “Dense Linear Algebraic Equation Subroutines”
- “Banded Linear Algebraic Equation Subroutines” on page 447
- “Sparse Linear Algebraic Equation Subroutines” on page 447
- “Linear Least Squares Subroutines” on page 448

**Note:** Some of the linear algebraic equations were designed in accordance with the Level 2 BLAS, Level 3 BLAS, and LAPACK de facto standard. If these subprograms do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subprograms, the updates could require modifications of the calling application program. For details on the Level 2 and 3 BLAS, see references [34] and [36]. For details on the LAPACK routines, see reference [8].

### Dense Linear Algebraic Equation Subroutines

The dense linear algebraic equation subroutines provide solutions to linear systems of equations for both real and complex general matrices and their transposes, positive definite real symmetric and complex Hermitian matrices, real symmetric indefinite matrices and triangular matrices. Some of these subroutines correspond to the Level 2 BLAS, Level 3 BLAS, and LAPACK routines described in references [34], [36], and [8].

Table 90. List of Dense Linear Algebraic Equation Subroutines

Descriptive Name	Short-Precision Subroutine	Long-Precision Subroutine	Page
General Matrix Factorization and Multiple Right-Hand Side Solve	SGESV <sup>△</sup> CGESV <sup>△</sup>	DGESV <sup>△</sup> ZGESV <sup>△</sup>	454
General Matrix Factorization	SGETRF <sup>△</sup> CGETRF <sup>△</sup>	DGETRF <sup>△</sup> ZGETRF <sup>△</sup>	458
	SGEF CGEF	DGEF ZGEF DGEFP <sup>§</sup>	467
General Matrix, Its Transpose, or Its Conjugate Transpose Multiple Right-Hand Side Solve	SGETRS <sup>△</sup> CGETRS <sup>△</sup>	DGETRS <sup>△</sup> ZGETRS <sup>△</sup>	462
	SGESM CGESM	DGESM ZGESM	474
General Matrix, Its Transpose, or Its Conjugate Transpose Solve	SGES CGES	DGES ZGES	470
General Matrix Factorization, Condition Number Reciprocal, and Determinant	SGEFCD	DGEFCD	479
Positive Definite Real Symmetric Matrix Factorization and Multiple Right-Hand Side Solve	SPPSV <sup>△</sup> CPPSV <sup>△</sup>	DPPSV <sup>△</sup> ZPPSV <sup>△</sup>	483

Table 90. List of Dense Linear Algebraic Equation Subroutines (continued)

Descriptive Name	Short-Precision Subroutine	Long-Precision Subroutine	Page
Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization and Multiple Right-Hand Side Solve	SPOSV <sup>△</sup> CPOSV <sup>△</sup>	DPOSV <sup>△</sup> ZPOSV <sup>△</sup>	489
Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization	SPOTRF <sup>△</sup> CPOTRF <sup>△</sup> SPOF CPOF SPPTRF <sup>△</sup> CPPTRF <sup>△</sup> SPPF	DPOTRF <sup>△</sup> ZPOTRF <sup>△</sup> DPOF ZPOF DPPTRF <sup>△</sup> ZPPTRF <sup>△</sup> DPPF DPPPF <sup>§</sup>	495
Positive Definite Real Symmetric or Complex Hermitian Matrix Multiple Right-Hand Side Solve	SPOTRS <sup>△</sup> CPOTRS <sup>△</sup> SPOSM CPOSM SPPTRS <sup>△</sup> CPPTRS <sup>△</sup>	DPOTRS <sup>△</sup> ZPOTRS <sup>△</sup> DPOSM ZPOSM DPPTRS <sup>△</sup> ZPPTRS <sup>△</sup>	507
Positive Definite Real Symmetric Matrix Solve	SPPS	DPPS	515
Positive Definite Real Symmetric Matrix Factorization, Condition Number Reciprocal, and Determinant	SPPFCD SPOFCD	DPPFCD DPOFCD	518
Symmetric Indefinite Matrix Factorization and Multiple Right-Hand Side Solve		DBSSV	524
Symmetric Indefinite Matrix Factorization		DBSTRF	530
Symmetric Indefinite Matrix Multiple Right-Hand Side Solve		DBSTRS	535
General Matrix Inverse, Condition Number Reciprocal, and Determinant	SGETRI <sup>△</sup> CGETRI <sup>△</sup> SGEICD	DGETRI <sup>△</sup> ZGETRI <sup>△</sup> DGEICD	539
Positive Definite Real Symmetric or Complex Hermitian Matrix Inverse, Condition Number Reciprocal, and Determinant	SPOTRI <sup>△</sup> CPOTRI <sup>△</sup> SPPTRI <sup>△</sup> SPPICD SPOICD	DPOTRI <sup>△</sup> ZPOTRI <sup>△</sup> DPPTRI <sup>△</sup> DPPICD DPOICD	547
Solution of a Triangular System of Equations with a Single Right-Hand Side	STRSV <sup>•</sup> CTRSV <sup>•</sup> STPSV <sup>•</sup> CTPSV <sup>•</sup>	DTRSV <sup>•</sup> ZTRSV <sup>•</sup> DTPSV <sup>•</sup> ZTPSV <sup>•</sup>	557
Solution of Triangular Systems of Equations with Multiple Right-Hand Sides	STRSM <sup>•</sup> CTRSM <sup>•</sup>	DTRSM <sup>•</sup> ZTRSM <sup>•</sup>	563
Triangular Matrix Inverse	STRTRI <sup>△</sup> CTRTRI <sup>△</sup> STPTRI <sup>△</sup> CTPTRI <sup>△</sup> STRI <sup>§</sup> STPI <sup>§</sup>	DTRTRI <sup>△</sup> ZTRTRI <sup>△</sup> DTPTRI <sup>△</sup> ZTPTRI <sup>△</sup> DTRI <sup>§</sup> DTPI <sup>§</sup>	570
<p>• Level 2 BLAS</p> <p>• Level 3 BLAS</p> <p>△ LAPACK</p> <p>§ This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.</p>			



## Banded Linear Algebraic Equation Subroutines

The banded linear algebraic equation subroutines provide solutions to linear systems of equations for real general band matrices, real positive definite symmetric band matrices, real or complex general tridiagonal matrices, real positive definite symmetric tridiagonal matrices, and real or complex triangular band matrices.

Table 91. List of Banded Linear Algebraic Equation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
General Band Matrix Factorization	SGBF	DGBF	579
General Band Matrix Solve	SGBS	DGBS	583
Positive Definite Symmetric Band Matrix Factorization	SPBF SPBCHF	DPBF DPBCHF	586
Positive Definite Symmetric Band Matrix Solve	SPBS SPBCHS	DPBS DPBCHS	590
General Tridiagonal Matrix Factorization	SGTF	DGTF	593
General Tridiagonal Matrix Solve	SGTS	DGTS	596
General Tridiagonal Matrix Combined Factorization and Solve with No Pivoting	SGTNP CGTNP	DGTNP ZGTNP	598
General Tridiagonal Matrix Factorization with No Pivoting	SGTNPF CGTNPF	DGTNPF ZGTNPF	601
General Tridiagonal Matrix Solve with No Pivoting	SGTNPS CGTNPS	DGTNPS ZGTNPS	604
Positive Definite Symmetric Tridiagonal Matrix Factorization	SPTF	DPTF	607
Positive Definite Symmetric Tridiagonal Matrix Solve	SPTS	DPTS	609
Triangular Band Equation Solve	STBSV <sup>†</sup> CTBSV <sup>†</sup>	DTBSV <sup>†</sup> ZTBSV <sup>†</sup>	611
† Level 2 BLAS			

## Sparse Linear Algebraic Equation Subroutines

The sparse linear algebraic equation subroutines provide direct and iterative solutions to linear systems of equations both for general sparse matrices and their transposes and for sparse symmetric matrices.

Table 92. List of Sparse Linear Algebraic Equation Subroutines

Descriptive Name	Long- Precision Subroutine	Page
General Sparse Matrix Factorization Using Storage by Indices, Rows, or Columns	DGSF	617
General Sparse Matrix or Its Transpose Solve Using Storage by Indices, Rows, or Columns	DGSS	623
General Sparse Matrix or Its Transpose Factorization, Determinant, and Solve Using Skyline Storage Mode	DGKFS	627
Symmetric Sparse Matrix Factorization, Determinant, and Solve Using Skyline Storage Mode	DSKFS	644
Iterative Linear System Solver for a General or Symmetric Sparse Matrix Stored by Rows	DSRIS	662
Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Matrix Storage Mode	DSMCG <sup>§</sup>	673

Table 92. List of Sparse Linear Algebraic Equation Subroutines (continued)

Descriptive Name	Long- Precision Subroutine	Page
Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Diagonal Storage Mode	DSDCG	681
General Sparse Matrix Iterative Solve Using Compressed-Matrix Storage Mode	DSMGCG <sup>§</sup>	689
General Sparse Matrix Iterative Solve Using Compressed-Diagonal Storage Mode	DSDGCG	696
<sup>§</sup> These subroutines are provided only for migration from earlier releases of ESSL and are not intended for use in new programs. Use DSRIS instead.		

## Linear Least Squares Subroutines

The linear least squares subroutines provide least squares solutions to linear systems of equations for real general matrices. Three methods are provided: one that uses the singular value decomposition; one that uses a QR decomposition with column pivoting; and another that uses a QR decomposition without column pivoting. Some of these subroutines correspond to the LAPACK routines described in reference [8].

Table 93. List of Linear Least Squares Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Singular Value Decomposition for a General Matrix	SGESVF	DGESVF	704
Linear Least Squares Solution for a General Matrix Using the Singular Value Decomposition	SGESVS	DGESVS	712
General Matrix QR Factorization		DGEQRF <sup>△</sup>	717
Linear Least Squares Solution for a General Matrix		DGELS <sup>△</sup>	721
Linear Least Squares Solution for a General Matrix with Column Pivoting	SGELLS	DGELLS	728
△ LAPACK			

## Dense and Banded Linear Algebraic Equation Considerations

This section provides some key points about using the dense and banded linear algebraic equation subroutines.

### Use Considerations

To solve a system of equations, you have two choices:

- Use the combined factorization-and-solve subroutine for the type of matrix you have.
- Use both the factorization subroutine and the solve subroutine for the type of matrix you have. When doing so, note the following:
  - Each factorization subroutine should be followed in your program by the corresponding solve subroutine. The output from the factorization subroutine should be used as input to the solve subroutine.
  - To solve a system of equations with one or more right-hand sides, follow the call to the factorization subroutine with one or more calls to a solve subroutine or one call to a multiple solve subroutine.

## Performance and Accuracy Considerations

1. Except in a few instances, the `_GTNP` subroutines provide better performance than the `_GTNPF` and `_GTNPS` subroutines. For details, see the subroutine descriptions.
2. The general subroutines (dense and banded) use partial pivoting for accuracy and fast performance.
3. The short-precision subroutines provide increased accuracy by accumulating intermediate results in long precision. Occasionally, for performance reasons, these intermediate results are stored.
4. There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see “What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?” on page 48.

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## Sparse Matrix Direct Solver Considerations

This section provides some key points about using the sparse matrix direct solver subroutines.

### Use Considerations

1. To solve a sparse system of equations by a direct method, you must use both the factorization and solve subroutines. The factorization subroutine should be followed in your program by the corresponding solve subroutine; that is, the output from the factorization subroutine should be used as input to the solve subroutine.
2. To solve a system of equations with one or more right-hand sides, follow the call to the factorization subroutine with one or more calls to the solve subroutine.
3. The amount of storage required for the arrays depends on the sparsity pattern of the matrix. The requirement that  $lna > 2nz$  on entry to DGSF does not guarantee a successful run of the program. Some programs may be terminated because of the large number of fill-ins generated upon factorization. Fill-ins generated in a program depend on the structure of each matrix. If a large number of fill-ins is anticipated when factoring a matrix, the value of  $lna$  should be large enough to accommodate your problem.

## Performance and Accuracy Considerations

1. To make the subroutine more efficient, an input matrix comprised of all nonzero elements is preferable. See the syntax description of each subroutine for details.
2. DGSF optionally checks the validity of the indices and pointers of the input matrix. Use of this option is suggested; however, it may affect performance. For details, see the syntax description for DGSF.
3. In DGSS, if there are multiple sparse right-hand sides to be solved, you should take advantage of the sparsity by selecting a proper value for  $jopt$  (such as  $jopt = 10$  or  $11$ ). If there is only one right-hand side to be solved, it is suggested that you do not exploit the sparsity.
4. In DGSF, the value you enter for the lower bound of all elements in the matrix (`RPARAM(1)`) affects the accuracy of the result. Specifying a larger number allows you to gain some performance; however, you may lose some accuracy in the solution.

5. In DGSF, the threshold pivot tolerance (RPARM(2)) is used to select pivots. A value that is close to 0.0 approaches no pivoting. A value close to 1.0 approaches partial pivoting. A value of 0.1 is considered to be a good compromise between numerical stability and sparsity.
6. If the ESSL subroutine performs storage compressions, you receive an attention message. When this occurs, the performance of this subroutine is affected. You can improve the performance by increasing the value specified for *lna*.
7. There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see “What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?” on page 48.

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## Sparse Matrix Skyline Solver Considerations

This section provides some key points about using the sparse matrix skyline solver subroutines.

### Use Considerations

1. To solve a system of equations with one or more right-hand sides, where the matrix is stored in skyline storage mode, you can use either of the following methods. The factored output matrix is the same for both of these methods.
  - Call the skyline subroutine with the combined factor-and-solve option.
  - Call the skyline subroutine with the factor-only option, followed in your program by a call to the same subroutine with the solve-only option. The factored output matrix resulting from the factorization should be used as input to the same subroutine to do the solve. You can solve for the right-hand sides in a single call or in individual calls.

You also have the option of doing a partial factorization, where the subroutine assumes that the initial part of the input matrix is already factored. It then factors the remaining rows and columns. If you want, you can factor a very large matrix progressively by using this option.

2. Forward elimination can be done with or without scaling the right-hand side by the diagonal matrix elements. To perform the computation without scaling, call DGKFS with the normal solve-only option, and define the upper triangular skyline matrix (AU) as a diagonal. To perform the computation with scaling, call DGKFS with the transpose solve-only, option and define the lower triangular skyline matrix (AL) as a diagonal.
3. Back substitution can be done with or without scaling the right-hand side by the diagonal matrix elements. To perform the computation without scaling, call DGKFS with the transpose solve-only option, and define the upper triangular skyline matrix (AU) as a diagonal. To perform the computation with scaling, call DGKFS with the normal solve-only option, and define the lower triangular skyline matrix (AL) as a diagonal.

### Performance and Accuracy Considerations

1. For optimal performance, use diagonal-out skyline storage mode for both your input and output matrices. If you specify profile-in skyline storage mode for your input matrix, and either you do not plan to use the factored output or you plan to do a solve only, it is more efficient to specify diagonal-out skyline storage mode for your output matrix. These rules apply to all the computations.

2. In some cases, elapsed time may be reduced significantly by using the combined factor-and-solve option to solve for all right-hand sides at once, in conjunction with the factorization, rather than doing the factorization and solve separately.
3. If you do a solve only, and you solve for more than one right-hand side, it is most efficient to call the skyline subroutine once with all right-hand sides, rather than once for each right-hand side.
4. The skyline subroutines allow some control over processing of the pivot (diagonal) elements of the matrix during the factorization phase. Pivot processing is controlled by IPARM(10) through IPARM(15) and RPARAM(10) through RPARAM(15). If a pivot occurs within a range that is designated to be fixed (IPARM(0) = 1, IPARM(10) = 1, and the appropriate element IPARM(11) through IPARM(15) = 1), it is replaced with the corresponding element of RPARAM(11) through RPARAM(15). Should this pivot fix-up occur, you receive an attention message. This message indicates that the matrix being factored may be unstable (singular or not definite). The results produced in this situation may be inaccurate, and you should review them carefully.

---

## Sparse Matrix Iterative Solver Considerations

This section provides some key points about using the sparse matrix iterative solver subroutines.

### Use Considerations

If you need to solve linear systems with different right-hand sides but with the same matrix using the preconditioned algorithms, you can reuse the incomplete factorization computed during the first call to the subroutine.

### Performance and Accuracy Considerations

1. The DSMCG and DSMGCG subroutines are provided for migration purposes from earlier releases of ESSL. You get better performance and a wider choice of algorithms if you use the DSRIS subroutine.
2. To select the sparse matrix subroutine that provides the best performance, you must consider the sparsity pattern of the matrix. From this, you can determine the most efficient storage mode for your sparse matrix. ESSL provides a number of versions of the sparse matrix iterative solve subroutines. They operate on sparse matrices stored in row-wise, diagonal, and compressed-matrix storage modes. These storage modes are described in "Sparse Matrix" on page 94.  
Storage-by-rows is generally applicable. You should use this storage mode unless your matrices are already set up in one of the other storage modes. If, however, your matrix has a regular sparsity pattern—that is, where the nonzero elements are concentrated along a few diagonals—you may want to use compressed-diagonal storage mode. This can save some storage space. Compressed-matrix storage mode is provided for migration purposes from earlier releases of ESSL and is not intended for use. (You get better performance and a wider choice of algorithms if you use the DSRIS subroutine, which uses storage-by-rows.)
3. The performance achieved in the sparse matrix iterative solver subroutines depends on the value specified for the relative accuracy  $\epsilon$ . For details, see Notes for each subroutine.
4. You can select the iterative algorithm you want to use to solve your linear system. The methods include conjugate gradient (CG), conjugate gradient

## SGEF, DGEF, CGEF, and ZGEF

squared (CGS), generalized minimum residual (GMRES), more smoothly converging variant of the CGS method (Bi-CGSTAB), or transpose-free quasi-minimal residual method (TFQMR).

5. For a general sparse or positive definite symmetric matrix, the iterative algorithm may fail to converge for one of the following reasons:
  - The value of  $\epsilon$  is too small, asking for too much precision.
  - The maximum number of iterations is too small, allowing too few iterations for the algorithm to converge.
  - The matrix is not positive real; that is, the symmetric part,  $(A+A^T)/2$ , is not positive definite.
  - The matrix is ill-conditioned, which may cause overflows during the computation.
6. These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

---

## Linear Least Squares Considerations

This section provides some key points about using the linear least squares subroutines.

### Use Considerations

If you want to use a singular value decomposition method to compute the minimal norm linear least squares solution of  $AX \cong B$ , calls to SGESVF or DGESVF should be followed by calls to SGESVS or DGESVS, respectively.

### Performance and Accuracy Considerations

1. Least squares solutions obtained by using a singular value decomposition require more storage and run time than those obtained using a QR decomposition with column pivoting. The singular value decomposition method, however, is a more reliable way to handle rank deficiency.
2. The short-precision subroutines provide increased accuracy by accumulating intermediate results in long precision. Occasionally, for performance reasons, these intermediate results are stored.
3. The accuracy of the resulting singular values and singular vectors varies between the short- and long-precision versions of each subroutine. The degree of difference depends on the size and conditioning of the matrix computation.
4. There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see “What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?” on page 48.

---

## Dense Linear Algebraic Equation Subroutines

This section contains the dense linear algebraic equation subroutine descriptions.

## SGESV, DGESV, CGESV, ZGESV — General Matrix Factorization and Multiple Right-Hand Side Solve

### Purpose

These subroutines solve the system of linear equations  $AX = B$  for  $X$ , where  $A$ ,  $B$ , and  $X$  are general matrices.

The matrix  $A$  is factored using Gaussian elimination with partial pivoting.

Table 94. Data Types

$A, B$	Subroutine
Short-precision real	SGESV <sup>△</sup>
Long-precision real	DGESV <sup>△</sup>
Short-precision complex	CGESV <sup>△</sup>
Long-precision complex	ZGESV <sup>△</sup>
△ LAPACK	

### Syntax

<b>Fortran</b>	CALL SGESV   DGESV   CGESV   ZGESV ( $n, nrhs, a, lda, ipvt, bx, ldb, info$ )
<b>C and C++</b>	sgesv   dgesv   cgesv   zgesv ( $n, nrhs, a, lda, ipvt, bx, ldb, info$ );

### On Entry

- $n$  is the order  $n$  of matrix  $A$  and the number of rows of matrix  $B$ .  
Specified as: a fullword integer;  $n \geq 0$ ,  $n \leq lda$ , and  $n \leq ldb$ .
- $nrhs$  is the number of right-hand sides; that is, the number of columns of matrix  $B$ .  
Specified as: a fullword integer;  $nrhs \geq 0$ .
- $a$  is the general matrix  $A$  to be factored.  
Specified as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 94.
- $lda$  is the leading dimension of the array specified for  $A$ .  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .
- $ipvt$  See "On Return" on page 455.
- $bx$  is the general matrix  $B$ , containing the  $nrhs$  right-hand sides of the system. The right-hand sides, each of length  $n$ , reside in the columns of matrix  $B$ .  
Specified as: an  $ldb$  by (at least)  $nrhs$  array, containing numbers of the data type indicated in Table 94.
- $ldb$  is the leading dimension of the array specified for  $B$ .  
Specified as: a fullword integer;  $ldb > 0$  and  $ldb \geq n$ .
- $info$  See "On Return" on page 455.



### On Return

- a* is the transformed matrix  $A$  of order  $n$ , containing the results of the factorization.  
Returned as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 94 on page 454. See "Function."
- ipvt* is the integer vector of length  $n$ , containing the pivot indices.  
Returned as: a one-dimensional array of (at least) length  $n$ , containing fullword integers, where  $1 \leq ipvt(i) \leq n$ .
- bx* is the matrix  $X$ , containing the *nrhs* solutions to the system. The solutions, each of length  $n$ , reside in the columns of  $X$ .  
Returned as: an  $ldb$  by (at least) *nrhs* array, containing numbers of the data type indicated in Table 94 on page 454.
- info* has the following meaning:  
If  $info = 0$ , the subroutine completed successfully.  
If  $info > 0$ , the factorization was unsuccessful and the solution was not computed.  $info$  is set equal to the first  $i$  where  $U_{ii}$  is singular and its inverse could not be computed.  
Returned as: a fullword integer;  $info \geq 0$ .

### Notes

1. In your C program, argument *info* must be passed by reference.
2. The matrices and vector used in this computation must have no common elements; otherwise, results are unpredictable.
3. The way these subroutines handle singularity differs from LAPACK. Like LAPACK, these subroutines use the *info* argument to provide information about the singularity of  $A$ , but they also provide an error message.
4. On both input and output, matrices  $A$  and  $B$  conform to LAPACK format.

### Function

These subroutines solve the system of linear equations  $AX = B$  for  $X$ , where  $A$ ,  $B$ , and  $X$  are general matrices.

The matrix  $A$  is factored using Gaussian elimination with partial pivoting to compute the  $LU$  factorization of  $A$ , where:

$$A=PLU$$

and

$L$  is a unit lower triangular matrix.

$U$  is an upper triangular matrix.

$P$  is the permutation matrix.

If  $n$  is 0, no computation is performed and the subroutine returns after doing some parameter checking. If  $n > 0$  and *nrhs* is 0, no solutions are computed and the subroutine returns after factoring the matrix.

See references [8], [38], and [64].

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

Matrix  $A$  is singular.

- The first column,  $i$ , of  $L$  with a corresponding  $U_{ii} = 0$  diagonal element is identified in the computational error message.
- The computational error message may occur multiple times with processing continuing after each error, because the default for the number of allowable errors for error code 2146 is set to be unlimited in the ESSL error option table.

### Input-Argument Errors

1.  $n < 0$
2.  $nrhs < 0$
3.  $n > lda$
4.  $lda \leq 0$
5.  $n > ldb$
6.  $ldb \leq 0$

## Examples

### Example 1

This example shows how to solve the system  $AX = B$ , where:

Matrix  $A$  is the same used as input in “Example 1” on page 460 for DGETRF.  
 Matrix  $B$  is the same used as input in “Example 1” on page 464 for DGETRS.

#### Call Statement and Input:

```

          N  NRHS  A  LDA  IPVT  BX  LDB  INFO
          |  |    |  |    |    |  |    |
CALL DGESV( 9 , 5 ,  A , 9 , IPVT, BX , 9 , INFO)
    
```

$A$  = (same as input  $A$  in “Example 1” on page 460)  
 $BX$  = (same as input  $BX$  in “Example 1” on page 464)

#### Output:

IPIV = (9, 9, 9, 9, 9, 9, 9, 9, 9)

$$A = \begin{bmatrix} 2.6 & 2.4 & 2.2 & 2.0 & 1.8 & 1.6 & 1.4 & 1.2 & 1.0 \\ 0.4 & 0.3 & 0.6 & 0.8 & 1.1 & 1.4 & 1.7 & 1.9 & 2.2 \\ 0.5 & -0.4 & 0.4 & 0.8 & 1.2 & 1.6 & 2.0 & 2.4 & 2.8 \\ 0.5 & -0.3 & 0.0 & 0.4 & 0.8 & 1.2 & 1.6 & 2.0 & 2.4 \\ 0.6 & -0.3 & 0.0 & 0.0 & 0.4 & 0.8 & 1.2 & 1.6 & 2.0 \\ 0.7 & -0.2 & 0.0 & 0.0 & 0.0 & 0.4 & 0.8 & 1.2 & 1.6 \\ 0.8 & -0.2 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 & 0.8 & 1.2 \\ 0.8 & -0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 & 0.8 \\ 0.9 & -0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 \end{bmatrix}$$

$$BX = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \\ 2.0 & 4.0 & 6.0 & 8.0 & 10.0 \\ 3.0 & 6.0 & 9.0 & 12.0 & 15.0 \\ 4.0 & 8.0 & 12.0 & 16.0 & 20.0 \\ 5.0 & 10.0 & 15.0 & 20.0 & 25.0 \\ 6.0 & 12.0 & 18.0 & 24.0 & 30.0 \end{bmatrix}$$

$$\begin{bmatrix} 7.0 & 14.0 & 21.0 & 28.0 & 35.0 \\ 8.0 & 16.0 & 24.0 & 32.0 & 40.0 \\ 9.0 & 18.0 & 27.0 & 36.0 & 45.0 \end{bmatrix}$$

INFO = 0

### Example 2

This example shows how to solve the system  $AX = B$ , where:

Matrix  $A$  is the same used as input in “Example 2” on page 460 for ZGETRF.  
 Matrix  $B$  is the same used as input in “Example 2” on page 465 for ZGETRS.

#### Call Statement and Input:

```

          N  NRHS  A  LDA  IPVT  BX  LDB  INFO
CALL ZGESV( 9 , 5 , A , 9 , IPVT, BX, 9 , INFO)
    
```

A = (same as input A in “Example 2” on page 460)  
 IPVT = (same as input IPVT in “Example 2” on page 465)  
 BX = (same as input BX in “Example 2” on page 465)

#### Output:

$$BX = \begin{bmatrix} (1.0,1.0) & (1.0,2.0) & (1.0,3.0) & (1.0,4.0) & (1.0,5.0) \\ (2.0,1.0) & (2.0,2.0) & (2.0,3.0) & (2.0,4.0) & (2.0,5.0) \\ (3.0,1.0) & (3.0,2.0) & (3.0,3.0) & (3.0,4.0) & (3.0,5.0) \\ (4.0,1.0) & (4.0,2.0) & (4.0,3.0) & (4.0,4.0) & (4.0,5.0) \\ (5.0,1.0) & (5.0,2.0) & (5.0,3.0) & (5.0,4.0) & (5.0,5.0) \\ (6.0,1.0) & (6.0,2.0) & (6.0,3.0) & (6.0,4.0) & (6.0,5.0) \\ (7.0,1.0) & (7.0,2.0) & (7.0,3.0) & (7.0,4.0) & (7.0,5.0) \\ (8.0,1.0) & (8.0,2.0) & (8.0,3.0) & (8.0,4.0) & (8.0,5.0) \\ (9.0,1.0) & (9.0,2.0) & (9.0,3.0) & (9.0,4.0) & (9.0,5.0) \end{bmatrix}$$

INFO = 0

## SGETRF, DGETRF, CGETRF and ZGETRF — General Matrix Factorization

### Purpose

These subroutines factor general matrix *A* using Gaussian elimination with partial pivoting. To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGETRS, DGETRS, CGETRS, or ZGETRS, respectively. To compute the inverse of matrix *A*, follow the call to these subroutines with a call to SGETRI, DGETRI, CGETRI, or ZGETRI, respectively.

Table 95. Data Types

<i>A</i>	Subroutine
Short-precision real	SGETRF <sup>△</sup>
Long-precision real	DGETRF <sup>△</sup>
Short-precision complex	CGETRF <sup>△</sup>
Long-precision complex	ZGETRF <sup>△</sup>
△ LAPACK	

**Note:** The output from these factorization subroutines should be used only as input to the following subroutines for performing a solve or inverse: SGETRS, DGETRS, CGETRS, ZGETRS, SGETRI, DGETRI, CGETRI, or ZGETRI, respectively.

### Syntax

<b>Fortran</b>	CALL SGETRF   DGETRF   CGETRF   ZGETRF ( <i>m</i> , <i>n</i> , <i>a</i> , <i>lda</i> , <i>ipvt</i> , <i>info</i> )
<b>C and C++</b>	sgetrf   dgetrf   cgetrf   zgetrf ( <i>m</i> , <i>n</i> , <i>a</i> , <i>lda</i> , <i>ipvt</i> , <i>info</i> );

### On Entry

- m* the number of rows in general matrix *A* used in the computation.  
Specified as: a fullword integer;  $0 \leq m \leq lda$ .
- n* the number of columns in general matrix *A* used in the computation.  
Specified as: a fullword integer;  $n \geq 0$ .
- a* is the *m* by *n* general matrix *A* to be factored.  
Specified as: an *lda* by (at least) *n* array, containing numbers of the data type indicated in Table 95.
- lda* is the leading dimension of matrix *A*.  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq m$ .
- ipvt* See "On Return."
- info* See "On Return."

### On Return

- a* is the *m* by *n* transformed matrix *A*, containing the results of the

factorization. See "Function." Returned as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 95 on page 458.

$ipvt$  is the integer vector  $ipvt$  of length  $\min(m,n)$ , containing the pivot indices. Returned as: a one-dimensional array of (at least) length  $\min(m,n)$ , containing fullword integers, where  $1 \leq ipvt(i) \leq m$ .

$info$  has the following meaning:

If  $info = 0$ , the factorization of general matrix  $A$  completed successfully.

If  $info > 0$ ,  $info$  is set equal to the first  $i$  where  $U_{ii}$  is singular and its inverse could not be computed.

Specified as: a fullword integer;  $info \geq 0$ .

## Notes

1. In your C program, argument  $info$  must be passed by reference.
2. The matrix  $A$  and vector  $ipvt$  must have no common elements; otherwise results are unpredictable.
3. The way these subroutines handle singularity differs from LAPACK. Like LAPACK, these subroutines use the  $info$  argument to provide information about the singularity of  $A$ , but they also provide an error message.
4. On both input and output, matrix  $A$  conforms to LAPACK format.

## Function

The matrix  $A$  is factored using Gaussian elimination with partial pivoting to compute the  $LU$  factorization of  $A$ , where:

$$A=PLU$$

and

$L$  is a unit lower triangular matrix.

$U$  is an upper triangular matrix.

$P$  is the permutation matrix.

On output, the transformed matrix  $A$  contains  $U$  in the upper triangle (if  $m \geq n$ ) or upper trapezoid (if  $m < n$ ) and  $L$  in the strict lower triangle (if  $m \leq n$ ) or lower trapezoid (if  $m > n$ ).  $ipvt$  contains the pivots representing permutation  $P$ , such that  $A = PLU$ .

If  $m$  or  $n$  is 0, no computation is performed and the subroutine returns after doing some parameter checking. See references [8],[38], and [64].

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

Matrix  $A$  is singular.

- The first column,  $i$ , of  $L$  with a corresponding  $U_{ii} = 0$  diagonal element is identified in the computational error message.

## SGETRF, DGETRF, CGETRF and ZGETRF

- The computational error message may occur multiple times with processing continuing after each error, because the default for the number of allowable errors for error code 2146 is set to be unlimited in the ESSL error option table.

### Input-Argument Errors

1.  $m < 0$
2.  $n < 0$
3.  $m > lda$
4.  $lda \leq 0$

## Examples

### Example 1

This example shows a factorization of a real general matrix  $A$  of order 9.

#### Call Statement and Input:

```
          M  N  A  LDA  IPVT  INFO
CALL DGETRF( 9 , 9 , A,  9 , IPVT, INFO )
```

$$A = \begin{bmatrix} 1.0 & 1.2 & 1.4 & 1.6 & 1.8 & 2.0 & 2.2 & 2.4 & 2.6 \\ 1.2 & 1.0 & 1.2 & 1.4 & 1.6 & 1.8 & 2.0 & 2.2 & 2.4 \\ 1.4 & 1.2 & 1.0 & 1.2 & 1.4 & 1.6 & 1.8 & 2.0 & 2.2 \\ 1.6 & 1.4 & 1.2 & 1.0 & 1.2 & 1.4 & 1.6 & 1.8 & 2.0 \\ 1.8 & 1.6 & 1.4 & 1.2 & 1.0 & 1.2 & 1.4 & 1.6 & 1.8 \\ 2.0 & 1.8 & 1.6 & 1.4 & 1.2 & 1.0 & 1.2 & 1.4 & 1.6 \\ 2.2 & 2.0 & 1.8 & 1.6 & 1.4 & 1.2 & 1.0 & 1.2 & 1.4 \\ 2.4 & 2.2 & 2.0 & 1.8 & 1.6 & 1.4 & 1.2 & 1.0 & 1.2 \\ 2.6 & 2.4 & 2.2 & 2.0 & 1.8 & 1.6 & 1.4 & 1.2 & 1.0 \end{bmatrix}$$

#### Output:

$$A = \begin{bmatrix} 2.6 & 2.4 & 2.2 & 2.0 & 1.8 & 1.6 & 1.4 & 1.2 & 1.0 \\ 0.4 & 0.3 & 0.6 & 0.8 & 1.1 & 1.4 & 1.7 & 1.9 & 2.2 \\ 0.5 & -0.4 & 0.4 & 0.8 & 1.2 & 1.6 & 2.0 & 2.4 & 2.8 \\ 0.5 & -0.3 & 0.0 & 0.4 & 0.8 & 1.2 & 1.6 & 2.0 & 2.4 \\ 0.6 & -0.3 & 0.0 & 0.0 & 0.4 & 0.8 & 1.2 & 1.6 & 2.0 \\ 0.7 & -0.2 & 0.0 & 0.0 & 0.0 & 0.4 & 0.8 & 1.2 & 1.6 \\ 0.8 & -0.2 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 & 0.8 & 1.2 \\ 0.8 & -0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 & 0.8 \\ 0.9 & -0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 \end{bmatrix}$$

```
IPVT    = (9, 9, 9, 9, 9, 9, 9, 9, 9)
INFO    = 0
```

### Example 2

This example shows a factorization of a complex general matrix  $A$  of order 9.

#### Call Statement and Input:

```
          M  N  A  LDA  IPVT  INFO
CALL ZGETRF( 9 , 9 , A,  9 , IPVT, INFO )
```

$$A = \begin{bmatrix} (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) & (3.6, -1.0) & (4.0, -1.0) & (4.4, -1.0) & (4.8, -1.0) & (5.2, -1.0) \\ (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) & (3.6, -1.0) & (4.0, -1.0) & (4.4, -1.0) & (4.8, -1.0) \\ (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) & (3.6, -1.0) & (4.0, -1.0) & (4.4, -1.0) \\ (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) & (3.6, -1.0) & (4.0, -1.0) \\ (3.6, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) & (3.6, -1.0) \\ (4.0, 1.0) & (3.6, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) \\ (4.4, 1.0) & (4.0, 1.0) & (3.6, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) \\ (4.8, 1.0) & (4.4, 1.0) & (4.0, 1.0) & (3.6, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) \\ (5.2, 1.0) & (4.8, 1.0) & (4.4, 1.0) & (4.0, 1.0) & (3.6, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) \end{bmatrix}$$

Output:

$$A = \begin{bmatrix} (5.2, 1.0) & (4.8, 1.0) & (4.4, 1.0) & (4.0, 1.0) & (3.6, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) \\ (0.4, 0.1) & (0.6, -2.0) & (1.1, -1.9) & (1.7, -1.9) & (2.3, -1.8) & (2.8, -1.8) & (3.4, -1.7) & (3.9, -1.7) & (4.5, -1.6) \\ (0.5, 0.1) & (0.0, -0.1) & (0.6, -1.9) & (1.2, -1.8) & (1.8, -1.7) & (2.5, -1.6) & (3.1, -1.5) & (3.7, -1.4) & (4.3, -1.3) \\ (0.6, 0.1) & (0.0, -0.1) & (-0.1, -0.1) & (0.7, -1.9) & (1.3, -1.7) & (2.0, -1.6) & (2.7, -1.5) & (3.4, -1.4) & (4.0, -1.2) \\ (0.6, 0.1) & (0.0, -0.1) & (-0.1, -0.1) & (-0.1, 0.0) & (0.7, -1.9) & (1.5, -1.7) & (2.2, -1.6) & (2.9, -1.5) & (3.7, -1.3) \\ (0.7, 0.1) & (0.0, -0.1) & (0.0, 0.0) & (-0.1, 0.0) & (-0.1, 0.0) & (0.8, -1.9) & (1.6, -1.8) & (2.4, -1.6) & (3.2, -1.5) \\ (0.8, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.8, -1.9) & (1.7, -1.8) & (2.5, -1.8) \\ (0.9, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.8, -2.0) & (1.7, -1.9) \\ (0.9, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.8, -2.0) \end{bmatrix}$$

IPVT = (9, 9, 9, 9, 9, 9, 9, 9, 9)  
INFO = 0

### Example 3

This example shows a factorization of a real general matrix  $A$  of order 9.

Call Statement and Input:

```

          M   N   A   LDA   IPVT   INFO
          |   |   |   |     |     |
CALL SGETRF( 9 , 9 , A, 9 , IPVT, INFO )
    
```

$$A = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 4.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 5.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 6.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 7.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 8.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 9.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 10.0 & 11.0 & 12.0 \end{bmatrix}$$

Output:

$$A = \begin{bmatrix} 4.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 5.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 6.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 7.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 8.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 9.0000 & 1.0000 & 1.0000 & 1.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 10.0000 & 11.0000 & 12.0000 \\ 0.2500 & 0.1500 & 0.1000 & 0.0714 & 0.0536 & -0.0694 & -0.0306 & 0.1806 & 0.3111 \\ 0.2500 & 0.1500 & 0.1000 & 0.0714 & -0.0714 & -0.0556 & -0.0194 & 0.9385 & -0.0031 \end{bmatrix}$$

IPVT = (3, 4, 5, 6, 7, 8, 9, 8, 9)

## SGETRS, DGETRS, CGETRS, and ZGETRS — General Matrix Multiple Right-Hand Side Solve

### Purpose

SGETRS and DGETRS solve one of the following systems of equations for multiple right-hand sides:

1.  $AX = B$
2.  $A^T X = B$

CGETRS and ZGETRS solve one of the following systems of equations for multiple right-hand sides:

1.  $AX = B$
2.  $A^T X = B$
3.  $A^H X = B$

In the formulas above:

$A$  represents the general matrix  $A$  containing the  $LU$  factorization.  
 $B$  represents the general matrix  $B$  containing the right-hand sides in its columns.  
 $X$  represents the general matrix  $B$  containing the solution vectors in its columns.

These subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to SGETRF, DGETRF, CGETRF, or ZGETRF, respectively.

Table 96. Data Types

$A, B$	Subroutine
Short-precision real	SGETRS <sup>△</sup>
Long-precision real	DGETRS <sup>△</sup>
Short-precision complex	CGETRS <sup>△</sup>
Long-precision complex	ZGETRS <sup>△</sup>
△ LAPACK	

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGETRF, DGETRF, CGETRF and ZGETRF, respectively.

### Syntax

Fortran	CALL SGETRS   DGETRS   CGETRS   ZGETRS ( <i>transa, n, nrhs, a, lda, ipvt, bx, ldb, info</i> )
C and C++	sgetrs   dgetrs   cgetrs   zgetrs ( <i>transa, n, nrhs, a, lda, ipvt, bx, ldb, info</i> );

### On Entry

*transa* indicates the form of matrix  $A$  to use in the computation, where:

If *transa* = 'N',  $A$  is used in the computation, resulting in solution 1.

If *transa* = 'T',  $A^T$  is used in the computation, resulting in solution 2.



## SGETRS, DGETRS, CGETRS, and ZGETRS

If  $transa = 'C'$ ,  $A^H$  is used in the computation, resulting in solution 3.

Specified as: a single character;  $transa = 'N', 'T',$  or  $'C'$ .

*n* is the order of factored matrix  $A$  and the number of rows in matrix  $B$ .

Specified as: a fullword integer;  $n \geq 0$ .

*nrhs* the number of right-hand sides—that is, the number of columns in matrix  $B$  used in the computation.

Specified as: a fullword integer;  $nrhs \geq 0$ .

*a* is the factorization of matrix  $A$ , produced by a preceding call to SGETRF, DGETRF, CGETRF, or ZGETRF, respectively.

Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 96 on page 462.

*lda* is the leading dimension of the array specified for  $a$ .

Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .

*ipvt* is the integer vector *ipvt* of length  $n$ , containing the pivot indices produced by a preceding call to SGETRF, DGETRF, CGETRF, or ZGETRF, respectively.

Specified as: a one-dimensional array of (at least) length  $n$ , containing fullword integers, where  $1 \leq ipvt(i) \leq n$ .

*bx* is the general matrix  $B$ , containing the *nrhs* right-hand sides of the system. The right-hand sides, each of length  $n$ , reside in the columns of matrix  $B$ .

Specified as: an *ldb* by (at least) *nrhs* array, containing numbers of the data type indicated in Table 96 on page 462.

*ldb* is the leading dimension of the array specified for  $B$ .

Specified as: a fullword integer;  $ldb > 0$  and  $ldb \geq n$ .

*info* See “On Return.”

**On Return**

*bx* is the matrix  $X$ , containing the *nrhs* solutions to the system. The solutions, each of length  $n$ , reside in the columns of  $X$ .

Returned as: an *ldb* by (at least) *nrhs* array, containing numbers of the data type indicated in Table 96 on page 462.

*info* *info* has the following meaning:

If  $info = 0$ , the solve of general matrix  $A$  completed successfully.

## Notes

1. In your C program, argument *info* must be passed by reference.
2. These subroutines accept lower case letters for the *transa* argument.
3. For SGETRS and DGETRS, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.

## SGETRS, DGETRS, CGETRS, and ZGETRS

4. The scalar data specified for input argument  $n$  must be the same for both `_GETRF` and `_GETRS`. In addition, the scalar data specified for input argument  $m$  in `_GETRF` **must be the same** as input argument  $n$  in both `_GETRF` and `_GETRS`.

If, however, you do **not** plan to call `_GETRS` after calling `_GETRF`, then input arguments  $m$  and  $n$  in `_GETRF` do not need to be equal.

5. The array data specified for input arguments  $a$  and  $ipvt$  for these subroutines must be the same as the corresponding output arguments for `SGETRF`, `DGETRF`, `CGETRF`, and `ZGETRF`, respectively.
6. The matrices and vector used in this computation must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
7. On both input and output, matrices  $A$  and  $B$  conform to LAPACK format.

### Function

One of the following systems of equations is solved for multiple right-hand sides:

1.  $AX = B$
2.  $A^T X = B$
3.  $A^H X = B$  (only for `CGETRS` and `ZGETRS`)

where  $A$ ,  $B$ , and  $X$  are general matrices. These subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to `SGETRF`, `DGETRF`, `CGETRF` or `ZGETRF`, respectively. For details on the factorization, see “`SGETRF`, `DGETRF`, `CGETRF` and `ZGETRF` — General Matrix Factorization” on page 458.

If  $n = 0$  or  $nrhs = 0$ , no computation is performed and the subroutine returns after doing some parameter checking. See references [8, [38], and [64].

### Error conditions

#### Computational Errors

None

**Note:** If the factorization performed by `SGETRF`, `DGETRF`, `CGETRF` or `ZGETRF` failed because a pivot element is zero, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

#### Input-Argument Errors

1.  $transa \neq 'N', 'T', \text{ or } 'C'$
2.  $n < 0$
3.  $nrhs < 0$
4.  $n > lda$
5.  $lda \leq 0$
6.  $n > ldb$
7.  $ldb \leq 0$

### Examples

#### Example 1

This example shows how to solve the system  $AX = B$ , where matrix  $A$  is the same matrix factored in the “Example 1” on page 460 for `DGETRF`.

**Call Statement and Input:**

## SGETRS, DGETRS, CGETRS, and ZGETRS

```

          TRANSA  N  NRHS  A  LDA  IPIV  BX  LDB  INFO
          |      |  |    |  |    |    |  |    |
CALL DGETRS('N' , 9 , 5 , A , 9 , IPIV, BX , 9 , INFO)

```

IPVT = (9, 9, 9, 9, 9, 9, 9, 9, 9)  
A = (same as output A in "Example 1" on page 460)

$$\text{BX} = \begin{bmatrix} 93.0 & 186.0 & 279.0 & 372.0 & 465.0 \\ 84.4 & 168.8 & 253.2 & 337.6 & 422.0 \\ 76.6 & 153.2 & 229.8 & 306.4 & 383.0 \\ 70.0 & 140.0 & 210.0 & 280.0 & 350.0 \\ 65.0 & 130.0 & 195.0 & 260.0 & 325.0 \\ 62.0 & 124.0 & 186.0 & 248.0 & 310.0 \\ 61.4 & 122.8 & 184.2 & 245.6 & 307.0 \\ 63.6 & 127.2 & 190.8 & 254.4 & 318.0 \\ 69.0 & 138.0 & 207.0 & 276.0 & 345.0 \end{bmatrix}$$

### Output:

$$\text{BX} = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \\ 2.0 & 4.0 & 6.0 & 8.0 & 10.0 \\ 3.0 & 6.0 & 9.0 & 12.0 & 15.0 \\ 4.0 & 8.0 & 12.0 & 16.0 & 20.0 \\ 5.0 & 10.0 & 15.0 & 20.0 & 25.0 \\ 6.0 & 12.0 & 18.0 & 24.0 & 30.0 \\ 7.0 & 14.0 & 21.0 & 28.0 & 35.0 \\ 8.0 & 16.0 & 24.0 & 32.0 & 40.0 \\ 9.0 & 18.0 & 27.0 & 36.0 & 45.0 \end{bmatrix}$$

INFO = 0

### Example 2

This example shows how to solve the system  $AX = b$ , where matrix  $A$  is the same matrix factored in the "Example 2" on page 460 for ZGETRF.

#### Call Statement and Input:

```

          TRANS  N  NRHS  A  LDA  IPIV  BX  LDB  INFO
          |     |  |    |  |    |    |  |    |
CALL ZGETRS('N' , 9 , 5 , A , 9 , IPIV, BX , 9 , INFO)

```

IPVT = (9, 9, 9, 9, 9, 9, 9, 9, 9)  
A = (same as output A in "Example 2" on page 460)

$$\text{BX} = \begin{bmatrix} (193.0, -10.6) & (200.0, 21.8) & (207.0, 54.2) & (214.0, 86.6) & (221.0, 119.0) \\ (173.8, -9.4) & (178.8, 20.2) & (183.8, 49.8) & (188.8, 79.4) & (193.8, 109.0) \\ (156.2, -5.4) & (159.2, 22.2) & (162.2, 49.8) & (165.2, 77.4) & (168.2, 105.0) \\ (141.0, 1.4) & (142.0, 27.8) & (143.0, 54.2) & (144.0, 80.6) & (145.0, 107.0) \\ (129.0, 11.0) & (128.0, 37.0) & (127.0, 63.0) & (126.0, 89.0) & (125.0, 115.0) \\ (121.0, 23.4) & (118.0, 49.8) & (115.0, 76.2) & (112.0, 102.6) & (109.0, 129.0) \\ (117.8, 38.6) & (112.8, 66.2) & (107.8, 93.8) & (102.8, 121.4) & (97.8, 149.0) \\ (120.2, 56.6) & (113.2, 86.2) & (106.2, 115.8) & (99.2, 145.4) & (92.2, 175.0) \\ (129.0, 77.4) & (120.0, 109.8) & (111.0, 142.2) & (102.0, 174.6) & (93.0, 207.0) \end{bmatrix}$$

## SGETRS, DGETRS, CGETRS, and ZGETRS

Output:

$$\text{BX} = \begin{bmatrix} (1.0,1.0) & (1.0,2.0) & (1.0,3.0) & (1.0,4.0) & (1.0,5.0) \\ (2.0,1.0) & (2.0,2.0) & (2.0,3.0) & (2.0,4.0) & (2.0,5.0) \\ (3.0,1.0) & (3.0,2.0) & (3.0,3.0) & (3.0,4.0) & (3.0,5.0) \\ (4.0,1.0) & (4.0,2.0) & (4.0,3.0) & (4.0,4.0) & (4.0,5.0) \\ (5.0,1.0) & (5.0,2.0) & (5.0,3.0) & (5.0,4.0) & (5.0,5.0) \\ (6.0,1.0) & (6.0,2.0) & (6.0,3.0) & (6.0,4.0) & (6.0,5.0) \\ (7.0,1.0) & (7.0,2.0) & (7.0,3.0) & (7.0,4.0) & (7.0,5.0) \\ (8.0,1.0) & (8.0,2.0) & (8.0,3.0) & (8.0,4.0) & (8.0,5.0) \\ (9.0,1.0) & (9.0,2.0) & (9.0,3.0) & (9.0,4.0) & (9.0,5.0) \end{bmatrix}$$

INFO = 0

## SGEF, DGEF, CGEF, and ZGEF — General Matrix Factorization

### Purpose

This subroutine factors a square general matrix  $A$  using Gaussian elimination with partial pivoting. To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGES/SGESM, DGES/DGESM, CGES/CGESM, or ZGES/ZGESM, respectively. To compute the inverse of matrix  $A$ , follow the call to these subroutines with a call to SGEICD or DGEICD, respectively.

Table 97. Data Types

$A$	Subroutine
Short-precision real	SGEF
Long-precision real	DGEF
Short-precision complex	CGEF
Long-precision complex	ZGEF

**Note:** The output from these factorization subroutines should be used only as input to the following subroutines for performing a solve or inverse: SGES/SGESM/SGEICD, DGES/DGESM/DGEICD, CGES/CGESM, and ZGES/ZGESM, respectively.

### Syntax

<b>Fortran</b>	CALL SGEF   DGEF   CGEF   ZGEF ( $a, lda, n, ipvt$ )
<b>C and C++</b>	sgef   dgef   cgef   zgef ( $a, lda, n, ipvt$ );

#### On Entry

$a$  is the  $n$  by  $n$  general matrix  $A$  to be factored.  
Specified as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 97.

$lda$  is the leading dimension of the array specified for  $a$ .  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .

$n$  is the order of matrix  $A$ .  
Specified as: a fullword integer;  $0 \leq n \leq lda$ .

$ipvt$  See "On Return."

#### On Return

$a$  is the  $n$  by  $n$  transformed matrix  $A$ , containing the results of the factorization. See "Function" on page 468. Returned as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 97.

$ipvt$  is the integer vector  $ipvt$  of length  $n$ , containing the pivot indices. Returned as: a one-dimensional array of (at least) length  $n$ , containing fullword integers.

## Notes

1. Calling SGEFCD or DGEFCD with  $ipvt = 0$  is equivalent to calling SGEF or DGEF.
2. On both input and output, matrix  $A$  conforms to LAPACK format.

## Function

The matrix  $A$  is factored using Gaussian elimination with partial pivoting ( $ipvt$ ) to compute the  $LU$  factorization of  $A$ , where ( $A = PLU$ ):

$L$  is a unit lower triangular matrix.

$U$  is an upper triangular matrix.

$P$  is the permutation matrix.

On output, the transformed matrix  $A$  contains  $U$  in the upper triangle and  $L$  in the strict lower triangle where  $ipvt$  contains the pivots representing permutation  $P$ , such that  $A = PLU$ .

If  $n$  is 0, no computation is performed. See references [38] and [40].

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

Matrix  $A$  is singular.

- One or more columns of  $L$  and the corresponding diagonal of  $U$  contain all zeros (all columns of  $L$  are checked). The first column,  $i$ , of  $L$  with a corresponding  $U = 0$  diagonal element is identified in the computational error message.
- The return code is set to 1.
- $i$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2103 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 51.

### Input-Argument Errors

1.  $lda \leq 0$
2.  $n < 0$
3.  $n > lda$

## Examples

### Example 1

This example shows a factorization of a real general matrix  $A$  of order 9.

#### Call Statement and Input:

```

      A  LDA  N  IPVT
      |  |  |  |
CALL SGEF( A , 9 , 9 , IPVT )

```

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 4.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 5.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 \end{bmatrix}$$

$$A = \begin{bmatrix} 0.0 & 0.0 & 6.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 7.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 8.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 9.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 10.0 & 11.0 & 12.0 \end{bmatrix}$$

Output:

$$A = \begin{bmatrix} 4.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 5.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 6.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 7.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 8.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 9.0000 & 1.0000 & 1.0000 & 1.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 10.0000 & 11.0000 & 12.0000 \\ 0.2500 & 0.1500 & 0.1000 & 0.0714 & 0.0536 & -0.0694 & -0.0306 & 0.1806 & 0.3111 \\ 0.2500 & 0.1500 & 0.1000 & 0.0714 & -0.0714 & -0.0556 & -0.0194 & 0.9385 & -0.0031 \end{bmatrix}$$

$$IPVT = (3, 4, 5, 6, 7, 8, 9, 8, 9)$$

### Example 2

This example shows a factorization of a complex general matrix  $A$  of order 4.

Call Statement and Input:

```

      A  LDA  N  IPVT
      |  |  |  |
CALL CGEF( A , 4 , 4 , IPVT )

```

$$A = \begin{bmatrix} (1.0, 2.0) & (1.0, 7.0) & (2.0, 4.0) & (3.0, 1.0) \\ (2.0, 0.0) & (1.0, 3.0) & (4.0, 4.0) & (2.0, 3.0) \\ (2.0, 1.0) & (5.0, 0.0) & (3.0, 6.0) & (0.0, 0.0) \\ (8.0, 5.0) & (1.0, 9.0) & (6.0, 6.0) & (8.0, 1.0) \end{bmatrix}$$

Output:

$$A = \begin{bmatrix} (8.0000, 5.0000) & (1.0000, 9.0000) & (6.0000, 6.0000) & (8.0000, 1.0000) \\ (0.2022, 0.1236) & (1.9101, 5.0562) & (1.5281, 2.0449) & (1.5056, -0.1910) \\ (0.2360, -0.0225) & (-0.0654, -0.9269) & (-0.3462, 6.2692) & (-1.6346, 1.3269) \\ (0.1798, -0.1124) & (0.2462, 0.1308) & (0.4412, -0.3655) & (0.2900, 2.3864) \end{bmatrix}$$

$$IPVT = (4, 4, 3, 4)$$

## SGES, DGES, CGES, and ZGES — General Matrix, Its Transpose, or Its Conjugate Transpose Solve

### Purpose

These subroutines solve the system  $Ax = b$  for  $x$ , where  $A$  is a general matrix and  $x$  and  $b$  are vectors. Using the *iopt* argument, they can also solve the real system  $A^T x = b$  or the complex system  $A^H x = b$  for  $x$ . These subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively.

Table 98. Data Types

$A, b, x$	Subroutine
Short-precision real	SGES
Long-precision real	DGES
Short-precision complex	CGES
Long-precision complex	ZGES

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.

### Syntax

Fortran	CALL SGES   DGES   CGES   ZGES ( <i>a, lda, n, ipvt, bx, iopt</i> )
C and C++	sges   dges   cges   zges ( <i>a, lda, n, ipvt, bx, iopt</i> );

### On Entry

- a* is the factorization of matrix  $A$ , produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively. Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 98.
- lda* is the leading dimension of the array specified for *a*.  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .
- n* is the order of matrix  $A$ .  
Specified as: a fullword integer;  $0 \leq n \leq lda$ .
- ipvt* is the integer vector *ipvt* of length  $n$ , containing the pivot indices produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively.  
Specified as: a one-dimensional array of (at least) length  $n$ , containing fullword integers.
- bx* is the vector  $b$  of length  $n$ , containing the right-hand side of the system.  
Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 98.
- iopt* determines the type of computation to be performed, where:  
If *iopt* = 0,  $A$  is used in the computation.



If  $iopt = 1$ ,  $A^T$  is used in SGES and DGES.  $A^H$  is used in CGES and ZGES.

**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix  $A$  should always be stored in its untransposed form.

Specified as: a fullword integer;  $iopt = 0$  or  $1$ .

### On Return

$bx$  is the solution vector  $x$  of length  $n$ , containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 98 on page 470.

### Notes

1. The scalar data specified for input arguments  $lda$  and  $n$  for these subroutines must be the same as the corresponding input arguments specified for SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.
2. The array data specified for input arguments  $a$  and  $iopt$  for these subroutines must be the same as the corresponding output arguments for SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.
3. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.

### Function

The system  $Ax = b$  is solved for  $x$ , where  $A$  is a general matrix and  $x$  and  $b$  are vectors. Using the  $iopt$  argument, this subroutine can also solve the real system  $A^T x = b$  or the complex system  $A^H x = b$  for  $x$ . These subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively. For a description of how  $A$  is factored, see “SGEF, DGEF, CGEF, and ZGEF — General Matrix Factorization” on page 467.

If  $n$  is 0, no computation is performed. See references [38] and [40].

### Error conditions

#### Computational Errors

None

**Note:** If the factorization performed by SGEF, DGEF, CGEF, ZGEF, SGEFCD, DGEFCD, or DGEFP failed because a pivot element is zero, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

#### Input-Argument Errors

1.  $lda \leq 0$
2.  $n < 0$
3.  $n > lda$
4.  $iopt \neq 0$  or  $1$

## Examples

### Example 1

**Part 1:** This part of the example shows how to solve the system  $Ax = b$ , where matrix  $A$  is the same matrix factored in the "Example 1" on page 468 for SGEF and DGEF.

**Call Statement and Input:**

```

          A LDA N  IPVT  BX IOPT
          |  |  |  |  |  |  |
CALL SGES( A , 9 , 9 , IPVT , BX , 0 )

```

```

IPVT      = (3, 4, 5, 6, 7, 8, 9, 8, 9)
BX        = (4.0, 5.0, 9.0, 10.0, 11.0, 12.0, 12.0, 12.0, 33.0)
A         = (same as output A in "Example 1" on page 468)

```

**Output:**

```

BX        = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)

```

**Part 2:** This part of the example shows how to solve the system  $A^T x = b$ , where matrix  $A$  is the input matrix factored in "Example 1" on page 468 for SGEF and DGEF. Most of the input is the same in Part 2 as in Part 1.

**Call Statement and Input:**

```

          A LDA N  IPVT  BX IOPT
          |  |  |  |  |  |  |
CALL SGES( A , 9 , 9 , IPVT , BX , 1 )

```

```

IPVT      = (3, 4, 5, 6, 7, 8, 9, 8, 9)
BX        = (6.0, 8.0, 10.0, 12.0, 13.0, 14.0, 15.0, 15.0, 15.0)
A         = (same as output A in "Example 1" on page 468)

```

**Output:**

```

BX        = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)

```

### Example 2

**Part 1:** This part of the example shows how to solve the system  $Ax = b$ , where matrix  $A$  is the same matrix factored in the "Example 2" on page 469 for CGEF and ZGEF.

**Call Statement and Input:**

```

          A LDA N  IPVT  BX IOPT
          |  |  |  |  |  |  |
CALL CGES( A , 4 , 4 , IPVT , BX , 0 )

```

```

IPVT      = (4, 4, 3, 4)
BX        = ((-10.0, 85.0), (-6.0, 61.0), (10.0, 38.0),
            (58.0, 168.0))
A         = (same as output A in "Example 1" on page 468)

```

**Output:**

```

BX        = ((9.0, 0.0), (5.0, 1.0), (1.0, 6.0), (3.0, 4.0))

```

**Part 2:** This part of the example shows how to solve the system  $A^H x = b$ , where matrix  $A$  is the input matrix factored in “Example 2” on page 469 for CGEF and ZGEF. Most of the input is the same in Part 2 as in Part 1.

**Call Statement and Input:**

```

          A  LDA  N  IPVT  BX  IOPT
          |  |  |  |  |  |
CALL CGES( A , 4 , 4 , IPVT , BX , 1 )

```

```

IPVT      = (4, 4, 3, 4)
BX        = ((71.0, 12.0), (61.0, -70.0), (123.0, -34.0),
             (68.0, 7.0))
A         = (same as output A in “Example 1” on page 468)

```

**Output:**

```

BX        = ((9.0, 0.0), (5.0, 1.0), (1.0, 6.0), (3.0, 4.0))

```

## SGESM, DGESM, CGESM, and ZGESM — General Matrix, Its Transpose, or Its Conjugate Transpose Multiple Right-Hand Side Solve

### Purpose

These subroutines solve the following systems of equations for multiple right-hand sides, where  $A$ ,  $X$ , and  $B$  are general matrices. SGESM and DGESM solve one of the following:

1.  $AX = B$
2.  $A^T X = B$

CGESM and ZGESM solve one of the following:

1.  $AX = B$
2.  $A^T X = B$
3.  $A^H X = B$

These subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively.

Table 99. Data Types

$A, B, X$	Subroutine
Short-precision real	SGESM
Long-precision real	DGESM
Short-precision complex	CGESM
Long-precision complex	ZGESM

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.

### Syntax

<b>Fortran</b>	CALL SGESM   DGESM   CGESM   ZGESM ( <i>trans, a, lda, n, ipvt, bx, ldb, nrhs</i> )
<b>C and C++</b>	sgesm   dgesm   cgesm   zgesm ( <i>trans, a, lda, n, ipvt, bx, ldb, nrhs</i> );

### On Entry

*trans* indicates the form of matrix  $A$  to use in the computation, where:

- If *transa* = 'N',  $A$  is used in the computation, resulting in equation 1.
- If *transa* = 'T',  $A^T$  is used in the computation, resulting in equation 2.
- If *transa* = 'C',  $A^H$  is used in the computation, resulting in equation 3.

Specified as: a single character. It must be 'N', 'T', or 'C'.

*a* is the factorization of matrix  $A$ , produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF,

	respectively. Specified as: an $lda$ by (at least) $n$ array, containing numbers of the data type indicated in Table 99 on page 474.
$lda$	is the leading dimension of the array specified for $a$ . Specified as: a fullword integer; $lda > 0$ and $lda \geq n$ .
$n$	is the order of matrix $A$ . Specified as: a fullword integer; $0 \leq n \leq lda$ .
$ipvt$	is the integer vector $ipvt$ of length $n$ , containing the pivot indices produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively. Specified as: a one-dimensional array of (at least) length $n$ , containing fullword integers.
$bx$	is the general matrix $B$ , containing the $nrhs$ right-hand sides of the system. The right-hand sides, each of length $n$ , reside in the columns of matrix $B$ . Specified as: an $ldb$ by (at least) $nrhs$ array, containing numbers of the data type indicated in Table 99 on page 474.
$ldb$	is the leading dimension of the array specified for $b$ . Specified as: a fullword integer; $ldb > 0$ and $ldb \geq n$ .
$nrhs$	is the number of right-hand sides in the system to be solved. Specified as: a fullword integer; $nrhs \geq 0$ .

### On Return

$bx$	is the matrix $X$ , containing the $nrhs$ solutions to the system. The solutions, each of length $n$ , reside in the columns of $X$ . Specified as: an $ldb$ by (at least) $nrhs$ array, containing numbers of the data type indicated in Table 99 on page 474.
------	--

### Notes

1. For SGESM and DGESM, if you specify 'C' for the *trans* argument, it is interpreted as though you specified 'T'.
2. The scalar data specified for input arguments  $lda$  and  $n$  for these subroutines must be the same as the corresponding input arguments specified for SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.
3. The array data specified for input arguments  $a$  and  $ipvt$  for these subroutines must be the same as the corresponding output arguments for SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.
4. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.

### Function

One of the following systems of equations is solved for multiple right-hand sides:

1.  $AX = B$
2.  $A^T X = B$
3.  $A^H X = B$  (only for CGESM and ZGESM)

## SGESM, DGESM, CGESM, ZGESM

where  $A$ ,  $B$ , and  $X$  are general matrices. These subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively. For a description of how  $A$  is factored, see “SGEF, DGEF, CGEF, and ZGEF — General Matrix Factorization” on page 467.

If  $n$  or  $nrhs$  is 0, no computation is performed. See references [38] and [40].

### Error conditions

#### Computational Errors

None

**Note:** If the factorization performed by SGEF, DGEF, CGEF, ZGEF, SGEFCD, DGEFCD, or DGEFP failed because a pivot element is zero, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

#### Input-Argument Errors

1.  $trans \neq 'N', 'T', \text{ or } 'C'$
2.  $lda, ldb \leq 0$
3.  $n < 0$
4.  $n > lda, ldb$
5.  $nrhs < 0$

### Examples

#### Example 1

**Part 1:** This part of the example shows how to solve the system  $AX = B$  for two right-hand sides, where matrix  $A$  is the same matrix factored in the “Example 1” on page 468 for SGEF and DGEF.

#### Call Statement and Input:

```
          TRANS  A  LDA  N  IPVT  BX  LDB  NRHS
          |      |  |   |  |     |  |   |
CALL SGESM( 'N' , A , 9 , 9 , IPVT , BX , 9 , 2 )
```

IPVT = (3, 4, 5, 6, 7, 8, 9, 8, 9)

A = (same as output A in “Example 1” on page 468)

BX = 
$$\begin{bmatrix} 4.0 & 10.0 \\ 5.0 & 15.0 \\ 9.0 & 24.0 \\ 10.0 & 35.0 \\ 11.0 & 48.0 \\ 12.0 & 63.0 \\ 12.0 & 70.0 \\ 12.0 & 78.0 \\ 33.0 & 266.0 \end{bmatrix}$$

#### Output:

$$\begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \end{bmatrix}$$

$$BX = \begin{bmatrix} 1.0 & 5.0 \\ 1.0 & 6.0 \\ 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

**Part 2:** This part of the example shows how to solve the system  $A^T X = B$  for two right-hand sides, where matrix  $A$  is the input matrix factored in “Example 1” on page 468 for SGEF and DGEF.

**Call Statement and Input:**

```

          TRANS  A  LDA  N  IPVT  BX  LDB  NRHS
          |      |  |   |  |     |  |   |   |
CALL SGESM( 'T' , A , 9 , 9 , IPVT , BX , 9 , 2 )
    
```

IPVT = (3, 4, 5, 6, 7, 8, 9, 8, 9)  
 A = (same as output A in “Example 1” on page 468)

$$BX = \begin{bmatrix} 6.0 & 15.0 \\ 8.0 & 26.0 \\ 10.0 & 40.0 \\ 12.0 & 57.0 \\ 13.0 & 76.0 \\ 14.0 & 97.0 \\ 15.0 & 120.0 \\ 15.0 & 125.0 \\ 15.0 & 129.0 \end{bmatrix}$$

**Output:**

$$BX = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \\ 1.0 & 5.0 \\ 1.0 & 6.0 \\ 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

**Example 2**

**Part 1:** This part of the example shows how to solve the system  $AX = B$  for two right-hand sides, where matrix  $A$  is the same matrix factored in the “Example 2” on page 469 for CGEF and ZGEF.

**Call Statement and Input:**

```

          TRANS  A  LDA  N  IPVT  BX  LDB  NRHS
          |      |  |   |  |     |  |   |   |
CALL CGESM( 'N' , A , 4 , 4 , IPVT , BX , 4 , 2 )
    
```

IPVT = (4, 4, 3, 4)  
 A = (same as output A in “Example 2” on page 469)

$$BX = \begin{bmatrix} (-10.0, 85.0) & (-11.0, 53.0) \\ (-6.0, 61.0) & (-6.0, 54.0) \\ (10.0, 38.0) & (2.0, 40.0) \\ (58.0, 168.0) & (15.0, 105.0) \end{bmatrix}$$

## SGESM, DGESM, CGESM, ZGESM

### Output:

$$BX = \begin{bmatrix} (9.0, 0.0) & (1.0, 1.0) \\ (5.0, 1.0) & (2.0, 2.0) \\ (1.0, 6.0) & (3.0, 3.0) \\ (3.0, 4.0) & (4.0, 4.0) \end{bmatrix}$$

**Part 2:** This part of the example shows how to solve the system  $A^T X = B$  for two right-hand sides, where matrix  $A$  is the input matrix factored in “Example 2” on page 469 for CGEF and ZGEF.

### Call Statement and Input:

```
          TRANS  A  LDA  N  IPVT  BX  LDB  NRHS
          |      |  |   |  |     |  |   |   |
CALL CGESM( 'T' , A , 4 , 4 , IPVT , BX , 4 , 2 )
```

IPVT = (4, 4, 3, 4)

A = (same as output A in “Example 2” on page 469)

$$BX = \begin{bmatrix} (71.0, 12.0) & (18.0, 68.0) \\ (61.0, -70.0) & (-27.0, 71.0) \\ (123.0, -34.0) & (-11.0, 97.0) \\ (68.0, 7.0) & (28.0, 50.0) \end{bmatrix}$$

### Output:

$$BX = \begin{bmatrix} (9.0, 0.0) & (1.0, 1.0) \\ (5.0, 1.0) & (2.0, 2.0) \\ (1.0, 6.0) & (3.0, 3.0) \\ (3.0, 4.0) & (4.0, 4.0) \end{bmatrix}$$

**Part 3:** This part of the example shows how to solve the system  $A^H X = B$  for two right-hand sides, where matrix  $A$  is the input matrix factored in “Example 2” on page 469 for CGEF and ZGEF.

### Call Statement and Input:

```
          TRANS  A  LDA  N  IPVT  BX  LDB  NRHS
          |      |  |   |  |     |  |   |   |
CALL CGESM( 'C' , A , 4 , 4 , IPVT , BX , 4 , 2 )
```

IPVT = (4, 4, 3, 4)

A = (same as output A in “Example 2” on page 469)

$$BX = \begin{bmatrix} (58.0, -3.0) & (45.0, 20.0) \\ (68.0, -31.0) & (83.0, -20.0) \\ (89.0, -22.0) & (98.0, 1.0) \\ (53.0, 15.0) & (45.0, 25.0) \end{bmatrix}$$

### Output:

$$BX = \begin{bmatrix} (1.0, 4.0) & (4.0, 5.0) \\ (2.0, 3.0) & (3.0, 4.0) \\ (3.0, 2.0) & (2.0, 3.0) \\ (4.0, 1.0) & (1.0, 2.0) \end{bmatrix}$$



## SGEFCD and DGEFCD — General Matrix Factorization, Condition Number Reciprocal, and Determinant

### Purpose

These subroutines factor general matrix  $A$  using Gaussian elimination. An estimate of the reciprocal of the condition number and the determinant of matrix  $A$  can also be computed. To solve a system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGES/SGESM or DGES/DGESM, respectively. To compute the inverse of matrix  $A$ , follow the call to these subroutines with a call to SGEICD and DGEICD, respectively.

Table 100. Data Types

$A$ , $aux$ , $rcond$ , $det$	Subroutine
Short-precision real	SGEFCD
Long-precision real	DGEFCD

**Note:** The output from these factorization subroutines should be used only as input to the following subroutines for performing a solve or inverse: SGES/SGESM/SGEICD and DGES/DGESM/DGEICD, respectively.

### Syntax

<b>Fortran</b>	CALL SGEFCD   DGEFCD ( $a$ , $lda$ , $n$ , $ipvt$ , $iopt$ , $rcond$ , $det$ , $aux$ , $naux$ )
<b>C and C++</b>	sgefcd   dgefcd ( $a$ , $lda$ , $n$ , $ipvt$ , $iopt$ , $rcond$ , $det$ , $aux$ , $naux$ );

### On Entry

- $a$  is a general matrix  $A$  of order  $n$ , whose factorization, reciprocal of condition number, and determinant are computed. Specified as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 100.
- $lda$  is the leading dimension of the array specified for  $a$ .  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .
- $n$  is the order of matrix  $A$ .  
Specified as: a fullword integer;  $0 \leq n \leq lda$ .
- $ipvt$  See "On Return" on page 480.
- $iopt$  indicates the type of computation to be performed, where:  
If  $iopt = 0$ , the matrix is factored.  
If  $iopt = 1$ , the matrix is factored, and the reciprocal of the condition number is computed.  
If  $iopt = 2$ , the matrix is factored, and the determinant is computed.  
If  $iopt = 3$ , the matrix is factored, and the reciprocal of the condition number and the determinant are computed.  
Specified as: a fullword integer;  $iopt = 0, 1, 2$ , or  $3$ .
- $rcond$  See "On Return" on page 480.

## SGEFCD, DGEFCD

<i>det</i>	See “On Return.”
<i>aux</i>	has the following meaning: If $naux = 0$ and error 2015 is unrecoverable, <i>aux</i> is ignored. Otherwise, it is a storage work area used by this subroutine. Its size is specified by <i>naux</i> . Specified as: an area of storage, containing numbers of the data type indicated in Table 100 on page 479.
<i>naux</i>	is the size of the work area specified by <i>aux</i> —that is, the number of elements in <i>aux</i> . Specified as: a fullword integer, where: If $naux = 0$ and error 2015 is unrecoverable, SGEFCD and DGEFCD dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program. Otherwise, $naux \geq n$ .

### On Return

<i>a</i>	is the transformed matrix <i>A</i> of order <i>n</i> , containing the results of the factorization. See “Function” on page 481. Returned as: an <i>lda</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 100 on page 479.
<i>ipvt</i>	is the integer vector <i>ipvt</i> of length <i>n</i> , containing the pivot indices. Returned as: a one-dimensional array of (at least) length <i>n</i> , containing fullword integers.
<i>rcond</i>	is an estimate of the reciprocal of the condition number, <i>rcond</i> , of matrix <i>A</i> . Returned as: a number of the data type indicated in Table 100 on page 479; $rcond \geq 0$ .
<i>det</i>	is the vector <i>det</i> , containing the two components, $det_1$ and $det_2$ , of the determinant of matrix <i>A</i> . The determinant is:

$$det_1(10^{det_2})$$

where  $1 \leq det_1 < 10$ . Returned as: an array of length 2, containing numbers of the data type indicated in Table 100 on page 479.

### Notes

1. In your C program, argument *rcond* must be passed by reference.
2. When *iopt* = 0, these subroutines provide the same function as a call to SGEF or DGEF, respectively.
3. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.
4. On both input and output, matrix **A** conforms to LAPACK format.

## Function

Matrix  $A$  is factored using Gaussian elimination with partial pivoting (*ipvt*) to compute the  $LU$  factorization of  $A$ , where ( $A=PLU$ ):

$L$  is a unit lower triangular matrix.

$U$  is an upper triangular matrix.

$P$  is the permutation matrix.

On output, the transformed matrix  $A$  contains  $U$  in the upper triangle and  $L$  in the strict lower triangle where *ipvt* contains the pivots representing permutation  $P$ , such that  $A = PLU$ .

An estimate of the reciprocal of the condition number, *rcond*, and the determinant, *det*, can also be computed by this subroutine. The estimate of the condition number uses an enhanced version of the algorithm described in references [72] and [73].

If  $n$  is 0, no computation is performed. See reference [38].

These subroutines call SGEF and DGEF, respectively, to perform the factorization. *ipvt* is an output vector of SGEF and DGEF. It is returned for use by SGES/SGESM and DGES/DGESM, the solve subroutines.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

Matrix  $A$  is singular.

- If your program is not terminated by SGEF and DGEF, then SGEFCD and DGEFCD, respectively, return 0 for *rcond* and *det*.
- One or more columns of  $L$  and the corresponding diagonal of  $U$  contain all zeros (all columns of  $L$  are checked). The first column,  $i$ , of  $L$  with a corresponding  $U = 0$  diagonal element is identified in the computational error message, issued by SGEF or DGEF, respectively.
- $i$  can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2103 in the ESSL error option table; otherwise, the default value causes your program to be terminated by SGEF or DGEF, respectively, when this error occurs. If your program is not terminated by SGEF or DGEF, respectively, the return code is set to 2. For details, see "What Can You Do about ESSL Computational Errors?" on page 51.

### Input-Argument Errors

1.  $lda \leq 0$
2.  $n < 0$
3.  $n > lda$
4.  $ipvt \neq 0, 1, 2, \text{ or } 3$
5. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example

This example shows a factorization of matrix  $A$  of order 9. The input is the same as used in SGEF and DGEF. See "Example 1" on page 468. The reciprocal of the condition number and the determinant of matrix  $A$  are also computed. The values used to estimate the reciprocal of the condition number in this example are obtained with the following values:

$$\|A\|_1 = \max(6.0, 8.0, 10.0, 12.0, 13.0, 14.0, 15.0, 15.0, 15.0) = 15.0$$

$$\text{Estimate of } \|A^{-1}\|_1 = 1091.87$$

This estimate is equal to the actual *rcond* of  $5.436(10^{-5})$ , which is computed by SGEICD and DGEICD. (See "Example 3" on page 544.) On output, the value in *det*,  $|A|$ , is equal to 336.

### Call Statement and Input:

	A	LDA	N	IPVT	IOPT	RCOND	DET	AUX	NAUX
CALL DGEFCD(									
	A	,	9	,	9	,	IPVT	,	3
	,	RCOND	,	DET	,	AUX	,	9	)

A           =(same as input A in  
"Example 1" on page 468)

### Output:

A           = (same as output A in "Example 1" on page 468)  
 IPVT       = (3, 4, 5, 6, 7, 8, 9, 8, 9)  
 RCOND      = 0.00005436  
 DET        = (3.36, 2.00)

## SPPSV, DPPSV, CPPSV, and ZPPSV — Positive Definite Real Symmetric and Complex Hermitian Matrix Factorization and Multiple Right-Hand Side Solve

### Purpose

These subroutines solve the system of linear equations  $AX = B$  for  $X$ , where  $X$  and  $B$  are general matrices and:

- for SPPSV and DPPSV,  $A$  is a positive definite real symmetric matrix.
- for CPPSV and ZPPSV,  $A$  is a positive definite complex Hermitian matrix.

The matrix  $A$ , stored in upper- or lower-packed storage mode, is factored using Cholesky factorization.

Table 101. Data Types

$A, B$	Subroutine
Short-precision real	SPPSV <sup>△</sup>
Long-precision real	DPPSV <sup>△</sup>
Short-precision complex	CPPSV <sup>△</sup>
Long-precision complex	ZPPSV <sup>△</sup>
△ LAPACK	

### Syntax

<b>Fortran</b>	CALL SPPSV   DPPSV   CPPSV   ZPPSV ( <i>uplo, n, nrhs, ap, bx, ldb, info</i> )
<b>C and C++</b>	sppsv   dppsv   cppsv   zppsv ( <i>uplo, n, nrhs, ap, bx, ldb, info</i> );

### On Entry

- uplo* indicates whether matrix  $A$  is stored in upper- or lower-packed storage mode, where:
- If *uplo* = 'U',  $A$  is stored in upper-packed storage mode.
- If *uplo* = 'L',  $A$  is stored in lower-packed storage mode.
- Specified as: a single character. It must be 'U' or 'L'.
- n* is the order  $n$  of matrix  $A$  and the number of rows of matrix  $B$ .
- Specified as: a fullword integer;  $n \geq 0$ .
- nrhs* is the number of right-hand sides; that is, the number of columns of matrix  $B$ .
- Specified as: a fullword integer;  $nrhs \geq 0$ .
- ap* is an array, referred to as AP, in which matrix  $A$ , to be factored, is stored in upper- or lower-packed storage mode.
- Specified as: a one-dimensional array of (at least) length  $n(n+1)/2$ , containing numbers of the data type indicated in Table 101.
- bx* is the general matrix  $B$ , containing the *nrhs* right-hand sides of the system. The right-hand sides, each of length  $n$ , reside in the columns of  $B$ .

## SPPSV, DPPSV, CPPSV, and ZPPSV

	Specified as: an <i>ldb</i> by (at least) <i>nrhs</i> array, containing numbers of the data type indicated in Table 101 on page 483.
<i>ldb</i>	is the leading dimension of the array specified for <i>B</i> . Specified as: a fullword integer; $ldb > 0$ and $ldb \geq n$ .
<i>info</i>	See "On Return."

### On Return

<i>ap</i>	is an array, referred to as AP, in which the transformed matrix <i>A</i> of order <i>n</i> , containing the results of the factorization, is stored in upper- or lower-packed storage mode. Returned as: a one-dimensional array of (at least) length $n(n+1)/2$ , containing numbers of the data type indicated in Table 101 on page 483. See "Function."
<i>bx</i>	is the general matrix <i>X</i> , containing the <i>nrhs</i> solutions to the system. The solutions, each of length <i>n</i> , reside in the columns of <i>X</i> . Returned as: an <i>ldb</i> by (at least) <i>nrhs</i> array, containing numbers of the data type indicated in Table 101 on page 483.
<i>info</i>	has the following meaning: If $info = 0$ , the subroutine completed successfully. If $info > 0$ , the factorization was unsuccessful. <i>B</i> is overwritten; that is, the original input is not preserved. <i>info</i> is set equal to the order <i>i</i> of the first minor encountered having a nonpositive determinant. Specified as: a fullword integer; $info \geq 0$ .

## Notes

1. These subroutines accept lowercase letters for the *uplo* argument.
2. In your C program, argument *info* must be passed by reference.
3. The matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.
4. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix *A* are assumed to be zero, so you do not have to set these values. On output, they are set to zero.
5. For a description of the storage modes used for the matrices, see:
  - For positive definite real symmetric matrices, see "Positive Definite or Negative Definite Symmetric Matrix" on page 73.
  - For positive definite complex Hermitian matrices, see "Positive Definite or Negative Definite Complex Hermitian Matrix" on page 75.
6. On both input and output, matrices *A*, *B*, and *X* conform to LAPACK format.
7. The way these subroutines handle computational errors differs from LAPACK. Like LAPACK, these subroutines use the *info* argument to provide information about the computational error, but they also provide an error message.

## Function

The system  $AX = B$  is solved for *X*, where *X* and *B* are general matrices and:

- for SPPSV and DPPSV, *A* is a positive definite real symmetric matrix.
- for CPPSV and ZPPSV, *A* is a positive definite complex Hermitian matrix.

The matrix  $A$ , stored in upper- or lower-packed storage mode, is factored using the Cholesky factorization method, where  $A$  is expressed as:

$$A = LL^T \text{ or } A = U^T U \quad \text{for SPPSV and DPPSV}$$

$$A = LL^H \text{ or } A = U^H U \quad \text{for CPPSV and ZPPSV}$$

where:

$L$  is a lower triangular matrix.

$U$  is an upper triangular matrix.

If  $n$  is 0, no computation is performed and the subroutine returns after doing some parameter checking. If  $n > 0$  and  $nrhs$  is 0, no solutions are computed and the subroutine returns after factoring the matrix.

See references [8], [38], and [40].

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

Matrix  $A$  is not positive definite.

- The order  $i$  of the **first** minor encountered having a nonpositive determinant is identified in the computational error message.
- The computational error message may occur multiple times with processing continuing after each error, because the default for the number of allowable errors for error code 2148 is set to be unlimited in the ESSL error option table.

### Input-Argument Errors

1.  $uplo \neq 'U'$  or  $'L'$
2.  $n < 0$
3.  $nrhs < 0$
4.  $n > ldb$
5.  $ldb \leq 0$

## Examples

### Example 1

This example shows how to solve the system  $AX = B$ , where matrix  $A$  is a positive definite real symmetric matrix of order 9, stored in lower-packed storage mode.

On input, matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 1.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 \\ 1.0 & 2.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 4.0 & 4.0 & 4.0 & 4.0 & 4.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 5.0 & 5.0 & 5.0 & 5.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 6.0 & 6.0 & 6.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 7.0 & 7.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 & 8.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 & 9.0 \end{bmatrix}$$

On output, all elements of this matrix  $A$  are 1.0.

## SPPSV, DPPSV, CPPSV, and ZPPSV

**Note:** The AP array is formatted in a triangular arrangement for readability; however, it is stored in lower-packed storage mode.

### Call Statement and Input:

```

          UPLO N  NRHS  AP  BX  LDB  INFO
          |   |   |   |   |   |   |
CALL SPPSV ( 'L', 9, 2,  AP, BX, 9,  INFO )

```

AP = (same as input AP in “Example 5” on page 503)

BX = (same as input BX in “Example 5” on page 512)

### Output:

```

AP = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0,
      1.0, 1.0,
      1.0)

```

```

BX = [
      1.0  1.0
      1.0  2.0
      1.0  3.0
      1.0  4.0
      1.0  5.0
      1.0  6.0
      1.0  7.0
      1.0  8.0
      1.0  9.0
]

```

INFO = 0

## Example 2

This example shows how to solve the system  $AX = B$ , where matrix  $A$  is a positive definite real symmetric matrix of order 9, stored in upper-packed storage mode.

On input, matrix  $A$  is:

```

[
  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
  1.0  2.0  2.0  2.0  2.0  2.0  2.0  2.0  2.0
  1.0  2.0  3.0  3.0  3.0  3.0  3.0  3.0  3.0
  1.0  2.0  3.0  4.0  4.0  4.0  4.0  4.0  4.0
  1.0  2.0  3.0  4.0  5.0  5.0  5.0  5.0  5.0
  1.0  2.0  3.0  4.0  5.0  6.0  6.0  6.0  6.0
  1.0  2.0  3.0  4.0  5.0  6.0  7.0  7.0  7.0
  1.0  2.0  3.0  4.0  5.0  6.0  7.0  8.0  8.0
  1.0  2.0  3.0  4.0  5.0  6.0  7.0  8.0  9.0
]

```

On output, all elements of this matrix  $A$  are 1.0.

**Note:** The AP array is formatted in a triangular arrangement for readability; however, it is stored in upper-packed storage mode.

### Call Statement and Input:

```

          UPLO N  NRHS  AP  BX  LDB  INFO
          |   |   |   |   |   |   |
CALL SPPSV ( 'U', 9, 2,  AP, BX, 9,  INFO )

```



AP = (same as input AP in “Example 6” on page 504)  
 BX = (same as input BX in “Example 6” on page 513)

**Output:**

```

AP = (
                                         1.0,
                                         1.0, 1.0,
                                         1.0, 1.0, 1.0,
                                         1.0, 1.0, 1.0, 1.0,
                                         1.0, 1.0, 1.0, 1.0,
                                         1.0, 1.0, 1.0, 1.0, 1.0,
                                         1.0, 1.0, 1.0, 1.0, 1.0,
                                         1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
                                         1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
                                         1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
    
```

```

BX = [
      [ 1.0  1.0
        1.0  2.0
        1.0  3.0
        1.0  4.0
        1.0  5.0
        1.0  6.0
        1.0  7.0
        1.0  8.0
        1.0  9.0 ]
    ]
    
```

INFO = 0

**Example 3**

This example shows how to solve the system  $AX = B$ , where matrix  $A$  is a positive definite complex Hermitian matrix of order 3, stored in lower-packed storage mode.

On input, matrix  $A$  is:

```

[ (25.0, 0.0) (-5.0, -5.0) (10.0, 5.0)
  (-5.0, 5.0) (51.0, 0.0) (4.0, -6.0)
  (10.0, -5.0) (4.0, 6.0) (71.0, 0.0) ]
    
```

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

**Call Statement and Input:**

```

          UPLO  N  NRHS  AP  BX  LDB  INFO
          |    |    |    |    |    |    |
CALL ZPPSV ( 'L', 3, 2,  AP, BX, 3,  INFO )
    
```

AP = (same as input AP in “Example 7” on page 504)  
 BX = (same as input BX in “Example 7” on page 513)

**Output:**

AP = ((5.0, 0.0), (-1.0, 1.0), (2.0, -1.0), (7.0, 0.0), (1.0, 1.0), (8.0, 0.0))

```

BX = [
      [ (2.0, -1.0) ( 2.0, 0.0)
        (1.0,  1.0) (-1.0, 2.0)
        (0.0, -2.0) ( 1.0, 1.0) ]
    ]
    
```

INFO = 0

**Example 4**

This example shows how to solve the system  $AX = B$ , where matrix  $A$  is a positive definite complex Hermitian matrix of order 3, stored in upper-packed storage mode.

On input, matrix  $A$  is:

$$\begin{bmatrix} (9.0, 0.0) & (3.0, 3.0) & (3.0, -3.0) \\ (3.0, -3.0) & (18.0, 0.0) & (8.0, -6.0) \\ (3.0, 3.0) & (8.0, 6.0) & (43.0, 0.0) \end{bmatrix}$$

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

**Call Statement and Input:**

```

                UPLO  N  NRHS  AP  BX  LDB  INFO
                |    |    |    |    |    |    |
CALL ZPPSV ( 'U', 3, 2,  AP, BX, 3,  INFO )
    
```

AP = (same as input AP in "Example 8" on page 505)

BX = (same as input BX in "Example 8" on page 514)

**Output:**

AP = ((3.0, 0.0), (1.0, 1.0), (4.0, 0.0), (1.0, -1.0), (2.0, -1.0), (6.0, 0.0))

$$BX = \begin{bmatrix} (2.0, -1.0) & (2.0, 0.0) \\ (1.0, -1.0) & (0.0, 1.0) \\ (3.0, 0.0) & (1.0, -1.0) \end{bmatrix}$$

INFO = 0

## SPOSV, DPOSV, CPOSV, and ZPOSV — Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization and Multiple Right-Hand Side Solve

### Purpose

These subroutines solve the system of linear equations  $AX = B$  for  $X$ , where  $X$  and  $B$  are general matrices and:

- for SPOSV and DPOSV,  $A$  is a positive definite real symmetric matrix.
- for CPOSV and ZPOSV,  $A$  is a positive definite complex Hermitian matrix.

The matrix  $A$ , stored in upper- or lower-storage mode, is factored using Cholesky factorization.

Table 102. Data Types

$A, B$	Subroutine
Short-precision real	SPOSV <sup>△</sup>
Long-precision real	DPOSV <sup>△</sup>
Short-precision complex	CPOSV <sup>△</sup>
Long-precision complex	ZPOSV <sup>△</sup>
<sup>△</sup> LAPACK	

### Syntax

<b>Fortran</b>	CALL SPOSV   DPOSV   CPOSV   ZPOSV ( <i>uplo, n, nrhs, a, lda, bx, ldb, info</i> )
<b>C and C++</b>	sposv   dposv   cposv   zposv ( <i>uplo, n, nrhs, a, lda, bx, ldb, info</i> );

### On Entry

- uplo* indicates whether matrix  $A$  is stored in upper or lower storage mode, where:
- If *uplo* = 'U',  $A$  is stored in upper storage mode.
- If *uplo* = 'L',  $A$  is stored in lower storage mode.
- Specified as: a single character. It must be 'U' or 'L'.
- n* is the order  $n$  of matrix  $A$  and the number of rows of matrix  $B$ .
- Specified as: a fullword integer;  $n \geq 0$ .
- nrhs* is the number of right-hand sides; that is, the number of columns of matrix  $B$ .
- Specified as: a fullword integer;  $nrhs \geq 0$ .
- a* is the positive definite matrix  $A$  to be factored.
- Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 102. See "Notes" on page 490.
- lda* is the leading dimension of the array specified for  $A$ .
- Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .

## SPOSV, DPOSV, CPOSV, ZPOSV

<i>bx</i>	is the general matrix $B$ , containing the <i>nrhs</i> right-hand sides of the system. The right-hand sides, each of length $n$ , reside in the columns of $B$ .  Specified as: an <i>ldb</i> by (at least) <i>nrhs</i> array, containing numbers of the data type indicated in Table 102 on page 489.
<i>ldb</i>	is the leading dimension of the array specified for $B$ .  Specified as: a fullword integer; $ldb > 0$ and $ldb \geq n$ .
<i>info</i>	See "On Return."

### On Return

<i>a</i>	is the transformed matrix $A$ of order $n$ , containing the results of the factorization.  Returned as: an <i>lda</i> by (at least) $n$ array, containing numbers of the data type indicated in Table 102 on page 489. See "Function."
<i>bx</i>	is the general matrix $X$ , containing the <i>nrhs</i> solutions to the system. The solutions, each of length $n$ , reside in the columns of $X$ .  Returned as: an <i>ldb</i> by (at least) <i>nrhs</i> array, containing numbers of the data type indicated in Table 102 on page 489.
<i>info</i>	has the following meaning:  If $info = 0$ , the subroutine completed successfully.  If $info > 0$ , the factorization was unsuccessful and the solution was not computed. <i>info</i> is set equal to the order $i$ of the first minor encountered having a nonpositive determinant.  Returned as: a fullword integer; $info \geq 0$ .

## Notes

1. In your C program, argument *info* must be passed by reference.
2. All subroutines accept lowercase letters for the *uplo* argument.
3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, they are set to zero.
4. The way these subroutines handle computational errors differs from LAPACK. Like LAPACK, these subroutines use the *info* argument to provide information about the computational error, but they also provide an error message.
5. On both input and output, matrices  $A$ ,  $B$ , and  $X$  conform to LAPACK format.
6. For a description of the storage modes used for the matrices, see:
  - For positive definite real symmetric matrices, see "Positive Definite or Negative Definite Symmetric Matrix" on page 73.
  - For positive definite complex Hermitian matrices, see "Positive Definite or Negative Definite Complex Hermitian Matrix" on page 75.
7. The matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.

## Function

These subroutines solve the system of linear equations  $AX = B$  for  $X$ , where  $X$  and  $B$  are general matrices and:

- for SPOSV and DPOSV,  $A$  is a positive definite real symmetric matrix.

- for CPOSV and ZPOSV,  $A$  is a positive definite complex Hermitian matrix.

The matrix  $A$  is factored using Cholesky factorization, where  $A$  is expressed as:

$$A=LL^T \text{ or } A=U^T U$$

for SPOSV and DPOSV

$$A=LL^H \text{ or } A=U^H U$$

for CPOSV and ZPOSV

where:

$L$  is a unit lower triangular matrix.

$U$  is an upper triangular matrix.

If  $n$  is 0, no computation is performed and the subroutine returns after doing some parameter checking. If  $n > 0$  and  $nrhs$  is 0, no solutions are computed and the subroutine returns after factoring the matrix.

See references [8], [38], and [73].

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

Matrix  $A$  is not positive definite.

The order  $i$  of the **first** minor encountered having a nonpositive determinant is identified in the computational error message.

The computational error message may occur multiple times with processing continuing after each error, because the default for the number of allowable errors for error code 2148 is set to be unlimited in the ESSL error option table.

### Input-Argument Errors

1.  $uplo \neq 'U'$  or  $'L'$
2.  $n < 0$
3.  $nrhs < 0$
4.  $n > lda$
5.  $lda \leq 0$
6.  $n > ldb$
7.  $ldb \leq 0$

## Examples

### Example 1

This example shows how to solve the system  $AX = B$ , where:

Matrix  $A$  is the same used as input in “Example 1” on page 500 for SPOTRF. Matrix  $B$  is the same used as input in “Example 1” on page 510 for SPOTRS.

**Call Statement and Input:**

```

          UPLO  N  NRHS  A  LDA  BX  LDB  INFO
          |    |    |    |    |    |    |    |
CALL SPOSV( 'L', 9 , 2 , A , 9 , BX , 9 , INFO)
    
```

## SPOSV, DPOSV, CPOSV, ZPOSV

A = (same as input A in "Example 1" on page 500)  
 BX = (same as input BX in "Example 1" on page 510)

### Output:

$$A = \begin{bmatrix} 1.0 & . & . & . & . & . & . & . & . \\ 1.0 & 1.0 & . & . & . & . & . & . & . \\ 1.0 & 1.0 & 1.0 & . & . & . & . & . & . \\ 1.0 & 1.0 & 1.0 & 1.0 & . & . & . & . & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . & . & . & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . & . & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \end{bmatrix}$$

$$BX = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \\ 1.0 & 5.0 \\ 1.0 & 6.0 \\ 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

INFO = 0

### Example 2

This example shows how to solve the system  $AX = B$ , where:

Matrix  $A$  is the same used as input in "Example 2" on page 501 for SPOTRF.  
 Matrix  $B$  is the same used as input in "Example 2" on page 510 for SPOTRS.

### Call Statement and Input:

```

          UPLO N  NRHS A  LDA BX  LDB INFO
          |   |   |   |   |   |   |   |
CALL SPOSV( 'U' , 9 , 2 , A , 9 , BX , 9 , INFO)

```

A = (same as input A in "Example 2" on page 501)  
 BX = (same as input BX in "Example 2" on page 510)

### Output:

$$A = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & . & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & . & . & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & . & . & . & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & . & . & . & . & 1.0 & 1.0 & 1.0 & 1.0 \\ . & . & . & . & . & . & 1.0 & 1.0 & 1.0 \\ . & . & . & . & . & . & . & 1.0 & 1.0 \\ . & . & . & . & . & . & . & . & 1.0 \end{bmatrix}$$

$$BX = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \\ 1.0 & 5.0 \\ 1.0 & 6.0 \end{bmatrix}$$

$$\begin{bmatrix} 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

INFO = 0

### Example 3

This example shows how to solve the system  $AX = B$ , where:

Matrix  $A$  is the same used as input in “Example 3” on page 502 for CPOTRF.  
 Matrix  $BX$  is the same used as input in “Example 3” on page 511 for CPOTRS.

#### Call Statement and Input:

```

          UPLO  N  NRHS  A  LDA  BX  LDB  INFO
          |    |    |    |    |    |    |
CALL CPOSV( 'L', 3, 2, A, 3, BX, 3, INFO)
    
```

$$A = \begin{bmatrix} ( 25.0, 0.0) & ( -5.0, -5.0) & (10.0, 5.0) \\ ( -5.0, 5.0) & ( 51.0, 0.0) & ( 4.0, -6.0) \\ ( 10.0, -5.0) & ( 4.0, 6.0) & (71.0, 0.0) \end{bmatrix}$$

$$BX = \begin{bmatrix} ( 60.0, -55.0) & ( 70.0, 10.0) \\ ( 34.0, 58.0) & (-51.0, 110.0) \\ ( 13.0, -152.0) & ( 75.0, 63.0) \end{bmatrix}$$

#### Output:

$$A = \begin{bmatrix} ( 5.0, 0.0) & (-5.0, -5.0) & (10.0, 5.0) \\ (-1.0, 1.0) & ( 7.0, 0.0) & ( 4.0, -6.0) \\ ( 2.0, -1.0) & ( 1.0, 1.0) & ( 8.0, 0.0) \end{bmatrix}$$

$$BX = \begin{bmatrix} ( 2.0, -1.0) & ( 2.0, 0.0) \\ ( 1.0, 1.0) & (-1.0, 2.0) \\ ( 0.0, -2.0) & ( 1.0, 1.0) \end{bmatrix}$$

INFO = 0

### Example 4

This example shows how to solve the system  $AX = B$ , where:

Matrix  $A$  is the same used as input in “Example 4” on page 502 for CPOTRF.  
 Matrix  $BX$  is the same used as input in “Example 4” on page 511 for CPOTRS.

#### Call Statement and Input:

```

          UPLO  N  NRHS  A  LDA  BX  LDB  INFO
          |    |    |    |    |    |    |
CALL CPOSV( 'U', 3, 2, A, 3, BX, 3, INFO)
    
```

$$A = \begin{bmatrix} (9.0, 0.0) & ( 3.0, 3.0) & ( 3.0, -3.0) \\ (3.0, -3.0) & (18.0, 0.0) & ( 8.0, -6.0) \\ (3.0, 3.0) & ( 8.0, 6.0) & (43.0, 0.0) \end{bmatrix}$$

$$BX = \begin{bmatrix} ( 33.0, -18.0) & (15.0, -3.0) \\ ( 45.0, -45.0) & ( 8.0, -2.0) \\ (152.0, 1.0) & (43.0, -29.0) \end{bmatrix}$$

## SPOSV, DPOSV, CPOSV, ZPOSV

### Output:

**Note:** The strict lower part of  $A$  is not referenced.

$$A = \begin{bmatrix} (3.0, 0.0) & (1.0, 1.0) & (1.0, -1.0) \\ (3.0, -3.0) & (4.0, 0.0) & (2.0, -1.0) \\ (3.0, 3.0) & (8.0, 6.0) & (6.0, 0.0) \end{bmatrix}$$

$$BX = \begin{bmatrix} (2.0, -1.0) & (2.0, 0.0) \\ (1.0, -1.0) & (0.0, 1.0) \\ (3.0, 0.0) & (1.0, -1.0) \end{bmatrix}$$

INFO = 0



---

## SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, ZPOF, SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPPF, and DPPF — Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization

### Purpose

These subroutines factor matrix  $A$  as explained below:

#### SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, and ZPOF

The SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, and ZPOF subroutines factor matrix  $A$  stored in upper or lower storage mode, where:

- For SPOTRF, DPOTRF, SPOF, and DPOF,  $A$  is a positive definite real symmetric matrix.
- For CPOTRF, ZPOTRF, CPOF, and ZPOF,  $A$  is a positive definite complex Hermitian matrix.

Matrix  $A$  is factored using Cholesky factorization.

To solve the system of equations with one or more right-hand sides, follow the call to SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, or ZPOF with a call to SPOTRS, DPOTRS, CPOTRS, ZPOTRS, SPOSM, DPOSM, CPOSM, or ZPOSM, respectively.

To find the inverse of matrix  $A$ , follow the call to SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, or DPOF with a call to SPOTRI, DPOTRI, CPOTRI, ZPOTRI, SPOICD, or DPOICD, respectively.

#### SPPTRF, DPPTRF, CPPTRF, and ZPPTRF

The SPPTRF, DPPTRF, CPPTRF, and ZPPTRF subroutines factor matrix  $A$ , stored in upper- or lower-packed storage mode, where:

- For SPPTRF and DPPTRF,  $A$  is a positive definite real symmetric matrix.
- For CPPTRF and ZPPTRF,  $A$  is a positive definite complex Hermitian matrix.

Matrix  $A$  is factored using Cholesky factorization.

To solve the system of equations with one or more right-hand sides, follow the call to SPPTRF, DPPTRF, CPPTRF, or ZPPTRF with a call to SPPTRS, DPPTRS, CPPTRS, or ZPPTRS, respectively.

To find the inverse of matrix  $A$ , follow the call to SPPTRF or DPPTRF with a call to SPPTRI or DPPTRI, respectively.

#### SPPF and DPPF

The SPPF and DPPF subroutines factor positive definite real symmetric matrix  $A$ , stored in lower-packed storage mode, using Gaussian elimination ( $LDL^T$ ) or Cholesky factorization. To solve a system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SPPS or DPPS, respectively. To find the inverse of matrix  $A$ , follow the call to these subroutines, performing Cholesky factorization, with a call to SPPICD or DPPICD, respectively.

**SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, ZPOF, SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPPF, and DPPF**

Table 103. Data Types

A	Subroutine
Short-precision real	SPOTRF <sup>△</sup> , SPOF, SPOTRF <sup>△</sup> , and SPPF
Long-precision real	DPOTRF <sup>△</sup> , DPOF, DPOTRF <sup>△</sup> , and DPPF
Short-precision complex	CPOTRF <sup>△</sup> , CPOF, and CPOTRF <sup>△</sup>
Long-precision complex	ZPOTRF <sup>△</sup> , ZPOF, and ZPOTRF <sup>△</sup>
<sup>△</sup> LAPACK	

**Note:** The output from each of these subroutines should be used only as input for specific other subroutines, as shown in the table below.

Output from this subroutine:	Should be used only as input to the following subroutine(s) for performing a solve or inverse:
SPOTRF	SPOTRS, SPOTRI
DPOTRF	DPOTRS, DPOTRI
CPOTRF	CPOTRS, CPOTRI
ZPOTRF	ZPOTRS, ZPOTRI
SPOF	SPOSM, SPOICD
DPOF	DPOSM, DPOICD
CPOF	CPOSM
ZPOF	ZPOSM
SPOTRF	SPOTRS, SPOTRI
DPOTRF	DPOTRS, DPOTRI
CPOTRF	CPOTRS
ZPOTRF	ZPOTRS
SPPF	SPPS, SPPICD
DPPF	DPPS, DPPICD

## Syntax

<b>Fortran</b>	CALL SPOTRF   DPOTRF   CPOTRF   ZPOTRF ( <i>uplo, n, a, lda, info</i> ) CALL SPOF   DPOF   CPOF   ZPOF ( <i>uplo, a, lda, n</i> ) CALL SPOTRF   DPOTRF   CPOTRF   ZPOTRF ( <i>uplo, n, ap, info</i> ) CALL SPPF   DPPF ( <i>ap, n, iopt</i> )
<b>C and C++</b>	spotrf   dpotrf   cpotrf   zpotrf ( <i>uplo, n, a, lda, info</i> ); spof   dpof   cpof   zpod ( <i>uplo, a, lda, n</i> ); spptrf   dpptrf   cpptrf   zpptrf ( <i>uplo, n, ap, info</i> ); sppf   dppf ( <i>ap, n, iopt</i> );

## On Entry

- uplo* indicates whether matrix  $A$  is stored in upper or lower storage mode, where:  
 If  $uplo = 'U'$ ,  $A$  is stored in upper storage mode.  
 If  $uplo = 'L'$ ,  $A$  is stored in lower storage mode.  
 Specified as: a single character. It must be 'U' or 'L'.
- ap* is an array, referred to as AP, in which matrix  $A$ , to be factored, is stored as follows:  
**SPPTRE, DPPTRE, CPPTRE, and ZPPTRE**  
 Upper-packed or lower-packed storage mode  
**SPPF and DPPF**  
 Lower-packed storage mode  
 Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 103 on page 496. See “Notes” on page 498.  
**For SPPTRE, DPPTRE, CPPTRE, and ZPPTRE:**  
 The array must have at least  $n(n+1)/2$  elements.  
**For SPPF and DPPF:**  
 If  $iopt = 0$  or 10, the array must have at least  $n(n+1)/2+n$  elements.  
 If  $iopt = 1$  or 11, the array must have at least  $n(n+1)/2$  elements.
- a* is the positive definite matrix  $A$ , to be factored.  
 Specified as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 103 on page 496.
- lda* is the leading dimension of the array specified for  $a$ .  
 Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .
- n* is the order  $n$  of matrix  $A$ .  
 Specified as: a fullword integer;  $n \geq 0$ .
- iopt* determines the type of computation to be performed, where:  
 If  $iopt = 0$ , the matrix is factored using the  $LDL^T$  method, and the output is stored in an internal format.  
 If  $iopt = 1$ , the matrix is factored using Cholesky factorization, and the output is stored in an internal format.  
 If  $iopt = 10$ , the matrix is factored using the  $LDL^T$  method, and the output is stored in lower-packed storage mode.  
 If  $iopt = 11$ , the matrix is factored using Cholesky factorization, and the output is stored in lower-packed storage mode.  
 Specified as: a fullword integer;  $iopt = 0, 1, 10, \text{ or } 11$ .
- info* See “On Return.”

## On Return

- ap* is an array, referred to as AP, in which the transformed matrix  $A$  of order  $n$ , containing the results of the factorization, is stored.

## SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, ZPOF, SPPTRF, DPPTRF, CPPTRF, ZPPTRF, SPPF, and DPPF

### For SPPTRF, DPPTRF, CPPTRF, and ZPPTRF:

The transformed matrix is stored in upper-packed or lower-packed storage mode.

### For SPPF and DPPF:

If  $iopt$  is 0 or 1, the transformed matrix is stored in an internal format and should only be used as input to the corresponding solve or inverse subroutine.

If  $iopt$  is 10 or 11, the transformed matrix is stored in lower-packed storage mode.

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 103 on page 496.

### For SPPTRF, DPPTRF, CPPTRF, and ZPPTRF:

The array contains at least  $n(n+1)/2$  elements.

### For SPPF and DPPF:

If  $iopt = 0$  or 10, the array contains  $n(n+1)/2+n$  elements.

If  $iopt = 1$  or 11, the array contains  $n(n+1)/2$  elements.

See "Notes" and see "Function" on page 499.

*a* is the transformed matrix  $A$  of order  $n$ , containing the results of the factorization. See "Function" on page 499.

Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 103 on page 496.

*info* has the following meaning:

If  $info = 0$ , the factorization completed successfully.

If  $info > 0$ ,  $info$  is set equal to the order  $i$  of the first minor encountered having a nonpositive determinant.

Specified as: a fullword integer;  $info \geq 0$ .

## Notes

1. In your C program, argument *info* must be passed by reference.
2. All subroutines accept lowercase letters for the *uplo* argument.
3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, they are set to zero.
4. In the input and output arrays specified for *ap*, the first  $n(n+1)/2$  elements are matrix elements. The additional  $n$  locations, required in the array when  $iopt = 0$  or 10, are used for working storage by this subroutine and should not be altered between calls to the factorization and solve subroutines.
5. If  $iopt = 0$  or 1, SPPF and DPPF in some cases utilize algorithms based on recursive packed storage format. As a result, on output, if  $iopt = 0$  or 1, the array specified for AP may be stored in this new format rather than the conventional lower packed format. (See references [54], [68], and [70]).  
The array specified for AP should not be altered between calls to the factorization and solve subroutines; otherwise unpredictable results may occur.
6. The way *\_POTRF* and *\_PPTRF* subroutines handle computational errors differs from LAPACK. Like LAPACK, these subroutines use the *info* argument to provide information about the computational error, but they also provide an error message.

7. On both input and output, matrix  $A$  conforms to LAPACK format.
8. For a description of the storage modes used for the matrices, see:
  - For positive definite symmetric matrices, see “Positive Definite or Negative Definite Symmetric Matrix” on page 73.
  - For positive definite complex Hermitian matrices, see “Positive Definite or Negative Definite Complex Hermitian Matrix” on page 75.

## Function

The functions for these subroutines are described in the sections below.

### For SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, and ZPOF

The positive definite matrix  $A$ , stored in upper or lower storage mode, is factored using Cholesky factorization, where  $A$  is expressed as:

$$A = LL^T \text{ or } A = U^T U \quad \text{for SPOTRF, DPOTRF, SPOF, and DPOF}$$

$$A = LL^H \text{ or } A = U^H U \quad \text{for CPOTRF, ZPOTRF, CPOF, and ZPOF}$$

where:

$L$  is a lower triangular matrix.

$U$  is an upper triangular matrix.

If  $n$  is 0, no computation is performed. See references [8] and [38].

### For SPOTRF, DPOTRF, CPOTRF, and ZPOTRF

The positive definite matrix  $A$ , stored in upper-packed or lower-packed storage mode, is factored using Cholesky factorization, where  $A$  is expressed as:

$$A = LL^T \text{ or } A = U^T U \quad \text{for SPOTRF and DPOTRF}$$

$$A = LL^H \text{ or } A = U^H U \quad \text{for CPOTRF and ZPOTRF}$$

where:

$L$  is a lower triangular matrix.

$U$  is an upper triangular matrix.

If  $n$  is 0, no computation is performed. See references [8], [38], and [69].

### For SPPF and DPPF

If  $iopt = 0$  or 10, the positive definite symmetric matrix  $A$ , stored in lower-packed storage mode, is factored using Gaussian elimination, where  $A$  is expressed as:

$$A = LDL^T$$

where:

$L$  is a unit lower triangular matrix.

$D$  is a diagonal matrix.

If  $iopt = 1$  or 11, the positive definite symmetric matrix  $A$ , stored in lower-packed storage mode, is factored using Cholesky factorization, where  $A$  is expressed as:

$$A = LL^T$$

where  $L$  is a lower triangular matrix.

If  $n$  is 0, no computation is performed. See references [8] and [38].

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

1. Matrix  $A$  is not positive definite (for SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPPTRF, DPPTRF, CPPTRF, and ZPPTRF).
  - The order  $i$  of the **first** minor encountered having a nonpositive determinant is identified in the computational error message.
  - The computational error message may occur multiple times with processing continuing after each error, because the default for the number of allowable errors for error code 2148 is set to be unlimited in the ESSL error option table.
2. Matrix  $A$  is not positive definite (for SPPF and DPPF when  $iopt = 0$  or 10).
  - Processing continues to the end of the matrix.
  - One or more elements of  $D$  contain values less than or equal to 0; all elements of  $D$  are checked. The index  $i$  of the **last** nonpositive element encountered is identified in the computational error message.
  - The return code is set to 1.
  - $i$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2104 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.
3. Matrix  $A$  is not positive definite (for SPPF and DPPF when  $iopt = 1$  or 11 and for SPOF, DPOF, CPOF, and ZPOF).
  - Processing stops at the first occurrence of a nonpositive definite diagonal element.
  - The order  $i$  of the **first** minor encountered having a nonpositive determinant is identified in the computational error message.
  - The return code is set to 1.
  - $i$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2115 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $uplo \neq 'U'$  or  $'L'$
2.  $n < 0$
3.  $n > lda$
4.  $lda \leq 0$
5.  $iopt \neq 0, 1, 10, \text{ or } 11$

## Examples

### Example 1

This example shows a factorization of the same positive definite symmetric matrix  $A$  of order 9 used in “Example 9” on page 505, but stored in lower storage mode.

**Call Statement and Input:**

```

          UPLO N   A   LDA   INFO
          |   |   |   |   |
CALL SPOTRF( 'L' , 9 , A , 9 , INFO )
    
```

or

```

          UPLO A   LDA   N
          |   |   |   |
CALL SPOF( 'L' , A , 9 , 9 )
    
```

$$A = \begin{bmatrix} 1.0 & . & . & . & . & . & . & . & . \\ 1.0 & 2.0 & . & . & . & . & . & . & . \\ 1.0 & 2.0 & 3.0 & . & . & . & . & . & . \\ 1.0 & 2.0 & 3.0 & 4.0 & . & . & . & . & . \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & . & . & . & . \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & . & . & . \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & . & . \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 & . \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 & 9.0 \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} 1.0 & . & . & . & . & . & . & . & . \\ 1.0 & 1.0 & . & . & . & . & . & . & . \\ 1.0 & 1.0 & 1.0 & . & . & . & . & . & . \\ 1.0 & 1.0 & 1.0 & 1.0 & . & . & . & . & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . & . & . & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . & . & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \end{bmatrix}$$

INFO = 0

**Example 2**

This example shows a factorization of the same positive definite symmetric matrix A of order 9 used in "Example 9" on page 505, but stored in upper storage mode.

**Call Statement and Input:**

```

          UPLO N   A   LDA   INFO
          |   |   |   |   |
CALL SPOTRF( 'U' , 9 , A , 9 , INFO )
    
```

or

```

          UPLO A   LDA   N
          |   |   |   |
CALL SPOF( 'U' , A , 9 , 9 )
    
```

$$A = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 \\ . & . & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 \\ . & . & . & 4.0 & 4.0 & 4.0 & 4.0 & 4.0 & 4.0 \\ . & . & . & . & 5.0 & 5.0 & 5.0 & 5.0 & 5.0 \\ . & . & . & . & . & 6.0 & 6.0 & 6.0 & 6.0 \\ . & . & . & . & . & . & 7.0 & 7.0 & 7.0 \\ . & . & . & . & . & . & . & 8.0 & 8.0 \\ . & . & . & . & . & . & . & . & 9.0 \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & . & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & . & . & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & . & . & . & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & . & . & . & . & 1.0 & 1.0 & 1.0 & 1.0 \\ . & . & . & . & . & . & 1.0 & 1.0 & 1.0 \\ . & . & . & . & . & . & . & 1.0 & 1.0 \\ . & . & . & . & . & . & . & . & 1.0 \end{bmatrix}$$

INFO = 0

### Example 3

This example shows a factorization of positive definite complex Hermitian matrix  $A$  of order 3, stored in lower storage mode, where on input matrix  $A$  is:

$$\begin{bmatrix} (25.0, 0.0) & (-5.0, -5.0) & (10.0, 5.0) \\ (-5.0, 5.0) & (51.0, 0.0) & (4.0, -6.0) \\ (10.0, -5.0) & (4.0, 6.0) & (71.0, 0.0) \end{bmatrix}$$

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

#### Call Statement and Input:

```

          UPLO N  A  LDA  INFO
          |   |   |   |   |
CALL CPOTRF( 'L' , 3 , A , 3 , INFO )
    
```

or

```

          UPLO A  LDA  N
          |   |   |   |
CALL CPOF( 'L' , A , 3 , 3 )
    
```

$$A = \begin{bmatrix} (25.0, .) & . & . \\ (-5.0, 5.0) & (51.0, .) & . \\ (10.0, -5.0) & (4.0, 6.0) & (71.0, .) \end{bmatrix}$$

#### Output:

$$A = \begin{bmatrix} (5.0, 0.0) & . & . \\ (-1.0, 1.0) & (7.0, 0.0) & . \\ (2.0, -1.0) & (1.0, 1.0) & (8.0, 0.0) \end{bmatrix}$$

INFO = 0

### Example 4

This example shows a factorization of positive definite complex Hermitian matrix  $A$  of order 3, stored in upper storage mode, where on input matrix  $A$  is:

$$\begin{bmatrix} (9.0, 0.0) & (3.0, 3.0) & (3.0, -3.0) \\ (3.0, -3.0) & (18.0, 0.0) & (8.0, -6.0) \\ (3.0, 3.0) & (8.0, 6.0) & (43.0, 0.0) \end{bmatrix}$$





**SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, ZPOF, SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPPF, and DPPF**

```
1.0, 1.0,
1.0)
```

```
INFO = 0
```

**Example 6**

This example shows a factorization (using the Cholesky factorization method) of the same positive definite symmetric matrix *A* of order 9 used in “Example 9” on page 505, but stored in upper-packed storage mode.

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in upper-packed storage mode.

**Call Statement and Input:**

```

          UPLO N  AP  INFO
          |   |  |   |
CALL SPOTRF( 'U', 9, AP, INFO )
AP = (
          1.0,
          1.0, 2.0,
          1.0, 2.0, 3.0,
          1.0, 2.0, 3.0, 4.0,
          1.0, 2.0, 3.0, 4.0, 5.0,
          1.0, 2.0, 3.0, 4.0, 5.0, 6.0,
          1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0,
          1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0,
          1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0)

```

**Output:**

```

AP = (
          1.0,
          1.0, 1.0,
          1.0, 1.0, 1.0,
          1.0, 1.0, 1.0, 1.0,
          1.0, 1.0, 1.0, 1.0, 1.0,
          1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
          1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
          1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
          1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
INFO = 0

```

**Example 7**

This example shows a factorization (using the Cholesky factorization method) of the same positive definite complex Hermitian matrix *A* of order 3 used in “Example 3” on page 502, but stored in lower-packed storage mode.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix *A* are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

**Call Statement and Input:**

```

          UPLO N  AP  INFO
          |   |  |   |
CALL ZPOTRF( 'L', 3, AP, INFO )
AP = ((25.0, .), (-5.0, 5.0), (10.0, -5.0), (51.0, .), (4.0, 6.0), (71.0, .))

```

**Output:**

```

AP = ((5.0, 0.0), (-1.0, 1.0), (2.0, -1.0), (7.0, 0.0), (1.0, 1.0), (8.0, 0.0))
INFO = 0

```

### Example 8

This example shows a factorization (using the Cholesky factorization method) of the same positive definite complex Hermitian matrix  $A$  of order 3 used in "Example 4" on page 502, but stored in upper-packed storage mode.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

#### Call Statement and Input:

```

          UPLO  N  AP  INFO
          |    |  |   |
CALL ZPPTRF( 'U' , 3 , AP , INFO )
AP = ((9.0, .), (3.0, 3.0), (18.0, .), (3.0, -3.0), (8.0, -6.0), (43.0, .))

```

#### Output:

```

AP = ((3.0, 0.0), (1.0, 1.0), (4.0, 0.0), (1.0, -1.0), (2.0, -1.0), (6.0, 0.0))
INFO = 0

```

### Example 9

This example shows a factorization (using the Gaussian elimination method) of positive definite symmetric matrix  $A$  of order 9, stored in lower-packed storage mode, where on input matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 1.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 \\ 1.0 & 2.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 4.0 & 4.0 & 4.0 & 4.0 & 4.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 5.0 & 5.0 & 5.0 & 5.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 6.0 & 6.0 & 6.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 7.0 & 7.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 & 8.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 & 9.0 \end{bmatrix}$$

On output, all elements of this matrix  $A$  are 1.0.

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in lower-packed storage mode.

#### Call Statement and Input:

```

          AP  N  IOPT
          |  |  |
CALL SPPF( AP, 9, 0 )
AP = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0,
      3.0, 3.0, 3.0, 3.0, 3.0, 3.0, 3.0, 3.0,
      4.0, 4.0, 4.0, 4.0, 4.0, 4.0,
      5.0, 5.0, 5.0, 5.0, 5.0,
      6.0, 6.0, 6.0, 6.0,
      7.0, 7.0, 7.0,
      8.0, 8.0,
      9.0,
      . , . , . , . , . , . , . , . , . )

```

#### Output:

```

AP = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,

```

**SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, ZPOF, SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPPF, and DPPF**

```

1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
1.0, 1.0, 1.0, 1.0, 1.0,
1.0, 1.0, 1.0, 1.0,
1.0, 1.0, 1.0,
1.0, 1.0,
1.0,
1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)

```

**Example 10**

This example shows a factorization (using the Cholesky factorization method) of the same positive definite symmetric matrix *A* of order 9 used in “Example 9” on page 505, stored in lower-packed storage mode.

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in lower-packed storage mode.

**Call Statement and Input:**

```

          AP  N  IOPT
          |  |  |
CALL SPPF( AP, 9, 1 )
AP = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0,
      3.0, 3.0, 3.0, 3.0, 3.0, 3.0, 3.0, 3.0,
      4.0, 4.0, 4.0, 4.0, 4.0, 4.0,
      5.0, 5.0, 5.0, 5.0, 5.0,
      6.0, 6.0, 6.0, 6.0,
      7.0, 7.0, 7.0,
      8.0, 8.0,
      9.0)

```

**Output:**

```

AP = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0, 1.0,
      1.0, 1.0, 1.0,
      1.0, 1.0,
      1.0)

```

## SPOTRS, DPOTRS, CPOTRS, ZPOTRS, SPOSM, DPOSM, CPOSM, ZPOSM, SPSTRS, DPSTRS, CPSTRS, and ZPSTRS —Positive Definite Real Symmetric or Complex Hermitian Matrix Multiple Right-Hand Side Solve

### Purpose

These subroutines solve the system  $AX = B$  for  $X$ , where  $X$  and  $B$  are general matrices and:

- For SPOTRS, DPOTRS, SPOSM, DPOSM, SPSTRS, and DPSTRS,  $A$  is a positive definite real symmetric matrix.
- For CPOTRS, ZPOTRS, CPOSM, ZPOSM, CPSTRS, and ZPSTRS,  $A$  is a positive definite complex Hermitian matrix.

SPOTRS, DPOTRS, CPOTRS, and ZPOTRS use the results of the factorization of matrix  $A$ , produced by a preceding call to SPOTRF, DPOTRF, CPOTRF, or ZPOTRF, respectively.

SPOSM, DPOSM, CPOSM, and ZPOSM use the results of the factorization of matrix  $A$ , produced by a preceding call to SPOF/SPOFCD, DPOF/DPOFCD, CPOF, or ZPOF, respectively.

SPSTRS, DPSTRS, CPSTRS, and ZPSTRS use the results of the factorization of matrix  $A$ , produced by a preceding call to SPSTRF, DPSTRF, CPSTRF, or ZPSTRF, respectively.

Table 104. Data Types

$A, B, X$	Subroutine
Short-precision real	SPOTRS <sup>△</sup> , SPOSM, and SPSTRS <sup>△</sup>
Long-precision real	DPOTRS <sup>△</sup> , DPOSM, and DPSTRS <sup>△</sup>
Short-precision complex	CPOTRS <sup>△</sup> , CPOSM, and CPSTRS <sup>△</sup>
Long-precision complex	ZPOTRS <sup>△</sup> , ZPOSM, and ZPSTRS <sup>△</sup>
<sup>△</sup> LAPACK	

**Note:** The input to these solve subroutines must be the output from the corresponding factorization subroutines.

### Syntax

<b>Fortran</b>	CALL SPOTRS   DPOTRS   CPOTRS   ZPOTRS ( <i>uplo, n, nrhs, a, lda, bx, ldb, info</i> ) CALL SPOSM   DPOSM   CPOSM   ZPOSM ( <i>uplo, a, lda, n, bx, ldb, nrhs</i> ) CALL SPSTRS   DPSTRS   CPSTRS   ZPSTRS ( <i>uplo, n, nrhs, ap, bx, ldb, info</i> )
<b>C and C++</b>	spotrs   dpotrs   cpotrs   zpotrs ( <i>uplo, n, nrhs, a, lda, bx, ldb, info</i> ); sposm   dposm   cposm   zposm ( <i>uplo, a, lda, n, bx, ldb, nrhs</i> ); spstrs   dpstrs   cpstrs   zpstrs ( <i>uplo, n, nrhs, ap, bx, ldb, info</i> );

### On Entry

<i>uplo</i>	<p>indicates whether the original matrix <i>A</i> is stored in upper or lower storage mode, where:</p> <p>If <i>uplo</i> = 'U', <i>A</i> is stored in upper storage mode.</p> <p>If <i>uplo</i> = 'L', <i>A</i> is stored in lower storage mode.</p> <p>Specified as: a single character. It must be 'U' or 'L'.</p>
<i>a</i>	<p>is the factorization of positive definite matrix <i>A</i>, produced by a preceding call to SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF/SPOFCD, DPOF/DPOFCD, CPOF, or ZPOF.</p> <p>Specified as: an <i>lda</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 104 on page 507.</p>
<i>ap</i>	<p>is an array, referred to as AP, in which the factorization of positive definite matrix <i>A</i>, produced by a preceding call to SPPTRF, DPPTRF, CPPTRF, or ZPPTRF, is stored in upper-packed or lower-packed storage mode.</p> <p>Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 104 on page 507.</p>
<i>lda</i>	<p>is the leading dimension of the array specified for <i>a</i>.</p> <p>Specified as: a fullword integer; <math>lda &gt; 0</math> and <math>lda \geq n</math>.</p>
<i>n</i>	<p>is the order of matrix <i>A</i> and the number of rows of matrix <i>B</i>.</p> <p>Specified as: a fullword integer; <math>n \geq 0</math>.</p>
<i>bx</i>	<p>is the general matrix <i>B</i>, containing the <i>nrhs</i> right-hand sides of the system. The right-hand sides, each of length <i>n</i>, reside in the columns of <i>B</i>.</p> <p>Specified as: an <i>ldb</i> by (at least) <i>nrhs</i> array, containing numbers of the data type indicated in Table 104 on page 507.</p>
<i>ldb</i>	<p>is the leading dimension of the array specified for <i>b</i>.</p> <p>Specified as: a fullword integer; <math>ldb &gt; 0</math> and <math>ldb \geq n</math>.</p>
<i>nrhs</i>	<p>is the number of right-hand sides; that is, the number of columns of matrix <i>B</i>.</p> <p>Specified as: a fullword integer; <math>nrhs \geq 0</math>.</p>
<i>info</i>	<p>See "On Return."</p>

### On Return

<i>bx</i>	<p>is the general matrix <i>X</i>, containing the <i>nrhs</i> solutions to the system. The solutions, each of length <i>n</i>, reside in the columns of <i>X</i>.</p> <p>Returned as: an <i>ldb</i> by (at least) <i>nrhs</i> array, containing numbers of the data type indicated in Table 104 on page 507.</p>
<i>info</i>	<p><i>info</i> has the following meaning:</p> <p>If <i>info</i> = 0, the solve completed successfully.</p>

### Notes

1. In your C program, argument *info* must be passed by reference.
2. All subroutines accept lowercase letters for the *uplo* argument.

3. The scalar data specified for input arguments *uplo*, *lda*, and *n* for these subroutines must be the same as the corresponding input arguments specified for SPOTRF/SPOF/SPOFCD/SPPTRE, DPOTRF/DPOF/DPOFCD/DPPTRF, CPOTRF/CPOF/CPPTRE, and ZPOTRF/ZPOF/ZPPTRE, respectively.
4. The array data specified for input argument *a* for these subroutines must be the same as the corresponding output arguments for SPOTRF/SPOF/SPOFCD, DPOTRF/DPOF/DPOFCD, CPOTRF/CPOF, and ZPOTRF/ZPOF, respectively.
5. The array data specified for input argument *ap* for these subroutines must be the same as the corresponding output arguments for SPPTRE, DPPTRF, CPPTRE, and ZPPTRE, respectively.
6. The matrices used in this computation must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
7. For a description of how the matrices are stored:
  - For positive definite real symmetric matrices, see “Positive Definite or Negative Definite Symmetric Matrix” on page 73.
  - For positive definite complex Hermitian matrices, see “Positive Definite or Negative Definite Complex Hermitian Matrix” on page 75.

## Function

The system  $AX = B$  is solved for  $X$ , where  $X$  and  $B$  are general matrices and  $A$  is a positive definite real symmetric matrix for SPOTRS/SPOSM/SPPTRS and DPOTRS/DPOSM/DPPTRS, and a positive definite complex Hermitian matrix for CPOTRS/CPOSM/CPPTRS and ZPOTRS/ZPOSM/ZPPTRS. These subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to SPOTRF/SPOF/SPOFCD/SPPTRE, DPOTRF/DPOF/DPOFCD/DPPTRF, CPOTRF/CPOF/CPPTRE, or ZPOTRF/ZPOF/ZPPTRE, respectively. For a description of how  $A$  is factored, see “SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, ZPOF, SPPTRE, DPPTRF, CPPTRE, ZPPTRE, SPPF, and DPPF — Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization” on page 495.

If  $n$  or  $nrhs$  is 0, no computation is performed. See references [8] and [38].

## Error conditions

### Computational Errors

None

**Note:** If the factorization performed by `_POTRF`, `_POF`, `_POFCD`, or `_PPTRF` failed because matrix  $A$  was not positive definite, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

### Input-Argument Errors

1.  $uplo \neq 'U'$  or  $'L'$
2.  $n < 0$
3.  $nrhs < 0$
4.  $n > lda$
5.  $lda \leq 0$
6.  $n > ldb$
7.  $ldb \leq 0$

## Examples

### Example 1

This example shows how to solve the system  $AX = B$  for two right-hand sides, where matrix  $A$  is the same matrix factored in the “Example 1” on page 500 for SPOTRF and SPOF.

#### Call Statement and Input:

```

          UPLO  N  NRHS  A  LDA  BX  LDB  INFO
          |    |    |    |    |    |    |    |
CALL SPOTRS( 'L' , 9 , 2 ,  A , 9 , BX , 9 , INFO )
    
```

or

```

          UPLO  A  LDA  N  BX  LDB  NRHS
          |    |    |    |    |    |    |
CALL SPOSM( 'L' , A , 9 , 9 , BX , 9 , 2 )
    
```

$A$  = (same as output  $A$  in “Example 1” on page 500)

$$BX = \begin{bmatrix} 9.0 & 45.0 \\ 17.0 & 89.0 \\ 24.0 & 131.0 \\ 30.0 & 170.0 \\ 35.0 & 205.0 \\ 39.0 & 235.0 \\ 42.0 & 259.0 \\ 44.0 & 276.0 \\ 45.0 & 285.0 \end{bmatrix}$$

#### Output:

$$BX = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \\ 1.0 & 5.0 \\ 1.0 & 6.0 \\ 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

INFO = 0

### Example 2

This example shows how to solve the system  $AX = B$  for two right-hand sides, where matrix  $A$  is the input matrix factored in “Example 2” on page 501 for SPOTRF and SPOF.

#### Call Statement and Input:

```

          UPLO  N  NRHS  A  LDA  BX  LDB  INFO
          |    |    |    |    |    |    |    |
CALL SPOTRS( 'U' , 9 , 2 ,  A , 9 , BX , 9 , INFO )
    
```

or

```

          UPLO  A  LDA  N  BX  LDB  NRHS
          |    |    |    |    |    |    |
CALL SPOSM( 'U' , A , 9 , 9 , BX , 9 , 2 )
    
```

$A$  = (same as output  $A$  in “Example 2” on page 501)



$$\text{BX} = \begin{bmatrix} 9.0 & 45.0 \\ 17.0 & 89.0 \\ 24.0 & 131.0 \\ 30.0 & 170.0 \\ 35.0 & 205.0 \\ 39.0 & 235.0 \\ 42.0 & 259.0 \\ 44.0 & 276.0 \\ 45.0 & 285.0 \end{bmatrix}$$

**Output:**

$$\text{BX} = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \\ 1.0 & 5.0 \\ 1.0 & 6.0 \\ 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

INFO = 0

### Example 3

This example shows how to solve the system  $AX = B$  for two right-hand sides, where matrix  $A$  is the same matrix factored in the “Example 3” on page 502 for CPOTRF and CPOF.

**Call Statement and Input:**

```

          UPLO  N  NRHS  A  LDA  BX  LDB  INFO
          |    |    |    |    |    |    |    |
CALL CPOTRS( 'L' , 3 , 2 , A , 3 , BX , 3 , INFO )

```

or

```

          UPLO  A  LDA  N  BX  LDB  NRHS
          |    |    |    |    |    |
CALL CPOSM( 'L' , A , 3 , 3 , BX , 3 , 2 )

```

A = (same as output A in “Example 3” on page 502)

$$\text{BX} = \begin{bmatrix} (60.0, -55.0) & (70.0, 10.0) \\ (34.0, 58.0) & (-51.0, 110.0) \\ (13.0, -152.0) & (75.0, 63.0) \end{bmatrix}$$

**Output:**

$$\text{BX} = \begin{bmatrix} (2.0, -1.0) & (2.0, 0.0) \\ (1.0, 1.0) & (-1.0, 2.0) \\ (0.0, -2.0) & (1.0, 1.0) \end{bmatrix}$$

INFO = 0

### Example 4

This example shows how to solve the system  $AX = B$  for two right-hand sides, where matrix  $A$  is the input matrix factored in “Example 4” on page 502 for CPOTRF and CPOF.

# SPOTRS, DPOTRS, CPOTRS, ZPOTRS, SPOSIM, DPOSIM, CPOSIM, ZPOSIM, SPPTRS, DPPTRS, CPPTRS, and ZPPTRS

## Call Statement and Input:

```

          UPLO  N  NRHS  A  LDA  BX  LDB  INFO
          |    |    |    |    |    |    |
CALL CPOTRS( 'U' , 3 , 2 , A , 3 , BX , 3 , INFO )

```

or

```

          UPLO  A  LDA  N  BX  LDB  NRHS
          |    |    |    |    |    |
CALL CPOSIM( 'U' , A , 3 , 3 , BX , 3 , 2 )

```

A = (same as output A in “Example 4” on page 502)

$$BX = \begin{bmatrix} ( 33.0, -18.0) & (15.0, -3.0) \\ ( 45.0, -45.0) & ( 8.0, -2.0) \\ (152.0, 1.0) & (43.0, -29.0) \end{bmatrix}$$

## Output:

$$BX = \begin{bmatrix} (2.0, -1.0) & (2.0, 0.0) \\ (1.0, -1.0) & (0.0, 1.0) \\ (3.0, 0.0) & (1.0, -1.0) \end{bmatrix}$$

INFO = 0

## Example 5

This example shows how to solve the system  $AX = B$  for two right-hand sides, where matrix  $A$  is the input matrix factored in “Example 5” on page 503 for SPPTRF and DPPTRF.

## Call Statement and Input:

```

          UPLO  N  NRHS  AP  BX  LDB  INFO
          |    |    |    |    |    |
CALL SPPTRS( 'L' , 9 , 2 , AP , BX , 9 , INFO )

```

A = (same as output A in “Example 5” on page 503)

$$BX = \begin{bmatrix} 9.0 & 45.0 \\ 17.0 & 89.0 \\ 24.0 & 131.0 \\ 30.0 & 170.0 \\ 35.0 & 205.0 \\ 39.0 & 235.0 \\ 42.0 & 259.0 \\ 44.0 & 276.0 \\ 45.0 & 285.0 \end{bmatrix}$$

## Output:

$$BX = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \\ 1.0 & 5.0 \\ 1.0 & 6.0 \\ 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

INFO = 0

### Example 6

This example shows how to solve the system  $AX = B$  for two right-hand sides, where matrix  $A$  is the same matrix factored in “Example 6” on page 504 for SPPTRF.

#### Call Statement and Input:

```

          UPLO N  NRHS AP  BX  LDB INFO
CALL SPPTRS( 'U' , 9 , 2 , AP , BX , 9 , INFO )

```

A = (same as output A in “Example 6” on page 504)

$$\text{BX} = \begin{bmatrix} 9.0 & 45.0 \\ 17.0 & 89.0 \\ 24.0 & 131.0 \\ 30.0 & 170.0 \\ 35.0 & 205.0 \\ 39.0 & 235.0 \\ 42.0 & 259.0 \\ 44.0 & 276.0 \\ 45.0 & 285.0 \end{bmatrix}$$

#### Output:

$$\text{BX} = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \\ 1.0 & 5.0 \\ 1.0 & 6.0 \\ 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

INFO = 0

### Example 7

This example shows how to solve the system  $AX = B$  for two right-hand sides, where matrix  $A$  is the same matrix factored in “Example 7” on page 504 for ZPPTRF.

#### Call Statement and Input:

```

          UPLO N  NRHS AP  BX  LDB INFO
CALL ZPPTRS( 'L' , 3 , 2 , AP , BX , 3 , INFO )

```

AP = (same as output AP in “Example 7” on page 504)

$$\text{BX} = \begin{bmatrix} (60.0, -55.0) & (70.0, 10.0) \\ (34.0, 58.0) & (-51.0, 110.0) \\ (13.0, -152.0) & (75.0, 63.0) \end{bmatrix}$$

#### Output:

**SPOTRS, DPOTRS, CPOTRS, ZPOTRS, SPOSIM, DPOSIM, CPOSIM, ZPOSIM, SPPTRS, DPPTRS, CPPTRS, and ZPPTRS**

$$BX = \begin{bmatrix} (2.0, -1.0) & (2.0, 0.0) \\ (1.0, 1.0) & (-1.0, 2.0) \\ (0.0, -2.0) & (1.0, 1.0) \end{bmatrix}$$

INFO = 0

**Example 8**

This example shows how to solve the system  $AX = B$  for two right-hand sides, where matrix  $A$  is the same matrix factored in "Example 8" on page 505 for ZPPTRF.

**Call Statement and Input:**

```

          UPLO N  NRHS  AP  BX  LDB  INFO
          |   |   |   |   |   |   |
CALL ZPPTRS( 'U' , 3 , 2 , AP , BX , 3 , INFO )

```

AP = (same as output AP in "Example 8" on page 505)

$$BX = \begin{bmatrix} (33.0, -18.0) & (15.0, -3.0) \\ (45.0, -45.0) & (8.0, -2.0) \\ (152.0, 1.0) & (43.0, -29.0) \end{bmatrix}$$

**Output:**

$$BX = \begin{bmatrix} (2.0, -1.0) & (2.0, 0.0) \\ (1.0, -1.0) & (0.0, 1.0) \\ (3.0, 0.0) & (1.0, -1.0) \end{bmatrix}$$

INFO = 0

## SPPS and DPPS — Positive Definite Real Symmetric Matrix Solve

### Purpose

These subroutines solve the system  $Ax = b$  for  $x$ , where  $A$  is a positive definite symmetric matrix, and  $x$  and  $b$  are vectors. The subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to SPPF/SPPFCD or DPPF/DPPFP/DPPFCD, respectively.

Table 105. Data Types

$A, b, x$	Subroutine
Short-precision real	SPPS
Long-precision real	DPPS

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SPPF/SPPFCD and DPPF/DPPFP/DPPFCD, respectively.

### Syntax

Fortran	CALL SPPS   DPPS ( $ap, n, bx, iopt$ )
C and C++	spps   dpps ( $ap, n, bx, iopt$ );

### On Entry

- $ap$  is the factorization of matrix  $A$ , produced by a preceding call to SPPF/SPPFCD or DPPF/DPPFP/DPPFCD, respectively.
- Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 105, where:
- If  $iopt = 0$ , the array must contain  $n(n+1)/2+n$  elements.
- If  $iopt = 1$ , the array must contain  $n(n+1)/2$  elements.
- $n$  is the order of matrix  $A$  used in the factorization, and the lengths of vectors  $b$  and  $x$ .
- Specified as: a fullword integer;  $n \geq 0$ .
- $bx$  is the vector  $b$  of length  $n$ , containing the right-hand side of the system.
- Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 105.
- $iopt$  indicates the type of factorization that was performed on matrix  $A$ , where:
- If  $iopt = 0$ , the matrix was factored using the  $LDL^T$  method.
- If  $iopt = 1$ , the matrix was factored using Cholesky factorization.
- Specified as: a fullword integer;  $iopt = 0$  or  $1$ .

### On Return

- $bx$  is the solution vector  $x$  of length  $n$ , containing the results of the computation.

Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 105 on page 515.

## Notes

1. The array data specified for input argument *ap* for these subroutines must be the same as the corresponding output argument for SPPF/SPPFCD and DPPF/DPPFP/DPPFCD, respectively.
2. The scalar data specified for input argument *n* for these subroutines must be the same as that specified for SPPF/SPPFCD and DPPF/DPPFP/DPPFCD, respectively.
3. When you call these subroutines after calling SPPF or DPPF, the value of input argument *iopt* must be as follows:

SPPF/DPPF Input <i>iopt</i>	SPPS/DPPS Input <i>iopt</i>
0 or 10	0
1 or 11	1

4. When you call these subroutines after calling SPPFCD or DPPFCD, the value of input argument *iopt* must be 0.
5. When you call these subroutines after calling DPPFP, the value of input argument *iopt* must be 1.
6. In the input array specified for *ap*, the first  $n(n+1)/2$  elements are matrix elements. The additional *n* locations, required in the array when *iopt* = 0, are used for working storage by this subroutine and should not be altered between calls to the factorization and solve subroutines.
7. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
8. For a description of how a positive definite symmetric matrix is stored in lower-packed storage mode in an array, see “Symmetric Matrix” on page 69.

## Function

The system  $Ax = b$  is solved for  $x$ , where  $A$  is a positive definite symmetric matrix, stored in lower-packed storage mode in array  $AP$ , and  $x$  and  $b$  are vectors. These subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to SPPF/SPPFCD or DPPF/DPPFP/DPPFCD, respectively.

If  $n$  is 0, no computation is performed. See references [38] and [40].

## Error conditions

### Computational Errors

None

**Note:** If a call to SPPF, DPPF, SPPFCD, DPPFCD, or DPPFP resulted in a nonpositive definite matrix, error 2104 or 2115, SPPS or DPPS results may be unpredictable or numerically unstable.

### Input-Argument Errors

1.  $n < 0$
2.  $iopt \neq 0$  or 1

## Examples

### Example 1

This example shows how to solve the system  $Ax = b$ , where matrix  $A$  is the same matrix factored in the “Example 9” on page 505 for SPPF and DPPF.

#### Call Statement and Input:

```

          AP  N  BX  IOPT
          |  |  |  |
CALL SPPS ( AP , 9 , BX , 0 )

```

AP = (same as output AP in “Example 9” on page 505 for SPPF and DPPF)

BX = (9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0)

#### Output:

BX = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)

### Example 2

This example shows how to solve the same system as in Example 1, where matrix  $A$  is the same matrix factored in the “Example 10” on page 506 for SPPF and DPPF.

#### Call Statement and Input:

```

          AP  N  BX  IOPT
          |  |  |  |
CALL SPPS( AP , 9 , BX , 1 )

```

AP = (same as output AP in “Example 10” on page 506 for SPPF and DPPF)

BX = (9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0)

#### Output:

BX = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)

## SPPFCD, DPPFCD, SPOFCD, and DPOFCD — Positive Definite Real Symmetric Matrix Factorization, Condition Number Reciprocal, and Determinant

### Purpose

The SPPFCD and DPPFCD subroutines factor positive definite symmetric matrix  $A$ , stored in lower-packed storage mode, using Gaussian elimination ( $LDL^T$ ). The reciprocal of the condition number and the determinant of matrix  $A$  can also be computed. To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SPPS or DPPS, respectively.

The SPOFCD and DPOFCD subroutines factor positive definite symmetric matrix  $A$ , stored in upper or lower storage mode, using Cholesky factorization ( $LL^T$  or  $U^T U$ ). The reciprocal of the condition number and the determinant of matrix  $A$  can also be computed. To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with a call to SPOSM or DPOSM, respectively. To find the inverse of matrix  $A$ , follow the call to these subroutines with a call to SPOICD or DPOICD, respectively.

Table 106. Data Types

$A$ , $aux$ , $rcond$ , $det$	Subroutine
Short-precision real	SPPFCD and SPOFCD
Long-precision real	DPPFCD and DPOFCD

**Note:** The output factorization from SPPFCD and DPPFCD should be used only as input to the solve subroutines SPPS and DPPS, respectively. The output from SPOFCD and DPOFCD should be used only as input to the following subroutines for performing a solve or inverse: SPOSM/SPOICD and DPOSM/DPOICD, respectively.

### Syntax

<b>Fortran</b>	CALL SPPFCD   DPPFCD ( $ap$ , $n$ , $iopt$ , $rcond$ , $det$ , $aux$ , $naux$ ) CALL SPOFCD   DPOFCD ( $uplo$ , $a$ , $lda$ , $n$ , $iopt$ , $rcond$ , $det$ , $aux$ , $naux$ )
<b>C and C++</b>	sppfcd   dppfcd ( $ap$ , $n$ , $iopt$ , $rcond$ , $det$ , $aux$ , $naux$ ); spofcd   dpoecd ( $uplo$ , $a$ , $lda$ , $n$ , $iopt$ , $rcond$ , $det$ , $aux$ , $naux$ );

### On Entry

$uplo$  indicates whether matrix  $A$  is stored in upper or lower storage mode, where:

If  $uplo = 'U'$ ,  $A$  is stored in upper storage mode.

If  $uplo = 'L'$ ,  $A$  is stored in lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

$ap$  is the array, referred to as AP, in which the matrix  $A$ , to be factored, is stored in lower-packed storage mode.



Specified as: a one-dimensional array of (at least) length  $n(n+1)/2+n$ , containing numbers of the data type indicated in Table 106 on page 518.

*a* is the positive definite symmetric matrix  $A$ , to be factored.

Specified as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 106 on page 518.

*lda* is the leading dimension of the array specified for  $a$ .

Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .

*n* is the order  $n$  of matrix  $A$ .

Specified as: a fullword integer, where:  
 For SPPFCD and DPPFCD,  $n \geq 0$ .  
 For SPOFCD and DPOFCD,  $0 \leq n \leq lda$ .

*iopt* indicates the type of computation to be performed, where:  
 If  $iopt = 0$ , the matrix is factored.  
 If  $iopt = 1$ , the matrix is factored, and the reciprocal of the condition number is computed.  
 If  $iopt = 2$ , the matrix is factored, and the determinant is computed.  
 If  $iopt = 3$ , the matrix is factored and the reciprocal of the condition number and the determinant are computed.

Specified as: a fullword integer;  $iopt = 0, 1, 2,$  or  $3$ .

*rcond* See "On Return."

*det* See "On Return."

*aux* has the following meaning:  
 If  $naux = 0$  and error 2015 is unrecoverable,  $aux$  is ignored.  
 Otherwise, is the storage work area used by these subroutines. Its size is specified by  $naux$ . Specified as: an area of storage, containing numbers of the data type indicated in Table 106 on page 518.

*naux* is the size of the work area specified by  $aux$ —that is, the number of elements in  $aux$ .

Specified as: a fullword integer, where:  
 If  $naux = 0$  and error 2015 is unrecoverable, SPPFCD, DPPFCD, SPOFCD, and DPOFCD dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.  
 Otherwise,  $naux \geq n$ .

### On Return

*ap* is the transformed matrix  $A$  of order  $n$ , containing the results of the factorization. See "Function" on page 520. Returned as: a one-dimensional array of (at least) length  $n(n+1)/2+n$ , containing numbers of the data type indicated in Table 106 on page 518.

*a* is the transformed matrix  $A$  of order  $n$ , containing the results of the

## SPPFCD, DPPFCD, SPOFCD, and DPOFCD

factorization. See “Function.” Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 106 on page 518.

*rcond* is the estimate of the reciprocal of the condition number, *rcond*, of matrix *A*. Returned as: a number of the data type indicated in Table 106 on page 518; *rcond*  $\geq$  0.

*det* is the vector *det*, containing the two components *det*<sub>1</sub> and *det*<sub>2</sub> of the determinant of matrix *A*. The determinant is:

$$det_1(10^{det_2})$$

where  $1 \leq det_1 < 10$ . Returned as: an array of length 2, containing numbers of the data type indicated in Table 106 on page 518.

## Notes

1. All subroutines accept lowercase letters for the *uplo* argument.
2. In your C program, argument *rcond* must be passed by reference.
3. When *iopt* = 0, SPPFCD and DPPFCD provide the same function as a call to SPPF or DPPF, respectively. When *iopt* = 1, SPOFCD and DPOFCD provide the same function as a call to SPOF or DPOF, respectively.
4. SPPFCD and DPPFCD in many cases utilize new algorithms based on recursive packed storage format. As a result, on output, the array specified for AP may be stored in this new format rather than the conventional lower packed format. (See references [54], [68], and [70]).  
The array specified for AP should not be altered between calls to the factorization and solve subroutines; otherwise unpredictable results may occur.
5. See “Notes” on page 516 for information on specifying a value for *iopt* in the SPPS and DPPS subroutines after calling SPPFCD and DPPFCD, respectively.
6. In the input and output arrays specified for *ap*, the first  $n(n+1)/2$  elements are matrix elements. The additional *n* locations in the array are used for working storage by this subroutine and should not be altered between calls to the factorization and solve subroutines.
7. For a description of how a positive definite symmetric matrix is stored in lower-packed storage mode in an array, see “Symmetric Matrix” on page 69. For a description of how a positive definite symmetric matrix is stored in upper or lower storage mode, see “Positive Definite or Negative Definite Symmetric Matrix” on page 73.
8. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## Function

The functions for these subroutines are described in the sections below.

### For SPPFCD and DPPFCD

The positive definite symmetric matrix *A*, stored in lower-packed storage mode, is factored using Gaussian elimination, where *A* is expressed as:

$$A = LDL^T$$

where:

$L$  is a unit lower triangular matrix.

$L^T$  is the transpose of matrix  $L$ .

$D$  is a diagonal matrix.

An estimate of the reciprocal of the condition number,  $rcond$ , and the determinant,  $det$ , can also be computed by this subroutine. The estimate of the condition number uses an enhanced version of the algorithm described in references [72] and [73].

If  $n$  is 0, no computation is performed. See references [38] and [40].

These subroutines call SPPF and DPPF, respectively, to perform the factorization using Gaussian elimination ( $LDL^T$ ). If you want to use the Cholesky factorization method, you must call SPPF and DPPF directly.

### For SPOFCD and DPOFCD

The positive definite symmetric matrix  $A$ , stored in upper or lower storage mode, is factored using Cholesky factorization, where  $A$  is expressed as:

$$A = LL^T \text{ or } A = U^TU$$

where:

$L$  is a lower triangular matrix.

$L^T$  is the transpose of matrix  $L$ .

$U$  is an upper triangular matrix.

$U^T$  is the transpose of matrix  $U$ .

If specified, the estimate of the reciprocal of the condition number and the determinant can also be computed. The estimate of the condition number uses an enhanced version of the algorithm described in references [72] and [73].

If  $n$  is 0, no computation is performed. See references [8] and [38].

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

- Matrix  $A$  is not positive definite (for SPPFCD and DPPFCD).
  - If matrix  $A$  is singular (at least one of the diagonal elements are 0), then  $rcond$  and  $det$ , if you requested them, are set to 0.
  - If matrix  $A$  is nonsingular and nonpositive definite (none of the diagonal elements are 0 and at least one diagonal element is negative), then  $rcond$  and  $det$ , if you requested them, are computed.
  - One or more elements of  $D$  contain values less than or equal to 0; all elements of  $D$  are checked. The index  $i$  of the last nonpositive element encountered is identified in the computational error message, issued by SPPF or DPPF, respectively.
  - $i$  can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2104 in the ESSL error option table; otherwise, the default value causes your program to be terminated by SPPF or DPPF,

## SPPFCD, DPPFCD, SPOFCD, and DPOFCD

respectively, when this error occurs. If your program is not terminated by SPPF or DPPF, respectively, the return code is set to 2. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

2. Matrix  $A$  is not positive definite (for SPOFCD and DPOFCD).
  - If matrix  $A$  is singular (at least one of the diagonal elements are 0), then  $rcond$  and  $det$ , if you requested them, are set to 0.
  - If matrix  $A$  is nonsingular and nonpositive definite (none of the diagonal elements are 0 and at least one diagonal element is negative), then  $rcond$  and  $det$ , if you requested them, are computed.
  - Processing stops at the first occurrence of a nonpositive definite diagonal element.
  - The order  $i$  of the **first** minor encountered having a nonpositive determinant is identified in the computational error message.
  - $i$  can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2115 in the ESSL error option table; otherwise, the default value causes your program to be terminated by SPPF or DPPF, respectively, when this error occurs. If your program is not terminated by SPPF or DPPF, respectively, the return code is set to 2. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $uplo \neq 'U'$  or  $'L'$
2.  $lda \leq 0$
3.  $lda < n$
4.  $n < 0$
5.  $iopt \neq 0, 1, 2,$  or  $3$
6. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example computes the factorization, reciprocal of the condition number, and determinant of matrix  $A$ . The input is the same as used in “Example 9” on page 505 for SPPF.

The values used to estimate the reciprocal of the condition number are obtained with the following values:

$$\|A\|_1 = \max(9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0) = 45.0$$

Estimate of  $\|A\| = 4.0$

On output, the value in  $det$ ,  $|A|$ , is equal to 1.

#### Call Statement and Input:

```
          AP   N   IOPT  RCOND   DET   AUX  NAUX
          |   |   |     |     |   |   |
CALL DPPFCD( AP , 9 , 3 , RCOND , DET , AUX , 9 )
```

AP           =(same as input AP in  
“Example 9” on page 505)

#### Output:

AP           =(same as output AP in "Example 9" on page 505)  
 RCOND       = 0.0055555  
 DET         = (1.0, 0.0)

**Example 2**

This example computes the factorization, reciprocal of the condition number, and determinant of matrix *A*. The input is the same as used in "Example 1" on page 500 for SPOF.

The values used to estimate the reciprocal of the condition number are obtained with the following values:

$$\|A\|_1 = \max(9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0) = 45.0$$

Estimate of  $\|A\| = 4.0$

On output, the value in *det*,  $|A|$ , is equal to 1.

**Call Statement and Input:**

```

                UPLO A  LDA  N  IOPT  RCOND  DET  AUX  NAUX
                |   |   |   |   |   |   |   |   |
CALL SPOFCD( 'L', A , 9 , 9 , 3 , RCOND , DET , AUX , 9 )
  
```

A           =(same as input A in "Example 1" on page 500)

**Output:**

A           =(same as output A in "Example 1" on page 500)  
 RCOND       = 0.0055555  
 DET         = (1.0, 0.0)

**Example 3**

This example computes the factorization, reciprocal of the condition number, and determinant of matrix *A*. The input is the same as used in "Example 2" on page 501 for SPOF.

The values used to estimate the reciprocal of the condition number are obtained with the following values:

$$\|A\|_1 = \max(9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0) = 45.0$$

Estimate of  $\|A\| = 4.0$

On output, the value in *det*,  $|A|$ , is equal to 1.

**Call Statement and Input:**

```

                UPLO A  LDA  N  IOPT  RCOND  DET  AUX  NAUX
                |   |   |   |   |   |   |   |   |
CALL SPOFCD( 'U', A , 9 , 9 , 3 , RCOND , DET , AUX , 9 )
  
```

A           =(same as input A in "Example 2" on page 501)

**Output:**

A           =(same as output A in "Example 2" on page 501)  
 RCOND       = 0.0055555  
 DET         = (1.0, 0.0)

## DBSSV — Symmetric Indefinite Matrix Factorization and Multiple Right-Hand Side Solve

### Purpose

The DBSSV subroutine solves a system of linear equations  $AX = B$  for  $X$ , where  $A$  is a real symmetric indefinite matrix, and  $X$  and  $B$  are real general matrices.

The matrix  $A$ , stored in upper- or lower-packed storage mode, is factored using the Bunch-Kaufman diagonal pivoting method, where  $A$  is expressed as:

$$A = UDU^T \quad \text{or}$$

$$A = LDL^T$$

where:

$U$  is a product of permutation and unit upper triangular matrices.

$L$  is a product of permutation and unit lower triangular matrices.

$D$  is a symmetric block diagonal matrix, consisting of  $1 \times 1$  and  $2 \times 2$  diagonal blocks.

Table 107. Data Types

$A, B$	$ipvt$	Subroutine
Long-precision real	Integer	DBSSV

### Syntax

Fortran	CALL DBSSV ( <i>uplo</i> , <i>n</i> , <i>nrhs</i> , <i>ap</i> , <i>ipvt</i> , <i>bx</i> , <i>ldb</i> , <i>nsinfo</i> )
C and C++	dbssv ( <i>uplo</i> , <i>n</i> , <i>nrhs</i> , <i>ap</i> , <i>ipvt</i> , <i>bx</i> , <i>ldb</i> , <i>nsinfo</i> );

### On Entry

- uplo* indicates whether matrix  $A$  is stored in upper- or lower-packed storage mode, where:
- If *uplo* = 'U',  $A$  is stored in upper-packed storage mode.
  - If *uplo* = 'L',  $A$  is stored in lower-packed storage mode.
- Specified as: a single character. It must be 'U' or 'L'.
- n* is the order  $n$  of matrix  $A$  and the number of rows of matrix  $B$ .
- Specified as: a fullword integer;  $n \geq 0$ .
- nrhs* is the number of right-hand sides; i.e., the number of columns of matrix  $B$ .
- Specified as: a fullword integer;  $nrhs \geq 0$ .
- ap* is array, referred to as AP, in which matrix  $A$ , to be factored, is stored in upper- or lower-packed storage mode.
- Specified as: a one-dimensional array of length *nsinfo*, containing numbers of the data type indicated in Table 107. See "Notes" on page 526.

<i>ipvt</i>	See “On Return.”
<i>bx</i>	is the matrix $B$ , containing the <i>nrhs</i> right-hand sides of the system. The right-hand sides, each of length $n$ , reside in the columns of matrix $B$ .  Specified as: an <i>ldb</i> by (at least) <i>nrhs</i> array, containing numbers of the data type indicated in Table 107 on page 524.
<i>ldb</i>	is the leading dimension of the array specified for $B$ .  Specified as: a fullword integer; $ldb > 0$ and $ldb \geq n$ .
<i>nsinfo</i>	is the number of elements in array, AP.  If $n \leq nco$ , $nsinfo = n(n + 1) / 2$  Where: <i>ics</i> is the size in doublewords of the data cache. The data cache size

$$nco = \sqrt{2.0(ics)}$$

can be obtained by utilizing the following C language code fragment:

```
#include <sys/systemcfg.h>
int ics;
    .
    .
    .
ics=_system_configuration.dcache_size/8;
```

Otherwise, to determine a sufficient amount of storage, use the following processor-independent formula:

```
n0 = 100
ns = (n + n0) (n + n0 + 1) / 2 + n(n0)
For uplo = 'L',
nsinfo ≥ ns
For uplo = 'U',
n1 = (n + 1) / 2
nt = n((n + 1) / 2)
nt1 = n1(n1 + 1)
ns1 = nt + nt1
nsinfo ≥ max(ns, ns1)
```

To determine the minimal amount of storage see “Notes” on page 526.

Specified as: a fullword integer;  $nsinfo > 0$ .

## On Return

<i>ap</i>	is the transformed matrix $A$ of order $n$ , containing the results of the factorization.  If $nsinfo \geq 0$ and $n > nco$ , additional information that can be used to obtain a minimum $nsinfo$ is stored in AP(1). See “Notes” on page 526 and “Function” on page 526.  Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 107 on page 524.
-----------	---

<i>ipvt</i>	is an integer vector of length $n$ , containing the pivot information necessary to construct the factored form of $A$ .  Returned as: a one-dimensional array of (at least) length $n$ , containing numbers of the data type indicated in Table 107 on page 524.
<i>bx</i>	is the matrix $X$ , containing the <i>nrhs</i> solutions to the system. The solutions, each of length $n$ , reside in the columns of $X$ .  Returned as: an <i>ldb</i> by (at least) <i>nrhs</i> array, containing numbers of the data type indicated in Table 107 on page 524.
<i>nsinfo</i>	indicates the result of the computation. <ul style="list-style-type: none"> <li>• If <i>nsinfo</i> = 0, the subroutine completed successfully.</li> <li>• If <i>nsinfo</i> &gt; 0, factorization was unsuccessful and array B was not updated. <i>nsinfo</i> is set to <math>i</math> where <math>d_{ii}</math> is exactly zero.</li> <li>• If <i>nsinfo</i> &lt; 0, factorization did not take place and the arrays, AP and B, remain unchanged. <math> nsinfo </math> is the minimal storage required for factorization to take place. Error message 2200 is issued and execution terminates, unless you have used ERRSET to make error code 2200 recoverable. See “What Can You Do about ESSL Input-Argument Errors?” on page 50.</li> </ul> <p>Specified as: a fullword integer.</p>

## Notes

1. This subroutine accepts lowercase letters for the *uplo* argument.
2. In your C program, argument *nsinfo* must be passed by reference.
3. In the input array specified for *ap*, the first  $n(n+1)/2$  elements are matrix elements. The additional locations, required in the array, are used for working storage.
4. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
5. On return, if *nsinfo*  $\geq 0$  and  $n > nco$ , *ap* contains additional information in AP(1) that can be used to obtain the minimal required *nsinfo*. This information can be accessed using the following code fragment:

```
REAL*8 AP(NSINFO)
INTEGER API(2)
EQUIVALENCE(API, AP)
      .
      .
      .
NSINFOMIN = API(2)
```

6. For a description of how a symmetric matrix is stored in upper- or lower-packed storage mode in an array, see “Symmetric Matrix” on page 69.

## Function

The system  $AX = B$  is solved for  $X$ , where  $A$  is a real symmetric indefinite matrix, and  $X$  and  $B$  are real general matrices.

The matrix  $A$ , stored in upper- or lower-packed storage mode, is factored using the Bunch-Kaufman diagonal pivoting method, where  $A$  is expressed as:

$$A = UDU^T \quad \text{or} \\ A = LDL^T$$



where:

$U$  is a product of permutation and unit upper triangular matrices.

$L$  is a product of permutation and unit lower triangular matrices.

$D$  is a symmetric block diagonal matrix, consisting of  $1 \times 1$  and  $2 \times 2$  diagonal blocks.

If  $n$  is 0, no computation is performed and the subroutine returns after doing some parameter checking. If  $n > 0$  and  $nrhs$  is 0, no solutions are computed and the subroutine returns after factoring the matrix.

See references [8] and [67].

## Error conditions

### Resource Errors

None.

### Computational Errors

Matrix  $A$  is singular.

- The factorization completed but the block diagonal matrix  $D$  is exactly singular.  $nsinfo$  is set to  $i$ , where  $d_{ii}$  is exactly zero. This diagonal element is identified in the computational error message.
- The computational error message may occur multiple times with processing continuing after each error, because the default for the number of allowable errors for error code 2147 is set to be unlimited in the ESSL error option table. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $uplo \neq 'U'$  or  $'L'$
2.  $n < 0$
3.  $n > ldb$
4.  $ldb \leq 0$
5.  $nrhs < 0$
6.  $nsinfo < (\text{minimum value})$ .
  - For the minimum value, see the  $nsinfo$  argument description.
  - Return code 1 is returned if error 2200 is recoverable.

## Examples

### Example 1

This example shows how to solve the system  $AX = B$ , for three right-hand sides, where matrix  $A$  is a real symmetric indefinite matrix of order 8, stored in lower-packed storage mode, and  $X$  and  $B$  are real general matrices.

On input, matrix  $A$  is:

$$A = \begin{bmatrix} 3.0 & 5.0 & -2.0 & 2.0 & 3.0 & -5.0 & -2.0 & -3.0 \\ 5.0 & 3.0 & 2.0 & -2.0 & 5.0 & -3.0 & 2.0 & -5.0 \\ -2.0 & 2.0 & 0.0 & 0.0 & -2.0 & 2.0 & 0.0 & 6.0 \\ 2.0 & -2.0 & 0.0 & 8.0 & -6.0 & -10.0 & -8.0 & -14.0 \\ 3.0 & 5.0 & -2.0 & -6.0 & 12.0 & 6.0 & 8.0 & 6.0 \\ -5.0 & -3.0 & 2.0 & -10.0 & 6.0 & 16.0 & 8.0 & 20.0 \end{bmatrix}$$

## DBSSV

$$\begin{bmatrix} -2.0 & 2.0 & 0.0 & -8.0 & 8.0 & 8.0 & 6.0 & 18.0 \\ -3.0 & -5.0 & 6.0 & -14.0 & 6.0 & 20.0 & 18.0 & 34.0 \end{bmatrix}$$

**Note:** The AP array is formatted in a triangular arrangement for readability; however, it is stored in lower-packed storage mode.

### Call Statement and Input:

```
          UPLO  N   NRHS  AP  IPVT  BX  LDB  NSINFO
CALL DBSSV ( 'L', 8,  3,  AP, IPVT, BX,  8,  36 )
AP = ( 3.0,  5.0, -2.0,  2.0,  3.0, -5.0, -2.0, -3.0,
       3.0,  2.0, -2.0,  5.0, -3.0,  2.0, -5.0,
       0.0,  0.0, -2.0,  2.0,  0.0,  6.0,
       8.0, -6.0, -10.0, -8.0, -14.0,
      12.0,  6.0,  8.0,  6.0,
      16.0,  8.0, 20.0,
       6.0, 18.0,
      34.0 )
```

$$BX = \begin{bmatrix} 1.0 & -38.0 & 47.0 \\ 7.0 & -10.0 & 73.0 \\ 6.0 & 52.0 & 2.0 \\ -30.0 & -228.0 & -42.0 \\ 32.0 & 183.0 & 105.0 \\ 34.0 & 297.0 & 9.0 \\ 32.0 & 244.0 & 44.0 \\ 62.0 & 497.0 & 61.0 \end{bmatrix}$$

### Output:

$$BX = \begin{bmatrix} 1.0 & 1.0 & 8.0 \\ 1.0 & 2.0 & 7.0 \\ 1.0 & 3.0 & 6.0 \\ 1.0 & 4.0 & 5.0 \\ 1.0 & 5.0 & 4.0 \\ 1.0 & 6.0 & 3.0 \\ 1.0 & 7.0 & 2.0 \\ 1.0 & 8.0 & 1.0 \end{bmatrix}$$

NSINFO = 0

**Note:** AP and IPVT are stored in an internal format.

### Example 2

This example shows how to solve the system  $AX = B$ , for three right-hand sides, where matrix  $A$  is a real symmetric indefinite matrix of order 8, stored in upper-packed storage mode, and  $X$  and  $B$  are real general matrices.

On input, matrix  $A$  is:

$$\begin{bmatrix} 34.0 & 18.0 & 17.0 & 6.0 & -14.0 & 6.0 & -5.0 & -3.0 \\ 18.0 & 6.0 & 6.0 & 8.0 & -8.0 & 0.0 & 2.0 & -2.0 \\ 17.0 & 6.0 & 9.0 & 9.0 & -8.0 & 0.0 & 2.0 & -2.0 \\ 6.0 & 8.0 & 9.0 & 12.0 & -6.0 & -2.0 & 5.0 & 3.0 \\ -14.0 & -8.0 & -8.0 & -6.0 & 8.0 & 0.0 & -2.0 & 2.0 \\ 6.0 & 0.0 & 0.0 & -2.0 & 0.0 & 0.0 & 2.0 & -2.0 \\ -5.0 & 2.0 & 2.0 & 5.0 & -2.0 & 2.0 & 3.0 & 5.0 \\ -3.0 & -2.0 & -2.0 & 3.0 & 2.0 & -2.0 & 5.0 & 3.0 \end{bmatrix}$$

**Note:** The AP array is formatted in a triangular arrangement for readability; however, it is stored in upper-packed storage mode.

**Call Statement and Input:**

```

          UPLO  N  NRHS  AP  IPVT  BX  LDB  NSINFO
          |    |    |    |    |    |    |    |
CALL DBSSV ( 'U', 8,  3,  AP, IPVT, BX,  8,  36 )

```

```

AP = ( 34.0,
      18.0, 6.0,
      17.0, 6.0, 9.0,
      6.0, 8.0, 9.0, 12.0,
     -14.0, -8.0, -8.0, -6.0, 8.0,
      6.0, 0.0, 0.0, -2.0, 0.0, 0.0,
     -5.0, 2.0, 2.0, 5.0, -2.0, 2.0, 3.0,
     -3.0, -2.0, -2.0, 3.0, 2.0, -2.0, 5.0, 3.0 )

```

```

BX = [ 59.0  52.0  479.0
      30.0  38.0  232.0
      33.0  50.0  247.0
      35.0 114.0  201.0
     -28.0 -36.0 -216.0
      4.0  -4.0  40.0
      12.0  88.0  20.0
      4.0  56.0 -20.0 ]

```

**Output:**

```

BX = [ 1.0  1.0  8.0
      1.0  2.0  7.0
      1.0  3.0  6.0
      1.0  4.0  5.0
      1.0  5.0  4.0
      1.0  6.0  3.0
      1.0  7.0  2.0
      1.0  8.0  1.0 ]

```

NSINFO = 0

**Note:** AP and IPVT are stored in an internal format.

## DBSTRF — Symmetric Indefinite Matrix Factorization

### Purpose

DBSTRF factors a real symmetric indefinite matrix  $A$ . The matrix  $A$ , stored in upper- or lower-packed storage mode, is factored using the Bunch-Kaufman diagonal pivoting method, where  $A$  is expressed as:

$$A = UDU^T \quad \text{or}$$

$$A = LDL^T$$

where:

$U$  is a product of permutation and unit upper triangular matrices.

$L$  is a product of permutation and unit lower triangular matrices.

$D$  is a symmetric block diagonal matrix, consisting of  $1 \times 1$  and  $2 \times 2$  diagonal blocks.

To solve a system of equations with one or more right-hand sides, follow the call to this subroutine with one or more calls to DBSTRS.

Table 108. Data Types

$A$	$ipvt$	Subroutine
Long-precision real	Integer	DBSTRF

**Note:** The output from DBSTRF should be used only as input to DBSTRS, for performing a solve.

### Syntax

Fortran	CALL DBSTRF ( <i>uplo</i> , <i>n</i> , <i>ap</i> , <i>ipvt</i> , <i>nsinfo</i> )
C and C++	dbstrf ( <i>uplo</i> , <i>n</i> , <i>ap</i> , <i>ipvt</i> , <i>nsinfo</i> );

### On Entry

<i>uplo</i>	indicates whether matrix $A$ is stored in upper- or lower-packed storage mode, where:  If <i>uplo</i> = 'U', $A$ is stored in upper-packed storage mode. If <i>uplo</i> = 'L', $A$ is stored in lower-packed storage mode. Specified as: a single character. It must be 'U' or 'L'.
<i>n</i>	is the order $n$ of matrix $A$ .  Specified as: a fullword integer; $n \geq 0$ .
<i>ap</i>	is array, referred to as $AP$ , in which matrix $A$ , to be factored, is stored in upper- or lower-packed storage mode.  Specified as: a one-dimensional array of length <i>nsinfo</i> , containing numbers of the data type indicated in Table 108. See "Notes" on page 532.
<i>ipvt</i>	See "On Return" on page 531.

*nsinfo* is the number of elements in array, AP.

If  $n \leq nco$ ,  $nsinfo = n(n + 1) / 2$

Where:

$$nco = \sqrt{2.0(ics)}$$

*ics* is the size in doublewords of the data cache. The data cache size can be obtained by utilizing the following C language code fragment:

```
#include <sys/systemcfg.h>
int ics;
.
.
.
ics=_system_configuration.dcache_size/8;
```

*ics* is the size in doublewords of the data cache. The data cache size can be obtained by utilizing the following C language code fragment:

```
#include <sys/systemcfg.h>
int ics;
.
.
.
ics=_system_configuration.dcache_size/8;
```

Otherwise, to determine a sufficient amount of storage, use the following processor-independent formula:

$$n0 = 100$$

$$ns = (n + n0) (n + n0 + 1) / 2 + n(n0)$$

For *uplo* = 'L',  
 $nsinfo \geq ns$

For *uplo* = 'U',  
 $n1 = (n + 1) / 2$   
 $nt = n((n + 1) / 2)$   
 $nt1 = n1(n1 + 1)$   
 $ns1 = nt + nt1$   
 $nsinfo \geq \max(ns, ns1)$

To determine the minimal amount of storage see "Notes" on page 532.

Specified as: a fullword integer;  $nsinfo > 0$ .

### On Return

*ap* is the transformed matrix *A* of order *n*, containing the results of the factorization.

If  $nsinfo \geq 0$  and  $n > nco$ , additional information that can be used to obtain a minimum *nsinfo* is stored in AP(1). See "Notes" on page 532 and "Function" on page 532.

	Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 108 on page 530.
<i>ipvt</i>	is an integer vector of length $n$ , containing the pivot information necessary to construct the factored form of $A$ .  Returned as: a one-dimensional array of (at least) length $n$ , containing numbers of the data type indicated in Table 108 on page 530.
<i>nsinfo</i>	indicates the result of the computation. <ul style="list-style-type: none"> <li>• If <math>nsinfo = 0</math>, the factorization completed successfully.</li> <li>• If <math>nsinfo &gt; 0</math>, factorization was unsuccessful and <math>nsinfo</math> is set to <math>i</math> where <math>d_{ii}</math> is exactly zero.</li> <li>• If <math>nsinfo &lt; 0</math>, factorization did not take place and the array <math>AP</math> remains unchanged. <math> nsinfo </math> is the minimal storage required for factorization to take place. Error message 2200 is issued and execution terminates, unless you have used ERRSET to make error code 2200 recoverable. See “What Can You Do about ESSL Input-Argument Errors?” on page 50.</li> </ul> <p>Specified as: a fullword integer.</p>

## Notes

1. This subroutine accepts lowercase letters for the *uplo* argument.
2. In your C program, argument *nsinfo* must be passed by reference.
3. In the input array specified for *ap*, the first  $n(n+1)/2$  elements are matrix elements. The additional locations, required in the array, are used for working storage.
4. The array specified for *ap* should not be altered between calls to the factorization and solve subroutines; otherwise, unpredictable results may occur.
5. On return, if  $nsinfo \geq 0$  and  $n > nco$ , *ap* contains additional information in  $AP(1)$  that can be used to obtain the minimal required *nsinfo*. This information can be accessed using the following code fragment:

```

REAL*8 AP(NSINFO)
INTEGER API(2)
EQUIVALENCE(API, AP)
      .
      .
      .
NSINFOMIN = API(2)

```
6. For a description of how a symmetric matrix is stored in upper- or lower-packed storage mode in an array, see “Symmetric Matrix” on page 69.

## Function

where:

$U$  is a product of permutation and unit upper triangular matrices.

$L$  is a product of permutation and unit lower triangular matrices.

$D$  is a symmetric block diagonal matrix, consisting of  $1 \times 1$  and  $2 \times 2$  diagonal blocks.

If  $n$  is 0, no computation is performed and the subroutine returns after doing some parameter checking.

See references [8] and [67].

## Error conditions

### Resource Errors

None.

### Computational Errors

Matrix  $A$  is singular.

- The factorization completed but the block diagonal matrix  $D$  is exactly singular.  $nsinfo$  is set to  $i$ , where  $d_{ii}$  is exactly zero. This diagonal element is identified in the computational error message.
- The computational error message may occur multiple times with processing continuing after each error, because the default for the number of allowable errors for error code 2147 is set to be unlimited in the ESSL error option table. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $uplo \neq 'U'$  or  $'L'$
2.  $n < 0$
3.  $nsinfo < (\text{minimum value})$ .
  - For the minimum value, see the  $nsinfo$  argument description.
  - Return code 1 is returned if error 2200 is recoverable.

## Examples

### Example 1

This example shows a factorization of a symmetric indefinite matrix  $A$  of order 8, stored in lower-packed storage mode, where on input matrix  $A$  is:

$$\begin{bmatrix} 3.0 & 5.0 & -2.0 & 2.0 & 3.0 & -5.0 & -2.0 & -3.0 \\ 5.0 & 3.0 & 2.0 & -2.0 & 5.0 & -3.0 & 2.0 & -5.0 \\ -2.0 & 2.0 & 0.0 & 0.0 & -2.0 & 2.0 & 0.0 & 6.0 \\ 2.0 & -2.0 & 0.0 & 8.0 & -6.0 & -10.0 & -8.0 & -14.0 \\ 3.0 & 5.0 & -2.0 & -6.0 & 12.0 & 6.0 & 8.0 & 6.0 \\ -5.0 & -3.0 & 2.0 & -10.0 & 6.0 & 16.0 & 8.0 & 20.0 \\ -2.0 & 2.0 & 0.0 & -8.0 & 8.0 & 8.0 & 6.0 & 18.0 \\ -3.0 & -5.0 & 6.0 & -14.0 & 6.0 & 20.0 & 18.0 & 34.0 \end{bmatrix}$$

**Note:** The AP array is formatted in a triangular arrangement for readability; however, it is stored in lower-packed storage mode.

### Call Statement and Input:

```

          UPLO N  AP  IPVT  NSINFO
          |   |   |   |   |
CALL DBSTRF ( 'L', 8, AP, IPVT, 36 )
AP = ( 3.0, 5.0, -2.0, 2.0, 3.0, -5.0, -2.0, -3.0,
       3.0, 2.0, -2.0, 5.0, -3.0, 2.0, -5.0,
       0.0, 0.0, -2.0, 2.0, 0.0, 6.0,
       8.0, -6.0, -10.0, -8.0, -14.0,
       12.0, 6.0, 8.0, 6.0,
       16.0, 8.0, 20.0,
       6.0, 18.0,
       34.0 )

```

**Output:** NSINFO = 0

## DBSTRF

**Note:** AP and IPVT are stored in an internal format and must be passed unchanged to the solve subroutine.

### Example 2

This example shows a factorization of a symmetric indefinite matrix  $A$  of order 8, stored in upper-packed storage mode, where on input matrix  $A$  is:

$$\begin{bmatrix} 34.0 & 18.0 & 17.0 & 6.0 & -14.0 & 6.0 & -5.0 & -3.0 \\ 18.0 & 6.0 & 6.0 & 8.0 & -8.0 & 0.0 & 2.0 & -2.0 \\ 17.0 & 6.0 & 9.0 & 9.0 & -8.0 & 0.0 & 2.0 & -2.0 \\ 6.0 & 8.0 & 9.0 & 12.0 & -6.0 & -2.0 & 5.0 & 3.0 \\ -14.0 & -8.0 & -8.0 & -6.0 & 8.0 & 0.0 & -2.0 & 2.0 \\ 6.0 & 0.0 & 0.0 & -2.0 & 0.0 & 0.0 & 2.0 & -2.0 \\ -5.0 & 2.0 & 2.0 & 5.0 & -2.0 & 2.0 & 3.0 & 5.0 \\ -3.0 & -2.0 & -2.0 & 3.0 & 2.0 & -2.0 & 5.0 & 3.0 \end{bmatrix}$$

**Note:** The AP array is formatted in a triangular arrangement for readability; however, it is stored in upper-packed storage mode.

### Call Statement and Input:

```
          UPLO  N   AP  IPVT  NSINFO
          |    |   |   |     |
CALL DBSTRF ( 'U', 8, AP, IPVT, 36 )
AP = ( 34.0,
      18.0, 6.0,
      17.0, 6.0, 9.0,
      6.0, 8.0, 9.0, 12.0,
      -14.0, -8.0, -8.0, -6.0, 8.0,
      6.0, 0.0, 0.0, -2.0, 0.0, 0.0,
      -5.0, 2.0, 2.0, 5.0, -2.0, 2.0, 3.0,
      -3.0, -2.0, -2.0, 3.0, 2.0, -2.0, 5.0, 3.0 )
```

**Output:** NSINFO = 0

**Note:** AP and IPVT are stored in an internal format and must be passed unchanged to the solve subroutine.



## DBSTRS — Symmetric Indefinite Matrix Multiple Right-Hand Side Solve

### Purpose

The DBSTRS subroutine solves a system of linear equations  $AX = B$  for  $X$ , where  $A$  is a real symmetric indefinite matrix, and  $X$  and  $B$  are real general matrices. This subroutine uses the results of the factorization of matrix  $A$ , produced by a preceding call to DBSTRF.

Table 109. Data Types

$A, B$	<i>ipvt</i>	Subroutine
Long-precision real	Integer	DBSTRS

**Note:** The input to this solve subroutine must be the output from the factorization subroutine DBSTRF.

### Syntax

<b>Fortran</b>	CALL DBSTRS ( <i>uplo, n, nrhs, ap, ipvt, bx, ldb, info</i> )
<b>C and C++</b>	dbstrs ( <i>uplo, n, nrhs, ap, ipvt, bx, ldb, info</i> );

### On Entry

<i>uplo</i>	<p>indicates whether original matrix <math>A</math> is stored in upper- or lower-packed storage mode, where:</p> <p>If <i>uplo</i> = 'U', <math>A</math> is stored in upper-packed storage mode.</p> <p>If <i>uplo</i> = 'L', <math>A</math> is stored in lower-packed storage mode.</p> <p>Specified as: a single character. It must be 'U' or 'L'.</p>
<i>n</i>	<p>is the order <math>n</math> of factored matrix <math>A</math> and the number of rows of matrix <math>B</math>.</p> <p>Specified as: a fullword integer; <math>n \geq 0</math>.</p>
<i>nrhs</i>	<p>is the number of right-hand sides; i.e., the number of columns of matrix <math>B</math>.</p> <p>Specified as: a fullword integer; <math>nrhs \geq 0</math>.</p>
<i>ap</i>	<p>is the factored matrix <math>A</math> produced by a preceding call to DBSTRF.</p> <p>Specified as: a one-dimensional array of length <i>nsinfo</i>, containing numbers of the data type indicated in Table 109. See Notes and "DBSTRF — Symmetric Indefinite Matrix Factorization" on page 530.</p>
<i>ipvt</i>	<p>is an integer vector of length <math>n</math>, containing the pivot information necessary to construct the factored form of <math>A</math>, produced by a preceding call to DBSTRF.</p> <p>Specified as: a one-dimensional array of (at least) length <math>n</math>, containing numbers of the data type indicated in Table 109. See Notes.</p>
<i>bx</i>	<p>is the general matrix <math>B</math>, containing the <i>nrhs</i> right-hand sides of the system. The right-hand sides, each of length <math>n</math>, reside in the columns of matrix <math>B</math>.</p>

Specified as: an *ldb* by (at least) *nrhs* array, containing numbers of the data type indicated in Table 109 on page 535.

*ldb* is the leading dimension of the array specified for *B*.

Specified as: a fullword integer;  $ldb > 0$  and  $ldb \geq n$ .

*info* See On Return.

### On Return

*bx* is the matrix *X*, containing the *nrhs* solutions to the system. The solutions, each of length *n*, reside in the columns of *X*.

Returned as: an *ldb* by (at least) *nrhs* array, containing numbers of the data type indicated in Table 109 on page 535.

*info* indicates the result of the computation.

- If *info* = 0, the subroutine completed successfully.

Returned as: a fullword integer.

## Notes

1. This subroutine accepts lowercase letters for the *uplo* argument.
2. In your C program, argument *info* must be passed by reference.
3. The array data specified for input arguments *ap* and *ipvt* for this subroutine must be the same as the corresponding output arguments for DBSTRF.
4. The scalar data specified for input arguments *uplo* and *n* must be the same as that specified for DBSTRF.
5. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.
6. For a description of how a symmetric matrix is stored in upper- or lower-packed storage mode in an array, see "Symmetric Matrix" on page 69.
7. To solve  $AX = B$  for *X*, where *B* and *X* are *n* by *nrhs* matrices, precede the call to DBSTRS with a call to DBSTRF.

## Function

The system  $AX = B$  is solved for *X*, where *A* is a real symmetric indefinite matrix, and *X* and *B* are real general matrices. This subroutine uses the results of the factorization of matrix *A*, produced by a preceding call to DBSTRF.

If *n* or *nrhs* is 0, no computation is performed and the subroutine returns after doing some parameter checking.

See references [8] and [67].

## Error conditions

### Resource Errors

None.

### Computational Errors

None.

**Note:** If the factorization performed by DBSTRF failed because matrix *A* is singular, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

## Input-Argument Errors

1.  $uplo \neq 'U'$  or  $'L'$
2.  $n < 0$
3.  $nrhs < 0$
4.  $n > ldb$
5.  $ldb \leq 0$

## Examples

### Example 1

This example shows how to solve the system  $AX = B$ , for three right-hand sides, where matrix  $A$  is the same matrix factored in the “Example 1” on page 533 for DBSTRF.

#### Call Statement and Input:

	UPLO	N	NRHS	AP	IPVT	BX	LDB	INFO
CALL DBSTRS (								
	'L'	8,	3,	AP,	IPVT,	BX,	8,	INFO )

AP = (for this subroutine must be the same as the corresponding output argument for DBSTRF. See “Example 1” on page 533 for DBSTRF.)

IPVT = (for this subroutine must be the same as the corresponding output argument for DBSTRF. See “Example 1” on page 533 for DBSTRF.)

$$BX = \begin{bmatrix} 1.0 & -38.0 & 47.0 \\ 7.0 & -10.0 & 73.0 \\ 6.0 & 52.0 & 2.0 \\ -30.0 & -228.0 & -42.0 \\ 32.0 & 183.0 & 105.0 \\ 34.0 & 297.0 & 9.0 \\ 32.0 & 244.0 & 44.0 \\ 62.0 & 497.0 & 61.0 \end{bmatrix}$$

#### Output:

$$BX = \begin{bmatrix} 1.0 & 1.0 & 8.0 \\ 1.0 & 2.0 & 7.0 \\ 1.0 & 3.0 & 6.0 \\ 1.0 & 4.0 & 5.0 \\ 1.0 & 5.0 & 4.0 \\ 1.0 & 6.0 & 3.0 \\ 1.0 & 7.0 & 2.0 \\ 1.0 & 8.0 & 1.0 \end{bmatrix}$$

INFO = 0

### Example 2

This example shows how to solve the system  $AX = B$ , for three right-hand sides, where matrix  $A$  is the same matrix factored in the “Example 2” on page 534 for DBSTRF.

#### Call Statement and Input:

	UPLO	N	NRHS	AP	IPVT	BX	LDB	INFO
CALL DBSTRS (								
	'U'	8,	3,	AP,	IPVT,	BX,	8,	INFO )

## DBSTRS

AP       =(for this subroutine must be the same  
          as the corresponding output argument for DBSTRF.  
          See "Example 2" on page 534 for DBSTRF.)

IPVT     =(for this subroutine must be the same  
          as the corresponding output argument for DBSTRF.  
          See "Example 2" on page 534 for DBSTRF.)

$$\text{BX} = \begin{bmatrix} 59.0 & 52.0 & 479.0 \\ 30.0 & 38.0 & 232.0 \\ 33.0 & 50.0 & 247.0 \\ 35.0 & 114.0 & 201.0 \\ -28.0 & -36.0 & -216.0 \\ 4.0 & -4.0 & 40.0 \\ 12.0 & 88.0 & 20.0 \\ 4.0 & 56.0 & -20.0 \end{bmatrix}$$

**Output:**

$$\text{BX} = \begin{bmatrix} 1.0 & 1.0 & 8.0 \\ 1.0 & 2.0 & 7.0 \\ 1.0 & 3.0 & 6.0 \\ 1.0 & 4.0 & 5.0 \\ 1.0 & 5.0 & 4.0 \\ 1.0 & 6.0 & 3.0 \\ 1.0 & 7.0 & 2.0 \\ 1.0 & 8.0 & 1.0 \end{bmatrix}$$

INFO = 0

## SGETRI, DGETRI, CGETRI, ZGETRI, SGEICD, and DGEICD — General Matrix Inverse, Condition Number Reciprocal, and Determinant

### Purpose

These subroutines find the inverse of general matrix  $A$ .

Subroutines SGEICD and DGEICD also find the reciprocal of the condition number and the determinant of general matrix  $A$ .

Table 110. Data Types

$A, aux, rcond, det, work$	Subroutine
Short-precision real	SGETRI <sup>△</sup> and SGEICD
Long-precision real	DGETRI <sup>△</sup> and DGEICD
Short-precision complex	CGETRI <sup>△</sup>
Long-precision complex	ZGETRI <sup>△</sup>
△LAPACK	

**Note:** The input to SGETRI, DGETRI, CGETRI, and ZGETRI must be the output from the factorization subroutines SGETRF, DGETRF, CGETRF, and ZGETRF, respectively.

If you call subroutines SGEICD and DGEICD with  $iopt = 4$ , the input must be the output from the factorization subroutines SGEF/SGEFCD/SGETRF or DGEF/DGEFCD/DGEFP/DGETRF, respectively.

### Syntax

<b>Fortran</b>	CALL SGETRI   DGETRI   CGETRI   ZGETRI ( $n, a, lda, ipvt, work, lwork, info$ ) CALL SGEICD   DGEICD ( $a, lda, n, iopt, rcond, det, aux, naux$ )
<b>C and C++</b>	sgetri   dgetri   cgetri   zgetri ( $n, a, lda, ipvt, work, lwork, info$ ); sgeicd   dgeicd ( $a, lda, n, iopt, rcond, det, aux, naux$ );

### On Entry

$a$  has the following meaning, where:

**For subroutines SGETRI, DGETRI, CGETRI, and ZGETRI:**

It is the transformed matrix  $A$  of order  $n$ , resulting from the factorization performed in a previous call to SGETRF, DGETRF, CGETRF, or ZGETRF, respectively, whose inverse is computed.

**For subroutines SGEICD and DGEICD:**

If  $iopt = 0, 1, 2,$  or  $3$ , it is matrix  $A$  of order  $n$ , whose inverse, reciprocal of condition number, and determinant are computed.

If  $iopt = 4$ , it is the transformed matrix  $A$  of order  $n$ , resulting from the factorization performed in a previous

## SGETRI, DGETRI, CGETRI, ZGETRI, SGEICD, and DGEICD

call to SGEF/SGEFCD or DGEF/DGEFCD/DGEFP, respectively, whose inverse is computed.

Specified as: an *lda* by (at least) *n* array, containing numbers of the data type indicated in Table 110 on page 539.

<i>lda</i>	is the leading dimension of the array specified for <i>a</i> . Specified as: a fullword integer; $lda > 0$ and $lda \geq n$ .
<i>n</i>	is the order of matrix <i>A</i> . Specified as: a fullword integer; $0 \leq n \leq lda$ .
<i>iopt</i>	indicates the type of computation to be performed, where: If <i>iopt</i> = 0, the inverse is computed for matrix <i>A</i> . If <i>iopt</i> = 1, the inverse and the reciprocal of the condition number are computed for matrix <i>A</i> . If <i>iopt</i> = 2, the inverse and the determinant are computed for matrix <i>A</i> . If <i>iopt</i> = 3, the inverse, the reciprocal of the condition number, and the determinant are computed for matrix <i>A</i> . If <i>iopt</i> = 4, the inverse is computed using the factored matrix <i>A</i> . Specified as: a fullword integer; <i>iopt</i> = 0, 1, 2, 3, 4.
<i>rcond</i>	See "On Return" on page 541.
<i>det</i>	See "On Return" on page 541.
<i>aux</i>	has the following meaning, and its size is specified by <i>naux</i> : If <i>iopt</i> = 0, 1, 2, or 3, then if <i>naux</i> = 0 and error 2015 is unrecoverable, <i>aux</i> is ignored. Otherwise, it is the storage work area used by this subroutine. If <i>iopt</i> = 4, <i>aux</i> has the following meaning: <ul style="list-style-type: none"><li>• For SGEICD, the first <i>n</i> locations in <i>aux</i> must contain the <i>ipvt</i> integer vector of length <i>n</i>, resulting from a previous call to SGEF, SGETRF, or SGEFCD.</li><li>• For DGEICD, the first <math>\text{ceiling}(n/2)</math> locations in <i>aux</i> must contain the <i>ipvt</i> integer vector of length <i>n</i>, resulting from a previous call to DGEF, DGETRF, DGEFCD, or DGEFP.</li></ul>
<i>naux</i>	Specified as: an area of storage, containing numbers of the data type indicated in Table 110 on page 539. is the size of the work area specified by <i>aux</i> ; that is, the number of elements in <i>aux</i> . Specified as: a fullword integer, where: If <i>iopt</i> $\neq$ 4, then if <i>naux</i> = 0 and error 2015 is unrecoverable, SGEICD and DGEICD dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program. Otherwise, $naux \geq 100n$ .

## SGETRI, DGETRI, CGETRI, ZGETRI, SGEICD, and DGEICD

**Note:** *naux* values specified for releases prior to ESSL Version 2 Release 2 will still work, but you may not achieve optimal performance.

*ipvt* is the integer vector *ipvt* of length *n*, containing the pivot indices resulting from a previous call to SGETRF, DGETRF, CGETRF, or ZGETRF.

Specified as: a one-dimensional array of (at least) length *n*, containing fullword integers, where  $1 \leq ipvt(i) \leq n$ .

*work*

has the following meaning:

If *lwork* = 0, *work* is ignored.

If *lwork* ≠ 0, *work* is the work area used by this subroutine, where:

- If *lwork* ≠ -1, its size is (at least) of length *lwork*.
- If *lwork* = -1, its size is (at least) of length 1.

Specified as: an area of storage containing numbers of data type indicated in Table 110 on page 539.

*lwork*

is the number of elements in array WORK.

Specified as: a fullword integer; where:

- If *lwork* = 0, SGETRI/DGETRI/CGETRI/ZGETRI dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program. This option is an extension to the LAPACK standard.
- If *lwork* = -1, SGETRI/DGETRI/CGETRI/ZGETRI performs a work area query and returns the optimal size of *work* in *work<sub>1</sub>*. No computation is performed and the subroutine returns after error checking is complete.
- Otherwise, it must be:  
 $lwork \geq \max(1, n)$
- For optimal performance,  $lwork \geq 100 * n$ .

*info*

See "On Return."

### On Return

*a*

is the resulting inverse of matrix *A* of order *n*. Returned as: an *lda* by (at least) *n* array, containing numbers of the data type indicated in Table 110 on page 539.

*rcond*

is the reciprocal of the condition number, *rcond*, of matrix *A*. Returned as: a real number of the data type indicated in Table 110 on page 539;  $rcond \geq 0$ .

*det*

is the vector *det*, containing the two components *det<sub>1</sub>* and *det<sub>2</sub>* of the determinant of matrix *A*. The determinant is:

$$det_1(10^{det_2})$$

where  $1 \leq det_1 < 10$ . Returned as: an array of length 2, containing numbers of the data type indicated in Table 110 on page 539.

*work*

is the work area used by this subroutine if *lwork* ≠ 0, where:

If *lwork* ≠ 0 and *lwork* ≠ -1, its size is (at least) of length *lwork*.

## SGETRI, DGETRI, CGETRI, ZGETRI, SGEICD, and DGEICD

If  $lwork = -1$ , its size is (at least) of length 1.

Returned as: an area of storage, where:

If  $lwork \geq 1$  or  $lwork = -1$ , then  $work_1$  is set to the optimal  $lwork$  value and contains numbers of the data type indicated in Table 110 on page 539. Except for  $work_1$ , the contents of  $work$  are overwritten on return.

*info* has the following meaning:

If  $info = 0$ , the inverse completed successfully.

If  $info > 0$ ,  $info$  is set equal to the first  $i$  where  $U_{ii}$  is exactly zero. The matrix is singular, and its inverse could not be computed.

Specified as: a fullword integer;  $info \geq 0$ .

### Notes

1. In your C program, arguments *rcond* and *info* must be passed by reference.
2. The input scalar arguments for SGETRI, DGETRI, CGETRI, and ZGETRI must be set to the same values as the corresponding input arguments in the previous call to SGETRF, DGETRF, CGETRF, and ZGETRF, respectively.  
If  $iopt = 4$ , the input scalar arguments for SGEICD and DGEICD must be set to the same values as the corresponding input arguments in the previous call to SGEF/SGEFCD or DGEF/DGEFCD/DGEFP, respectively.
3. You have the option of having the value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.
4. The way \_GETRI subroutines handle computational errors differs from LAPACK. Like LAPACK, these subroutines use the *info* argument to provide information about the computational error, but they also provide an error message.
5. On both input and output, matrix *A* conforms to LAPACK format.
6. For best performance, specify  $lwork = 0$ .

### Function

These subroutines compute the inverse of general square matrix *A*, where:

- $A^{-1}$  is the inverse of matrix *A*, where  $AA^{-1} = A^{-1}A = I$ , and *I* is the identity matrix.

Additionally, the subroutines SGEICD and DGEICD compute the reciprocal of the condition number and the determinant of a general square matrix *A*, using partial pivoting to preserve accuracy, where:

- $1/(\|A\|_1)(\|A^{-1}\|_1)$  is the reciprocal of the condition number, where  $\|A\|_1$  is the one-norm of matrix *A*.
- $|A|$  is the determinant of matrix *A*, where  $|A|$  is expressed as:

$$\det_1(10^{det_2})$$

The *iopt* argument is used to determine the combination of output items produced by SGEICD and DGEICD: the inverse, the reciprocal of the condition number, and the determinant.

If *n* is 0, no computation is performed. See references [38], [40], and [46].



## Error conditions

### Resource Errors

1. Unable to allocate internal work area.
2. If  $iopt = 0, 1, 2,$  or  $3,$  then error 2015 is unrecoverable,  $naux = 0,$  and unable to allocate work area.

### Computational Errors

Matrix  $A$  is singular or nearly singular.

For SGETRI, DGETRI, CGETRI, and ZGETRI:

- The index  $i$  of the first pivot element having a value equal to zero is identified in the computational error message.
- The computational error message may occur multiple times with processing continuing after each error, because the default for the number of allowable errors for error code 2149 is set to be unlimited in the ESSL error option table.

For SGEICD and DGEICD:

- The index  $i$  of the first pivot element having a value equal to 0 is identified in the computational error message.
- These subroutines return 0 for  $rcond$  and  $det,$  if you requested them.
- The return code is set to 2.
- $i$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2105 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $lda \leq 0$
2.  $n < 0$
3.  $n > lda$
4.  $iopt \neq 0, 1, 2, 3,$  or  $4$
5.  $lwork \neq 0, lwork \neq -1,$  and  $lwork < \max(1, n)$
6. Error 2015 is recoverable or  $naux \neq 0,$  and  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example computes the inverse of matrix  $A,$  where matrix  $A$  is the transformed matrix factored by SGETRF in “Example 3” on page 461 and the input contents of IPVT are the same as the output contents of IPVT in “Example 3” on page 461.

**Note:** Because  $lwork$  is 0, SGETRI dynamically allocates the work area used by this subroutine.

**Call Statement and Input:**

```

          N  A  LDA  IPVT  WORK  LWORK  INFO
          |  |  |    |    |    |    |
CALL SGETRI( 9 , A , 9 , IPVT , WORK , 0 , INFO )

```

A = (same as output A in “Example 3” on page 461)

IPVT = (same as output IPVT in “Example 3” on page 461)

## SGETRI, DGETRI, CGETRI, ZGETRI, SGEICD, and DGEICD

Output:

$$A = \begin{bmatrix} 0.333 & -0.667 & 0.333 & 0.000 & 0.000 & 0.000 & 0.042 & -0.042 & 0.000 \\ 56.833 & -52.167 & -1.167 & -0.500 & -0.500 & -0.357 & 6.836 & -0.479 & -0.500 \\ -55.167 & 51.833 & 0.833 & 0.500 & 0.500 & 0.214 & -6.735 & 0.521 & 0.500 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.143 & -0.143 & 0.000 & 0.000 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & -0.125 & 0.125 & 0.000 \\ -226.000 & 206.000 & 5.000 & 3.000 & 2.000 & 1.429 & -27.179 & 1.750 & 2.000 \\ 560.000 & -520.000 & -10.000 & -6.000 & -4.000 & -2.857 & 67.857 & -5.000 & -5.000 \\ -325.000 & 305.000 & 5.000 & 3.000 & 2.000 & 1.429 & -39.554 & 3.125 & 3.000 \end{bmatrix}$$

INFO = 0

### Example 2

This example computes the inverse of matrix  $A$ , where  $A$  is the transformed matrix factored by ZGETRF in "Example 2" on page 460 and the input contents of IPVT are the same as the output contents of IPVT in "Example 2" on page 460.

**Note:** Because  $lwork$  is 0, ZGETRI dynamically allocates the work area used by this subroutine.

### Call Statement and Input:

```

          N   A   LDA   IPVT   WORK   LWORK   INFO
          |   |   |     |     |     |     |
CALL ZGETRI( 9 , A , 9 , IPVT , WORK , 0 , INFO )

```

A = (same as output A in "Example 2" on page 460)

IPVT = (same as output IPVT in "Example 2" on page 460)

Output:

$$A = \begin{bmatrix} (-0.2, -0.4) & (-0.1, 0.1) & (-0.1, 0.1) & (0.0, 0.1) & (0.1, 0.1) & (0.1, 0.1) & (0.1, 0.1) & (0.1, 0.0) & (0.1, 0.0) & (0.0, -0.3) \\ (0.2, 0.4) & (0.0, -0.6) & (-0.1, 0.0) & (-0.1, 0.0) & (-0.1, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.1, 0.0) \\ (0.0, 0.0) & (0.2, 0.4) & (0.0, -0.6) & (-0.1, 0.0) & (-0.1, 0.0) & (-0.1, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.1, 0.0) \\ (0.0, 0.0) & (0.0, 0.0) & (0.2, 0.4) & (0.0, -0.6) & (-0.1, 0.0) & (-0.1, 0.0) & (-0.1, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.1, 0.1) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.2, 0.4) & (0.0, -0.6) & (-0.1, 0.0) & (-0.1, 0.0) & (-0.1, 0.0) & (-0.1, 0.0) & (0.1, 0.1) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.2, 0.4) & (0.0, -0.6) & (-0.1, 0.0) & (-0.1, 0.0) & (-0.1, 0.0) & (0.0, 0.1) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.2, 0.4) & (0.0, -0.6) & (-0.1, 0.0) & (-0.1, 0.0) & (-0.1, 0.1) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.2, 0.4) & (0.0, -0.6) & (-0.1, 0.1) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.2, 0.4) & (-0.2, -0.4) \end{bmatrix}$$

INFO = 0

### Example 3

This example computes the inverse, the reciprocal of the condition number, and the determinant of matrix  $A$ . The values used to compute the reciprocal of the condition number in this example are obtained with the following values:

$$\|A\|_1 = \max(6.0, 8.0, 10.0, 12.0, 13.0, 14.0, 15.0, 15.0, 15.0) = 15.0$$

$$\|A^{-1}\|_1 = 1226.33$$

On output, the value in  $det, |A|$ , is equal to 336.

## SGETRI, DGETRI, CGETRI, ZGETRI, SGEICD, and DGEICD

### Call Statement and Input:

```

          A  LDA  N  IOPT  RCOND  DET  AUX  NAUX
          |  |  |  |  |  |  |  |
CALL DGEICD( A , 9 , 9 , 3 , RCOND , DET , AUX , 293 )
    
```

$$A = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 4.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 5.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 6.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 7.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 8.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 9.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 10.0 & 11.0 & 12.0 \end{bmatrix}$$

### Output:

$$A = \begin{bmatrix} 0.333 & -0.667 & 0.333 & 0.000 & 0.000 & 0.000 & 0.042 & -0.042 & 0.000 \\ 56.833 & -52.167 & -1.167 & -0.500 & -0.500 & -0.357 & 6.836 & -0.479 & -0.500 \\ -55.167 & 51.833 & 0.833 & 0.500 & 0.500 & 0.214 & -6.735 & 0.521 & 0.500 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.143 & -0.143 & 0.000 & 0.000 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & -0.125 & 0.125 & 0.000 \\ -226.000 & 206.000 & 5.000 & 3.000 & 2.000 & 1.429 & -27.179 & 1.750 & 2.000 \\ 560.000 & -520.000 & -10.000 & -6.000 & -4.000 & -2.857 & 67.857 & -5.000 & -5.000 \\ -325.000 & 305.000 & 5.000 & 3.000 & 2.000 & 1.429 & -39.554 & 3.125 & 3.000 \end{bmatrix}$$

```

RCOND  = 0.00005436
DET     = (3.36, 2.00)
    
```

### Example 4

This example computes the inverse of matrix  $A$ , where:  $iopt = 4$ ; matrix  $A$  is the transformed matrix factored by SGEF in “Example 1” on page 468; and the input contents of AUX are the same as the output contents of IPVT in “Example 1” on page 468.

### Call Statement and Input:

```

          A  LDA  N  IOPT  RCOND  DET  AUX  NAUX
          |  |  |  |  |  |  |  |
CALL SGEICD( A , 9 , 9 , 4 , RCOND , DET , AUX , 300 )
    
```

```

A      = (same as output A in “Example 1” on page 468)
AUX    = (same as output IPVT in “Example 1” on page 468)
    
```

### Output:

$$A = \begin{bmatrix} 0.333 & -0.667 & 0.333 & 0.000 & 0.000 & 0.000 & 0.042 & -0.042 & 0.000 \\ 56.833 & -52.167 & -1.167 & -0.500 & -0.500 & -0.357 & 6.836 & -0.479 & -0.500 \\ -55.167 & 51.833 & 0.833 & 0.500 & 0.500 & 0.214 & -6.735 & 0.521 & 0.500 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.143 & -0.143 & 0.000 & 0.000 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & -0.125 & 0.125 & 0.000 \\ -226.000 & 206.000 & 5.000 & 3.000 & 2.000 & 1.429 & -27.179 & 1.750 & 2.000 \\ 560.000 & -520.000 & -10.000 & -6.000 & -4.000 & -2.857 & 67.857 & -5.000 & -5.000 \\ -325.000 & 305.000 & 5.000 & 3.000 & 2.000 & 1.429 & -39.554 & 3.125 & 3.000 \end{bmatrix}$$

**SPOTRI, DPOTRI, CPOTRI, ZPOTRI, SPOICD, DPOICD, SPPTRI, DPPTRI, SPPICD, and DPPICD**

## SPOTRI, DPOTRI, CPOTRI, ZPOTRI, SPOICD, DPOICD, SPPTRI, DPPTRI, SPPICD, and DPPICD — Positive Definite Real Symmetric or Complex Hermitian Matrix Inverse, Condition Number Reciprocal, and Determinant

### Purpose

These subroutines find the inverse of a positive definite real symmetric or complex Hermitian matrix  $A$  using Cholesky factorization, where:

- For SPOTRI, DPOTRI, CPOTRI, ZPOTRI, SPOICD, and DPOICD,  $A$  is stored in upper or lower storage mode.
- For SPPTRI and DPPTRI,  $A$  is stored in upper- or lower-packed storage mode.
- For SPPICD and DPPICD,  $A$  is stored in lower-packed storage mode.

Subroutines SPOICD, DPOICD, SPPICD, and DPPICD also find the reciprocal of the condition number and the determinant of matrix  $A$ .

Table 111. Data Types

$A$ , $aux$ , $rcond$ , $det$	Subroutine
Short-precision real	SPOTRI <sup>△</sup> , SPOICD, SPPTRI <sup>△</sup> , and SPPICD
Long-precision real	DPOTRI <sup>△</sup> , DPOICD, DPPTRI <sup>△</sup> , and DPPICD
Short-precision complex	CPOTRI <sup>△</sup>
Long-precision complex	ZPOTRI <sup>△</sup>
<sup>△</sup> LAPACK	

**Note:** For each of the `_POTRI` and `_PPTRI` subroutines, the input must be the output from the corresponding `_POTRF` or `_PPTRF` Cholesky factorization subroutine.

If you call the subroutines SPOICD, DPOICD, SPPICD, and DPPICD with `iopt=4`, the input must be the output from SPPE, DPPE, SPOF/SPOFCD, or DPOF/DPOFCD, respectively, where Cholesky factorization was performed.

### Syntax

<b>Fortran</b>	CALL SPOTRI   DPOTRI   CPOTRI   ZPOTRI ( <i>uplo</i> , <i>n</i> , <i>a</i> , <i>lda</i> , <i>info</i> ) CALL SPOICD   DPOICD ( <i>uplo</i> , <i>a</i> , <i>lda</i> , <i>n</i> , <i>iopt</i> , <i>rcond</i> , <i>det</i> , <i>aux</i> , <i>naux</i> ) CALL SPPTRI   DPPTRI ( <i>uplo</i> , <i>n</i> , <i>ap</i> , <i>info</i> ) CALL SPPICD   DPPICD ( <i>ap</i> , <i>n</i> , <i>iopt</i> , <i>rcond</i> , <i>det</i> , <i>aux</i> , <i>naux</i> )
<b>C and C++</b>	<code>spotri   dpotri   cpotri   zpotri (uplo, n, a, lda, info);</code> <code>spoicd   dpoicd (uplo, a, lda, n, iopt, rcond, det, aux, naux);</code> <code>spptri   dpptri (uplo, n, ap, info);</code> <code>sppicd   dppicd (ap, n, iopt, rcond, det, aux, naux);</code>

**On Entry**

*uplo* indicates whether matrix *A* is stored in upper or lower storage mode, where:

If *uplo* = 'U', *A* is stored in upper storage mode.

If *uplo* = 'L', *A* is stored in lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

*ap* is the array, referred to as AP, where:

**For SPPTRI and DPPTRI:**

AP contains the transformed matrix *A* of order *n*, resulting from the Cholesky factorization performed in a previous call to SPPTRF or DPPTRF, respectively, whose inverse is computed.

**For SPPICD and DPPICD:**

If *iopt* = 0, 1, 2, or 3, then AP contains the positive definite real symmetric matrix *A*, whose inverse, condition number reciprocal, and determinant are computed, where matrix *A* is stored in lower-packed storage mode.

If *iopt* = 4, then AP contains the transformed matrix *A* of order *n*, resulting from the Cholesky factorization performed in a previous call to SPPF or DPPF, respectively, whose inverse is computed.

Specified as: a one-dimensional array of (at least) length  $n(n+1)/2$ , containing numbers of the data type indicated in Table 111 on page 547.

*a* has the following meaning, where:

**For SPOTRI, DPOTRI, CPOTRI, and ZPOTRI:**

It is the transformed matrix *A* of order *n*, containing results of the factorization from a previous call to SPOTRF, DPOTRF, CPOTRF, or ZPOTRF, respectively, whose inverse is computed.

**For SPOICD and DPOICD:**

If *iopt* = 0, 1, 2, or 3, it is the positive definite real symmetric matrix *A*, whose inverse, condition number reciprocal, and determinant are computed, where matrix *A* is stored in upper or lower storage mode.

If *iopt* = 4, it is the transformed matrix *A* of order *n*, containing results of the factorization from a previous call to SPOF/SPOFCD or DPOF/DPOFCD, respectively, whose inverse is computed.

Specified as: an *lda* by (at least) *n* array, containing numbers of the data type indicated in Table 111 on page 547.

*lda* is the leading dimension of the array specified for *a*.

Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .

*n* is the order *n* of matrix *A*.

Specified as: a fullword integer;  $n \geq 0$ .

*iopt* indicates the type of computation to be performed, where:  
 If  $iopt = 0$ , the inverse is computed for matrix  $A$ .  
 If  $iopt = 1$ , the inverse and the reciprocal of the condition number are computed for matrix  $A$ .  
 If  $iopt = 2$ , the inverse and the determinant are computed for matrix  $A$ .  
 If  $iopt = 3$ , the inverse, the reciprocal of the condition number, and the determinant are computed for matrix  $A$ .  
 If  $iopt = 4$ , the inverse is computed for the Cholesky factored matrix  $A$ .  
 Specified as: a fullword integer;  $iopt = 0, 1, 2, 3, \text{ or } 4$ .

*rcond* See "On Return."

*det* See "On Return."

*aux* has the following meaning:  
 If  $naux = 0$  and error 2015 is unrecoverable, *aux* is ignored.  
 Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*. Specified as: an area of storage, containing numbers of the data type indicated in Table 111 on page 547.

*naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.  
 Specified as: a fullword integer, where:  
 If  $naux = 0$  and error 2015 is unrecoverable, SPOICD, DPOICD, SPPICD, and DPPICD dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.  
 Otherwise,  $naux \geq n$ .

*info* See "On Return."

### On Return

*ap* is an array, referred to as AP, in which the transformed matrix  $A$  of order  $n$ , containing the inverse of the matrix, is stored.  
**For SPPTRI and DPPTRI:**  
 The transformed matrix is stored in upper- or lower-packed storage mode.  
**For SPPICD and DPPICD:**  
 The transformed matrix is stored in lower-packed storage mode.  
 Returned as: a one-dimensional array of at least length  $n(n+1)/2$ , containing numbers of the data type indicated in Table 111 on page 547.

*a* is the transformed matrix  $A$  of order  $n$ , containing the inverse of the matrix in upper or lower storage mode. Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 111 on page 547.

## SPOTRI, DPOTRI, CPOTRI, ZPOTRI, SPOICD, DPOICD, SPPTRI, DPPTRI, SPPICD, and DPPICD

*rcond* is the reciprocal of the condition number, *rcond*, of matrix *A*.  
Returned as: a real number of the data type indicated in Table 111 on page 547;  $rcond \geq 0$ .

*det* is the vector *det*, containing the two components  $det_1$  and  $det_2$  of the determinant of matrix *A*. The determinant is:

$$det_1(10^{det_2})$$

where  $1 \leq det_1 < 10$ . Returned as: an array of length 2, containing numbers of the data type indicated in Table 111 on page 547.

*info* has the following meaning:

If  $info = 0$ , the inverse completed successfully.

If  $info > 0$ , *info* is set equal to the first *i* where  $A_{ii}$  is zero; the matrix is not positive definite, and its inverse could not be completed.

Specified as: a fullword integer;  $info \geq 0$ .

### Notes

1. In your C program, the arguments *info* and *rcond* must be passed by reference.
2. For SPOICD, DPOICD, SPPICD, and DPPICD, when you specify *iopt* = 4, you must do the following:
  - For SPOICD and DPOICD, specify the same storage mode for matrix *A* that was specified in the previous call to SPOF/SPOFCD or DPOF/DPOFCD, respectively.
  - For SPPICD and DPPICD, use Cholesky factorization in the previous call to SPPF or DPPF, respectively.
3. The scalar data specified for input arguments *uplo*, *lda*, and *n* for these subroutines must be the same as the input arguments specified for the corresponding factorization subroutines.
4. All subroutines accept lowercase letters for the *uplo* argument.
5. SPPICD and DPPICD in some cases utilize algorithms based on recursive packed storage format. (See references [54], [68], and [70]).
6. The way \_POTRI and \_PPTRI subroutines handle computational errors differs from LAPACK. Like LAPACK, these subroutines use the *info* argument to provide information about the computational error, but they also provide an error message.
7. On both input and output, matrix *A* conforms to LAPACK format.
8. For a description of how a positive definite symmetric matrix is stored in upper- or lower-packed storage mode in an array or in upper or lower storage mode, see "Symmetric Matrix" on page 69.
9. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

### Function

These subroutines find the inverse of positive definite matrix *A*, where:

- $A^{-1}$  is the inverse of matrix *A*, where  $AA^{-1} = A^{-1}A = I$ .



- For positive definite real symmetric matrix  $A$ :  
 $A = LL^T$  or  $U^T U$   
 $A^{-1} = L^{-T} L^{-1}$  or  $U^{-1} U^{-T}$
- For positive definite complex Hermitian matrix  $A$ :  
 $A = LL^H$  or  $U^H U$   
 $A^{-1} = L^{-H} L^{-1}$  or  $U^{-1} U^{-H}$

**Note:** SPPICD and DPPICD only support a matrix in lower-packed storage mode.

Additionally, the subroutines SPOICD, DPOICD, SPPICD, and DPPICD find the reciprocal of the condition number and the determinant of positive definite symmetric matrix  $A$  using Cholesky factorization, where:

- $1/(\|A\|_1)(\|A^{-1}\|_1)$  is the reciprocal of the condition number, where  $\|A\|_1$  is the one-norm of matrix  $A$ .
- $|A|$  is the determinant of matrix  $A$ , where  $|A|$  is expressed as:

$$\det_1(10^{det_2})$$

- The *iopt* argument is used to determine the combination of output items produced: the inverse, the reciprocal of the condition number, and the determinant.

If  $n$  is 0, no computation is performed. See references [38], [40], and [46].

## Error conditions

### Resource Errors

- Unable to allocate internal work area.
- Error 2015 is unrecoverable, *naux* = 0, and unable to allocate work area.

### Computational Errors

**Note:** If the Cholesky factorization performed by one of the `_POTRF` and `_PPTRF` subroutines failed because matrix  $A$  was not positive definite, the results returned by the corresponding `_POTRI` or `_PPTRI` subroutine are unpredictable.

If the Cholesky factorization performed by `SPPF`, `DPPF`, `SPOF/SPOFCD`, or `DPOF/DPOFCD` failed because matrix  $A$  was not positive definite, the results returned by `SPOICD`, `DPOICD`, `SPPICD`, or `DPPICD`, respectively, with *iopt*=4, are unpredictable.

**For SPOTRI, DPOTRI, CPOTRI, ZPOTRI, SPPTRI, and DPPTRI:**

The inverse of matrix  $A$  could not be computed.

- One or more of the diagonal elements of the factored matrix  $A$  are zero. The first diagonal element that is found to be exactly zero is identified in the computational error message and returned in *info*. If one or more of the diagonal elements of the factored matrix  $A$  are negative, the results are unpredictable.

- The computational error message may occur multiple times with processing continuing after each error because the default for the number of allowable errors for error code 2151 is set to be unlimited in the ESSL error option table.

**For SPOICD, DPOICD, SPPICD, and DPPICD:**

Matrix *A* is not positive definite.

- These subroutines do not perform the inverse, determinant, and reciprocal of the condition number computations.
- For *iopt* = 1, 2, or 3, the leading minor of order *i* has a nonpositive determinant. The order *i* is identified in the computational error message.
- *i* can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2115 in the error option table; otherwise, the default value causes your program to terminate. If your program is not terminated, the return code is set to 2. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

The inverse of matrix *A* could not be computed.

- For *iopt* = 4, for \_POICD and \_PPICD, one or more of the diagonal elements of the factored matrix *A* are zero. *i* is the first diagonal element that is found to be exactly zero and is identified in the computational error message. If one or more of the diagonal elements of the factored matrix *A* are negative, the results are unpredictable.
- *i* can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2150 in the error option table; otherwise, the default value causes your program to terminate. If your program is not terminated, the return code is set to 3. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

**Input-Argument Errors**

1. *uplo* ≠ 'U' or 'L'
2. *n* < 0
3. *lda* ≤ 0
4. *lda* < *n*
5. *iopt* ≠ 0, 1, 2, 3, or 4
6. Error 2015 is recoverable or *naux* ≠ 0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Examples**

**Example 1**

This example uses SPOTRI to compute the inverse of matrix *A*, where *iopt* = 4, and matrix *A* is the transformed matrix factored by SPOTRF in “Example 9” on page 505.

**Call Statement and Input:**

```

          UPLO N  A  LDA  INFO
          |   |  |   |   |
CALL SPOTRI( 'U' , 9 , A , 9 , INFO )
    
```

A           =(same as output A in “Example 2” on page 501 for SPOTRF)

Output:

$$A = \begin{bmatrix} 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ . & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ . & . & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ . & . & . & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ . & . & . & . & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 \\ . & . & . & . & . & 2.0 & -1.0 & 0.0 & 0.0 \\ . & . & . & . & . & . & 2.0 & -1.0 & 0.0 \\ . & . & . & . & . & . & . & 2.0 & -1.0 \\ . & . & . & . & . & . & . & . & 1.0 \end{bmatrix}$$

INFO = 0

### Example 2

This example uses CPOTRI to compute the inverse of the matrix  $A$ , stored in lower storage mode. Matrix  $A$  is the transformed matrix factored by CPOTRF in “Example 3” on page 502.

Call Statement and Input:

```

          UPLO N  A  LDA  INFO
          |   |  |   |   |
CALL CPOTRI( 'L' , 3 , A , 3 , INFO )

```

$A$  = (same as output  $A$  in “Example 3” on page 502 for CPOTRF)

Output:

$$A = \begin{bmatrix} (.05, .00) & . & . \\ (.00, -.01) & (.02, .00) & . \\ (-.01, .00) & (.00, .00) & (.02, .00) \end{bmatrix}$$

INFO = 0

### Example 3

This example uses CPOTRI to compute the inverse of the matrix  $A$ , stored in upper storage mode. Matrix  $A$  is the transformed matrix factored by CPOTRF in “Example 4” on page 502.

Call Statement and Input:

```

          UPLO N  A  LDA  INFO
          |   |  |   |   |
CALL CPOTRI( 'U' , 3 , A , 3 , INFO )

```

$A$  = (same as output  $A$  in “Example 4” on page 502 for CPOTRF)

Output:

$$A = \begin{bmatrix} (.13, .00) & (-.02, -.03) & (.00, .01) \\ . & (.07, .00) & (-.01, .01) \\ . & . & (.03, .00) \end{bmatrix}$$

INFO = 0

### Example 4

This example uses SPOICD to compute the inverse, reciprocal of the condition number, and determinant of matrix  $A$ , stored in upper storage mode. Matrix  $A$  is:

**SPOTRI, DPOTRI, CPOTRI, ZPOTRI, SPOICD, DPOICD, SPPTRI, DPPTRI, SPPICD, and DPPICD**

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 1.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 \\ 1.0 & 2.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 4.0 & 4.0 & 4.0 & 4.0 & 4.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 5.0 & 5.0 & 5.0 & 5.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 6.0 & 6.0 & 6.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 7.0 & 7.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 & 8.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 & 8.0 & 9.0 \end{bmatrix}$$

The values used to compute the reciprocal of the condition number in this example are obtained with the following values:

$$\|A\|_1 = \max(9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0) = 45.0$$

$$\|A^{-1}\|_1 = 4.0$$

On output, the value in *det*,  $|A|$ , is equal to 1, and RCOND = 1/180.

**Call Statement and Input:**

```

          UPLO  A  LDA  N  IOPT  RCOND  DET  AUX  NAUX
CALL SPOICD( 'U' , A , 9 , 9 , 3 , RCOND , DET , AUX , 9 )
    
```

$$A = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ . & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 \\ . & . & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 \\ . & . & . & 4.0 & 4.0 & 4.0 & 4.0 & 4.0 & 4.0 \\ . & . & . & . & 5.0 & 5.0 & 5.0 & 5.0 & 5.0 \\ . & . & . & . & . & 6.0 & 6.0 & 6.0 & 6.0 \\ . & . & . & . & . & . & 7.0 & 7.0 & 7.0 \\ . & . & . & . & . & . & . & 8.0 & 8.0 \\ . & . & . & . & . & . & . & . & 9.0 \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ . & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ . & . & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ . & . & . & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ . & . & . & . & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 \\ . & . & . & . & . & 2.0 & -1.0 & 0.0 & 0.0 \\ . & . & . & . & . & . & 2.0 & -1.0 & 0.0 \\ . & . & . & . & . & . & . & 2.0 & -1.0 \\ . & . & . & . & . & . & . & . & 1.0 \end{bmatrix}$$

RCOND = 0.005555556  
 DET = (1.0, 0.0)

**Example 5**

This example uses SPPTRI to compute the inverse of matrix *A*, where matrix *A* is the transformed matrix factored in “Example 5” on page 503 by SPPTRF.

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in lower-packed storage mode.

**Call Statement and Input:**

```

          UPLO N  AP  INFO
          |   |   |   |
CALL SPPTRI( 'L' , 9 , AP , INFO )

```

AP       =(same as output AP in “Example 5” on page 503 for SPPTRF)

**Output:**

```

AP  = (2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
       2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
       2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
       2.0, -1.0, 0.0, 0.0, 0.0, 0.0,
       2.0, -1.0, 0.0, 0.0,
       2.0, -1.0, 0.0,
       2.0, -1.0,
       1.0)

```

INFO = 0

**Example 6**

This example uses SPPTRI to compute the inverse of matrix *A*, where matrix *A* is the transformed matrix factored in “Example 6” on page 504 by SPPTRF.

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in upper-packed storage mode.

**Call Statement and Input:**

```

          UPLO N  AP  INFO
          |   |   |   |
CALL SPPTRI( 'U' , 9 , AP , INFO )

```

AP       =(same as output AP in “Example 6” on page 504 for SPPTRF)

**Output:**

```

AP  = (
                                     2.0,
                                     -1.0, 2.0,
                                     0.0, -1.0, 2.0,
                                     0.0, 0.0, -1.0, 2.0,
                                     0.0, 0.0, 0.0, -1.0, 2.0,
                                     0.0, 0.0, 0.0, 0.0, -1.0, 2.0,
                                     0.0, 0.0, 0.0, 0.0, 0.0, -1.0, 2.0,
                                     0.0, 0.0, 0.0, 0.0, 0.0, 0.0, -1.0, 2.0,
                                     0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, -1.0, 2.0,
                                     0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, -1.0, 1.0)

```

INFO = 0

**Example 7**

This example uses SPPICD to compute the inverse, reciprocal of the condition number, and determinant of the same matrix *A* used in “Example 4” on page 553; however, matrix *A* is stored in lower-packed storage mode in this example.

The values used to compute the reciprocal of the condition number in this example are obtained with the following values:

$$\|A\|_1 = \max(9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0) = 45.0$$

$$\|A^{-1}\|_1 = 4.0$$

On output, the value in *det*,  $|A|$ , is equal to 1, and RCOND = 1/180.

**SPOTRI, DPOTRI, CPOTRI, ZPOTRI, SPOICD, DPOICD, SPPTRI, DPPTRI, SPPICD, and DPPICD**

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in lower-packed storage mode.

**Call Statement and Input:**

```

          AP  N  IOPT RCOND  DET  AUX  NAUX
          |  |  |    |    |    |    |
CALL SPPICD( AP , 9 , 3 , RCOND , DET , AUX , 9 )

```

```

AP = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
      2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0,
      3.0, 3.0, 3.0, 3.0, 3.0, 3.0, 3.0,
      4.0, 4.0, 4.0, 4.0, 4.0, 4.0,
      5.0, 5.0, 5.0, 5.0,
      6.0, 6.0, 6.0, 6.0,
      7.0, 7.0, 7.0,
      8.0, 8.0,
      9.0)

```

**Output:**

```

AP = (2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
      2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
      2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0,
      2.0, -1.0, 0.0, 0.0, 0.0, 0.0,
      2.0, -1.0, 0.0, 0.0, 0.0,
      2.0, -1.0, 0.0,
      2.0, -1.0,
      1.0)

```

```

RCOND = 0.005556
DET    = (1.0, 0.0)

```

**Example 8**

This example uses SPPICD to compute the inverse of matrix *A*, where *iopt* = 4, and matrix *A* is the transformed matrix factored in “Example 10” on page 506 by SPPF.

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in lower-packed storage mode.

**Call Statement and Input:**

```

          AP  N  IOPT RCOND  DET  AUX  NAUX
          |  |  |    |    |    |    |
CALL SPPICD(AP , 9 , 4 , RCOND , DET , AUX , 9)

```

AP = (same as output AP in “Example 10” on page 506 for SPPF)

**Output:**

```

AP = (2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
      2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
      2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0,
      2.0, -1.0, 0.0, 0.0, 0.0, 0.0,
      2.0, -1.0, 0.0, 0.0, 0.0,
      2.0, -1.0, 0.0, 0.0,
      2.0, -1.0, 0.0,
      2.0, -1.0,
      1.0)

```

## STRSV, DTRSV, CTRSV, ZTRSV, STPSV, DTPSV, CTPSV, and ZTPSV — Solution of a Triangular System of Equations with a Single Right-Hand Side

### Purpose

STRSV, DTRSV, STPSV, and DTPSV perform one of the following solves for a triangular system of equations with a single right-hand side, using the vector  $x$  and triangular matrix  $A$  or its transpose:

Solution	Equation
1. $x \leftarrow A^{-1}x$	$Ax = b$
2. $x \leftarrow A^{-T}x$	$A^T x = b$

CTRSV, ZTRSV, CTPSV, and ZTPSV perform one of the following solves for a triangular system of equations with a single right-hand side, using the vector  $x$  and and triangular matrix  $A$ , its transpose, or its conjugate transpose:

Solution	Equation
1. $x \leftarrow A^{-1}x$	$Ax = b$
2. $x \leftarrow A^{-T}x$	$A^T x = b$
3. $x \leftarrow A^{-H}x$	$A^H x = b$

Matrix  $A$  can be either upper or lower triangular, where:

- For the `_TRSV` subroutines, it is stored in upper- or lower-triangular storage mode, respectively.
- For the `_TPSV` subroutines, it is stored in upper- or lower-triangular-packed storage mode, respectively.

**Note:** The term  $b$  used in the systems of equations listed above represents the right-hand side of the system. It is important to note that in these subroutines the right-hand side of the equation is actually provided in the input-output argument  $x$ .

Table 112. Data Types

$A, x$	Subroutine
Short-precision real	STRSV and STPSV
Long-precision real	DTRSV and DTPSV
Short-precision complex	CTRSV and CTPSV
Long-precision complex	ZTRSV and ZTPSV

### Syntax

<b>Fortran</b>	CALL STRSV   DTRSV   CTRSV   ZTRSV ( <i>uplo, transa, diag, n, a, lda, x, incx</i> ) CALL STPSV   DTPSV   CTPSV   ZTPSV ( <i>uplo, transa, diag, n, ap, x, incx</i> )
<b>C and C++</b>	strsv   dtrsv   ctrsv   ztrsv ( <i>uplo, transa, diag, n, a, lda, x, incx</i> ); stpsv   dtpsv   ctpsv   ztpsv ( <i>uplo, transa, diag, n, ap, x, incx</i> );

## STRSV, DTRSV, CTRSV, ZTRSV, STPSV, DTPSV, CTPSV, and ZTPSV

### On Entry

<i>uplo</i>	indicates whether matrix $A$ is an upper or lower triangular matrix, where: If $uplo = 'U'$ , $A$ is an upper triangular matrix. If $uplo = 'L'$ , $A$ is a lower triangular matrix. Specified as: a single character. It must be 'U' or 'L'.
<i>transa</i>	indicates the form of matrix $A$ used in the system of equations, where: If $transa = 'N'$ , $A$ is used, resulting in solution 1. If $transa = 'T'$ , $A^T$ is used, resulting in solution 2. If $transa = 'C'$ , $A^H$ is used, resulting in solution 3. Specified as: a single character. It must be 'N', 'T', or 'C'.
<i>diag</i>	indicates the characteristics of the diagonal of matrix $A$ , where: If $diag = 'U'$ , $A$ is a unit triangular matrix. If $diag = 'N'$ , $A$ is not a unit triangular matrix. Specified as: a single character. It must be 'U' or 'N'.
<i>n</i>	is the order of triangular matrix $A$ . Specified as: a fullword integer; $n \geq 0$ and $n \leq lda$ .
<i>a</i>	is the upper or lower triangular matrix $A$ of order $n$ , stored in upper- or lower-triangular storage mode, respectively. Specified as: an $lda$ by (at least) $n$ array, containing numbers of the data type indicated in Table 112 on page 557.
<i>lda</i>	is the leading dimension of the array specified for $a$ . Specified as: a fullword integer; $lda > 0$ and $lda \geq n$ .
<i>ap</i>	is the upper or lower triangular matrix $A$ of order $n$ , stored in upper- or lower-triangular-packed storage mode, respectively. Specified as: a one-dimensional array of (at least) length $n(n+1)/2$ , containing numbers of the data type indicated in Table 112 on page 557.
<i>x</i>	is the vector $x$ of length $n$ , containing the right-hand side of the triangular system to be solved. Specified as: a one-dimensional array of (at least) length $1+(n-1) incx $ , containing numbers of the data type indicated in Table 112 on page 557.
<i>incx</i>	is the stride for vector $x$ . Specified as: a fullword integer; $incx > 0$ or $incx < 0$ .

### On Return

<i>x</i>	is the solution vector $x$ of length $n$ , containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 112 on page 557.
----------	---



## Notes

1. These subroutines accept lowercase letters for the *uplo*, *transa*, and *diag* arguments.
2. For STRSV, DTRSV, STPSV, and DTPSV, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
3. Matrix  $A$  and vector  $x$  must have no common elements; otherwise, results are unpredictable.
4. ESSL assumes certain values in your array for parts of a triangular matrix. As a result, you do not have to set these values. For unit diagonal matrices, the elements of the diagonal are assumed to be 1.0 for real matrices and (1.0, 0.0) for complex matrices. When using upper- or lower-triangular storage, the unreferenced elements in the lower and upper triangular part, respectively, are assumed to be zero.
5. For a description of triangular matrices and how they are stored in upper- and lower-triangular storage mode and in upper- and lower-triangular-packed storage mode, see “Triangular Matrix” on page 77.

## Function

These subroutines solve a triangular system of equations with a single right-hand side. The solution  $x$  may be any of the following, where triangular matrix  $A$ , its transpose, or its conjugate transpose is used, and where  $A$  can be either upper- or lower-triangular:

$$x \leftarrow A^{-1}x$$

$$x \leftarrow A^{-T}x$$

$$x \leftarrow A^{-H}x \text{ (only for CTRSV, ZTRSV, CTPSV, and ZTPSV)}$$

where:

$x$  is a vector of length  $n$ .

$A$  is an upper or lower triangular matrix of order  $n$ . For `_TRSV`, it is stored in upper- or lower-triangular storage mode, respectively. For `_TPSV`, it is stored in upper- or lower-triangular-packed storage mode, respectively.

If  $n$  is 0, no computation is performed. See references [34], [38], and [40].

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1. *uplo*  $\neq$  'L' or 'U'
2. *transa*  $\neq$  'T', 'N', or 'C'
3. *diag*  $\neq$  'N' or 'U'
4.  $n < 0$
5.  $lda \leq 0$
6.  $lda < n$
7.  $incx = 0$

## Examples

### Example 1

This example shows the solution  $x \leftarrow A^{-1}x$ . Matrix  $A$  is a real 4 by 4 lower unit triangular matrix, stored in lower-triangular storage mode. Vector  $x$  is a vector of length 4.

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

#### Call Statement and Input:

```

          UPLO TRANSA DIAG  N  A  LDA  X  INCX
CALL STRSV( 'L' , 'N' , 'U' , 4 , A , 4 , X , 1 )

```

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ 1.0 & \cdot & \cdot & \cdot \\ 2.0 & 3.0 & \cdot & \cdot \\ 3.0 & 4.0 & 3.0 & \cdot \end{bmatrix}$$

$$X = (1.0, 3.0, 11.0, 24.0)$$

#### Output:

$$X = (1.0, 2.0, 3.0, 4.0)$$

### Example 2

This example shows the solution  $x \leftarrow A^{-T}x$ . Matrix  $A$  is a real 4 by 4 upper nonunit triangular matrix, stored in upper-triangular storage mode. Vector  $x$  is a vector of length 4.

#### Call Statement and Input:

```

          UPLO TRANSA DIAG  N  A  LDA  X  INCX
CALL STRSV( 'U' , 'T' , 'N' , 4 , A , 4 , X , 1 )

```

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 2.0 \\ \cdot & 2.0 & 2.0 & 5.0 \\ \cdot & \cdot & 3.0 & 3.0 \\ \cdot & \cdot & \cdot & 1.0 \end{bmatrix}$$

$$X = (5.0, 18.0, 32.0, 41.0)$$

#### Output:

$$X = (5.0, 4.0, 3.0, 2.0)$$

### Example 3

This example shows the solution  $x \leftarrow A^{-H}x$ . Matrix  $A$  is a complex 4 by 4 upper unit triangular matrix, stored in upper-triangular storage mode. Vector  $x$  is a vector of length 4.

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of (1.0, 0.0) for the diagonal elements.

#### Call Statement and Input:

## STRSV, DTRSV, CTRSV, ZTRSV, STPSV, DTPSV, CTPSV, and ZTPSV

```

          UPLO TRANSA DIAG  N  A  LDA  X  INCX
          |      |      |   |   |   |   |
CALL CTRSV( 'U' , 'C' , 'U' , 4 , A , 4 , X , 1 )

```

$$A = \begin{bmatrix} . & (2.0, 2.0) & (3.0, 3.0) & (2.0, 2.0) \\ . & . & (2.0, 2.0) & (5.0, 5.0) \\ . & . & . & (3.0, 3.0) \\ . & . & . & . \end{bmatrix}$$

$$X = ((5.0, 5.0), (24.0, 4.0), (49.0, 3.0), (80.0, 2.0))$$

**Output:**

$$X = ((5.0, 5.0), (4.0, 4.0), (3.0, 3.0), (2.0, 2.0))$$

### Example 4

This example shows the solution  $x \leftarrow A^{-1}x$ . Matrix  $A$  is a real 4 by 4 lower unit triangular matrix, stored in lower-triangular-packed storage mode. Vector  $x$  is a vector of length 4. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & . & . & . \\ 1.0 & 1.0 & . & . \\ 2.0 & 3.0 & 1.0 & . \\ 3.0 & 4.0 & 3.0 & 1.0 \end{bmatrix}$$

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

**Call Statement and Input:**

```

          UPLO TRANSA DIAG  N  AP  X  INCX
          |      |      |   |   |   |
CALL STPSV( 'L' , 'N' , 'U' , 4 , AP , X , 1 )

```

$$\begin{aligned} AP &= ( . , 1.0, 2.0, 3.0, . , 3.0, 4.0, . , 3.0, . ) \\ X &= (1.0, 3.0, 11.0, 24.0) \end{aligned}$$

**Output:**

$$X = (1.0, 2.0, 3.0, 4.0)$$

### Example 5

This example shows the solution  $x \leftarrow A^{-T}x$ . Matrix  $A$  is a real 4 by 4 upper nonunit triangular matrix, stored in upper-triangular-packed storage mode. Vector  $x$  is a vector of length 4. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 2.0 & 3.0 & 2.0 \\ . & 2.0 & 2.0 & 5.0 \\ . & . & 3.0 & 3.0 \\ . & . & . & 1.0 \end{bmatrix}$$

**Call Statement and Input:**

```

          UPLO TRANSA DIAG  N  AP  X  INCX
          |      |      |   |   |   |
CALL STPSV( 'U' , 'T' , 'N' , 4 , AP , X , 1 )

```

$$\begin{aligned} AP &= (1.0, 2.0, 2.0, 3.0, 2.0, 3.0, 2.0, 5.0, 3.0, 1.0) \\ X &= (5.0, 18.0, 32.0, 41.0) \end{aligned}$$

**Output:**

## STRSV, DTRSV, CTRSV, ZTRSV, STPSV, DTPSV, CTPSV, and ZTPSV

X = (5.0, 4.0, 3.0, 2.0)

### Example 6

This example shows the solution  $x \leftarrow A^{-H}x$ . Matrix  $A$  is a complex 4 by 4 upper unit triangular matrix, stored in upper-triangular-packed storage mode. Vector  $x$  is a vector of length 4. Matrix  $A$  is:

$$\begin{bmatrix} (1.0, 0.0) & (2.0, 2.0) & (3.0, 3.0) & (2.0, 2.0) \\ . & (1.0, 0.0) & (2.0, 2.0) & (5.0, 5.0) \\ . & . & (1.0, 0.0) & (3.0, 3.0) \\ . & . & . & (1.0, 0.0) \end{bmatrix}$$

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of (1.0, 0.0) for the diagonal elements.

### Call Statement and Input:

```
          UPLO  TRANSA  DIAG  N  AP  X  INCX
          |    |      |    |  |  |  |
CALL CTPSV( 'U' , 'C' , 'U' , 4 , AP , X , 1 )
```

```
AP      = ( . , (2.0, 2.0), . , (3.0, 3.0), (2.0, 2.0), . ,
           (2.0, 2.0), (5.0, 5.0), (3.0, 3.0), . )
X       = ((5.0, 5.0), (24.0, 4.0), (49.0, 3.0), (80.0, 2.0))
```

### Output:

```
X       = ((5.0, 5.0), (4.0, 4.0), (3.0, 3.0), (2.0, 2.0))
```

## STRSM, DTRSM, CTRSM, and ZTRSM — Solution of Triangular Systems of Equations with Multiple Right-Hand Sides

### Purpose

STRSM and DTRSM perform one of the following solves for a triangular system of equations with multiple right-hand sides, using scalar  $\alpha$ , rectangular matrix  $B$ , and triangular matrix  $A$  or its transpose:

Solution	Equation
1. $B \leftarrow \alpha(A^{-1})B$	$AX = \alpha B$
2. $B \leftarrow \alpha(A^{-T})B$	$A^T X = \alpha B$
3. $B \leftarrow \alpha B(A^{-1})$	$XA = \alpha B$
4. $B \leftarrow \alpha B(A^{-T})$	$XA^T = \alpha B$

CTRSM and ZTRSM perform one of the following solves for a triangular system of equations with multiple right-hand sides, using scalar  $\alpha$ , rectangular matrix  $B$ , and triangular matrix  $A$ , its transpose, or its conjugate transpose:

Solution	Equation
1. $B \leftarrow \alpha(A^{-1})B$	$AX = \alpha B$
2. $B \leftarrow \alpha(A^{-T})B$	$A^T X = \alpha B$
3. $B \leftarrow \alpha B(A^{-1})$	$XA = \alpha B$
4. $B \leftarrow \alpha B(A^{-T})$	$XA^T = \alpha B$
5. $B \leftarrow \alpha(A^{-H})B$	$A^H X = \alpha B$
6. $B \leftarrow \alpha B(A^{-H})$	$XA^H = \alpha B$

**Note:** The term  $X$  used in the systems of equations listed above represents the output solution matrix. It is important to note that in these subroutines the solution matrix is actually returned in the input-output argument  $b$ .

Table 113. Data Types

$A, B, \alpha$	Subroutine
Short-precision real	STRSM
Long-precision real	DTRSM
Short-precision complex	CTRSM
Long-precision complex	ZTRSM

### Syntax

<b>Fortran</b>	CALL STRSM   DTRSM   CTRSM   ZTRSM ( <i>side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb</i> )
<b>C and C++</b>	strsm   dtrsm   ctrsm   ztrsm ( <i>side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb</i> );

### On Entry

*side*

indicates whether the triangular matrix  $A$  is located to the left or right of rectangular matrix  $B$  in the system of equations, where:

If *side* = 'L',  $A$  is to the left of  $B$ , resulting in solution 1, 2, or 5.

If *side* = 'R',  $A$  is to the right of  $B$ , resulting in solution 3, 4, or 6.

Specified as: a single character. It must be 'L' or 'R'.

## STRSM, DTRSM, CTRSM, and ZTRSM

<i>uplo</i>	indicates whether matrix <i>A</i> is an upper or lower triangular matrix, where: If <i>uplo</i> = 'U', <i>A</i> is an upper triangular matrix. If <i>uplo</i> = 'L', <i>A</i> is a lower triangular matrix. Specified as: a single character. It must be 'U' or 'L'.
<i>transa</i>	indicates the form of matrix <i>A</i> used in the system of equations, where: If <i>transa</i> = 'N', <i>A</i> is used, resulting in solution 1 or 3. If <i>transa</i> = 'T', $A^T$ is used, resulting in solution 2 or 4. If <i>transa</i> = 'C', $A^H$ is used, resulting in solution 5 or 6. Specified as: a single character. It must be 'N', 'T', or 'C'.
<i>diag</i>	indicates the characteristics of the diagonal of matrix <i>A</i> , where: If <i>diag</i> = 'U', <i>A</i> is a unit triangular matrix. If <i>diag</i> = 'N', <i>A</i> is not a unit triangular matrix. Specified as: a single character. It must be 'U' or 'N'.
<i>m</i>	is the number of rows in rectangular matrix <i>B</i> , and: If <i>side</i> = 'L', <i>m</i> is the order of triangular matrix <i>A</i> . Specified as: a fullword integer, where: If <i>side</i> = 'L', $0 \leq m \leq lda$ and $m \leq ldb$ . If <i>side</i> = 'R', $0 \leq m \leq ldb$ .
<i>n</i>	is the number of columns in rectangular matrix <i>B</i> , and: If <i>side</i> = 'R', <i>n</i> is the order of triangular matrix <i>A</i> . Specified as: a fullword integer; $n \geq 0$ , and: If <i>side</i> = 'R', $n \leq lda$ .
<i>alpha</i>	is the scalar $\alpha$ . Specified as: a number of the data type indicated in Table 113 on page 563.
<i>a</i>	is the triangular matrix <i>A</i> , of which only the upper or lower triangular portion is used, where: If <i>side</i> = 'L', <i>A</i> is order <i>m</i> . If <i>side</i> = 'R', <i>A</i> is order <i>n</i> . Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 113 on page 563, where: If <i>side</i> = 'L', its size must be <i>lda</i> by (at least) <i>m</i> . If <i>side</i> = 'R', its size must be <i>lda</i> by (at least) <i>n</i> .
<i>lda</i>	is the leading dimension of the array specified for <i>a</i> . Specified as: a fullword integer; $lda > 0$ , and: If <i>side</i> = 'L', $lda \geq m$ . If <i>side</i> = 'R', $lda \geq n$ .

- $b$  is the  $m$  by  $n$  rectangular matrix  $B$ , which contains the right-hand sides of the triangular system to be solved.  
Specified as: an  $ldb$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 113 on page 563.
- $ldb$  is the leading dimension of the array specified for  $b$ .  
Specified as: a fullword integer;  $ldb > 0$  and  $ldb \geq m$ .

### On Return

- $b$  is the  $m$  by  $n$  matrix  $B$ , containing the results of the computation.  
Returned as: an  $ldb$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 113 on page 563.

### Notes

1. These subroutines accept lowercase letters for the *transa*, *side*, *diag*, and *uplo* arguments.
2. For STRSM and DTRSM, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
3. Matrices  $A$  and  $B$  must have no common elements or results are unpredictable.
4. If matrix  $A$  is upper triangular (*uplo* = 'U'), these subroutines refer to only the upper triangular portion of the matrix. If matrix  $A$  is lower triangular, (*uplo* = 'L'), these subroutines refer to only the lower triangular portion of the matrix. The unreferenced elements are assumed to be zero.
5. The elements of the diagonal of a unit triangular matrix are always one, so you do not need to set these values. The ESSL subroutines always assume that the values in these positions are 1.0 for STRSM and DTRSM and (1.0, 0.0) for CTRSM and ZTRSM.
6. For a description of triangular matrices and how they are stored, see "Triangular Matrix" on page 77.

### Function

These subroutines solve a triangular system of equations with multiple right-hand sides. The solution  $B$  may be any of the following, where  $A$  is a triangular matrix and  $B$  is a rectangular matrix:

1.  $B \leftarrow \alpha(A^{-1})B$
2.  $B \leftarrow \alpha(A^{-T})B$
3.  $B \leftarrow \alpha B(A^{-1})$
4.  $B \leftarrow \alpha B(A^{-T})$
5.  $B \leftarrow \alpha(A^{-H})B$  (only for CTRSM and ZTRSM)
6.  $B \leftarrow \alpha B(A^{-H})$  (only for CTRSM and ZTRSM)

where:

$\alpha$  is a scalar.

$B$  is an  $m$  by  $n$  rectangular matrix.

$A$  is an upper or lower triangular matrix, where:

If *side* = 'L', it has order  $m$ , and equation 1, 2, or 5 is performed.

If *side* = 'R', it has order  $n$ , and equation 3, 4, or 6 is performed.

If  $n$  or  $m$  is 0, no computation is performed. See references [34] and [38].

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

None

**Note:** If the triangular matrix  $A$  is singular, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

### Input-Argument Errors

1.  $m < 0$
2.  $n < 0$
3.  $lda, ldb \leq 0$
4.  $side \neq 'L'$  or  $'R'$
5.  $uplo \neq 'L'$  or  $'U'$
6.  $transa \neq 'T', 'N',$  or  $'C'$
7.  $diag \neq 'N'$  or  $'U'$
8.  $side = 'L'$  and  $m > lda$
9.  $m > ldb$
10.  $side = 'R'$  and  $n > lda$

## Examples

### Example 1

This example shows the solution  $B \leftarrow \alpha(A^{-1})B$ , where  $A$  is a real 5 by 5 upper triangular matrix that is not unit triangular, and  $B$  is a real 5 by 3 rectangular matrix.

#### Call Statement and Input:

```

          SIDE  UPLO  TRANSA  DIAG  M  N  ALPHA  A  LDA  B  LDB
CALL STRSM( 'L' , 'U' , 'N' , 'N' , 5 , 3 , 1.0 , A , 7 , B , 6 )

```

$$A = \begin{bmatrix} 3.0 & -1.0 & 2.0 & 2.0 & 1.0 \\ . & -2.0 & 4.0 & -1.0 & 3.0 \\ . & . & -3.0 & 0.0 & 2.0 \\ . & . & . & 4.0 & -2.0 \\ . & . & . & . & 1.0 \\ . & . & . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} 6.0 & 10.0 & -2.0 \\ -16.0 & -1.0 & 6.0 \\ -2.0 & 1.0 & -4.0 \\ 14.0 & 0.0 & -14.0 \\ -1.0 & 2.0 & 1.0 \\ . & . & . \end{bmatrix}$$

#### Output:

$$B = \begin{bmatrix} 2.0 & 3.0 & 1.0 \\ 5.0 & 5.0 & 4.0 \\ 0.0 & 1.0 & 2.0 \end{bmatrix}$$



$$\begin{bmatrix} 3.0 & 1.0 & -3.0 \\ -1.0 & 2.0 & 1.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 2

This example shows the solution  $B \leftarrow \alpha(A^{-T})B$ , where  $A$  is a real 5 by 5 upper triangular matrix that is not unit triangular, and  $B$  is a real 5 by 4 rectangular matrix.

#### Call Statement and Input:

```

          SIDE UPLO TRANSA DIAG M N ALPHA A LDA B LDB
CALL STRSM( 'L' , 'U' , 'T' , 'N' , 5 , 4 , 1.0 , A , 7 , B , 6 )

```

$$A = \begin{bmatrix} -1.0 & -4.0 & -2.0 & 2.0 & 3.0 \\ \cdot & -2.0 & 2.0 & 2.0 & 2.0 \\ \cdot & \cdot & -3.0 & -1.0 & 4.0 \\ \cdot & \cdot & \cdot & 1.0 & 0.0 \\ \cdot & \cdot & \cdot & \cdot & -2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} -1.0 & -2.0 & -3.0 & -4.0 \\ 2.0 & -2.0 & -14.0 & -12.0 \\ 10.0 & 5.0 & -8.0 & -7.0 \\ 14.0 & 15.0 & 1.0 & 8.0 \\ -3.0 & 4.0 & 3.0 & 16.0 \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

#### Output:

$$B = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 4.0 \\ 3.0 & 3.0 & -1.0 & 2.0 \\ -2.0 & -1.0 & 0.0 & 1.0 \\ 4.0 & 4.0 & -3.0 & -3.0 \\ 2.0 & 2.0 & 2.0 & 2.0 \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 3

This example shows the solution  $B \leftarrow \alpha B(A^{-1})$ , where  $A$  is a real 5 by 5 lower triangular matrix that is not unit triangular, and  $B$  is a real 3 by 5 rectangular matrix.

#### Call Statement and Input:

```

          SIDE UPLO TRANSA DIAG M N ALPHA A LDA B LDB
CALL STRSM( 'R' , 'L' , 'N' , 'N' , 3 , 5 , 1.0 , A , 7 , B , 4 )

```

$$A = \begin{bmatrix} 2.0 & \cdot & \cdot & \cdot & \cdot \\ 2.0 & 3.0 & \cdot & \cdot & \cdot \\ 2.0 & 1.0 & 1.0 & \cdot & \cdot \\ 0.0 & 3.0 & 0.0 & -2.0 & \cdot \\ 2.0 & 4.0 & -1.0 & 2.0 & -1.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

## STRSM, DTRSM, CTRSM, and ZTRSM

$$B = \begin{bmatrix} 10.0 & 4.0 & 0.0 & 0.0 & 1.0 \\ 10.0 & 14.0 & -4.0 & 6.0 & -3.0 \\ -8.0 & 2.0 & -5.0 & 4.0 & -2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$B = \begin{bmatrix} 3.0 & 4.0 & -1.0 & -1.0 & -1.0 \\ 2.0 & 1.0 & -1.0 & 0.0 & 3.0 \\ -2.0 & -1.0 & -3.0 & 0.0 & 2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 4

This example shows the solution  $B \leftarrow \alpha B(A^{-1})$ , where  $A$  is a real 6 by 6 upper triangular matrix that is unit triangular, and  $B$  is a real 1 by 6 rectangular matrix.

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal element.

**Call Statement and Input:**

```

          SIDE UPLO TRANSA DIAG M N ALPHA A LDA B LDB
          |   |   |   |   | | |   |   |   |   |
CALL STRSM( 'R' , 'U' , 'N' , 'U' , 1 , 6 , 1.0 , A , 7 , B , 2 )

```

$$A = \begin{bmatrix} \cdot & 2.0 & -3.0 & 1.0 & 2.0 & 4.0 \\ \cdot & \cdot & 0.0 & 1.0 & 1.0 & -2.0 \\ \cdot & \cdot & \cdot & 4.0 & -1.0 & 1.0 \\ \cdot & \cdot & \cdot & \cdot & 0.0 & -1.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & 2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & 4.0 & -2.0 & 10.0 & 2.0 & -6.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

**Output:**

$$B = \begin{bmatrix} 1.0 & 2.0 & 1.0 & 3.0 & -1.0 & -2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 5

This example shows the solution  $B \leftarrow \alpha B(A^{-1})$ , where  $A$  is a complex 5 by 5 lower triangular matrix that is not unit triangular, and  $B$  is a complex 3 by 5 rectangular matrix.

**Call Statement and Input:**

```

          SIDE UPLO TRANSA DIAG M N ALPHA A LDA B LDB
          |   |   |   |   | | |   |   |   |   |
CALL CTRSM( 'R' , 'L' , 'N' , 'N' , 3 , 5 , ALPHA , A , 7 , B , 4 )

```

ALPHA = (1.0, 0.0)

$$\begin{bmatrix} (2.0, -3.0) & \cdot & \cdot & \cdot & \cdot \\ (2.0, -4.0) & (3.0, -1.0) & \cdot & \cdot & \cdot \\ (2.0, 2.0) & (1.0, 2.0) & (1.0, 1.0) & \cdot & \cdot \end{bmatrix}$$

$$A = \begin{bmatrix} (0.0, 0.0) & (3.0, -1.0) & (0.0, -1.0) & (-2.0, 1.0) & . \\ (2.0, 2.0) & (4.0, 0.0) & (-1.0, 2.0) & (2.0, -4.0) & (-1.0, -4.0) \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} (22.0, -41.0) & (7.0, -26.0) & (9.0, 0.0) & (-15.0, -3.0) & (-15.0, 8.0) \\ (29.0, -18.0) & (24.0, -10.0) & (9.0, 6.0) & (-12.0, -24.0) & (-19.0, -8.0) \\ (-15.0, 2.0) & (-3.0, -21.0) & (-2.0, 4.0) & (-4.0, -12.0) & (-10.0, -6.0) \\ . & . & . & . & . \\ . & . & . & . & . \end{bmatrix}$$

Output:

$$B = \begin{bmatrix} (3.0, 0.0) & (4.0, 0.0) & (-1.0, -2.0) & (-1.0, -1.0) & (-1.0, -4.0) \\ (2.0, -1.0) & (1.0, 2.0) & (-1.0, -3.0) & (0.0, 2.0) & (3.0, -4.0) \\ (-2.0, 1.0) & (-1.0, -3.0) & (-3.0, 1.0) & (0.0, 0.0) & (2.0, -2.0) \\ . & . & . & . & . \\ . & . & . & . & . \end{bmatrix}$$

### Example 6

This example shows the solution  $B \leftarrow \alpha(A^{-H})B$ , where  $A$  is a complex 5 by 5 upper triangular matrix that is not unit triangular, and  $B$  is a complex 5 by 1 rectangular matrix.

Call Statement and Input:

```

                SIDE  UPLO  TRANSA  DIAG  M  N  ALPHA  A  LDA  B  LDB
CALL CTRSM( 'L' , 'U' , 'C' , 'N' , 5 , 1 , ALPHA , A , 6 , B , 6 )

```

ALPHA = (1.0, 0.0)

$$A = \begin{bmatrix} (-4.0, 1.0) & (4.0, -3.0) & (-1.0, 3.0) & (0.0, 0.0) & (-1.0, 0.0) \\ . & (-2.0, 0.0) & (-3.0, -1.0) & (-2.0, -1.0) & (4.0, 3.0) \\ . & . & (-5.0, 3.0) & (-3.0, -3.0) & (-5.0, -5.0) \\ . & . & . & (4.0, -4.0) & (2.0, 0.0) \\ . & . & . & . & (2.0, -1.0) \\ . & . & . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} (-8.0, -19.0) \\ (8.0, 21.0) \\ (44.0, -8.0) \\ (13.0, -7.0) \\ (19.0, 2.0) \\ . \end{bmatrix}$$

Output:

$$B = \begin{bmatrix} (3.0, 4.0) \\ (-4.0, 2.0) \\ (-5.0, 0.0) \\ (1.0, 3.0) \\ (3.0, 1.0) \\ . \end{bmatrix}$$

## STRTRI, DTRTRI, CTRTRI, ZTRTRI, STPTRI, DTPTRI, CTPTRI, and ZTPTRI — Triangular Matrix Inverse

### Purpose

These subroutines find the inverse of triangular matrix  $A$ :

$$A \leftarrow A^{-1}$$

Matrix  $A$  can be either upper or lower triangular, where:

- For STRTRI, DTRTRI, CTRTRI, and ZTRTRI, it is stored in upper- or lower-triangular storage mode.
- For STPTRI, DTPTRI, CTPTRI, and ZTPTRI, it is stored in upper- or lower-triangular-packed storage mode.

Table 114. Data Types

$A$	Subroutine
Short-precision real	STRTRI <sup>△</sup> and STPTRI <sup>△</sup>
Long-precision real	DTRTRI <sup>△</sup> and DTPTRI <sup>△</sup>
Short-precision complex	CTRTRI <sup>△</sup> and CTPTRI <sup>△</sup>
Long-precision complex	ZTRTRI <sup>△</sup> and ZTPTRI <sup>△</sup>
<sup>△</sup> LAPACK	

### Syntax

<b>Fortran</b>	CALL STRTRI   DTRTRI   CTRTRI   ZTRTRI ( <i>uplo, diag, n, a, lda, info</i> ) CALL STPTRI   DTPTRI   CTPTRI   ZTPTRI ( <i>uplo, diag, n, ap, info</i> )
<b>C and C++</b>	strtri   dtrtri   ctrtri   zrtri ( <i>uplo, diag, n, a, lda, info</i> ); stptri   dtptri   ctptri   ztptri ( <i>uplo, diag, n, ap, info</i> );

### On Entry

*uplo* indicates whether matrix  $A$  is an upper or lower triangular matrix, where:

If *uplo* = 'U',  $A$  is an upper triangular matrix.

If *uplo* = 'L',  $A$  is a lower triangular matrix.

Specified as: a single character. It must be 'U' or 'L'.

*diag* indicates the characteristics of the diagonal of matrix  $A$ , where:

If *diag* = 'U',  $A$  is a unit triangular matrix.

If *diag* = 'N',  $A$  is not a unit triangular matrix.

Specified as: a single character. It must be 'U' or 'N'.

*a* is the upper or lower triangular matrix  $A$  of order  $n$ , stored in upper- or lower-triangular storage mode, respectively. Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 114.

*lda* is the leading dimension of the arrays specified for *a*.

## STRTRI, DTRTRI, CTRTRI, ZTRTRI, STPTRI, DTPTRI, CTPTRI, and ZTPTRI

	Specified as: a fullword integer; $lda > 0$ and $lda \geq n$ .
<i>ap</i>	is the upper or lower triangular matrix $A$ of order $n$ , stored in upper- or lower-triangular-packed storage mode, respectively.  Specified as: a one-dimensional array of (at least) length $n(n+1)/2$ , containing numbers of the data type indicated in Table 114 on page 570.
<i>n</i>	is the order of matrix $A$ .  Specified as: a fullword integer; $n \geq 0$ .
<i>info</i>	See "On Return."

### On Return

<i>a</i>	is the inverse of the upper or lower triangular matrix $A$ of order $n$ , stored in upper- or lower-triangular storage mode, respectively. Returned as: an $lda$ by (at least) $n$ array, containing numbers of the data type indicated in Table 114 on page 570.
<i>ap</i>	is the inverse of the upper or lower triangular matrix $A$ of order $n$ , stored in upper- or lower-triangular-packed storage mode, respectively. Returned as: a one-dimensional array of (at least) length $n(n+1)/2$ , containing numbers of the data type indicated in Table 114 on page 570.
<i>info</i>	has the following meaning:  If $info = 0$ , the inverse completed successfully.  If $info > 0$ , $info$ is set equal to the first $i$ where $A_{ii}$ is zero. Matrix $A$ is singular and its inverse could not be computed.  Specified as: a fullword integer; $info \geq 0$ .

### Notes

1. In C programs, the argument *info* must be passed by reference.
2. These subroutines accept lowercase letters for the *uplo* and *diag* arguments.
3. If matrix  $A$  is upper triangular (*uplo* = 'U'), these subroutines refer to only the upper triangular portion of the matrix. If matrix  $A$  is lower triangular, (*uplo* = 'L'), these subroutines refer to only the lower triangular portion of the matrix. The unreferenced elements are assumed to be zero.
4. The elements of the diagonal of a unit triangular matrix are always one, so you do not need to set these values.
5. The way `_TRTRI` and `_TPTRI` subroutines handle computational errors differs from LAPACK. Like LAPACK, these subroutines use the *info* argument to provide information about the computational error, but they also provide an error message.
6. On both input and output, matrix  $A$  conforms to LAPACK format.
7. For a description of triangular matrices and how they are stored in upper- and lower-triangular storage mode and in upper- and lower-triangular-packed storage mode, see "Triangular Matrix" on page 77.

### Function

These subroutines find the inverse of triangular matrix  $A$ , where  $A$  is either upper or lower triangular:

## STRTRI, DTRTRI, CTRTRI, ZTRTRI, STPTRI, DTPTRI, CTPTRI, and ZTPTRI

$$A \leftarrow A^{-1}$$

where:

$A$  is the triangular matrix of order  $n$ .

$A^{-1}$  is the inverse of the triangular matrix of order  $n$ .

If  $n$  is 0, no computation is performed. See references [8] and [38].

### Error conditions

#### Resource Errors

Unable to allocate internal work area.

#### Computational Errors

Matrix  $A$  is singular.

- One or more of the diagonal elements of matrix  $A$  are zero. The first column,  $i$ , of matrix  $A$ , in which a zero diagonal element is found, is identified in the computational error message and returned in the argument *info*.
- The computational error message may occur multiple times with processing continuing after each error, because the default for the number of allowable errors for error code 2146 is set to be unlimited in the ESSL error option table.

#### Input-Argument Errors

1.  $uplo \neq 'U'$  or  $'L'$
2.  $diag \neq 'U'$  or  $'N'$
3.  $n < 0$
4.  $lda \leq 0$
5.  $lda < n$

### Examples

#### Example 1

This example shows how the inverse of matrix  $A$  is computed, where  $A$  is a 5 by 5 upper triangular matrix that is not unit triangular and is stored in upper-triangular storage mode.

Matrix  $A$  is:

$$\begin{bmatrix} 1.00 & 3.00 & 4.00 & 5.00 & 6.00 \\ 0.00 & 2.00 & 8.00 & 9.00 & 1.00 \\ 0.00 & 0.00 & 4.00 & 8.00 & 4.00 \\ 0.00 & 0.00 & 0.00 & -2.00 & 6.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & -1.00 \end{bmatrix}$$

Matrix  $A^{-1}$  is:

$$\begin{bmatrix} 1.00 & -1.50 & 2.00 & 3.75 & 35.00 \\ 0.00 & 0.50 & -1.00 & -1.75 & -14.00 \\ 0.00 & 0.00 & 0.25 & 1.00 & 7.00 \\ 0.00 & 0.00 & 0.00 & -0.50 & -3.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & -1.00 \end{bmatrix}$$

#### Call Statement and Input:

## STRTRI, DTRTRI, CTRTRI, ZTRTRI, STPTRI, DTPTRI, CTPTRI, and ZTPTRI

```

          UPLO  DIAG  N  A  LDA  INFO
          |    |    |  |  |    |
CALL STRTRI( 'U' , 'N' , 5 , A, 5, INFO )

```

$$A = \begin{bmatrix} 1.00 & 3.00 & 4.00 & 5.00 & 6.00 \\ . & 2.00 & 8.00 & 9.00 & 1.00 \\ . & . & 4.00 & 8.00 & 4.00 \\ . & . & . & -2.00 & 6.00 \\ . & . & . & . & -1.00 \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} 1.00 & -1.50 & 2.00 & 3.75 & 35.00 \\ . & 0.50 & -1.00 & -1.75 & -14.00 \\ . & . & 0.25 & 1.00 & 7.00 \\ . & . & . & -0.50 & -3.00 \\ . & . & . & . & -1.00 \end{bmatrix}$$

INFO = 0

### Example 2

This example shows how the inverse of matrix  $A$  is computed, where  $A$  is a 5 by 5 lower triangular matrix that is unit triangular and is stored in lower-triangular storage mode.

Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 3.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 4.0 & 8.0 & 1.0 & 0.0 & 0.0 \\ 5.0 & 9.0 & 8.0 & 1.0 & 0.0 \\ 6.0 & 1.0 & 4.0 & 6.0 & 1.0 \end{bmatrix}$$

Matrix  $A^{-1}$  is:

$$\begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ -3.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 20.0 & -8.0 & 1.0 & 0.0 & 0.0 \\ -138.0 & 55.0 & -8.0 & 1.0 & 0.0 \\ 745.0 & -299.0 & 44.0 & -6.0 & 1.0 \end{bmatrix}$$

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of one for the diagonal elements.

**Call Statement and Input:**

```

          UPLO  DIAG  N  A  LDA  INFO
          |    |    |  |  |    |
CALL STRTRI( 'L' , 'U' , 5 , A, 5, INFO )

```

$$A = \begin{bmatrix} . & . & . & . & . \\ 3.0 & . & . & . & . \\ 4.0 & 8.0 & . & . & . \\ 5.0 & 9.0 & 8.0 & . & . \\ 6.0 & 1.0 & 4.0 & 6.0 & . \end{bmatrix}$$

**Output:**

## STRTRI, DTRTRI, CTRTRI, ZTRTRI, STPTRI, DTPTRI, CTPTRI, and ZTPTRI

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ -3.0 & \cdot & \cdot & \cdot & \cdot \\ 20.0 & -8.0 & \cdot & \cdot & \cdot \\ -138.0 & 55.0 & -8.0 & \cdot & \cdot \\ 745.0 & -299.0 & 44.0 & -6.0 & \cdot \end{bmatrix}$$

INFO = 0

### Example 3

This example shows how the inverse of matrix  $A$  is computed, where  $A$  is a 5 by 5 upper triangular matrix that is not unit triangular and is stored in upper-triangular storage mode.

Matrix  $A$  is:

$$\begin{bmatrix} (-4.00, 1.00) & (4.00, -3.00) & (-1.00, 3.00) & (0.00, 0.00) & (-1.00, 0.00) \\ (0.00, 0.00) & (-2.00, 0.00) & (-3.00, -1.00) & (-2.00, -1.00) & (4.00, 3.00) \\ (0.00, 0.00) & (0.00, 0.00) & (-5.00, 3.00) & (-3.00, -3.00) & (-5.00, -5.00) \\ (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (4.00, -4.00) & (2.00, 0.00) \\ (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (2.00, -1.00) \end{bmatrix}$$

Matrix  $A^{-1}$  is:

$$\begin{bmatrix} (-0.24, -0.06) & (-0.56, 0.24) & (0.41, 0.09) & (-0.22, 0.13) & (1.32, 2.12) \\ (0.00, 0.00) & (-0.50, 0.00) & (0.18, 0.21) & (-0.22, -0.06) & (0.21, 1.87) \\ (0.00, 0.00) & (0.00, 0.00) & (-0.15, -0.09) & (0.07, -0.11) & (0.02, -0.47) \\ (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (0.12, 0.12) & (-0.05, -0.15) \\ (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (0.40, 0.20) \end{bmatrix}$$

### Call Statement and Input:

```

          UPLO  DIAG  N  A  LDA  INFO
          |    |    |  |  |    |
CALL ZTRTRI( 'U' , 'N' , 5 , A, 5, INFO )

```

$$A = \begin{bmatrix} (-4.00, 1.00) & (4.00, -3.00) & (-1.00, 3.00) & (0.00, 0.00) & (-1.00, 0.00) \\ \cdot & (-2.00, 0.00) & (-3.00, -1.00) & (-2.00, -1.00) & (4.00, 3.00) \\ \cdot & \cdot & (-5.00, 3.00) & (-3.00, -3.00) & (-5.00, -5.00) \\ \cdot & \cdot & \cdot & (4.00, -4.00) & (2.00, 0.00) \\ \cdot & \cdot & \cdot & \cdot & (2.00, -1.00) \end{bmatrix}$$

### Output:

$$A = \begin{bmatrix} (-0.24, -0.06) & (-0.56, 0.24) & (0.41, 0.09) & (-0.22, 0.13) & (1.32, 2.12) \\ \cdot & (-0.50, 0.00) & (0.18, 0.21) & (-0.22, -0.06) & (0.21, 1.87) \\ \cdot & \cdot & (-0.15, -0.09) & (0.07, -0.11) & (0.02, -0.47) \\ \cdot & \cdot & \cdot & (0.12, 0.12) & (-0.05, -0.15) \\ \cdot & \cdot & \cdot & \cdot & (0.40, 0.20) \end{bmatrix}$$

INFO = 0



## STRTRI, DTRTRI, CTRTRI, ZTRTRI, STPTRI, DTPTRI, CTPTRI, and ZTPTRI

### Example 4

This example shows how the inverse of matrix  $A$  is computed, where  $A$  is a 5 by 5 lower triangular matrix that is unit triangular and is stored in lower-triangular storage mode.

Matrix  $A$  is:

$$\begin{bmatrix} (1.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) \\ (4.00, -3.00) & (1.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) \\ (-1.00, 3.00) & (-3.00, -1.00) & (1.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) \\ (0.00, 0.00) & (-2.00, -1.00) & (-3.00, -3.00) & (1.00, 0.00) & (0.00, 0.00) \\ (-1.00, 0.00) & (4.00, 3.00) & (-5.00, -5.00) & (2.00, 0.00) & (1.00, 0.00) \end{bmatrix}$$

Matrix  $A^{-1}$  is:

$$\begin{bmatrix} (1.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) \\ (-4.00, 3.00) & (1.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) \\ (-14.00, 2.00) & (3.00, 1.00) & (1.00, 0.00) & (0.00, 0.00) & (0.00, 0.00) \\ (-59.00, -34.00) & (8.00, 13.00) & (3.00, 3.00) & (1.00, 0.00) & (0.00, 0.00) \\ (64.00, 8.00) & (-10.00, -9.00) & (-1.00, -1.00) & (-2.00, 0.00) & (1.00, 0.00) \end{bmatrix}$$

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of one for the diagonal elements.

#### Call Statement and Input:

```

          UPLO  DIAG  N   A   LDA  INFO
          |    |    |   |   |    |
CALL ZTRTRI( 'L' , 'U' , 5 , A, 5,  INFO )

```

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ (4.00, -3.00) & \cdot & \cdot & \cdot & \cdot \\ (-1.00, 3.00) & (-3.00, 1.00) & \cdot & \cdot & \cdot \\ (0.00, 0.00) & (-2.00, -1.00) & (-3.00, -3.00) & \cdot & \cdot \\ (-1.00, 0.00) & (4.00, 3.00) & (-5.00, -5.00) & (2.00, 0.00) & \cdot \end{bmatrix}$$

#### Output:

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ (-4.00, 3.00) & \cdot & \cdot & \cdot & \cdot \\ (-14.00, 2.00) & (3.00, 1.00) & \cdot & \cdot & \cdot \\ (-59.00, -34.00) & (8.00, 13.00) & (3.00, 3.00) & \cdot & \cdot \\ (64.00, 8.00) & (-10.00, -9.00) & (-1.00, -1.00) & (-2.00, 0.00) & \cdot \end{bmatrix}$$

INFO = 0

### Example 5

This example shows how the inverse of matrix  $A$  is computed, where  $A$  is the same matrix shown in “Example 1” on page 572 and is stored in upper-triangular-packed storage mode. The inverse matrix computed here is the same as the inverse matrix shown in “Example 1” on page 572 and is stored in upper-triangular-packed storage mode.

#### Call Statement and Input:

## STRTRI, DTRTRI, CTRTRI, ZTRTRI, STPTRI, DTPTRI, CTPTRI, and ZTPTRI

```
          UPLO  DIAG  N  AP  INFO
          |    |    |  |  |
CALL STPTRI( 'U' , 'N' , 5 , AP, INFO )
AP   = ( 1.00, 3.00, 2.00, 4.00, 8.00, 4.00, 5.00, 9.00, 8.00,
        -2.00, 6.00, 1.00, 4.00, 6.00, -1.00)
```

### Output:

```
AP   = ( 1.00, -1.50, 0.50, 2.00, -1.00, 0.25, 3.75, -1.75, 1.00,
        -0.50, 35.00, -14.00, 7.00, -3.00, -1.00)
INFO =  0
```

### Example 6

This example shows how the inverse of matrix  $A$  is computed, where  $A$  is the same matrix shown in “Example 2” on page 573 and is stored in lower-triangular-packed storage mode. The inverse matrix computed here is the same as the inverse matrix shown in “Example 2” on page 573 and is stored in lower-triangular-packed storage mode.

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of one for the diagonal elements.

### Call Statement and Input:

```
          UPLO  DIAG  N  AP  INFO
          |    |    |  |  |
CALL STPTRI( 'L' , 'U' , N , AP, INFO )
AP   = ( . , 3.0, 4.0, 5.0, 6.0, . , 8.0, 9.0, 1.0, . , 8.0, 4.0,
        . , 6.0, . )
```

### Output:

```
AP   = ( . , -3.0, 20.0, -138.0, 745.0, . , -8.0, 55.0, -299.0,
        . , -8.0, 44.0, . , -6.0, . )
INFO =  0
```

### Example 7

This example shows how the inverse of matrix  $A$  is computed, where  $A$  is the same matrix shown in “Example 3” on page 574 and is stored in upper-triangular-packed storage mode. The inverse matrix computed here is the same as the inverse matrix shown in “Example 3” on page 574 and is stored in upper-triangular-packed storage mode.

### Call Statement and Input:

```
          UPLO  DIAG  N  AP  INFO
          |    |    |  |  |
CALL ZTPTRI( 'U' , 'N' , 5 , AP, INFO )

AP   = ( (-4.00, 1.00),
        ( 4.00, -3.00), (-2.00, 0.00),
        (-1.00, 3.00), (-3.00, -1.00), (-5.00, 3.00),
        ( 0.00, 0.00), (-2.00, -1.00), (-3.00, -3.00), (4.00, -4.00),
        (-1.00, 0.00), ( 4.00, 3.00), (-5.00, -5.00), (2.00, 0.00), (2.00, -1.00) )
```

## STRTRI, DTRTRI, CTRTRI, ZTRTRI, STPTRI, DTPTRI, CTPTRI, and ZTPTRI

### Output:

```
AP = ( (-0.24, -0.06),
        (-0.56, 0.24), (-0.50, 0.00),
        ( 0.41, 0.09), ( 0.18, 0.21), (-0.15, -0.09),
        (-0.22, 0.13), (-0.22, -0.06), ( 0.07, -0.11), ( 0.12, 0.12),
        ( 1.32, 2.12), ( 0.21, 1.87), ( 0.02, -0.47), (-0.05, -0.15), (0.40, 0.20) )
```

```
INFO = 0
```

### Example 8

This example shows how the inverse of matrix  $A$  is computed, where  $A$  is the same matrix shown in “Example 4” on page 575 and is stored in lower-triangular-packed storage mode. The inverse matrix computed here is the same as the inverse matrix shown in “Example 4” on page 575 and is stored in lower-triangular-packed storage mode.

**Note:** Because matrix  $A$  is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of one for the diagonal elements.

### Call Statement and Input:

```
          UPLO  DIAG  N   AP  INFO
          |    |    |   |   |
CALL ZTPTRI( 'L' , 'U' , 5 , AP, INFO )
```

```
AP = ( ., ( 4.00, -3.00), (-1.00, 3.00), (0.00, 0.00), (-1.00, 0.00),
        ., (-3.00, -1.00), (-2.00, -1.00), (4.00, 3.00),
        ., (-3.00, -3.00), (-5.00, -5.00),
        ., ( 2.00, 0.00),
        . )
```

### Output:

```
AP = ( ., (-4.00, 3.00), (-14.00, 2.00), (-59.00, -34.00), (64.00, 8.00),
        ., ( 3.00, 1.00), ( 8.00, 13.00), (-10.00, -9.00),
        ., ( 3.00, 3.00), ( -1.00, -1.00),
        ., (-2.00, 0.00),
        . )
```

```
INFO = 0
```

---

## Banded Linear Algebraic Equation Subroutines

This section contains the banded linear algebraic equation subroutine descriptions.

## SGBF and DGBF — General Band Matrix Factorization

### Purpose

These subroutines factor general band matrix  $A$ , stored in general-band storage mode, using Gaussian elimination. To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGBS or DGBS, respectively.

Table 115. Data Types

$A$	Subroutine
Short-precision real	SGBF
Long-precision real	DGBF

**Note:** The output from these factorization subroutines should be used only as input to the solve subroutines SGBS and DGBS, respectively.

### Syntax

Fortran	CALL SGBF   DGBF ( $agb, lda, n, ml, mu, ipvt$ )
C and C++	$sgbf$   $dgbf$ ( $agb, lda, n, ml, mu, ipvt$ );

### On Entry

$agb$	is the general band matrix $A$ of order $n$ , stored in general-band storage mode, to be factored. It has an upper band width $mu$ and a lower band width $ml$ . Specified as: an $lda$ by (at least) $n$ array, containing numbers of the data type indicated in Table 115, where $lda \geq 2ml+mu+16$ .
$lda$	is the leading dimension of the array specified for $agb$ . Specified as: a fullword integer; $lda > 0$ and $lda \geq 2ml+mu+16$ .
$n$	is the order of the matrix $A$ . Specified as: a fullword integer; $n > ml$ and $n > mu$ .
$ml$	is the lower band width $ml$ of the matrix $A$ . Specified as: a fullword integer; $0 \leq ml < n$ .
$mu$	is the upper band width $mu$ of the matrix $A$ . Specified as: a fullword integer; $0 \leq mu < n$ .
$ipvt$	See "On Return."

### On Return

$agb$	is the transformed matrix $A$ of order $n$ , containing the results of the factorization. See "Function" on page 580. Returned as: an $lda$ by (at least) $n$ array, containing numbers of the data type indicated in Table 115.
$ipvt$	is the integer vector $ipvt$ of length $n$ , containing the pivot information necessary to construct matrix $L$ from the information contained in the output array $agb$ . Returned as: a one-dimensional array of (at least) length $n$ , containing fullword integers.

## Notes

1. *ipvt* is not a permutation vector in the strict sense. It is used to record column interchanges in  $L$  due to partial pivoting and to improve performance.
2. The entire  $lda$  by  $n$  array specified for *agb* must remain unchanged between calls to the factorization and solve subroutines.
3. This subroutine can be used for tridiagonal matrices ( $ml = mu = 1$ ); however, the tridiagonal subroutines SGTF/DGTF and SGTS/DGTS are faster.
4. For a description of how a general band matrix is stored in general-band storage mode in an array, see “General Band Matrix” on page 80.

## Function

The general band matrix  $A$ , stored in general-band storage mode, is factored using Gaussian elimination with partial pivoting to compute the  $LU$  factorization of  $A$ , where:

$ipvt$  is a vector containing the pivoting information.

$L$  is a unit lower triangular band matrix.

$U$  is an upper triangular band matrix.

The transformed matrix  $A$  contains  $U$  in packed format, along with the multipliers necessary to construct, with the help of  $ipvt$ , a matrix  $L$ , such that  $A = LU$ . This factorization can then be used by SGBS or DGBS, respectively, to solve the system of equations. See reference [40].

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

Matrix  $A$  is singular.

- One or more columns of  $L$  and the corresponding diagonal of  $U$  contain all zeros (all columns of  $L$  are checked). The last column,  $i$ , of  $L$  with a corresponding  $U = 0$  diagonal element is identified in the computational error message.
- The return code is set to 1.
- $i$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2103 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $lda \leq 0$
2.  $ml < 0$
3.  $ml \geq n$
4.  $mu < 0$
5.  $mu \geq n$
6.  $lda < 2ml + mu + 16$

## Examples

### Example

This example shows a factorization of a general band matrix  $A$  of order 9, with a lower band width of 2 and an upper band width of 3. On input matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 4.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 5.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 6.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 7.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 8.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 9.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 10.0 & 11.0 & 12.0 \end{bmatrix}$$

Matrix  $A$  is stored in general-band storage mode in the two-dimensional array AGB of size LDA by N, where  $LDA = 2ml+mu+16 = 23$ . The array AGB is declared as `AGB(1:23,1:9)`.

**Note:** Matrix  $A$  is the same matrix used in the examples in subroutines SGEF and DGEF (see “Example 1” on page 468) and SGEFCD and DGEFCD (see “Example” on page 482).

#### Call Statement and Input:

```

          AGB  LDA  N  ML  MU  IPVT )
          |   |   |   |   |   |
CALL SGBF( AGB , 23 , 9 , 2 , 3 , IPVT )

```

$$\text{AGB} = \begin{bmatrix} 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 \\ 0.0000 & 0.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 \\ 0.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 \\ 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 12.0000 \\ 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 1.0000 & 11.0000 & 0.0000 \\ 4.0000 & 5.0000 & 6.0000 & 7.0000 & 8.0000 & 9.0000 & 10.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \end{bmatrix}$$

**SGBF and DGBF**

**Output:**

	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	1.0000	1.0000	1.0000
	0.0000	0.0000	0.0000	0.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	0.0000	0.0000	0.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	0.0000	0.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	12.0000
	0.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	11.0000	0.3111
	0.2500	0.2000	0.1600	0.1400	0.1250	0.1100	0.1000	5.5380	-325.00
	0.0000	0.1500	0.0000	0.0714	0.0000	-0.0556	-0.0306	0.9385	0.0000
	0.2500	0.1500	0.1000	0.0714	-0.0714	-0.0694	-0.0194	0.0000	0.0000
	0.2500	0.0000	0.1000	0.0000	0.0536	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AGB =	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

IPVT = (2, -65534, -131070, -196606, -262142, -327678, -327678, -327680, -327680)



## SGBS and DGBS — General Band Matrix Solve

### Purpose

These subroutines solve the system  $Ax = b$  for  $x$ , where  $A$  is a general band matrix, and  $x$  and  $b$  are vectors. They use the results of the factorization of matrix  $A$ , produced by a preceding call to SGBF or DGBF, respectively.

Table 116. Data Types

$A, b, x$	Subroutine
Short-precision real	SGBS
Long-precision real	DGBS

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGBF and DGBF, respectively.

### Syntax

Fortran	CALL SGBS   DGBS ( <i>agb, lda, n, ml, mu, ipvt, bx</i> )
C and C++	sgbs   dgbs ( <i>agb, lda, n, ml, mu, ipvt, bx</i> );

### On Entry

- agb* is the factorization of general band matrix  $A$ , produced by a preceding call to SGBF or DGBF. Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 116, where  $lda \geq 2ml + mu + 16$ .
- lda* is the leading dimension of the array specified for *agb*. Specified as: a fullword integer;  $lda > 0$  and  $lda \geq 2ml + mu + 16$ .
- n* is the order of the matrix  $A$ . Specified as: a fullword integer;  $n > ml$  and  $n > mu$ .
- ml* is the lower band width  $ml$  of the matrix  $A$ . Specified as: a fullword integer;  $0 \leq ml < n$ .
- mu* is the upper band width  $mu$  of the matrix  $A$ . Specified as: a fullword integer;  $0 \leq mu < n$ .
- ipvt* is the integer vector *ipvt* of length  $n$ , produced by a preceding call to SGBF or DGBF. It contains the pivot information necessary to construct matrix  $L$  from the information contained in the array specified for *agb*.  
Specified as: a one-dimensional array of (at least) length  $n$ , containing fullword integers.
- bx* is the vector  $b$  of length  $n$ , containing the right-hand side of the system. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 116.

### On Return

- bx* is the solution vector  $x$  of length  $n$ , containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 116.

## Notes

1. The scalar data specified for input arguments  $lda$ ,  $n$ ,  $ml$ , and  $mu$  for these subroutines must be the same as that specified for SGBF and DGBF, respectively.
2. The array data specified for input arguments  $agb$  and  $ipvt$  for these subroutines must be the same as the corresponding output arguments for SGBF and DGBF, respectively.
3. The entire  $lda$  by  $n$  array specified for  $agb$  must remain unchanged between calls to the factorization and solve subroutines.
4. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.
5. This subroutine can be used for tridiagonal matrices ( $ml = mu = 1$ ); however, the tridiagonal subroutines, SGTF/DGTF and SGTS/DGTS, are faster.
6. For a description of how a general band matrix is stored in general-band storage mode in an array, see "General Band Matrix" on page 80.

## Function

The real system  $Ax = b$  is solved for  $x$ , where  $A$  is a real general band matrix, stored in general-band storage mode, and  $x$  and  $b$  are vectors. These subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to SGBF or DGBF, respectively. The transformed matrix  $A$ , used by this computation, consists of the upper triangular matrix  $U$  and the multipliers necessary to construct  $L$  using  $ipvt$ , as defined in "Function" on page 580. See reference [40].

## Error conditions

### Computational Errors

**Note:** If the factorization performed by SGBF or DGBF failed due to a singular matrix argument, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

### Input-Argument Errors

1.  $lda \leq 0$
2.  $ml < 0$
3.  $ml \geq n$
4.  $mu < 0$
5.  $mu \geq n$
6.  $lda < 2ml+mu+16$

## Examples

### Example

This example shows how to solve the system  $Ax = b$ , where general band matrix  $A$  is the same matrix factored in "Example" on page 580 for SGBF and DGBF. The input for AGB and IPVT in this example is the same as the output for that example.

#### Call Statement and Input:

```

          AGB  LDA  N  ML  MU  IPVT  BX
          |   |   |   |   |   |   |
CALL SGBS( AGB , 23 , 9 , 2 , 3 , IPVT , BX )

```

```

IPVT      = (2, -65534, -131070, -196606, -262142, -327678, -327678,
             -327680, -327680)

```

BX = (4.0000, 5.0000, 9.0000, 10.0000, 11.0000, 12.0000,  
12.0000, 12.0000, 33.0000)  
AGB = (same as output AGB in  
"Example" on page 580)

**Output:**

BX = (1.0000, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000,  
0.9999, 1.0001)

## SPBF, DPBF, SPBCHF, and DPBCHF — Positive Definite Symmetric Band Matrix Factorization

### Purpose

These subroutines factor positive definite symmetric band matrix  $A$ , stored in lower-band-packed storage mode, using:

- Gaussian elimination for SPBF and DPBF
- Cholesky factorization for SPBCHF and DPBCHF

To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SPBS, DPBS, SPBCHS, or DPBCHS, respectively.

Table 117. Data Types

$A$	Subroutine
Short-precision real	SPBF and SPBCHF
Long-precision real	DPBF and DPBCHF

### Notes:

1. The output from these factorization subroutines should be used only as input to the solve subroutines SPBS, DPBS, SPBCHS, and DPBCHS, respectively.
2. For optimal performance:
  - For wide band widths, use `_PBCHF`.
  - For narrow band widths, use either `_PBF` or `_PBCHF`.
  - For very narrow band widths:
    - Use either SPBF or SPBCHF.
    - Use DPBF.

### Syntax

<b>Fortran</b>	CALL SPBF   DPBF   SPBCHF   DPBCHF ( <i>apb</i> , <i>lda</i> , <i>n</i> , <i>m</i> )
<b>C and C++</b>	spbf   dpbf   spbchf   dpbchf ( <i>apb</i> , <i>lda</i> , <i>n</i> , <i>m</i> );

### On Entry

- apb* is the positive definite symmetric band matrix  $A$  of order  $n$ , stored in lower-band-packed storage mode, to be factored. It has a half band width of  $m$ . Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 117. See “Notes” on page 587.
- lda* is the leading dimension of the array specified for *apb*. Specified as: a fullword integer;  $lda > 0$  and  $lda > m$ .
- n* is the order  $n$  of matrix  $A$ . Specified as: a fullword integer;  $n > m$ .
- m* is the half band width of the matrix  $A$ . Specified as: a fullword integer;  $0 \leq m < n$ .

### On Return

- apb* is the transformed matrix  $A$  of order  $n$ , containing the results of the factorization. See “Function” on page 587. Returned as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 117. For further details, see “Notes” on page 587.

## Notes

1. These subroutines can be used for tridiagonal matrices ( $m = 1$ ); however, the tridiagonal subroutines, SPTF/DPTF and SPTS/DPTS, are faster.
2. For SPBF and DPBF when  $m > 0$ , location APB(2, $n$ ) is sometimes set to 0.
3. For a description of how a positive definite symmetric band matrix is stored in lower-band-packed storage mode in an array, see “Positive Definite Symmetric Band Matrix” on page 87.

## Function

The positive definite symmetric band matrix  $A$ , stored in lower-band-packed storage mode, is factored using Gaussian elimination in SPBF and DPBF and Cholesky factorization in SPBCHF and DPBCHF. The transformed matrix  $A$  contains the results of the factorization in packed format. This factorization can then be used by SPBS, DPBS, SPBCHS, and DPBCHS, respectively, to solve the system of equations.

For performance reasons, divides are done in a way that reduces the effective exponent range for which DPBF works properly, when processing narrow band widths; therefore, you may want to scale your problem.

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

1. Matrix  $A$  is not positive definite (for SPBF and DPBF).
  - One or more elements of  $D$  contain values less than or equal to 0; all elements of  $D$  are checked. The index  $i$  of the last nonpositive element encountered is identified in the computational error message.
  - The return code is set to 1.
  - $i$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2104 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see Chapter 4, “Coding Your Program,” on page 111.
2. Matrix  $A$  is not positive definite (for SPBCHF and DPBCHF).
  - The leading minor of order  $i$  has a nonpositive determinant. The order  $i$  is identified in the computational error message.
  - The return code is set to 1.
  - $i$  can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2115 in the ESSL error option table; otherwise, the default value causes your program to be terminate when this error occurs. For details, see Chapter 4, “Coding Your Program,” on page 111.

### Input-Argument Errors

1.  $lda \leq 0$
2.  $m < 0$
3.  $m \geq n$
4.  $m \geq lda$

## Examples

### Example 1

This example shows a factorization of a real positive definite symmetric band matrix  $A$  of order 9, using Gaussian elimination, where on input, matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 2.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 3.0 & 2.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 2.0 & 3.0 & 2.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 2.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 2.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 2.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & 3.0 \end{bmatrix}$$

and on output, matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 \end{bmatrix}$$

where array location  $APB(2,9)$  is set to 0.0.

#### Call Statement and Input:

```

      APB  LDA  N  M
      |    |  |  |
CALL SPBF( APB , 3 , 9 , 2 )
    
```

$$APB = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 & 3.0 \\ 1.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & 2.0 & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . & . \end{bmatrix}$$

#### Output:

$$APB = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . & . \end{bmatrix}$$

### Example 2

This example shows a Cholesky factorization of the same matrix used in Example 1.

#### Call Statement and Input:

```

      APB  LDA  N  M
      |    |  |  |
CALL SPBCHF( APB , 3 , 9 , 2 )
    
```

$APB$  = (same as input  $APB$  in Example 1)

Output:

$$\text{APB} = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & . & . \end{bmatrix}$$

## SPBS, DPBS, SPBCHS, and DPBCHS — Positive Definite Symmetric Band Matrix Solve

### Purpose

These subroutines solve the system  $Ax = b$  for  $x$ , where  $A$  is a positive definite symmetric band matrix, and  $x$  and  $b$  are vectors. They use the results of the factorization of matrix  $A$ , produced by a preceding call to SPBF, DPBF, SPBCHF, and DPBCHF, respectively, where:

- Gaussian elimination was used by SPBF and DPBF.
- Cholesky factorization was used by SPBCHF and DPBCHF.

Table 118. Data Types

$A, b, x$	Subroutine
Short-precision real	SPBS and SPBCHS
Long-precision real	DPBS and DPBCHS

### Notes:

1. The input to these solve subroutines must be the output from the factorization subroutines SPBF, DPBF, SPBCHF, and DPBCHF, respectively.
2. For performance tradeoffs, see “SPBF, DPBF, SPBCHF, and DPBCHF — Positive Definite Symmetric Band Matrix Factorization” on page 586.

### Syntax

Fortran	CALL SPBS   DPBS   SPBCHS   DPBCHS ( <i>apb, lda, n, m, bx</i> )
C and C++	spbs   dpbs   spbchs   dpbchs ( <i>apb, lda, n, m, bx</i> );

### On Entry

<i>apb</i>	is the factorization of matrix $A$ , produced by a preceding call to SPBF or DPBF. Specified as: an <i>lda</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 118. See “Notes” on page 591.
<i>lda</i>	is the leading dimension of the array specified for <i>apb</i> . Specified as: a fullword integer; $lda > 0$ and $lda > m$ .
<i>n</i>	is the order $n$ of matrix $A$ . Specified as: a fullword integer; $n > m$ .
<i>m</i>	is the half band width of the matrix $A$ . Specified as: a fullword integer; $0 \leq m < n$ .
<i>bx</i>	is the vector $b$ of length $n$ , containing the right-hand side of the system. Specified as: a one-dimensional array of (at least) length $n$ , containing numbers of the data type indicated in Table 118.

### On Return

<i>bx</i>	is the solution vector $x$ of length $n$ , containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 118.
-----------	---



## Notes

1. The scalar data specified for input arguments  $lda$ ,  $n$ , and  $m$  for these subroutines must be the same as that specified for SPBF, DPBF, SPBCHF, and DPBCHF, respectively.
2. The array data specified for input argument  $apb$  for these subroutines must be the same as the corresponding output argument for SPBF, DPBF, SPBCHF, and DPBCHF, respectively.
3. These subroutines can be used for tridiagonal matrices ( $m = 1$ ); however, the tridiagonal subroutines, SPTF/DPTF and SPTS/DPTS, are faster.
4. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
5. For a description of how a positive definite symmetric band matrix is stored in lower-band-packed storage mode in an array, see “Positive Definite Symmetric Band Matrix” on page 87.

## Function

The system  $Ax = b$  is solved for  $x$ , where  $A$  is a positive definite symmetric band matrix, stored in lower-band-packed storage mode, and  $x$  and  $b$  are vectors. These subroutines use the results of the factorization of matrix  $A$ , produced by a preceding call to SPBF, DPBF, SPBCHF, or DPBCHF, respectively.

## Error conditions

### Computational Errors

None

**Note:** If the factorization subroutine resulted in a nonpositive definite matrix, error 2104 for SPBF and DPBF or error 2115 for SPBCHF and DPBCHF, results of these subroutines may be unpredictable.

### Input-Argument Errors

1.  $lda \leq 0$
2.  $m < 0$
3.  $m \geq n$
4.  $m \geq lda$

## Examples

### Example 1

This example shows how to solve the system  $Ax = b$ , where matrix  $A$  is the same matrix factored in the “Example 1” on page 588 for SPBF and DPBF, using Gaussian elimination.

#### Call Statement and Input:

```

          APB  LDA  N   M   BX
          |   |   |   |   |
CALL SPBS( APB , 3 , 9 , 2 , BX )

```

APB = (same as output APB in “Example 1” on page 588)

BX = (3.0, 6.0, 9.0, 9.0, 9.0, 9.0, 9.0, 8.0, 6.0)

#### Output:

BX = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)

## SPBS, DPBS, SPBCHS, and DPBCHS

This example shows how to solve the system  $Ax = b$ , where matrix  $A$  is the same matrix factored in the "Example 2" on page 588 for SPBCHF and DPBCHF, using Cholesky factorization.

### Call Statement and Input:

```
          APB  LDA  N   M   BX
          |   |   |   |   |
CALL SPBCHS( APB , 3 , 9 , 2 , BX )
```

APB = (same as output APB in  
"Example 2" on page 588)

BX = (3.0, 6.0, 9.0, 9.0, 9.0, 9.0, 9.0, 8.0, 6.0)

### Output:

BX = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)

## SGTF and DGTF — General Tridiagonal Matrix Factorization

### Purpose

These subroutines compute the standard Gaussian factorization with partial pivoting for tridiagonal matrix  $A$ , stored in tridiagonal storage mode. To solve a tridiagonal system with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGTS or DGTS, respectively.

Table 119. Data Types

$c, d, e, f$	Subroutine
Short-precision real	SGTF
Long-precision real	DGTF

**Note:** The output from these factorization subroutines should be used only as input to the solve subroutines SGTS and DGTS, respectively.

### Syntax

Fortran	CALL SGTF   DGTF ( $n, c, d, e, f, ipvt$ )
C and C++	sgtf   dgtf ( $n, c, d, e, f, ipvt$ );

### On Entry

- $n$  is the order  $n$  of tridiagonal matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- $c$  is the vector  $c$ , containing the lower subdiagonal of matrix  $A$  in positions 2 through  $n$  in an array, referred to as C. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 119.
- $d$  is the vector  $d$ , containing the main diagonal of matrix  $A$ , in positions 1 through  $n$  in an array, referred to as D. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 119.
- $e$  is the vector  $e$ , containing the upper subdiagonal of matrix  $A$ , in positions 1 through  $n-1$  in an array, referred to as E. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 119.
- $f$  See "On Return."
- $ipvt$  See "On Return."

### On Return

- $c$  is the vector  $c$ , containing part of the factorization of matrix  $A$  in positions 1 through  $n$  in an array, referred to as C. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 119.
- $d$  is the vector  $d$ , containing part of the factorization of matrix  $A$  in an array, referred to as D. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 119.

## SGTF and DGTF

$e$	is the vector $e$ , containing part of the factorization of the matrix $A$ in positions 1 through $n$ in an array, referred to as E. Returned as: a one-dimensional array of (at least) length $n$ , containing numbers of the data type indicated in Table 119 on page 593.
$f$	is the vector $f$ , containing part of the factorization of matrix $A$ in the first $n$ positions in an array, referred to as F. Returned as: a one-dimensional array of (at least) length $n$ , containing numbers of the data type indicated in Table 119 on page 593.
$ipvt$	is the integer vector $ipvt$ of length $n$ , containing the pivot information. Returned as: a one-dimensional array of (at least) length $n$ , containing fullword integers.

## Notes

1. For a description of how tridiagonal matrices are stored, see “General Tridiagonal Matrix” on page 92.
2.  $ipvt$  is not a permutation vector in the strict sense. It is used to record column interchanges in the tridiagonal matrix due to partial pivoting.
3. The factorization matrix  $A$  is stored in nonstandard format.

## Function

The standard Gaussian elimination with partial pivoting of tridiagonal matrix  $A$  is computed. The factorization is returned by overwriting input arrays C, D, and E, and by writing into output array F, along with pivot information in vector  $ipvt$ . This factorization can then be used by SGTS or DGTS, respectively, to solve tridiagonal systems of linear equations. See references [45], [56], [57], and [94]. If  $n$  is 0, no computation is performed.

## Error conditions

### Computational Errors

Matrix  $A$  is singular or nearly singular.

- A pivot element has a value that cannot be reciprocated or is equal to 0. The index  $i$  of the element is identified in the computational error message.
- The return code is set to 1.
- $i$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2105 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

$n < 0$

## Examples

### Example

This example shows how to factor the following tridiagonal matrix  $A$  of order 4:

$$\begin{bmatrix} 2.0 & 2.0 & 0.0 & 0.0 \\ 1.0 & 3.0 & 2.0 & 0.0 \\ 0.0 & 1.0 & 3.0 & 2.0 \\ 0.0 & 0.0 & 1.0 & 3.0 \end{bmatrix}$$

**Call Statement and Input:**

	N	C	D	E	F	IPVT
CALL DGTF(	4	,	C	,	D	,
		,	E	,	F	,
			,		,	IPVT
						)

C = ( . , 1.0, 1.0, 1.0)  
D = (2.0, 3.0, 3.0, 3.0)  
E = (2.0, 2.0, 2.0, . )

**Output:**

C = ( . , -0.5, -0.5, -0.5)  
D = (-0.5, -0.5, -0.5, -0.5)  
E = (2.0, 2.0, 2.0, . )  
IPVT = (X'00', X'00', X'00', X'00')

*Notes:*

1. F is stored in an internal format and is passed unchanged to the solve subroutine.
2. A "." means you do not have to store a value in that position in the array. However, these storage positions are required and may be overwritten during the computation.

## SGTS and DGTS — General Tridiagonal Matrix Solve

### Purpose

These subroutines solve a tridiagonal system of linear equations using the factorization of tridiagonal matrix  $A$ , stored in tridiagonal storage mode, produced by SGTF or DGTF, respectively.

Table 120. Data Types

$c, d, e, f, b, x$	Subroutine
Short-precision real	SGTS
Long-precision real	DGTS

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGTF and DGTF, respectively.

### Syntax

Fortran	CALL SGTS   DGTS ( $n, c, d, e, f, ipvt, bx$ )
C and C++	sgts   dgts ( $n, c, d, e, f, ipvt, bx$ );

### On Entry

- $n$  is the order  $n$  of tridiagonal matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- $c$  is the vector  $c$ , containing part of the factorization of matrix  $A$  from SGTF or DGTF, respectively, in an array, referred to as C. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 120.
- $d$  is the vector  $d$ , containing part of the factorization of matrix  $A$  from SGTF or DGTF, respectively, in an array, referred to as D. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 120.
- $e$  is the vector  $e$ , containing part of the factorization of matrix  $A$  from SGTF or DGTF, respectively, in an array, referred to as E. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 120.
- $f$  is the vector  $f$ , containing part of the factorization of matrix  $A$  from SGTF or DGTF, respectively, in an array, referred to as F. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 120.
- $ipvt$  is the integer vector  $ipvt$  of length  $n$ , containing the pivot information, produced by a preceding call to SGTF and DGTF, respectively. Specified as: a one-dimensional array of (at least) length  $n$ , containing fullword integers.
- $bx$  is the vector  $b$  of length  $n$ , containing the right-hand side of the system in the first  $n$  positions in an array, referred to as BX. Specified as: a one-dimensional array of (at least) length  $n+1$ , containing numbers of the data type indicated in Table 120. For details on specifying the length, see “Notes” on page 597.

**On Return**

*bx* is the solution vector  $x$  (at least) of length  $n$ , containing the solution of the tridiagonal system in the first  $n$  positions in an array, referred to as BX. Returned as: a one-dimensional array, of (at least) length  $(n+1)$ , containing numbers of the data type indicated in Table 120 on page 596. For details about the length, see “Notes.”

**Notes**

1. For a description of how tridiagonal matrices are stored, see “General Tridiagonal Matrix” on page 92.
2. Array BX can have a length of  $n$  if memory location  $BX(n+1)$  is addressable—that is, not in read-protected storage. If it is in read-protected storage, array BX must have a length of  $n+1$ . In both cases, the vector  $b$  (on input) and vector  $x$  (on output) reside in positions 1 through  $n$  in array BX. Array location  $BX(n+1)$  is not altered by these subroutines.

**Function**

Given the factorization produced by SGTF or DGTF, respectively, these subroutines use the standard forward elimination and back substitution to solve the tridiagonal system  $Ax = b$ , where  $A$  is a general tridiagonal matrix. See references [45], [56], [57], and [94].

**Error conditions**

**Computational Errors**

None

**Input-Argument Errors**

$n < 0$

**Examples**

**Example**

This example solves the tridiagonal system  $Ax = b$ , where matrix  $A$  is the same matrix factored in “Example” on page 594 for SGTF and DGTF, and where:

$$b = (4.0, 6.0, 6.0, 4.0)$$

$$x = (1.0, 1.0, 1.0, 1.0)$$

**Call Statement and Input:**

	N	C	D	E	F	IPVT	BX
CALL DGTS(	4	,	C	,	D	,	E
		,	F	,	IPVT	,	BX
			)				

C = (same as output C in “Example” on page 594)  
 D = (same as output D in “Example” on page 594)  
 E = (same as output E in “Example” on page 594)  
 F = (same as output F in “Example” on page 594)  
 IPVT = (same as output IPVT in “Example” on page 594)  
 BX = (4.0, 6.0, 6.0, 4.0, . )

**Output:**

BX = (1.0, 1.0, 1.0, 1.0, . )

## SGTNP, DGTNP, CGTNP, and ZGTNP — General Tridiagonal Matrix Combined Factorization and Solve with No Pivoting

### Purpose

These subroutines solve the tridiagonal system  $Ax = b$  using Gaussian elimination, where tridiagonal matrix  $A$  is stored in tridiagonal storage mode.

Table 121. Data Types

$c, d, e, b, x$	Subroutine
Short-precision real	SGTNP
Long-precision real	DGTNP
Short-precision complex	CGTNP
Long-precision complex	ZGTNP

**Note:** In general, these subroutines provide better performance than the `_GTNPF` and `_GTNPS` subroutines; however, in the following instances, you get better performance by using `_GTNPF` and `_GTNPS`:

- For small  $n$
- When performing a single factorization followed by multiple solves

### Syntax

Fortran	CALL SGTNP   DGTNP   CGTNP   ZGTNP ( $n, c, d, e, bx$ )
C and C++	sgtnp   dgtnp   cgtnp   zgtnp ( $n, c, d, e, bx$ );

### On Entry

- $n$  is the order  $n$  of tridiagonal matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- $c$  is the vector  $c$ , containing the lower subdiagonal of matrix  $A$  in positions 2 through  $n$  in an array, referred to as C. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 121. On output, C is overwritten; that is, the original input is not preserved.
- $d$  is the vector  $d$ , containing the main diagonal of matrix  $A$  in positions 1 through  $n$  in an array, referred to as D. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 121. On output, D is overwritten; that is, the original input is not preserved.
- $e$  is the vector  $e$ , containing the upper subdiagonal of matrix  $A$  in positions 1 through  $n-1$  in an array, referred to as E. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 121. On output, E is overwritten; that is, the original input is not preserved.
- $bx$  is the vector  $b$ , containing the right-hand side of the system in the first  $n$  positions in an array, referred to as BX. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 121.



**On Return**

$bx$  is the solution vector  $x$  of length  $n$ , containing the solution of the tridiagonal system in the first  $n$  positions in an array, referred to as BX. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 121 on page 598.

**Notes**

For a description of how tridiagonal matrices are stored, see “General Tridiagonal Matrix” on page 92.

**Function**

The solution of the tridiagonal system  $Ax = b$  is computed by Gaussian elimination.

No pivoting is done. Therefore, these subroutines should not be used when pivoting is necessary to maintain the numerical accuracy of the solution. Overflow may occur if small main diagonal elements are generated. Underflow or accuracy loss may occur if large main diagonal elements are generated.

For performance reasons, complex divides are done without scaling. Computing the inverse in this way restricts the range of numbers for which the ZGTNP subroutine works properly.

For performance reasons, divides are done in a way that reduces the effective exponent range for which DGTNP and ZGTNP work properly; therefore, you may want to scale your problem, such that the diagonal elements are close to 1.0 for DGTNP and (1.0, 0.0) for ZGTNP.

**Error conditions****Computational Errors**

None

**Input-Argument Errors**

$n < 0$

**Examples****Example 1**

This example shows a factorization of the real tridiagonal matrix  $A$ , of order 4:

$$\begin{bmatrix} 7.0 & 4.0 & 0.0 & 0.0 \\ 1.0 & 8.0 & 5.0 & 0.0 \\ 0.0 & 2.0 & 9.0 & 6.0 \\ 0.0 & 0.0 & 3.0 & 10.0 \end{bmatrix}$$

It then finds the solution of the tridiagonal system  $Ax = b$ , where  $b$  is:

(11.0, 14.0, 17.0, 13.0)

and  $x$  is:

(1.0, 1.0, 1.0, 1.0)

On output, arrays C, D, and E are overwritten.

## SGTNP, DGTNP CGTNP, and ZGTNP

### Call Statement and Input:

```
          N   C   D   E   BX
          |   |   |   |   |
CALL DGTNP( 4 , C , D , E , BX )

C       = ( . , 1.0, 2.0, 3.0)
D       = (7.0, 8.0, 9.0, 10.0)
E       = (4.0, 5.0, 6.0, . )
BX      = (11.0, 14.0, 17.0, 13.0)
```

### Output:

```
BX      = (1.0, 1.0, 1.0, 1.0)
```

### Example 2

This example shows a factorization of the complex tridiagonal matrix  $A$ , of order 4:

$$\begin{bmatrix} (7.0, 7.0) & (4.0, 4.0) & (0.0, 0.0) & (0.0, 0.0) \\ (1.0, 1.0) & (8.0, 8.0) & (5.0, 5.0) & (0.0, 0.0) \\ (0.0, 0.0) & (2.0, 2.0) & (9.0, 9.0) & (6.0, 6.0) \\ (0.0, 0.0) & (0.0, 0.0) & (3.0, 3.0) & (10.0, 10.0) \end{bmatrix}$$

It then finds the solution of the tridiagonal system  $Ax = b$ , where  $b$  is:

```
((-11.0,19.0), (-14.0,50.0), (-17.0,93.0), (-13.0,85.0))
```

and  $x$  is:

```
((1.0,-1.0), (2.0,-2.0), (3.0,-3.0), (4.0,-4.0))
```

On output, arrays C, D, and E are overwritten.

### Call Statement and Input:

```
          N   C   D   E   BX
          |   |   |   |   |
CALL ZGTNP( 4 , C , D , E , BX )

C       = ( . , (1.0, 1.0), (2.0, 2.0), (3.0, 3.0))
D       = ((7.0, 7.0), (8.0, 8.0), (9.0, 9.0), (10.0, 10.0))
E       = ((4.0, 4.0), (5.0, 5.0), (6.0, 6.0), . )
BX      = ((-11.0, 19.0), (-14.0, 50.0), (-17.0, 93.0), (-13.0, 85.0))
```

### Output:

```
BX      = ((0.0, 1.0), (1.0, 2.0), (2.0, 3.0), (3.0, 4.0))
```

## SGTNPF, DGTNPF, CGTNPF, and ZGTNPF — General Tridiagonal Matrix Factorization with No Pivoting

### Purpose

These subroutines factor tridiagonal matrix  $A$ , stored in tridiagonal storage mode, using Gaussian elimination. To solve a tridiagonal system of linear equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGTNPS, DGTNPS, CGTNPS, or ZGTNPS, respectively.

Table 122. Data Types

$c, d, e$	Subroutine
Short-precision real	SGTNPF
Long-precision real	DGTNPF
Short-precision complex	CGTNPF
Long-precision complex	ZGTNPF

### Notes:

1. The output from these factorization subroutines should be used only as input to the solve subroutines SGTNPS, DGTNPS, CGTNPS, and ZGTNPS, respectively.
2. In general, the `_GTNP` subroutines provide better performance than the `_GTNPF` and `_GTNPS` subroutines; however, in the following instances, you get better performance by using `_GTNPF` and `_GTNPS`:
  - For small  $n$
  - When performing a single factorization followed by multiple solves

### Syntax

Fortran	CALL SGTNPF   DGTNPF   CGTNPF   ZGTNPF ( $n, c, d, e, iopt$ )
C and C++	sgtnpf   dgtnpf   cgtnpf   zgtnpf ( $n, c, d, e, iopt$ );

### On Entry

- $n$  is the order  $n$  of tridiagonal matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- $c$  is the vector  $c$ , containing the lower subdiagonal of matrix  $A$  in positions 2 through  $n$  in an array, referred to as C. Specified as: a one-dimensional array, of (at least) length  $n$ , containing numbers of the data type indicated in Table 122.
- $d$  is the vector  $d$ , containing the main diagonal of matrix  $A$  in positions 1 through  $n$  in an array, referred to as D. Specified as: a one-dimensional array, of (at least) length  $n$ , containing numbers of the data type indicated in Table 122.
- $e$  is the vector  $e$ , containing the upper subdiagonal of matrix  $A$  in positions 1 through  $n-1$  in an array, referred to as E. Specified as: a one-dimensional array, of (at least) length  $n$ , containing numbers of the data type indicated in Table 122.
- $iopt$  indicates the type of computation to be performed, where:

## SGTNPF, DGTNPF CGTNPF, and ZGTNPF

If  $iopt = 0$  or  $1$ , Gaussian elimination is used to factor the matrix.

Specified as: a fullword integer;  $iopt = 0$  or  $1$ .

### On Return

- $c$  is the vector  $c$ , containing part of the factorization of matrix  $A$  in positions 1 through  $n$  in an array, referred to as C. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 122 on page 601.
- $d$  is the vector  $d$ , containing part of the factorization of matrix  $A$  in an array, referred to as D. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 122 on page 601.
- $e$  is the vector  $e$ , containing part of the factorization of matrix  $A$  in positions 1 through  $n$  in an array, referred to as E. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 122 on page 601. It has the same length as E on entry.

### Notes

For a description of how tridiagonal matrices are stored, see “General Tridiagonal Matrix” on page 92.

### Function

The factorization of a diagonally-dominant tridiagonal matrix  $A$  is computed using Gaussian elimination. This factorization can then be used by SGTNPS, DGTNPS, CGTNPS, or ZGTNPS respectively, to solve the tridiagonal systems of linear equations. See reference [80].

No pivoting is done by these subroutines. Therefore, these subroutines should not be used when pivoting is necessary to maintain the numerical accuracy of the solution. Overflow may occur if small main diagonal elements are generated. Underflow or accuracy loss may occur if large main diagonal elements are generated.

For performance reasons, complex divides are done without scaling. Computing the inverse in this way restricts the range of numbers for which ZGTNPF works properly.

For performance reasons, divides are done in a way that reduces the effective exponent range for which DGTNPF and ZGTNPF work properly; therefore, you may want to scale your problem, such that the diagonal elements are close to 1.0 for DGTNPF and (1.0, 0.0) for ZGTNPF.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

1.  $n < 0$
2.  $iopt \neq 0$  or  $1$

## Examples

### Example 1

This example shows a factorization of the tridiagonal matrix  $A$ , of order 4:

$$\begin{bmatrix} 1.0 & 1.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 1.0 & 0.0 \\ 0.0 & 1.0 & 3.0 & 1.0 \\ 0.0 & 0.0 & 1.0 & 1.0 \end{bmatrix}$$

#### Call Statement and Input:

```

      N   C   D   E   IOPT
      |   |   |   |   |
CALL DGTNPF( 4 , C , D , E , 0 )

```

```

C      = ( . , 1.0, 1.0, 1.0)
D      = (1.0, 2.0, 3.0, 1.0)
E      = (1.0, 1.0, 1.0, . )

```

#### Output:

```

C      = ( . , -1.0, -1.0, 1.0)
D      = (-1.0, -1.0, -1.0, -1.0)
E      = (1.0, 1.0, -1.0, . )

```

### Example 2

This example shows a factorization of the tridiagonal matrix  $A$ , of order 4:

$$\begin{bmatrix} (7.0, 7.0) & (4.0, 4.0) & (0.0, 0.0) & (0.0, 0.0) \\ (1.0, 1.0) & (8.0, 8.0) & (5.0, 5.0) & (0.0, 0.0) \\ (0.0, 0.0) & (2.0, 2.0) & (9.0, 9.0) & (6.0, 6.0) \\ (0.0, 0.0) & (0.0, 0.0) & (3.0, 3.0) & (10.0, 10.0) \end{bmatrix}$$

#### Call Statement and Input:

```

      N   C   D   E   IOPT
      |   |   |   |   |
CALL ZGTNPF( 4 , C , D , E , 0 )

```

```

C      = ( . , (1.0, 1.0), (2.0, 2.0), (3.0, 3.0))
D      = ((7.0, 7.0), (8.0, 8.0), (9.0, 9.0), (10.0, 10.0))
E      = ((4.0, 4.0), (5.0, 5.0), (6.0, 6.0), . )

```

#### Output:

```

C      = ( . , (-0.142, 0.0), (-0.269, 0.0), (3.0, 3.0))
D      = ((-0.0714, 0.0714), (-0.0673, 0.0673), (-0.0854, 0.0854),
          (-0.05, 0.05))
E      = ((4.0, 4.0), (5.0, 5.0), (-0.6, 0.0), . )

```

#### Notes:

1. A "." means you do not have to store a value in that position in the array. However, these storage positions are required and may be overwritten during the computation.

## SGTNPS, DGTNPS, CGTNPS, and ZGTNPS — General Tridiagonal Matrix Solve with No Pivoting

### Purpose

These subroutines solve a tridiagonal system of equations using the factorization of matrix  $A$ , stored in tridiagonal storage mode, produced by SGTNPF, DGTNPF, CGTNPF, or ZGTNPF, respectively.

Table 123. Data Types

$c, d, e, b, x$	Subroutine
Short-precision real	SGTNPS
Long-precision real	DGTNPS
Short-precision complex	CGTNPS
Long-precision complex	ZGTNPS

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGTNPF, DGTNPF, CGTNPF, and ZGTNPF, respectively.

### Syntax

Fortran	CALL SGTNPS   DGTNPS   CGTNPS   ZGTNPS ( $n, c, d, e, bx$ )
C and C++	sgtnps   dgtmps   cgtmps   zgtmps ( $n, c, d, e, bx$ );

### On Entry

- $n$  is the order  $n$  of tridiagonal matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- $c$  is the vector  $c$ , containing part of the factorization of matrix  $A$  from SGTNPF, DGTNPF, CGTNPF, and ZGTNPF, respectively, in an array, referred to as C. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 123.
- $d$  is the vector  $d$ , containing part of the factorization of matrix  $A$  from SGTNPF, DGTNPF, CGTNPF, and ZGTNPF, respectively, in an array, referred to as D. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 123.
- $e$  is the vector  $e$ , containing part of the factorization of matrix  $A$  from SGTNPF, DGTNPF, CGTNPF, and ZGTNPF, respectively, in an array, referred to as E. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 123.
- $bx$  is the vector  $b$ , containing the right-hand side of the system in the first  $n$  positions in an array, referred to as BX. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 123.

**On Return**

$bx$  is the solution vector  $x$  of length  $n$ , containing the solution of the tridiagonal system in the first  $n$  positions in an array, referred to as BX. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 123 on page 604.

**Notes**

For a description of how tridiagonal matrices are stored, see “General Tridiagonal Matrix” on page 92.

**Function**

The solution of tridiagonal system  $Ax = b$  is computed using the factorization produced by SGTNPF, DGTNPF, CGTNPF, or ZGTNPF, respectively. The factorization is based on Gaussian elimination. See reference [80].

**Error conditions****Computational Errors**

None

**Input-Argument Errors**

$n < 0$

**Examples****Example 1**

This example finds the solution of tridiagonal system  $Ax = b$ , where matrix  $A$  is the same matrix factored in “Example 1” on page 603 for SGTNPF and DGTNPF.  $b$  is:

(2.0, 4.0, 5.0, 2.0)

and  $x$  is:

(1.0, 1.0, 1.0, 1.0)

**Call Statement and Input:**

```

      N   C   D   E   BX
      |   |   |   |   |
CALL DGTNPS( 4 , C , D , E , BX )

```

C = (same as output C in “Example 1” on page 603)  
D = (same as output D in “Example 1” on page 603)  
E = (same as output E in “Example 1” on page 603)  
BX = (2.0, 4.0, 5.0, 2.0)

**Output:**

BX = (1.0, 1.0, 1.0, 1.0)

**Example 2**

This example finds the solution of tridiagonal system  $Ax = b$ , where matrix  $A$  is the same matrix factored in “Example 2” on page 603 for CGTNPF and ZGTNPF.  $b$  is:

((-11.0,19.0), (-14.0,50.0), (-17.0,93.0), (-13.0,85.0))

## SGTNPS, DGTNPS, CGTNPS, and ZGTNPS

and  $x$  is:

$((0.0,1.0), (1.0,2.0), (2.0,3.0), (3.0,4.0))$

### Call Statement and Input:

```
          N   C   D   E   BX
          |   |   |   |   |
CALL ZGTNPS( 4 , C , D , E , BX )
```

C = (same as output C in "Example 2" on page 603)

D = (same as output D in "Example 2" on page 603)

E = (same as output E in "Example 2" on page 603)

BX =  $((-11.0, 19.0), (-14.0, 50.0), (-17.0, 93.0), (-13.0, 8))$

### Output:

BX =  $((0.0, 1.0), (1.0, 2.0), (2.0, 3.0), (3.0, 4.0))$



## SPTF and DPTF — Positive Definite Symmetric Tridiagonal Matrix Factorization

### Purpose

These subroutines factor symmetric tridiagonal matrix  $A$ , stored in symmetric-tridiagonal storage mode, using Gaussian elimination. To solve a tridiagonal system of linear equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SPTS or DPTS, respectively.

Table 124. Data Types

$c, d$	Subroutine
Short-precision real	SPTF
Long-precision real	DPTF

**Note:** The output from these factorization subroutines should be used only as input to the solve subroutines SPTS and DPTS, respectively.

### Syntax

Fortran	CALL SPTF   DPTF ( $n, c, d, iopt$ )
C and C++	sptf   dptf ( $n, c, d, iopt$ );

### On Entry

- $n$  is the order  $n$  of tridiagonal matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- $c$  is the vector  $c$ , containing the off-diagonal of matrix  $A$  in positions 2 through  $n$  in an array, referred to as C. Specified as: a one-dimensional array, of (at least) length  $n$ , containing numbers of the data type indicated in Table 124.
- $d$  is the vector  $d$ , containing the main diagonal of matrix  $A$  in positions 1 through  $n$  in an array referred to as D. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 124.
- $iopt$  indicates the type of computation to be performed, where:
- If  $iopt = 0$  or 1, Gaussian elimination is used to factor the matrix.
- Specified as: a fullword integer;  $iopt = 0$  or 1.

### On Return

- $c$  is the vector  $c$ , containing part of the factorization of matrix  $A$  in an array, referred to as C. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 124.
- $d$  is the vector  $d$ , containing part of the factorization of matrix  $A$  in positions 1 through  $n$  in an array, referred to as D. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 124. It has the same length as D on entry.

## Notes

For a description of how positive definite symmetric tridiagonal matrices are stored, see "Positive Definite Symmetric Tridiagonal Matrix" on page 94.

## Function

The factorization of positive definite symmetric tridiagonal matrix  $A$  is computed using Gaussian elimination. This factorization can then be used by SPTS or DPTS, respectively, to solve the tridiagonal systems of linear equations. See reference [80].

No pivoting is done. Therefore, these subroutines should not be used when pivoting is necessary to maintain the numerical accuracy of the solution. Overflow may occur if small pivots are generated.

For performance reasons, divides are done in a way that reduces the effective exponent range for which DPTF works properly; therefore, you may want to scale your problem, such that the diagonal elements are close to 1.0 for DPTF.

## Error conditions

### Computational Errors

None

**Note:** There is no test for positive definiteness in these subroutines.

### Input-Argument Errors

1.  $n < 0$
2.  $iopt \neq 0$  or 1

## Examples

### Example

This example shows a factorization of the tridiagonal matrix  $A$ , of order 4:

$$\begin{bmatrix} 1.0 & 1.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 1.0 & 0.0 \\ 0.0 & 1.0 & 3.0 & 1.0 \\ 0.0 & 0.0 & 1.0 & 1.0 \end{bmatrix}$$

### Call Statement and Input:

```

      N   C   D   IOPT
      |   |   |   |
CALL DPTF( 4 , C , D , 0 )

```

```

C      = ( . , 1.0, 1.0, 1.0)
D      = (1.0, 2.0, 3.0, 1.0)

```

### Output:

```

C      = ( . , -1.0, -1.0, -1.0)
D      = (-1.0, -1.0, -1.0, -1.0)

```

### Notes:

1. A "." means you do not have to store a value in that position in the array. However, these storage positions are required and may be overwritten during the computation.

## SPTS and DPTS — Positive Definite Symmetric Tridiagonal Matrix Solve

### Purpose

These subroutines solve a positive definite symmetric tridiagonal system of equations using the factorization of matrix  $A$ , stored in symmetric-tridiagonal storage mode, produced by SPTF and DPTF, respectively.

Table 125. Data Types

$c, d, b, x$	Subroutine
Short-precision real	SPTS
Long-precision real	DPTS

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SPTF and DPTF, respectively.

### Syntax

<b>Fortran</b>	CALL SPTS   DPTS ( $n, c, d, bx$ )
<b>C and C++</b>	spts   dpts ( $n, c, d, bx$ );

### On Entry

- $n$  is the order  $n$  of tridiagonal matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- $c$  is the vector  $c$ , containing part of the factorization of matrix  $A$  from SPTF or DPTF, respectively, in an array, referred to as C. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 125.
- $d$  is the vector  $d$ , containing part of the factorization of matrix  $A$  from SPTF or DPTF, respectively, in an array, referred to as D. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 125.
- $bx$  is the vector  $b$ , containing the right-hand side of the system in the first  $n$  positions in an array, referred to as BX. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 125.

### On Return

- $bx$  is the solution vector  $x$  of length  $n$ , containing the solution of the tridiagonal system in the first  $n$  positions in an array, referred to as BX. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 125.

### Notes

For a description of how tridiagonal matrices are stored, see “Positive Definite or Negative Definite Symmetric Matrix” on page 73.

## Function

The solution of positive definite symmetric tridiagonal system  $Ax = b$  is computed using the factorization produced by SPTF or DPTF, respectively. The factorization is based on Gaussian elimination. See reference [80].

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example

This example finds the solution of tridiagonal system  $Ax = b$ , where matrix  $A$  is the same matrix factored in "Example" on page 608 for SPTF and DPTF.  $b$  is:

(2.0, 4.0, 5.0, 2.0)

and  $x$  is:

(1.0, 1.0, 1.0, 1.0)

### Call Statement and Input:

```

          N   C   D   BX
          |   |   |   |
CALL DPTS( 4 , C , D , BX )

```

```

C       = ( . , -1.0, -1.0, -1.0)
D       = (-1.0, -1.0, -1.0, -1.0)
BX      = (2.0, 4.0, 5.0, 2.0)

```

### Output:

```

BX      = (1.0, 1.0, 1.0, 1.0)

```

## STBSV, DTBSV, CTBSV, and ZTBSV — Triangular Band Equation Solve

### Purpose

STBSV and DTBSV solve one of the following triangular banded systems of equations with a single right-hand side, using the vector  $x$  and triangular band matrix  $A$  or its transpose:

Solution	Equation
1. $x \leftarrow A^{-1}x$	$Ax = b$
2. $x \leftarrow A^{-T}x$	$A^T x = b$

CTBSV and ZTBSV solve one of the following triangular banded systems of equations with a single right-hand side, using the vector  $x$  and triangular band matrix  $A$ , its transpose, or its conjugate transpose:

Solution	Equation
1. $x \leftarrow A^{-1}x$	$Ax = b$
2. $x \leftarrow A^{-T}x$	$A^T x = b$
3. $x \leftarrow A^{-H}x$	$A^H x = b$

Matrix  $A$  can be either upper or lower triangular and is stored in upper- or lower-triangular-band-packed storage mode, respectively.

Table 126. Data Types

$A, x$	Subprogram
Short-precision real	STBSV
Long-precision real	DTBSV
Short-precision complex	CTBSV
Long-precision complex	ZTBSV

### Syntax

<b>Fortran</b>	CALL STBSV   DTBSV   CTBSV   ZTBSV ( <i>uplo, trans, diag, n, k, a, lda, x, incx</i> )
<b>C and C++</b>	stbsv   dtbsv   ctbsv   ztbsv ( <i>uplo, trans, diag, n, k, a, lda, x, incx</i> );

### On Entry

*uplo* indicates whether matrix  $A$  is an upper or lower triangular band matrix, where:

If *uplo* = 'U',  $A$  is an upper triangular matrix.

If *uplo* = 'L',  $A$  is a lower triangular matrix.

Specified as: a single character. It must be 'U' or 'L'.

*trans* indicates the form of matrix  $A$  used in the system of equations, where:

If *trans* = 'N',  $A$  is used, resulting in solution 1.

If *trans* = 'T',  $A^T$  is used, resulting in solution 2.

If *trans* = 'C',  $A^H$  is used, resulting in solution 3.

## STBSV, DTBSV, CTBSV, and ZTBSV

	Specified as: a single character. It must be 'N', 'T', or 'C'.
<i>diag</i>	indicates the characteristics of the diagonal of matrix <i>A</i> , where: If <i>diag</i> = 'U', <i>A</i> is a unit triangular matrix. If <i>diag</i> = 'N', <i>A</i> is not a unit triangular matrix. Specified as: a single character. It must be 'U' or 'N'.
<i>n</i>	is the order of triangular band matrix <i>A</i> . Specified as: a fullword integer; $n \geq 0$ .
<i>k</i>	is the upper or lower band width <i>k</i> of the matrix <i>A</i> . Specified as: a fullword integer; $k \geq 0$ .
<i>a</i>	is the upper or lower triangular band matrix <i>A</i> of order <i>n</i> , stored in upper- or lower-triangular-band-packed storage mode, respectively. Specified as: an <i>lda</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 126 on page 611.
<i>lda</i>	is the leading dimension of the array specified for <i>a</i> . Specified as: a fullword integer; $lda > 0$ and $lda \geq k+1$ .
<i>x</i>	is the vector <i>x</i> of length <i>n</i> , containing the right-hand side of the triangular system to be solved. Specified as: a one-dimensional array of (at least) length $1+(n-1) incx $ , containing numbers of the data type indicated in Table 126 on page 611.
<i>incx</i>	is the stride for vector <i>x</i> . Specified as: a fullword integer; $incx > 0$ or $incx < 0$ .

### On Return

<i>x</i>	is the solution vector <i>x</i> of length <i>n</i> , containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 126 on page 611.
----------	---

### Notes

1. These subroutines accept lowercase letters for the *uplo*, *trans*, and *diag* arguments.
2. For STBSV and DTBSV, if you specify 'C' for the *trans* argument, it is interpreted as though you specified 'T'.
3. Matrix *A* and vector *x* must have no common elements; otherwise, results are unpredictable.
4. For unit triangular matrices, the elements of the diagonal are assumed to be 1.0 for real matrices and (1.0, 0.0) for complex matrices, and you do not need to set these values in the array.
5. For both upper and lower triangular band matrices, if you specify  $k \geq n$ , ESSL assumes, **for purposes of the computation only**, that the upper or lower band width of matrix *A* is  $n-1$ ; that is, it processes matrix *A* of order *n*, as though it is a (nonbanded) triangular matrix. However, ESSL uses the original value for **for the purposes of finding the locations** of element  $a_{11}$  and all other elements in the array specified for *A*, as described in "Triangular Band Matrix" on page 88. For an illustration of this technique, see "Example 3" on page 614.
6. For a description of triangular band matrices and how they are stored in upper- and lower-triangular-band-packed storage mode, see "Triangular Band Matrix" on page 88.
7. If you are using a lower triangular band matrix, it may save your program some time if you use this alternate approach instead of using

lower-triangular-band-packed storage mode. Leave matrix  $A$  in full-matrix storage mode when you pass it to ESSL and specify the  $lda$  argument to be  $lda+1$ , which is the leading dimension of matrix  $A$  plus 1. ESSL then processes the matrix elements in the same way as though you had set them up in lower-triangular-band-packed storage mode.

## Function

These subroutines solve a triangular banded system of equations with a single right-hand side. The solution,  $x$ , may be any of the following, where triangular band matrix  $A$ , its transpose, or its conjugate transpose is used, and where  $A$  can be either upper- or lower-triangular:

1.  $x \leftarrow A^{-1}x$
2.  $x \leftarrow A^{-T}x$
3.  $x \leftarrow A^{-H}x$  (for CTBSV and ZTBSV only)

where:

$x$  is a vector of length  $n$ .

$A$  is an upper or lower triangular band matrix of order  $n$ , stored in upper- or lower-triangular-band-packed storage mode, respectively.

See references [36], [48], and [40]. If  $n$  is 0, no computation is performed.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $n < 0$
2.  $k < 0$
3.  $lda \leq 0$
4.  $lda < k+1$
5.  $incx = 0$
6.  $uplo \neq 'L'$  or  $'U'$
7.  $trans \neq 'T', 'N',$  or  $'C'$
8.  $diag \neq 'N'$  or  $'U'$

## Examples

### Example 1

This example shows the solution  $x \leftarrow A^{-1}x$ . Matrix  $A$  is a real 9 by 9 upper triangular band matrix with an upper band width of 2 that is not unit triangular, stored in upper-triangular-band-packed storage mode. Vector  $x$  is a vector of length 9, where matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 4.0 & 2.0 & 3.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 4.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 4.0 & 2.0 & 2.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 3.0 & 1.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 3.0 & 2.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 3.0 & 1.0 & 0.0 \end{bmatrix}$$

## STBSV, DTBSV, CTBSV, and ZTBSV

$$\begin{bmatrix} 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 2.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{bmatrix}$$

### Call Statement and Input:

```

          UPLO TRANS  DIAG  N  K  A  LDA  X  INCX
CALL STBSV( 'U' , 'N' , 'N' , 9 , 2 , A , 3 , X , 1 )

```

$$A = \begin{bmatrix} . & . & 1.0 & 3.0 & 1.0 & 2.0 & 1.0 & 2.0 & 0.0 \\ . & 1.0 & 2.0 & 1.0 & 2.0 & 1.0 & 2.0 & 1.0 & 2.0 \\ 1.0 & 4.0 & 4.0 & 4.0 & 3.0 & 3.0 & 3.0 & 2.0 & 1.0 \end{bmatrix}$$

$$X = (2.0, 7.0, 1.0, 8.0, 2.0, 8.0, 1.0, 8.0, 3.0)$$

### Output:

$$X = (1.0, 1.0, 0.0, 1.0, 0.0, 2.0, 0.0, 1.0, 3.0)$$

### Example 2

This example shows the solution  $x \leftarrow A^{-T}x$ , solving the same system as in Example 1. Matrix  $A$  is a real 9 by 9 lower triangular band matrix with a lower band width of 2 that is not unit triangular, stored in lower-triangular-band-packed storage mode. Vector  $x$  is a vector of length 9 where matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 4.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 4.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 3.0 & 1.0 & 4.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 1.0 & 3.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \end{bmatrix}$$

### Call Statement and Input:

```

          UPLO TRANS  DIAG  N  K  A  LDA  X  INCX
CALL STBSV( 'L' , 'T' , 'N' , 9 , 2 , A , 3 , X , 1 )

```

$$A = \begin{bmatrix} 1.0 & 4.0 & 4.0 & 4.0 & 3.0 & 3.0 & 3.0 & 2.0 & 1.0 \\ 1.0 & 2.0 & 1.0 & 2.0 & 1.0 & 2.0 & 1.0 & 2.0 & . \\ 1.0 & 3.0 & 1.0 & 2.0 & 1.0 & 2.0 & 0.0 & . & . \end{bmatrix}$$

$$X = (\text{same as input } X \text{ in Example 1})$$

### Output:

$$X = (\text{same as output } X \text{ in Example 1})$$

### Example 3

This example shows the solution  $x \leftarrow A^{-T}x$ , where  $k > n$ . Matrix  $A$  is a real 4 by 4 upper triangular band matrix with an upper band width of 3, even though  $k$  is specified as 5. It is not unit triangular and is stored in upper-triangular-band-packed storage mode. Vector  $x$  is a vector of length 4 where matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 2.0 & 3.0 & 2.0 \\ 0.0 & 2.0 & 2.0 & 5.0 \end{bmatrix}$$



$$\begin{bmatrix} 0.0 & 0.0 & 3.0 & 3.0 \\ 0.0 & 0.0 & 0.0 & 1.0 \end{bmatrix}$$

**Call Statement and Input:**

```

          UPLO TRANS  DIAG  N  K  A  LDA  X  INCX
CALL STBSV( 'U' , 'T' , 'N' , 4 , 5 , A , 6 , X , 1 )
    
```

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 2.0 \\ \cdot & \cdot & 3.0 & 5.0 \\ \cdot & 2.0 & 2.0 & 3.0 \\ 1.0 & 2.0 & 3.0 & 1.0 \end{bmatrix}$$

$$X = (5.0, 18.0, 32.0, 41.0)$$

**Output:**

$$X = (5.0, 4.0, 3.0, 2.0)$$

**Example 4**

This example shows the solution  $x \leftarrow A^{-T}x$ . Matrix  $A$  is a complex 7 by 7 lower triangular band matrix with a lower band width of 3 that is not unit triangular, stored in lower-triangular-band-packed storage mode. Vector  $x$  is a vector of length 7. Matrix  $A$  is:

$$\begin{bmatrix} (1.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) \\ (1.0, 2.0) & (2.0, 1.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) \\ (1.0, 3.0) & (2.0, 2.0) & (3.0, 1.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) \\ (1.0, 4.0) & (2.0, 3.0) & (3.0, 3.0) & (4.0, 1.0) & (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) \\ (0.0, 0.0) & (2.0, 4.0) & (3.0, 3.0) & (4.0, 2.0) & (2.0, 1.0) & (0.0, 0.0) & (0.0, 0.0) \\ (0.0, 0.0) & (0.0, 0.0) & (3.0, 3.0) & (4.0, 3.0) & (5.0, 1.0) & (3.0, 1.0) & (0.0, 0.0) \\ (0.0, 0.0) & (0.0, 0.0) & (0.0, 0.0) & (4.0, 4.0) & (5.0, 2.0) & (6.0, 1.0) & (2.0, 1.0) \end{bmatrix}$$

**Call Statement and Input:**

```

          UPLO TRANS  DIAG  N  K  A  LDA  X  INCX
CALL CTBSV( 'L' , 'T' , 'N' , 7 , 3 , A , 4 , X , 1 )
    
```

$$A = \begin{bmatrix} (1.0, 0.0) & (2.0, 1.0) & (3.0, 1.0) & (4.0, 1.0) & (2.0, 1.0) & (3.0, 1.0) & (2.0, 1.0) \\ (1.0, 2.0) & (2.0, 2.0) & (3.0, 3.0) & (4.0, 2.0) & (5.0, 1.0) & (6.0, 1.0) & \cdot \\ (1.0, 3.0) & (2.0, 3.0) & (3.0, 3.0) & (4.0, 3.0) & (5.0, 2.0) & \cdot & \cdot \\ (1.0, 4.0) & (2.0, 4.0) & (3.0, 3.0) & (4.0, 4.0) & \cdot & \cdot & \cdot \end{bmatrix}$$

$$X = ((2.0, 2.0), (7.0, 1.0), (1.0, 1.0), (8.0, 1.0), (2.0, 0.0), (8.0, 1.0), (1.0, 2.0))$$

**Output:**

$$X = ((-12.048, -13.136), (6.304, -1.472), (-1.880, 1.040), (2.600, -1.800), (-2.160, 1.880), (0.800, -1.400), (0.800, 0.600))$$

---

## Sparse Linear Algebraic Equation Subroutines

This section contains the sparse linear algebraic equation subroutine descriptions.

## DGSF — General Sparse Matrix Factorization Using Storage by Indices, Rows, or Columns

### Purpose

This subroutine factors sparse matrix  $A$  by Gaussian elimination, using a modified Markowitz count with threshold pivoting. The sparse matrix can be stored by indices, rows, or columns. To solve the system of equations, follow the call to this subroutine with a call to DGSS.

### Syntax

Fortran	CALL DGSF ( <i>iopt</i> , <i>n</i> , <i>nz</i> , <i>a</i> , <i>ia</i> , <i>ja</i> , <i>lna</i> , <i>iparm</i> , <i>rparm</i> , <i>oparm</i> , <i>aux</i> , <i>naux</i> )
C and C++	dgsf ( <i>iopt</i> , <i>n</i> , <i>nz</i> , <i>a</i> , <i>ia</i> , <i>ja</i> , <i>lna</i> , <i>iparm</i> , <i>rparm</i> , <i>oparm</i> , <i>aux</i> , <i>naux</i> );

### On Entry

- iopt* indicates the storage technique used for sparse matrix  $A$ , where:
- If  $iopt = 0$ , it is stored by indices.
  - If  $iopt = 1$ , it is stored by rows.
  - If  $iopt = 2$ , it is stored by columns.
- Specified as: a fullword integer;  $iopt = 0, 1, \text{ or } 2$ .
- n* is the order  $n$  of sparse matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- nz* is the number of elements in sparse matrix  $A$ , stored in an array, referred to as  $A$ .
- Specified as: a fullword integer;  $nz > 0$ .
- a* is the sparse matrix  $A$ , to be factored, stored in an array, referred to as  $A$ .
- Specified as: an array of length  $lna$ , containing long-precision real numbers.
- ia* is the array, referred to as  $IA$ , where:
- If  $iopt = 0$ , it contains the row numbers that correspond to the elements in array  $A$ .
  - If  $iopt = 1$ , it contains the row pointers.
  - If  $iopt = 2$ , it contains the row numbers that correspond to the elements in array  $A$ .
- Specified as: an array of length  $lna$ , containing fullword integers;  $IA(i) \geq 1$ . See "Sparse Matrix" on page 94 for more information on storage techniques.
- ja* is the array, referred to as  $JA$ , where:
- If  $iopt = 0$ , it contains the column numbers that correspond to the elements in array  $A$ .
  - If  $iopt = 1$ , it contains the column numbers that correspond to the elements in array  $A$ .
  - If  $iopt = 2$ , it contains the column pointers.

Specified as: an array of length  $lna$ , containing fullword integers;  $JA(i) \geq 1$ . See "Sparse Matrix" on page 94 for more information on storage techniques.

*lna*

is the length of the arrays specified for  $a$ ,  $ia$ , and  $ja$ .

Specified as: a fullword integer;  $lna > 2nz$ . If you do not specify a sufficient amount, it results in an error. See "Error conditions" on page 620.

The size of  $lna$  depends on the structure of the input matrix. The requirement that  $lna > 2nz$  does not guarantee a successful run of the program. If the input matrix is expected to have many fill-ins,  $lna$  should be set larger. Larger  $lna$  may result in a performance improvement.

For details on how  $lna$  relates to storage compressions, see "Performance and Accuracy Considerations" on page 449.

*iparm*

is an array of parameters,  $IPARM(i)$ , where:

- $IPARM(1)$  determines whether the default values for  $iparm$  and  $rparm$  are used by this subroutine.

If  $IPARM(1) = 0$ , the following default values are used:

$IPARM(2) = 10$   
 $IPARM(3) = 1$   
 $IPARM(4) = 0$   
 $RPARM(1) = 10^{-12}$   
 $RPARM(2) = 0.1$

If  $IPARM(1) = 1$ , the default values are not used.

- $IPARM(2)$  determines the number of minimal Markowitz counts that are examined to determine a pivot. (See reference [105].)
- $IPARM(3)$  has the following meaning, where:

If  $IPARM(3) = 0$ , this subroutine checks the values in arrays  $IA$  and  $JA$ .

If  $IPARM(3) = 1$ , this subroutine assumes that the input values are correct in arrays  $IA$  and  $JA$ .

- $IPARM(4)$  has the following meaning, where:

If  $IPARM(4) = 0$ , this computation is not performed.

If  $IPARM(4) = 1$ , this subroutine computes:

The absolute value of the smallest pivot element

The absolute value of the largest element in  $U$ .

These values are stored in  $OPARM(2)$  and  $OPARM(3)$ , respectively.

- $IPARM(5)$  is reserved.

Specified as: an array of (at least) length 5, containing fullword integers, where the  $iparm$  values must be:

$IPARM(1) = 0$  or  $1$   
 $IPARM(2) \geq 1$   
 $IPARM(3) = 0$  or  $1$   
 $IPARM(4) = 0$  or  $1$

*rparm*

is an array of parameters,  $RPARM(i)$ , where:

- RPARAM(1) contains the lower bound of the absolute value of all elements in the matrix. If a pivot element is less than this number, the matrix is reported as singular. Any computed element whose absolute value is less than this number is set to 0.
- RPARAM(2) is the threshold pivot tolerance used to control the choice of pivots.
- RPARAM(3) is reserved.
- RPARAM(4) is reserved.
- RPARAM(5) is reserved.

Specified as: a one-dimensional array of (at least) length 5, containing long-precision real numbers, where the *rparm* values must be:

$$\begin{aligned} \text{RPARAM}(1) &\geq 0.0 \\ 0.0 &\leq \text{RPARAM}(2) \leq 1.0 \end{aligned}$$

For additional information about *rparm*, see “Performance and Accuracy Considerations” on page 449.

*oparm* See “On Return.”

*aux* is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing long-precision real numbers.

*naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.

Specified as: a fullword integer;  $naux \geq 10n+100$ .

### On Return

*a* is the transformed array, referred to as *A*, containing the factored matrix *A*, required as input to DGSS. Returned as: a one-dimensional array of length *lna*, containing long-precision real numbers.

*ia* is the transformed array, referred to as *IA*, required as input to DGSS. Returned as: a one-dimensional array of length *lna*, containing fullword integers.

*ja* is the transformed array, referred to as *JA*, required as input to DGSS. Returned as: a one-dimensional array of length *lna*, containing fullword integers.

*oparm* is an array of parameters, *OPARM*(*i*), where:

- *OPARM*(1) is the amount of fill-ins for the sparse processing portion of the algorithm.
- *OPARM*(2) contains the absolute value of the smallest pivot element of the matrix. This value is computed and set only if *IPARM*(4) = 1.
- *OPARM*(3) contains the absolute value of the largest element encountered in *U* after the factorization. This value is computed and set only if *IPARM*(4) = 1.
- *OPARM*(4) is reserved.

- OPARM(5) is reserved.

Returned as: a one-dimensional array of length 5, containing long-precision real numbers.

*aux* is the storage work area used by this subroutine. It contains the information required as input for DGSS.

Specified as: an area of storage, containing long-precision real numbers.

## Notes

1. For a description of the three storage techniques used by this subroutine for sparse matrices, see “Sparse Matrix” on page 94.
2. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## Function

The matrix  $A$  is factored by Gaussian elimination, using a modified Markowitz count with threshold pivoting to compute the sparse LU factorization of  $A$ :

$$LU = PAQ$$

where:

$A$  is a general sparse matrix of order  $n$ , stored by indices, columns, or rows in arrays  $A$ ,  $IA$ , and  $JA$ .

$L$  is a unit lower triangular matrix.

$U$  is an upper triangular matrix.

$P$  is a permutation matrix.

$Q$  is a permutation matrix.

To solve the system of equations, follow the call to this subroutine with a call to DGSS. If  $n$  is 0, no computation is performed. See references [12], [49], and [97].

## Error conditions

### Computational Errors

1. If this subroutine has to perform storage compressions, an attention message is issued. When this occurs, the performance of this subroutine is affected. The performance can be improved by increasing the value specified for *lna*.
2. The following errors with their corresponding return codes can occur in this subroutine. Where a value of  $i$  is indicated, it can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for that particular error code in the ESSL error option table; otherwise, the default value causes your program to terminate when the error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.
  - For error 2117, return code 2 indicates that the pivot element in a column,  $i$ , is smaller than the value specified in RPARAM(1).

- For error 2118, return code 3 indicates that pivot element in a row,  $i$ , is smaller than the value specified in RPARAM(1).
- For error 2120, return code 4 indicates that a row,  $i$ , is found empty on factorization. The matrix is singular.
- For error 2121, return code 5 indicates that a column is found empty on factorization. The matrix is singular.
- For error 2119, return code 6 indicates that the storage space indicated by  $lna$  is insufficient.
- For error 2122, return code 7 indicates that no pivot element was found in the active submatrix.

### Input-Argument Errors

1.  $iopt \neq 0, 1, \text{ or } 2$
2.  $n < 0$
3.  $nz \leq 0$
4.  $lna \leq 2nz$
5. IPARM(1)  $\neq 0$  or 1
6. IPARM(2)  $\leq 0$
7. IPARM(3)  $\neq 0$  or 1
8. IPARM(4)  $\neq 0$  or 1
9. RPARAM(1)  $< 0.0$
10. RPARAM(2)  $< 0.0$  or RPARAM(2)  $> 1.0$
11.  $iopt = 1$  and  $ia(i) \geq ia(i+1), i = 1, n$
12.  $iopt = 2$  and  $ja(i) \geq ja(i+1), i = 1, n$
13.  $iopt = 0$  or 1 and  $ja(i) < 1$  or  $ja(i) > n, i = 1, nz$
14.  $iopt = 0$  or 1 and  $ia(i) < 1$  or  $ia(i) > n, i = 1, nz$
15. There are duplicate indices in a row or column of the input matrix.
16. The matrix is singular if a row or column of the input matrix is empty.
17.  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example

This example factors 5 by 5 sparse matrix  $A$ , which is stored by indices in arrays  $A$ ,  $IA$ , and  $JA$ . The three storage techniques are shown in this example, and the output is the same regardless of the storage technique used. The matrix is factored using Gaussian elimination with threshold pivoting. Matrix  $A$  is:

$$\begin{bmatrix} 2.0 & 0.0 & 4.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 0.0 & 0.0 & 3.0 \\ 0.0 & 0.0 & 3.0 & 4.0 & 0.0 \\ 2.0 & 2.0 & 0.0 & 1.0 & 5.0 \\ 0.0 & 0.0 & 1.0 & 1.0 & 0.0 \end{bmatrix}$$

**Note:** In this example, only nonzero elements are used as input to the matrix.

### Call Statement and Input (Storage-By-Indices):

```

          IOPT  N  NZ  A  IA  JA  LNA  IPARM  RPARM  OPARM  AUX  NAUX
CALL DGSF( 0 , 5, 13, A, IA, JA, 27 , IPARM, RPARM, OPARM, AUX, 150 )
A        = (2.0, 1.0, 1.0, 3.0, 4.0, 1.0, 5.0, 2.0, 2.0, 1.0, 1.0,
           4.0, 3.0, . . . , . . . , . . . , . . . , . . . , . . . ,
           . . . )
IA       = (1, 2, 2, 3, 3, 4, 4, 4, 4, 5, 5, 1, 2, . . . , . . . ,
           . . . , . . . , . . . , . . . , . . . , . . . )

```





## DGSS — General Sparse Matrix or Its Transpose Solve Using Storage by Indices, Rows, or Columns

### Purpose

This subroutine solves either of the following systems:

$$\begin{aligned} Ax &= b \\ A^T x &= b \end{aligned}$$

where  $A$  is a sparse matrix,  $A^T$  is the transpose of sparse matrix  $A$ , and  $x$  and  $b$  are vectors. DGSS uses the results of the factorization of matrix  $A$ , produced by a preceding call to DGSF.

**Note:** The input to this solve subroutine must be the output from the factorization subroutine, DGSF.

### Syntax

Fortran	CALL DGSS ( <i>jopt</i> , <i>n</i> , <i>a</i> , <i>ia</i> , <i>ja</i> , <i>lna</i> , <i>bx</i> , <i>aux</i> , <i>naux</i> )
C and C++	dgss ( <i>jopt</i> , <i>n</i> , <i>a</i> , <i>ia</i> , <i>ja</i> , <i>lna</i> , <i>bx</i> , <i>aux</i> , <i>naux</i> );

### On Entry

- jopt* indicates the type of computation to be performed, where:
- If *jopt* = 0,  $Ax = b$  is solved, where the right-hand side is not sparse.
  - If *jopt* = 1,  $A^T x = b$  is solved, where the right-hand side is not sparse.
  - If *jopt* = 10,  $Ax = b$  is solved, where the right-hand side is sparse.
  - If *jopt* = 11,  $A^T x = b$  is solved, where the right-hand side is sparse.
- Specified as: a fullword integer; *jopt* = 0, 1, 10, or 11.
- n* is the order  $n$  of sparse matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- a* is the factorization of sparse matrix  $A$ , stored in array  $A$ , produced by a preceding call to DGSF.
- Specified as: an array of length *lna*, containing long-precision real numbers.
- ia* is the array, referred to as IA, produced by a preceding call to DGSF.
- Specified as: an array of length *lna*, containing fullword integers.
- ja* is the array, referred to as JA, produced by a preceding call to DGSF.
- Specified as: an array of length *lna*, containing fullword integers.
- lna* is the length of the arrays  $A$ , IA, and JA. In DGSS, *lna* must be identical to the value specified in DGSF; otherwise, results are unpredictable.
- Specified as: a fullword integer;  $lna > 0$ .

- bx* is the vector  $\mathbf{b}$  of length  $n$ , containing the right-hand side of the system.  
Specified as: a one-dimensional array of (at least) length  $n$ , containing long-precision real numbers.
- aux* is the storage work area passed to this subroutine by a preceding call to DGSS. Its size is specified by *naux*.  
Specified as: an area of storage, containing long-precision real numbers.
- naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.  
Specified as: a fullword integer;  $naux \geq 10n+100$ .

### On Return

- ia* is the transformed array, referred to as IA, which can be used as input in subsequent calls to this subroutine. This may result in a performance increase.  
Specified as: an array of length  $lna$ , containing fullword integers.
- bx* is the solution vector  $\mathbf{x}$  of length  $n$ , containing the results of the computation.  
Specified as: a one-dimensional array, containing long-precision real numbers.

### Notes

1. The input arguments  $n$ ,  $lna$ , and  $naux$ , must be the same as those specified for DGSS. Whereas, the input arguments  $a$ ,  $ia$ ,  $ja$ , and  $aux$  must be those produced on output by DGSS. Otherwise, results are unpredictable.
2. You have the option of having the minimum required value for  $naux$  dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

### Function

The system  $A\mathbf{x} = \mathbf{b}$  is solved for  $\mathbf{x}$ , where  $A$  is a sparse matrix and  $\mathbf{x}$  and  $\mathbf{b}$  are vectors. Depending on the value specified for the *jopt* argument, DGSS can also solve the system  $A^T\mathbf{x} = \mathbf{b}$ , where  $A^T$  is the transpose of sparse matrix  $A$ .

If the value specified for the *jopt* argument is 0 or 10, the following equation is solved:

$$A\mathbf{x} = \mathbf{b}$$

If the value specified for the *jopt* argument is 1 or 11, the following equation is solved:

$$A^T\mathbf{x} = \mathbf{b}$$

DGSS uses the results of the factorization of matrix  $A$ , produced by a preceding call to DGSS. The transformed matrix  $A$  consists of the upper triangular matrix  $U$  and the lower triangular matrix  $L$ .

See references [12], [49], and [97].

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $jopt \neq 0, 1, 10, \text{ or } 11$
2.  $n < 0$
3.  $lna \leq 0$
4.  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to solve the system  $Ax = b$ , where matrix  $A$  is a 5 by 5 sparse matrix. The right-hand side is not sparse.

**Note:** The input for this subroutine is the same as the output from DGSE, except for BX.

Matrix  $A$  is:

$$\begin{bmatrix} 2.0 & 0.0 & 4.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 0.0 & 0.0 & 3.0 \\ 0.0 & 0.0 & 3.0 & 4.0 & 0.0 \\ 2.0 & 2.0 & 0.0 & 1.0 & 5.0 \\ 0.0 & 0.0 & 1.0 & 1.0 & 0.0 \end{bmatrix}$$

### Call Statement and Input:

```

          JOPT  N   A   IA   JA   LNA  BX   AUX   NAUX
CALL DGSS( 0 , 5 , A , IA , JA , 27 , BX , AUX , 150 )
A        = (0.5, . , 0.3, 1.0, . , 1.0, . , 3.0, . , . , . , 1.0,
           1.0, . , . , . , . , . , . , . , -1.7, -0.5, -1.0, -1.0,
           4.0, -3.0, -4.0)
IA       = (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, . , . , . , . , . ,
           . , . , . , . , 2, 1, 1, 3, 3, 5, 5)
JA       = (1, 0, 5, 2, 0, 4, 0, 2, 0, 0, 0, 3, 4, . , . , . , . , . ,
           . , . , . , . , 4, 2, 4, 4, 1, 3, 1)
BX       = (1.0, 1.0, 1.0, 1.0, 1.0)

```

### Output:

```

IA       = (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, . , . , . , . , . ,
           . , . , . , . , 2, 1, 1, 3, 3, 5, 5)
BX       = (-5.500000, 9.500000, 3.000000, -2.000000, -1.000000)

```

**Note:** On input, a “.” means that you do not have to store a value in that position in the array. However, the storage position is required and may be overwritten during the computation. On output, a “.” means that the value in that position in the array is not significant.

### Example 2

This example shows how to solve the system  $A^T x = b$ , using the same matrix  $A$  used in Example 1. The input is also the same as in Example 1, except for the  $jopt$  argument. The right-hand side is not sparse.

### Call Statement and Input:

```

          JOPT N  A  IA  JA  LNA  BX  AUX  NAUX
          |   |   |   |   |   |   |   |
CALL DGSS( 1 , 5 , A , IA , JA , 27 , BX , AUX , 150 )

BX      = ( 1.0, 1.0, 1.0, 1.0, 1.0)

```

**Output:**

```

IA      = ( 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, . , . , . , . , . ,
          . , . , . , . , 2, 1, 1, 3, 3, 5, 5)
BX      = ( 0.000000, -3.000000, -2.000000, 2.000000, 7.000000)

```

**Note:** On input, a “.” means that you do not have to store a value in that position in the array. However, the storage position is required and may be overwritten during the computation. On output, a “.” means that the value in that position in the array is not significant.

**Example 3**

This example shows how to solve the system  $Ax = b$ , using the same matrix  $A$  as in Examples 1 and 2. The input is also the same as in Examples 1 and 2, except for the *jopt* and *bx* arguments. The right-hand side is sparse.

**Call Statement and Input:**

```

          JOPT N  A  IA  JA  LNA  BX  AUX  NAUX
          |   |   |   |   |   |   |   |
CALL DGSS( 10 , 5 , A , IA , JA , 27 , BX , AUX , 150 )

BX      = ( 0.0, 0.0, 0.0, 1.0, 0.0)

```

**Output:**

```

IA      = ( 1, 4, 2, 5, 3, 5, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
          0, 2, 1, 1, 3, 3, 5, 5)
BX      = ( 0.000000, 3.000000, 0.000000, 0.000000, -1.000000)

```

**Note:** On input, a “.” means that you do not have to store a value in that position in the array. However, the storage position is required and may be overwritten during the computation. On output, a “.” means that the value in that position in the array is not significant.

**Example 4**

This example shows how to solve the system  $A^T x = b$ , using the same matrix  $A$  as in Examples 1, 2, and 3. The input is also the same as in Examples 1, 2, and 3, except for the *jopt* argument. The right-hand side is sparse.

**Call Statement and Input:**

```

          JOPT N  A  IA  JA  LNA  BX  AUX  NAUX
          |   |   |   |   |   |   |   |
CALL DGSS( 11 , 5 , A , IA , JA , 27 , BX , AUX , 150 )

BX      = ( 0.0, 0.0, 0.0, 1.0, 0.0)

```

**Output:**

```

IA      = ( 1, 4, 2, 5, 3, 5, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
          0, 2, 1, 1, 3, 3, 5, 5)
BX      = ( 0.000000, 0.000000, 1.000000, 0.000000, -3.000000 )

```

**Note:** On input, a “.” means that you do not have to store a value in that position in the array. However, the storage position is required and may be overwritten during the computation. On output, a “.” means that the value in that position in the array is not significant.

## DGKFS — General Sparse Matrix or Its Transpose Factorization, Determinant, and Solve Using Skyline Storage Mode

### Purpose

This subroutine can perform either or both of the following functions for general sparse matrix  $A$ , stored in skyline storage mode, and for vectors  $x$  and  $b$ :

- Factor  $A$  and, optionally, compute the determinant of  $A$ .
- Solve the system  $Ax = b$  or  $A^T x = b$  using the results of the factorization of matrix  $A$ , produced on this call or a preceding call to this subroutine.

You also have the choice of using profile-in or diagonal-out skyline storage mode for  $A$  on input or output.

**Note:** The input to the solve performed by this subroutine must be the output from the factorization performed by this subroutine.

### Syntax

Fortran	CALL DGKFS ( <i>n, au, nu, idu, al, nl, idl, iparm, rparm, aux, nau, bx, ldbx, mbx</i> )
C and C++	dgkfs ( <i>n, au, nu, idu, al, nl, idl, iparm, rparm, aux, nau, bx, ldbx, mbx</i> );

### On Entry

- n* is the order of general sparse matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- au* is the array, referred to as AU, containing one of three forms of the upper triangular part of general sparse matrix  $A$ , depending on the type of computation performed, where:
- If you are doing a **factor and solve** or a **factor only**, and if  $IPARM(3) = 0$ , then AU contains the unfactored upper triangle of general sparse matrix  $A$ .
  - If you are doing a **factor only**, and if  $IPARM(3) > 0$ , then AU contains the partially factored upper triangle of general sparse matrix  $A$ . The first  $IPARM(3)$  columns in the upper triangle of  $A$  are already factored. The remaining columns are factored in this computation.
  - If you are doing a **solve only**, then AU contains the factored upper triangle of general sparse matrix  $A$ , produced by a preceding call to this subroutine.
- In each case:
- If  $IPARM(4) = 0$ , diagonal-out skyline storage mode is used for  $A$ .  
If  $IPARM(4) = 1$ , profile-in skyline storage mode is used for  $A$ .
- Specified as: a one-dimensional array of (at least) length  $nu$ , containing long-precision real numbers.
- nu* is the length of array AU.  
Specified as: a fullword integer;  $nu \geq 0$  and  $nu \geq (IDU(n+1)-1)$ .
- idu* is the array, referred to as IDU, containing the relative positions of the diagonal elements of matrix  $A$  (in one of its three forms) in array AU.

Specified as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.

*al* is the array, referred to as AL, containing one of three forms of the lower triangular part of general sparse matrix *A*, depending on the type of computation performed, where:

- If you are doing a **factor and solve** or a **factor only**, and if  $IPARM(3) = 0$ , then AL contains the unfactored lower triangle of general sparse matrix *A*.
- If you are doing a **factor only**, and if  $IPARM(3) > 0$ , then AL contains the partially factored lower triangle of general sparse matrix *A*. The first  $IPARM(3)$  rows in the lower triangle of *A* are already factored. The remaining rows are factored in this computation.
- If you are doing a **solve only**, then AL contains the factored lower triangle of general sparse matrix *A*, produced by a preceding call to this subroutine.

**Note:** In all these cases, entries in AL for diagonal elements of *A* are not assumed to have meaningful values.

In each case:

If  $IPARM(4) = 0$ , diagonal-out skyline storage mode is used for *A*.

If  $IPARM(4) = 1$ , profile-in skyline storage mode is used for *A*.

Specified as: a one-dimensional array of (at least) length  $nl$ , containing long-precision real numbers.

*nl* is the length of array AL.

Specified as: a fullword integer;  $nl \geq 0$  and  $nl \geq (IDL(n+1)-1)$ .

*idl* is the array, referred to as IDL, containing the relative positions of the diagonal elements of matrix *A* (in one of its three forms) in array AL.

Specified as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.

*iparm* is an array of parameters,  $IPARM(i)$ , where:

- $IPARM(1)$  indicates whether certain default values for *iparm* and *rparm* are used by this subroutine, where:

If  $IPARM(1) = 0$ , the following default values are used. For restrictions, see "Notes" on page 634.

$IPARM(2) = 0$   
 $IPARM(3) = 0$   
 $IPARM(4) = 0$   
 $IPARM(5) = 0$   
 $IPARM(10) = 0$   
 $IPARM(11) = -1$   
 $IPARM(12) = -1$   
 $IPARM(13) = -1$   
 $IPARM(14) = -1$   
 $IPARM(15) = 0$   
 $RPARAM(10) = 10^{-12}$

If  $IPARM(1) = 1$ , the default values are not used.

- IPARM(2) indicates the type of computation performed by this subroutine. The following table gives the IPARM(2) values for each variation:

Type of Computation	$Ax = b$	$Ax = b$ and Determinant(A)	$A^T x = b$	$A^T x = b$ and Determinant(A)
Factor and Solve	0	10	100	110
Factor Only	1	11	N/A	N/A
Solve Only	2	N/A	102	N/A

- IPARM(3) indicates whether a full or partial factorization is performed on matrix  $A$ , where:  
 If IPARM(3) = 0, and:  
 If you are doing a **factor and solve** or a **factor only**, then a full factorization is performed for matrix  $A$  on rows and columns 1 through  $n$ .  
 If you are doing a **solve only**, this argument has no effect on the computation, but must be set to 0.

If IPARM(3) > 0, and you are doing a **factor only**, then a partial factorization is performed on matrix  $A$ . Rows 1 through IPARM(3) of columns 1 through IPARM(3) in matrix  $A$  must be in factored form from a preceding call to this subroutine. The factorization is performed on rows IPARM(3)+1 through  $n$  and columns IPARM(3)+1 through  $n$ . For an illustration, see “Notes” on page 634.

- IPARM(4) indicates the input storage mode used for matrix  $A$ . This determines the arrangement of data in arrays AU, IDU, AL, and IDL on input, where:  
 If IPARM(4) = 0, diagonal-out skyline storage mode is used.  
 If IPARM(4) = 1, profile-in skyline storage mode is used.
- IPARM(5) indicates the output storage mode used for matrix  $A$ . This determines the arrangement of data in arrays AU, IDU, AL, and IDL on output, where:  
 If IPARM(5) = 0, diagonal-out skyline storage mode is used.  
 If IPARM(5) = 1, profile-in skyline storage mode is used.
- IPARM(6) through IPARM(9) are reserved.
- IPARM(10) has the following meaning, where:  
 If you are doing a **factor and solve** or a **factor only**, then IPARM(10) indicates whether certain default values for *iparm* and *rparm* are used by this subroutine, where:  
 If IPARM(10) = 0, the following default values are used. For restrictions, see “Notes” on page 634.

IPARM(11) = -1  
 IPARM(12) = -1  
 IPARM(13) = -1  
 IPARM(14) = -1  
 IPARM(15) = 0  
 RPARAM(10) =  $10^{-12}$

If IPARM(10) = 1, the default values are not used.

If you are doing a **solve only**, this argument is not used.

- IPARM(11) through IPARM(15) have the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, then IPARM(11) through IPARM(15) control the type of processing to apply to pivot elements occurring in regions 1 through 5, respectively. The pivot elements are  $u_{kk}$  for  $k = 1, n$  when doing a full factorization, and they are  $k = \text{IPARM}(3)+1, n$  when doing a partial factorization. The region in which a pivot element falls depends on the sign and magnitude of the pivot element. The regions are determined by RPARAM(10). For a description of the regions and associated pivot values, see "Notes" on page 634. For each region  $i$  for  $i = 1, 5$ , where the pivot occurs in region  $i$ , the processing applied to the pivot element is determined by IPARM(10+i), where:

If IPARM(10+i) = -1, the pivot element is trapped and computational error 2126 is generated. See "Error conditions" on page 636.

If IPARM(10+i) = 0, for  $i = 1, 2, 4$ , and 5, processing continues normally.

**Note:** A value of 0 is not permitted for region 3, because if processing continues, a divide-by-zero exception occurs.

If IPARM(10+i) = 1, the pivot element is replaced with the value in RPARAM(10+i), and processing continues normally.

If you are doing a **solve only**, these arguments are not used.

- IPARM(16) through IPARM(25), see "On Return" on page 632.

Specified as: a one-dimensional array of (at least) length 25, containing fullword integers, where:

IPARM(1) = 0 or 1

IPARM(2) = 0, 1, 2, 10, 11, 100, 102, or 110

If IPARM(2) = 0, 2, 10, 100, 102, or 110, then IPARM(3) = 0

If IPARM(2) = 1 or 11, then  $0 \leq \text{IPARM}(3) \leq n$

IPARM(4), IPARM(5) = 0 or 1

If IPARM(2) = 0, 1, 10, 11, 100, or 110, then:

IPARM(10) = 0 or 1

IPARM(11), IPARM(12) = -1, 0, or 1

IPARM(13) = -1 or 1

IPARM(14), IPARM(15) = -1, 0, or 1

*rparam*

is an array of parameters, RPARAM( $i$ ), where:

- RPARAM(1) through RPARAM(9) are reserved.
- RPARAM(10) has the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, RPARAM(10) is the tolerance value for small pivots. This sets the bounds for the pivot regions, where pivots are processed according to the options you specify for the five regions in IPARM(11) through IPARM(15), respectively. The suggested value is  $10^{-15} \leq \text{RPARAM}(10) \leq 1$ .

If you are doing a **solve only**, this argument is not used.

- RPARAM(11) through RPARAM(15) have the following meaning, where:



If you are doing a **factor and solve** or a **factor only**, RPARAM(11) through RPARAM(15) are the fix-up values to use for the pivots in regions 1 through 5, respectively. For each RPARAM(10+i) for  $i = 1, 5$ , where the pivot occurs in region  $i$ :

If  $\text{IPARM}(10+i) = 1$ , the pivot is replaced with RPARAM(10+i), where  $|\text{RPARAM}(10+i)|$  should be a sufficiently large nonzero value to avoid overflow when calculating the reciprocal of the pivot. The suggested value is  $10^{-15} \leq |\text{RPARAM}(10+i)| \leq 1$ .

If  $\text{IPARM}(10+i) \neq 1$ , RPARAM(10+i) is not used.

If you are doing a **solve only**, these arguments are not used.

- RPARAM(16) through RPARAM(25), see “On Return” on page 632.

Specified as: a one-dimensional array of (at least) length 25, containing long-precision real numbers, where if  $\text{IPARM}(2) = 0, 1, 10, 11, 100$ , or 110, then:

$\text{RPARAM}(10) \geq 0.0$

$\text{RPARAM}(11)$  through  $\text{RPARAM}(15) \neq 0.0$

*aux* has the following meaning:

If  $naux = 0$  and error 2015 is unrecoverable, *aux* is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing long-precision real numbers.

*naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.

Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, DGKFS dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,

If you are doing a **factor only**, use  $naux \geq 5n$ .

If you are doing a **factor and solve** or a **solve only**, use  $naux \geq 5n+4mbx$ .

*bx* has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, *bx* is the array, containing the *mbx* right-hand side vectors  $\mathbf{b}$  of the system  $\mathbf{Ax} = \mathbf{b}$  or  $\mathbf{A}^T\mathbf{x} = \mathbf{b}$ . Each vector  $\mathbf{b}$  is length  $n$  and is stored in the corresponding column of the array.

If you are doing a **factor only**, this argument is not used in the computation.

Specified as: an *ldbx* by (at least) *mbx* array, containing long-precision real numbers.

*ldbx* has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, *ldbx* is the leading dimension of the array specified for *bx*.

If you are doing a **factor only**, this argument is not used in the computation.

Specified as: a fullword integer;  $ldb_x \geq n$  and:

If  $mbx \neq 0$ , then  $ldb_x > 0$ .

If  $mbx = 0$ , then  $ldb_x \geq 0$ .

*mbx* has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, *mbx* is the number of right-hand side vectors, *b*, in the array specified for *bx*.

If you are doing a **factor only**, this argument is not used in the computation.

Specified as: a fullword integer;  $mbx \geq 0$ .

### On Return

*au* is the array, referred to as AU, containing the upper triangular part of the **LU** factored form of general sparse matrix *A*, where:

If  $IPARM(5) = 0$ , diagonal-out skyline storage mode is used for *A*.

If  $IPARM(5) = 1$ , profile-in skyline storage mode is used for *A*.

(If  $mbx = 0$  and you are doing a solve only, then *au* is unchanged on output.) Returned as: a one-dimensional array of (at least) length *nu*, containing long-precision real numbers.

*idu* is the array, referred to as IDU, containing the relative positions of the diagonal elements of the factored output matrix *A* in array AU. (If  $mbx = 0$  and you are doing a solve only, then *idu* is unchanged on output.) Returned as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.

*al* is the array, referred to as AL, containing the lower triangular part of the **LU** factored form of general sparse matrix *A*, where:

If  $IPARM(5) = 0$ , diagonal-out skyline storage mode is used for *A*.

If  $IPARM(5) = 1$ , profile-in skyline storage mode is used for *A*.

**Note:** You should assume that entries in AL for diagonal elements of *A* do not have meaningful values.

(If  $mbx = 0$  and you are doing a solve only, then *al* is unchanged on output.) Returned as: a one-dimensional array of (at least) length *nl*, containing long-precision real numbers.

*idl* is the array, referred to as IDL, containing the relative positions of the diagonal elements of the factored output matrix *A* in array AL. (If  $mbx = 0$  and you are doing a solve only, then *idl* is unchanged on output.) Returned as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.

*iparm* is an array of parameters,  $IPARM(i)$ , where:

- $IPARM(1)$  through  $IPARM(15)$  are unchanged.
- $IPARM(16)$  has the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, and:

If  $IPARM(16) = -1$ , your factorization did not complete successfully, resulting in computational error 2126.

If  $\text{IPARM}(16) > 0$ , it is the row number  $k$ , in which the maximum absolute value of the ratio  $a_{kk}/u_{kk}$  occurred, where:

If  $\text{IPARM}(3) = 0$ ,  $k$  can be any of the rows, 1 through  $n$ , in the full factorization.

If  $\text{IPARM}(3) > 0$ ,  $k$  can be any of the rows,  $\text{IPARM}(3)+1$  through  $n$ , in the partial factorization.

If you are doing a **solve only**, this argument is not used in the computation and is unchanged.

- $\text{IPARM}(17)$  through  $\text{IPARM}(20)$  are reserved.
- $\text{IPARM}(21)$  through  $\text{IPARM}(25)$  have the following meaning, where:

If you are doing a **factor and solve** or a **factor only**,  $\text{IPARM}(21)$  through  $\text{IPARM}(25)$  have the following meanings for each region  $i$  for  $i = 1,5$ , respectively:

If  $\text{IPARM}(20+i) = -1$ , your factorization did not complete successfully, resulting in computational error 2126.

If  $\text{IPARM}(20+i) \geq 0$ , it is the number of pivots in region  $i$  for the columns that were factored in matrix  $A$ , where:

If  $\text{IPARM}(3) = 0$ , columns 1 through  $n$  were factored in the full factorization.

If  $\text{IPARM}(3) > 0$ , columns  $\text{IPARM}(3)+1$  through  $n$  were factored in the partial factorization.

If you are doing a **solve only**, these arguments are not used in the computation and are unchanged.

Returned as: a one-dimensional array of (at least) length 25, containing fullword integers.

*rparm*

is an array of parameters,  $\text{RPARAM}(i)$ , where:

- $\text{RPARAM}(1)$  through  $\text{RPARAM}(15)$  are unchanged.
- $\text{RPARAM}(16)$  has the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, and:

If  $\text{RPARAM}(16) = 0.0$ , your factorization did not complete successfully, resulting in computational error 2126.

If  $|\text{RPARAM}(16)| > 0.0$ , it is the ratio for row  $k$ ,  $a_{kk}/u_{kk}$ , having the maximum absolute value. Row  $k$  is indicated in  $\text{IPARM}(16)$ , and:

If  $\text{IPARM}(3) = 0$ , the ratio corresponds to one of the rows, 1 through  $n$ , in the full factorization.

If  $\text{IPARM}(3) > 0$ , the ratio corresponds to one of the rows,  $\text{IPARM}(3)+1$  through  $n$ , in the partial factorization.

If you are doing a **solve only**, this argument is not used in the computation and is unchanged.

- $\text{RPARAM}(17)$  and  $\text{RPARAM}(18)$  have the following meaning, where:

If you are **computing the determinant** of matrix  $A$ , then  $\text{RPARAM}(17)$  is the mantissa,  $\text{detbas}$ , and  $\text{RPARAM}(18)$  is the power of 10,  $\text{detpow}$ , used to express the value of the determinant:  $\text{detbas}(10^{\text{detpow}})$ , where  $1 \leq \text{detbas} < 10$ . Also:

If  $\text{IPARM}(3) = 0$ , the determinant is computed for columns 1 through  $n$  in the full factorization.

If  $IPARM(3) > 0$ , the determinant is computed for columns  $IPARM(3)+1$  through  $n$  in the partial factorization.

If you are **not computing the determinant** of matrix  $A$ , these arguments are not used in the computation and are unchanged.

- $RPARAM(19)$  through  $RPARAM(25)$  are reserved.

Returned as: a one-dimensional array of (at least) length 25, containing long-precision real numbers.

$bx$  has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**,  $bx$  is the array, containing the  $mbx$  solution vectors  $x$  of the system  $Ax = b$  or  $A^T x = b$ . Each vector  $x$  is length  $n$  and is stored in the corresponding column of the array. (If  $mbx = 0$ , then  $bx$  is unchanged on output.)

If you are doing a **factor only**, this argument is not used in the computation and is unchanged.

Returned as: an  $ldb_x$  by (at least)  $mbx$  array, containing long-precision real numbers.

## Notes

1. If you set either  $IPARM(1) = 0$  or  $IPARM(10) = 0$ , indicating you want to use the default values for  $IPARM(11)$  through  $IPARM(15)$  and  $RPARAM(10)$ , then:
  - Matrix  $A$  must be positive definite.
  - No pivots are fixed, using  $RPARAM(11)$  through  $RPARAM(15)$  values.
  - No small pivots are tolerated; that is, the value should be  $|pivot| > RPARAM(10)$ .
2. Many of the input and output parameters for  $iparm$  and  $rparm$  are defined for the five pivot regions handled by this subroutine. The limits of the regions are based on  $RPARAM(10)$ , as shown in Figure 11. The pivot values in each region are:

- Region 1:  $pivot < -RPARAM(10)$
- Region 2:  $-RPARAM(10) \leq pivot < 0$
- Region 3:  $pivot = 0$
- Region 4:  $0 < pivot \leq RPARAM(10)$
- Region 5:  $pivot > RPARAM(10)$

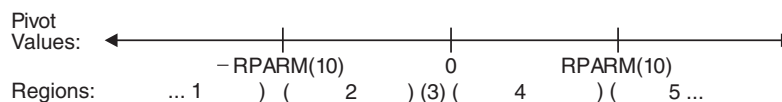


Figure 11. Five Pivot Regions

3. The  $IPARM(4)$  and  $IPARM(5)$  arguments allow you to specify the same or different skyline storage modes for your input and output arrays for matrix  $A$ . This allows you to change storage modes as needed. However, if you are concerned with performance, you should use diagonal-out skyline storage mode for both input and output, if possible, because there is less overhead. For a description of how sparse matrices are stored in skyline storage mode, see “Profile-In Skyline Storage Mode” on page 104 and “Diagonal-Out Skyline Storage Mode” on page 102.
4. Following is an illustration of the portion of matrix  $A$  factored in the partial factorization when  $IPARM(3) > 0$ . In this case, the subroutine assumes that rows

and columns 1 through IPARM(3) are already factored and that rows and columns IPARM(3)+1 through  $n$  are to be factored in this computation.

$$\begin{array}{c}
 \overline{\uparrow} \\
 \text{factored} \\
 \downarrow \\
 \overline{\uparrow} \\
 \text{to be} \\
 \text{factored} \\
 \downarrow
 \end{array}
 \left[ \begin{array}{ccccccc}
 & & & & \leftarrow \text{factored} \rightarrow & & \leftarrow \text{to be factored} \rightarrow \\
 & a_{11} & \cdot & \cdot & \cdot & a_{1j} & a_{1,j+1} & \cdot & \cdot & \cdot & a_{1n} \\
 & \cdot & \cdot & & & \cdot & & & & & \cdot \\
 & \cdot & & \cdot & & \cdot & & & & & \cdot \\
 & \cdot & & & & \cdot & & & & & \cdot \\
 & a_{j1} & \cdot & \cdot & \cdot & a_{jj} & & & & & \cdot \\
 & a_{j+1,1} & & & & & & & & & \cdot \\
 & \cdot & & & & & & \cdot & & & \cdot \\
 & \cdot & & & & & & \cdot & & & \cdot \\
 & \cdot & & & & & & & \cdot & & \cdot \\
 & a_{n1} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a_{nn}
 \end{array} \right]
 \quad \text{where } j = \text{IPARM}(3)$$

You use the partial factorization function when, for design or storage reasons, you must factor the matrix  $A$  in stages. When doing a partial factorization, you must use the same skyline storage mode for all parts of the matrix as it is progressively factored.

5. Your various arrays must have no common elements; otherwise, results are unpredictable.
6. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

### Function

This subroutine can factor, compute the determinant of, and solve general sparse matrix  $A$ , stored in skyline storage mode. For all computations, input matrix  $A$  can be stored in either diagonal-out or profile-in skyline storage mode. Output matrix  $A$  can also be stored in either of these modes and can be different from the mode used for input.

Matrix  $A$  is factored into the following form using specified pivot processing:

$$A = LU$$

where:

- $U$  is an upper triangular matrix.
- $L$  is a lower triangular matrix.

The transformed matrix  $A$ , factored into its  $LU$  form, is stored in packed format in arrays AU and AL. The inverse of the diagonal of matrix  $U$  is stored in the corresponding elements of array AU. The off-diagonal elements of the upper triangular matrix  $U$  are stored in the corresponding off-diagonal elements of array AU. The off-diagonal elements of the lower triangular matrix  $L$  are stored in the corresponding off-diagonal elements of array AL. (The diagonal elements stored in array AL do not have meaningful values.)

The partial factorization of matrix  $A$ , which you can do when you specify the factor-only option, assumes that the first IPARM(3) rows and columns are already factored in the input matrix. It factors the remaining  $n$ -IPARM(3) rows and columns in matrix  $A$ . (See “Notes” on page 634 for an illustration.) It updates only the elements in arrays AU and AL corresponding to the part of matrix  $A$  that is factored.

The determinant can be computed with any of the factorization computations. With a full factorization, you get the determinant for the whole matrix. With a partial factorization, you get the determinant for only that part of the matrix factored in this computation.

The system  $Ax = b$  or  $A^T x = b$ , having multiple right-hand sides, is solved for  $x$ , using the transformed matrix  $A$  produced by this call or a subsequent call to this subroutine.

See references [11], [14], [27], [49], and [74]. If  $n$  is 0, no computation is performed. If  $mbx$  is 0, no solve is performed.

## Error conditions

### Resource Errors

- Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.
- Unable to allocate internal work area.

### Computational Errors

1. If a pivot occurs in region  $i$  for  $i = 1, 5$  and IPARM(10+ $i$ ) = 1, the pivot value is replaced with RPARAM(10+ $i$ ), an attention message is issued, and processing continues.
2. Unacceptable pivot values occurred in the factorization of matrix  $A$ .
  - One or more diagonal elements of  $U$  contains unacceptable pivots and no valid fixup is applicable. The row number  $i$  of the first unacceptable pivot element is identified in the computational error message.
  - The return code is set to 2.
  - $i$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2126 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $n < 0$
2.  $nu < 0$
3.  $IDU(n+1) > nu+1$
4.  $IDU(i+1) \leq IDU(i)$  for  $i = 1, n$
5.  $IDU(i+1) > IDU(i)+i$  and IPARM(4) = 0 for  $i = 1, n$
6.  $IDU(i) > IDU(i-1)+i$  and IPARM(4) = 1 for  $i = 2, n$
7.  $nl < 0$
8.  $IDL(n+1) > nl+1$
9.  $IDL(i+1) \leq IDL(i)$  for  $i = 1, n$
10.  $IDL(i+1) > IDL(i)+i$  and IPARM(4) = 0 for  $i = 1, n$
11.  $IDL(i) > IDL(i-1)+i$  and IPARM(4) = 1 for  $i = 2, n$
12. IPARM(1)  $\neq$  0 or 1
13. IPARM(2)  $\neq$  0, 1, 2, 10, 11, 100, 102, or 110
14. IPARM(3)  $< 0$
15. IPARM(3)  $> n$

- 16. IPARM(3) > 0 and IPARM(2) ≠ 1 or 11
- 17. IPARM(4), IPARM(5) ≠ 0 or 1
- 18. IPARM(2) = 0, 1, 10, 11, 100, or 110 and:
  - IPARM(10) ≠ 0 or 1
  - IPARM(11), IPARM(12) ≠ -1, 0, or 1
  - IPARM(13) ≠ -1 or 1
  - IPARM(14), IPARM(15) ≠ -1, 0, or 1
  - RPARM(10) < 0.0
  - RPARM(10+i) = 0.0 and IPARM(10+i) = 1 for i = 1,5
- 19. IPARM(2) = 0, 2, 10, 100, 102, or 110 and:
  - ldb<sub>x</sub> ≤ 0 and mb<sub>x</sub> ≠ 0 and n ≠ 0
  - ldb<sub>x</sub> < 0 and mb<sub>x</sub> = 0
  - ldb<sub>x</sub> < n and mb<sub>x</sub> ≠ 0
  - mb<sub>x</sub> < 0
- 20. Error 2015 is recoverable or nau<sub>x</sub> ≠ 0, and nau<sub>x</sub> is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to factor a 9 by 9 general sparse matrix *A* and solve the system  $Ax = b$  with three right-hand sides. The default values are used for IPARM and RPARM. Input matrix *A*, shown here, is stored in diagonal-out skyline storage mode. Matrix *A* is:

$$\begin{bmatrix} 2.0 & 2.0 & 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 2.0 & 4.0 & 4.0 & 2.0 & 2.0 & 0.0 & 0.0 & 0.0 & 2.0 \\ 2.0 & 4.0 & 6.0 & 4.0 & 4.0 & 0.0 & 2.0 & 0.0 & 4.0 \\ 2.0 & 4.0 & 6.0 & 6.0 & 6.0 & 2.0 & 4.0 & 0.0 & 6.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 4.0 & 4.0 & 4.0 & 2.0 & 4.0 \\ 0.0 & 2.0 & 4.0 & 6.0 & 8.0 & 6.0 & 8.0 & 4.0 & 10.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 4.0 & 6.0 & 8.0 & 6.0 & 8.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 4.0 & 6.0 & 8.0 & 8.0 & 10.0 \\ 2.0 & 4.0 & 6.0 & 6.0 & 8.0 & 6.0 & 10.0 & 8.0 & 16.0 \end{bmatrix}$$

Output matrix *A*, shown here, is in *LU* factored form with  $U^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Matrix *B* is:

$$\begin{bmatrix} 0.5 & 2.0 & 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 0.5 & 2.0 & 2.0 & 2.0 & 0.0 & 0.0 & 0.0 & 2.0 \\ 1.0 & 1.0 & 0.5 & 2.0 & 2.0 & 0.0 & 2.0 & 0.0 & 2.0 \\ 1.0 & 1.0 & 1.0 & 0.5 & 2.0 & 2.0 & 2.0 & 0.0 & 2.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 0.5 & 2.0 & 2.0 & 2.0 & 2.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.5 & 2.0 & 2.0 & 2.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 0.5 & 2.0 & 2.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.5 & 2.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.5 \end{bmatrix}$$

### Call Statement and Input:

```

      N  AU  NU  IDU  AL  NL  IDL  IPARM  RPARM  AUX  NAUX  BX  LDBX  MBX
CALL DGKFS( 9 , AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 57 , BX , 12 , 3 )
    
```

# DGKFS

```

AU      = (2.0, 4.0, 2.0, 6.0, 4.0, 2.0, 6.0, 4.0, 2.0, 4.0, 6.0,
           4.0, 2.0, 6.0, 4.0, 2.0, 8.0, 8.0, 4.0, 4.0, 2.0, 8.0,
           6.0, 4.0, 2.0, 16.0, 10.0, 8.0, 10.0, 4.0, 6.0, 4.0, 2.0)
IDU     = (1, 2, 4, 7, 10, 14, 17, 22, 26, 34)
AL      = (0.0, 0.0, 2.0, 0.0, 4.0, 2.0, 0.0, 6.0, 4.0, 2.0, 0.0,
           2.0, 0.0, 8.0, 6.0, 4.0, 2.0, 0.0, 6.0, 4.0, 2.0, 0.0,
           8.0, 6.0, 4.0, 2.0, 0.0, 8.0, 10.0, 6.0, 8.0, 6.0, 6.0,
           4.0, 2.0)
IDL     = (1, 2, 4, 7, 11, 13, 18, 22, 27, 36)
IPARM   = (0, ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,
           ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .)

RPARM   =(not relevant)

```

```

BX      = [
           6.00  12.00  18.00
           16.00 32.00  48.00
           26.00 52.00  78.00
           36.00 72.00 108.00
           20.00 40.00  60.00
           48.00 96.00 144.00
           34.00 68.00 102.00
           38.00 76.00 114.00
           66.00 132.00 198.00
           .      .      .
           .      .      .
           .      .      .
         ]

```

## Output:

```

AU      = (0.5, 0.5, 2.0, 0.5, 2.0, 2.0, 0.5, 2.0, 2.0, 0.5,
           2.0,
           2.0, 2.0, 0.5, 2.0, 2.0, 0.5, 2.0, 2.0, 2.0, 2.0, 0.5,
           2.0, 2.0, 2.0, 0.5, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0)
IDU     =(same as input)
AL      = (0.0, 0.0, 1.0, 0.0, 1.0, 1.0, 0.0, 1.0, 1.0, 1.0, 0.0,
           1.0, 0.0, 1.0, 1.0, 1.0, 1.0, 0.0, 1.0, 1.0, 1.0, 0.0,
           1.0, 1.0, 1.0, 1.0, 0.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
           1.0, 1.0)
IDL     =(same as input)
IPARM   = (0, ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,
           ., 9, ., ., ., ., ., 0, 0, 0, 0, 9)
RPARM   = (., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,
           ., 8.0, ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .)

```

```

BX      = [
           1.00  2.00  3.00
           1.00  2.00  3.00
           1.00  2.00  3.00
           1.00  2.00  3.00
           1.00  2.00  3.00
           1.00  2.00  3.00
           1.00  2.00  3.00
           1.00  2.00  3.00
           1.00  2.00  3.00
           .      .      .
           .      .      .
           .      .      .
         ]

```

## Example 2

This example shows how to factor the 9 by 9 general sparse matrix  $A$  from Example 1, solve the system  $A^T x = b$  with three right-hand sides, and compute the



determinant of  $A$ . The default values for pivot processing are used for IPARM. Input matrix  $A$  is stored in profile-in skyline storage mode. Output matrix  $A$  is in  $LU$  factored form with  $U^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. It is the same as output matrix  $A$  in Example 1.

**Call Statement and Input:**

```

      N  AU  NU  IDU  AL  NL  IDL  IPARM  RPARM  AUX  NAUX  BX  LDBX  MBX
      |  |  |  |  |  |  |  |  |  |  |  |  |  |
CALL DGKFS( 9, AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 57, BX, 12, 3 )
    
```

```

AU      = (2.0, 2.0, 4.0, 2.0, 4.0, 6.0, 2.0, 4.0, 6.0, 2.0, 4.0,
           6.0, 4.0, 2.0, 4.0, 6.0, 2.0, 4.0, 4.0, 8.0, 8.0, 2.0,
           4.0, 6.0, 8.0, 2.0, 4.0, 6.0, 4.0, 10.0, 8.0, 10.0, 16.0)
IDU     = (1, 3, 6, 9, 13, 16, 21, 25, 33, 34)
AL      = (0.0, 2.0, 0.0, 2.0, 4.0, 0.0, 2.0, 4.0, 6.0, 0.0, 2.0,
           0.0, 2.0, 4.0, 6.0, 8.0, 0.0, 2.0, 4.0, 6.0, 0.0, 2.0,
           4.0, 6.0, 8.0, 0.0, 2.0, 4.0, 6.0, 6.0, 8.0, 6.0, 10.0,
           8.0, 0.0)
IDL     = (1, 3, 6, 10, 12, 17, 21, 26, 35, 36)
IPARM   = (1, 110, 0, 1, 0, ., ., ., ., ., ., 0, ., ., ., ., ., ., ., ., .,
           ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .)
    
```

RPARM = (not relevant)

```

BX      = [ 10.00  20.00  30.00
            20.00  40.00  60.00
            28.00  56.00  84.00
            30.00  60.00  90.00
            40.00  80.00  120.00
            30.00  60.00  90.00
            44.00  88.00  132.00
            28.00  56.00  84.00
            60.00  120.00  180.00
            .      .      .
            .      .      .
            .      .      .
    
```

**Output:**

```

AU      = (same as output AU in Example 1)
IDU     = (same as output IDU in Example 1)
AL      = (same as output AL in Example 1)
IDL     = (same as output IDL in Example 1)
IPARM   = (1, 110, 0, 1, 0, ., ., ., ., ., ., 0, ., ., ., ., ., ., ., ., .,
           9, ., ., ., ., ., 0, 0, 0, 0, 9)
RPARM   = (., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,
           ., 8.0, 5.12, 2.0, ., ., ., ., ., ., ., ., ., .)
BX      = (same as output BX in Example 1)
    
```

**Example 3**

This example shows how to factor a 9 by 9 negative-definite general sparse matrix  $A$ , solve the system  $Ax = b$  with three right-hand sides, and compute the determinant of  $A$ . (Default values for pivot processing are not used for IPARM because  $A$  is negative-definite.) Input matrix  $A$ , shown here, is stored in diagonal-out skyline storage mode:

```

[ -2.0  -2.0  -2.0  0.0  0.0  0.0  0.0  0.0  0.0
  -2.0  -4.0  -4.0  -2.0  -2.0  0.0  0.0  0.0  -2.0
  -2.0  -4.0  -6.0  -4.0  -4.0  0.0  -2.0  0.0  -4.0 ]
    
```

$$\begin{bmatrix} -2.0 & -4.0 & -6.0 & -6.0 & -6.0 & -2.0 & -4.0 & 0.0 & -6.0 \\ 0.0 & 0.0 & 0.0 & -2.0 & -4.0 & -4.0 & -4.0 & -2.0 & -4.0 \\ 0.0 & -2.0 & -4.0 & -6.0 & -8.0 & -6.0 & -8.0 & -4.0 & -10.0 \\ 0.0 & 0.0 & 0.0 & -2.0 & -4.0 & -6.0 & -8.0 & -6.0 & -8.0 \\ 0.0 & 0.0 & 0.0 & -2.0 & -4.0 & -6.0 & -8.0 & -8.0 & -10.0 \\ -2.0 & -4.0 & -6.0 & -6.0 & -8.0 & -6.0 & -10.0 & -8.0 & -16.0 \end{bmatrix}$$

Output matrix  $A$ , shown here, is in  $LU$  factored form with  $U^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Matrix  $A$  is:

$$\begin{bmatrix} -0.5 & -2.0 & -2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & -0.5 & -2.0 & -2.0 & -2.0 & 0.0 & 0.0 & 0.0 & -2.0 \\ 1.0 & 1.0 & -0.5 & -2.0 & -2.0 & 0.0 & -2.0 & 0.0 & -2.0 \\ 1.0 & 1.0 & 1.0 & -0.5 & -2.0 & -2.0 & -2.0 & 0.0 & -2.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & -0.5 & -2.0 & -2.0 & -2.0 & -2.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & -0.5 & -2.0 & -2.0 & -2.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & -0.5 & -2.0 & -2.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & -0.5 & -2.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & -0.5 \end{bmatrix}$$

**Call Statement and Input:**

```
CALL DGKFS( N, AU, NU, IDU, AL, NL, IDL, IPARM, RPARM, AUX, NAUX, BX, LDBX, MBX
            | | | | | | | | | | | | | | |
            9, AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 57, BX, 12, 3 )
```

```
AU      = (-2.0, -4.0, -2.0, -6.0, -4.0, -2.0, -6.0, -4.0, -2.0,
           -4.0, -6.0, -4.0, -2.0, -6.0, -4.0, -2.0, -8.0, -8.0,
           -4.0, -4.0, -2.0, -8.0, -6.0, -4.0, -2.0, -16.0, -10.0,
           -8.0, -10.0, -4.0, -6.0, -4.0, -2.0)
IDU     = (1, 2, 4, 7, 10, 14, 17, 22, 26, 34)
AL      = (0.0, 0.0, -2.0, 0.0, -4.0, -2.0, 0.0, -6.0, -4.0, -2.0,
           0.0, -2.0, 0.0, -8.0, -6.0, -4.0, -2.0, 0.0, -6.0, -4.0,
           -2.0, 0.0, -8.0, -6.0, -4.0, -2.0, 0.0, -8.0, -10.0,
           -6.0, -8.0, -6.0, -6.0, -4.0, -2.0)
IDL     = (1, 2, 4, 7, 11, 13, 18, 22, 27, 36)
IPARM   = (1, 10, 0, 0, 0, . . . . ., 1, 0, -1, -1, -1, -1, . . .
           . . . . .)
```

```
RPARM   = (. . . . ., 10-15, . . . . .,
           . . . . .)
BX      =(same as input BX in Example 1)
```

**Output:**

```
AU      = (-0.5, -0.5, -2.0, -0.5, -2.0, -2.0, -0.5, -2.0, -2.0,
           -0.5, -2.0, -2.0, -2.0, -0.5, -2.0, -2.0, -0.5, -2.0,
           -2.0, -2.0, -2.0, -0.5, -2.0, -2.0, -2.0, -0.5, -2.0,
           -2.0, -2.0, -2.0, -2.0, -2.0, -2.0)
IDU     =(same as input)
AL      = (0.0, 0.0, 1.0, 0.0, 1.0, 1.0, 0.0, 1.0, 1.0, 1.0, 0.0,
           1.0, 0.0, 1.0, 1.0, 1.0, 1.0, 0.0, 1.0, 1.0, 1.0, 0.0,
           1.0, 1.0, 1.0, 1.0, 0.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
           1.0, 1.0)
IDL     =(same as input)
IPARM   = (1, 10, 0, 0, 0, . . . . ., 1, 0, -1, -1, -1, -1, 9,
           . . . . ., 9, 0, 0, 0, 0)
RPARM   = (. . . . ., 10-15, . . . . .,
           . . . . ., 8.0, -5.12, 2.0, . . . . .)
```

$$\text{BX} = \begin{bmatrix} -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Example 4**

This example shows how to factor the first six rows and columns, referred to as matrix *A1*, of the 9 by 9 general sparse matrix *A* from Example 1 and compute the determinant of *A1*. Input matrix *A1*, shown here, is stored in diagonal-out skyline storage mode. Input matrix *A1* is:

$$\begin{bmatrix} 2.0 & 2.0 & 2.0 & 0.0 & 0.0 & 0.0 \\ 2.0 & 4.0 & 4.0 & 2.0 & 2.0 & 0.0 \\ 2.0 & 4.0 & 6.0 & 4.0 & 4.0 & 0.0 \\ 2.0 & 4.0 & 6.0 & 6.0 & 6.0 & 2.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 4.0 & 4.0 \\ 0.0 & 2.0 & 4.0 & 6.0 & 8.0 & 6.0 \end{bmatrix}$$

Output matrix *A1*, shown here, is in *LU* factored form with *U*<sup>-1</sup> on the diagonal, and is stored in diagonal-out skyline storage mode. Output matrix *A1* is:

$$\begin{bmatrix} 0.5 & 2.0 & 2.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 0.5 & 2.0 & 2.0 & 2.0 & 0.0 \\ 1.0 & 1.0 & 0.5 & 2.0 & 2.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 0.5 & 2.0 & 2.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 0.5 & 2.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.5 \end{bmatrix}$$

**Call Statement and Input:**

```

          N  AU  NU  IDU  AL  NL  IDL  IPARM  RPARM  AUX  NAUX  BX  LDBX  MBX
CALL DGKFS( 6, AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 45, BX, LDBX, MBX )

```

- AU = (same as input AU in Example 1)
- IDU = (1, 2, 4, 7, 10, 14, 17)
- AL = (same as input AL in Example 1)
- IDL = (1, 2, 4, 7, 11, 13, 18)
- IPARM = (1, 11, 0, 0, 0, ., ., ., ., ., 0, ., ., ., ., ., ., .)
- RPARM = (not relevant)
- BX = (not relevant)
- LDBX = (not relevant)
- MBX = (not relevant)

**Output:**

```

AU = (0.5, 0.5, 2.0, 0.5, 2.0, 2.0, 0.5, 2.0, 2.0, 0.5,
2.0,
2.0, 2.0, 0.5, 2.0, 2.0, 8.0, 8.0, 4.0, 4.0, 2.0, 8.0,

```

```

        6.0, 4.0, 2.0, 16.0, 10.0, 8.0, 10.0, 4.0, 6.0, 4.0, 2.0)
IDU    =(same as input)
AL     = (0.0, 0.0, 1.0, 0.0, 1.0, 1.0, 0.0, 1.0, 1.0, 1.0, 0.0,
        1.0, 0.0, 1.0, 1.0, 1.0, 1.0, 0.0, 6.0, 4.0, 2.0, 0.0,
        8.0, 6.0, 4.0, 2.0, 0.0, 8.0, 10.0, 6.0, 8.0, 6.0, 6.0,
        4.0, 2.0)
IDL    =(same as input)
IPARM  = (1, 11, 0, 0, 0, ., ., ., ., ., 0, ., ., ., ., ., ., ., 3,
        ., ., ., ., ., 0, 0, 0, 0, 6)
RPARAM = (., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,
        ., 3.0, 6.4, 1.0, ., ., ., ., ., ., ., .)
BX     =(same as input)
LDBX   =(same as input)
MBX    =(same as input)

```

**Example 5**

This example shows how to do a partial factorization of the 9 by 9 general sparse matrix *A* from Example 1, where the first six rows and columns were factored in Example 4. It factors the remaining three rows and columns and computes the determinant of that part of the matrix. The input matrix, referred to as *A2*, shown here, is made up of the output factored matrix *A1* plus the three remaining unfactored rows and columns of matrix *A*. Matrix *A2* is:

$$\begin{bmatrix}
 0.5 & 2.0 & 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
 1.0 & 0.5 & 2.0 & 2.0 & 2.0 & 0.0 & 0.0 & 0.0 & 2.0 \\
 1.0 & 1.0 & 0.5 & 2.0 & 2.0 & 0.0 & 2.0 & 0.0 & 4.0 \\
 1.0 & 1.0 & 1.0 & 0.5 & 2.0 & 2.0 & 4.0 & 0.0 & 6.0 \\
 0.0 & 0.0 & 0.0 & 1.0 & 0.5 & 2.0 & 4.0 & 2.0 & 4.0 \\
 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.5 & 8.0 & 4.0 & 10.0 \\
 0.0 & 0.0 & 0.0 & 2.0 & 4.0 & 6.0 & 8.0 & 6.0 & 8.0 \\
 0.0 & 0.0 & 0.0 & 2.0 & 4.0 & 6.0 & 8.0 & 8.0 & 10.0 \\
 2.0 & 4.0 & 6.0 & 6.0 & 8.0 & 6.0 & 10.0 & 8.0 & 16.0
 \end{bmatrix}$$

Both parts of input matrix *A2* are stored in diagonal-out skyline storage mode.

Output matrix *A2* is the same as output matrix *A* in Example 1 and is stored in diagonal-out skyline storage mode.

**Call Statement and Input:**

```

          N  AU  NU  IDU  AL  NL  IDL  IPARM  RPARAM  AUX  NAUX  BX  LDBX  MBX
CALL DGKFS( 9, AU, 33, IDU, AL, 35, IDL, IPARM, RPARAM, AUX, 45, BX, LDBX, MBX )

```

```

AU       =(same as output AU in Example 4)
IDU     =(same as input IDU in Example 1)
AL      =(same as output AL in Example 4)
IDL     =(same as input IDL in Example 1)
IPARM   = (1, 11, 6, 0, 0, ., ., ., ., ., 0, ., ., ., ., ., ., ., ., ., .,
        ., ., ., ., ., ., ., ., ., ., .)
RPARAM  =(not relevant)
BX      =(not relevant)
LDBX    =(not relevant)
MBX     =(not relevant)

```

**Output:**

AU        =(same as output AU in Example 1)  
 IDU       =(same as output IDU in Example 1)  
 AL        =(same as output AL in Example 1)  
 IDL       =(same as output IDL in Example 1)  
 IPARM     = (1, 11, 6, 0, 0, ., ., ., ., ., ., 0, ., ., ., ., ., ., ., ., 9,  
           ., ., ., ., ., ., 0, 0, 0, 0, 3)  
 RPARM     = (.,  
           ., ., 8.0, 8.0, 0.0, ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .)  
 BX        =(same as input)  
 LDBX      =(same as input)  
 MBX       =(same as input)

**Example 6**

This example shows how to solve the system  $Ax = b$  with one right-hand side for a general sparse matrix  $A$ . Input matrix  $A$ , used here, is the same as factored output matrix  $A$  from Example 1, stored in profile-in skyline storage mode. Here, output matrix  $A$  is unchanged on output and is stored in profile-in skyline storage mode.

**Call Statement and Input:**

```

      N  AU  NU  IDU  AL  NL  IDL  IPARM  RPARM  AUX  NAUX  BX  LDBX  MBX
CALL DGKFS( 9, AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 49, BX, 9, 1 )
  
```

AU        = (0.5, 2.0, 0.5, 2.0, 2.0, 0.5, 2.0, 2.0, 0.5, 2.0,  
 2.0,  
           2.0, 0.5, 2.0, 2.0, 0.5, 2.0, 2.0, 2.0, 2.0, 0.5, 2.0,  
           2.0, 2.0, 0.5, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 0.5)  
 IDU       = (1, 3, 6, 9, 13, 16, 21, 25, 33, 34)  
 AL        = (0.0, 1.0, 0.0, 1.0, 1.0, 0.0, 1.0, 1.0, 1.0, 0.0, 1.0,  
           0.0, 1.0, 1.0, 1.0, 1.0, 0.0, 1.0, 1.0, 1.0, 0.0, 1.0,  
           1.0, 1.0, 1.0, 0.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,  
           1.0, 0.0)  
 IDL       = (1, 3, 6, 10, 12, 17, 21, 26, 35, 36)  
 IPARM     = (1, 2, 0, 1, 1, ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,  
           ., .)  
 RPARM     =(not relevant)  
 BX        = (12.0, 58.0, 114.0, 176.0, 132.0, 294.0, 240.0, 274.0,  
           406.0)

**Output:**

AU        =(same as input)  
 IDU       =(same as input)  
 AL        =(same as input)  
 IDL       =(same as input)  
 IPARM     =(same as input)  
 RPARM     =(not relevant)  
 BX        = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0)

## DSKFS — Symmetric Sparse Matrix Factorization, Determinant, and Solve Using Skyline Storage Mode

### Purpose

This subroutine can perform either or both of the following functions for symmetric sparse matrix  $A$ , stored in skyline storage mode, and for vectors  $x$  and  $b$ :

- Factor  $A$  and, optionally, compute the determinant of  $A$ .
- Solve the system  $Ax = b$  using the results of the factorization of matrix  $A$ , produced on this call or a preceding call to this subroutine.

You have the choice of using either Gaussian elimination or Cholesky decomposition. You also have the choice of using profile-in or diagonal-out skyline storage mode for  $A$  on input or output.

**Note:** The input to the solve performed by this subroutine must be the output from the factorization performed by this subroutine.

### Syntax

Fortran	CALL DSKFS ( <i>n, a, na, idiag, iparm, rparm, aux, naux, bx, ldbx, mbx</i> )
C and C++	dskfs ( <i>n, a, na, idiag, iparm, rparm, aux, naux, bx, ldbx, mbx</i> );

### On Entry

*n* is the order of symmetric sparse matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .

*a* is the array, referred to as  $A$ , containing one of three forms of the upper triangular part of symmetric sparse matrix  $A$ , depending on the type of computation performed, where:

- If you are doing a **factor and solve** or a **factor only**, and if  $IPARM(3) = 0$ , then  $A$  contains the unfactored upper triangle of symmetric sparse matrix  $A$ .
- If you are doing a **factor only**, and if  $IPARM(3) > 0$ , then  $A$  contains the partially factored upper triangle of symmetric sparse matrix  $A$ . The first  $IPARM(3)$  columns in the upper triangle of  $A$  are already factored. The remaining columns are factored in this computation.
- If you are doing a **solve only**, then  $A$  contains the factored upper triangle of sparse matrix  $A$ , produced by a preceding call to this subroutine.

In each case:

If  $IPARM(4) = 0$ , diagonal-out skyline storage mode is used for  $A$ .

If  $IPARM(4) = 1$ , profile-in skyline storage mode is used for  $A$ .

Specified as: a one-dimensional array of (at least) length  $na$ , containing long-precision real numbers.

*na* is the length of array  $A$ .

Specified as: a fullword integer;  $na \geq 0$  and  $na \geq (IDIAG(n+1)-1)$ .

*idiag* is the array, referred to as IDIAG, containing the relative positions of the diagonal elements of matrix *A* (in one of its three forms) in array *A*.

Specified as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.

*iparm* is an array of parameters,  $IPARM(i)$ , where:

- $IPARM(1)$  indicates whether certain default values for *iparm* and *rparm* are used by this subroutine, where:

If  $IPARM(1) = 0$ , the following default values are used. For restrictions, see “Notes” on page 651.

- $IPARM(2) = 0$
- $IPARM(3) = 0$
- $IPARM(4) = 0$
- $IPARM(5) = 0$
- $IPARM(10) = 0$
- $IPARM(11) = -1$
- $IPARM(12) = -1$
- $IPARM(13) = -1$
- $IPARM(14) = -1$
- $IPARM(15) = 0$
- $RPARM(10) = 10^{-12}$

If  $IPARM(1) = 1$ , the default values are not used.

- $IPARM(2)$  indicates the type of computation performed by this subroutine. The following table gives the  $IPARM(2)$  values for each variation:

Type of Computation	Gaussian Elimination $Ax = b$	Gaussian Elimination $Ax = b$ and Determinant( <i>A</i> )	Cholesky Decomposition $Ax = b$	Cholesky Decomposition $Ax = b$ and Determinant( <i>A</i> )
Factor and Solve	0	10	100	110
Factor Only	1	11	101	111
Solve Only	2	N/A	102	N/A

- $IPARM(3)$  indicates whether a full or partial factorization is performed on matrix *A*, where:

If  $IPARM(3) = 0$ , and:

If you are doing a **factor and solve** or a **factor only**, then a full factorization is performed for matrix *A* on rows and columns 1 through *n*.

If you are doing a **solve only**, this argument has no effect on the computation, but must be set to 0.

If  $IPARM(3) > 0$ , and you are doing a **factor only**, then a partial factorization is performed on matrix *A*. Rows 1 through  $IPARM(3)$  of columns 1 through  $IPARM(3)$  in matrix *A* must be in factored form from a preceding call to this subroutine. The factorization is performed on rows  $IPARM(3)+1$  through *n* and columns  $IPARM(3)+1$  through *n*. For an illustration, see “Notes” on page 651.

- IPARM(4) indicates the input storage mode used for matrix  $A$ . This determines the arrangement of data in arrays  $A$  and IDIAG on input, where:  
If IPARM(4) = 0, diagonal-out skyline storage mode is used.  
If IPARM(4) = 1, profile-in skyline storage mode is used.
- IPARM(5) indicates the output storage mode used for matrix  $A$ . This determines the arrangement of data in arrays  $A$  and IDAIG on output, where:  
If IPARM(5) = 0, diagonal-out skyline storage mode is used.  
If IPARM(5) = 1, profile-in skyline storage mode is used.
- IPARM(6) through IPARM(9) are reserved.
- IPARM(10) has the following meaning, where:  
If you are doing a **factor and solve** or a **factor only**, then IPARM(10) indicates whether certain default values for  $iparm$  and  $rparm$  are used by this subroutine, where:

If IPARM(10) = 0, the following default values are used.  
For restrictions, see “Notes” on page 651.

IPARM(11) = -1  
 IPARM(12) = -1  
 IPARM(13) = -1  
 IPARM(14) = -1  
 IPARM(15) = 0  
 RPARAM(10) =  $10^{-12}$

If IPARM(10) = 1, the default values are not used.

If you are doing a **solve only**, this argument is not used.

- IPARM(11) through IPARM(15) have the following meaning, where:  
If you are doing a **factor and solve** or a **factor only**, then IPARM(11) through IPARM(15) control the type of processing to apply to pivot elements occurring in regions 1 through 5, respectively. The pivot elements are  $d_{kk}$  for Gaussian elimination and  $r_{kk}$  for Cholesky decomposition for  $k = 1, n$  when doing a full factorization, and they are  $k = \text{IPARM}(3)+1, n$  when doing a partial factorization. The region in which a pivot element falls depends on the sign and magnitude of the pivot element. The regions are determined by RPARAM(10). For a description of the regions and associated pivot values, see “Notes” on page 651. For each region  $i$  for  $i = 1,5$ , where the pivot occurs in region  $i$ , the processing applied to the pivot element is determined by IPARM(10+ $i$ ), where:  
If IPARM(10+ $i$ ) = -1, the pivot element is trapped and computational error 2126 is generated. See “Error conditions” on page 653.  
If IPARM(10+ $i$ ) = 0, processing continues normally.

**Note:** A value of 0 is not permitted for region 3, because if processing continues, a divide-by-zero exception occurs. In addition, if you are doing a Cholesky decomposition, a value of 0 is not permitted in regions 1 and 2, because a square root exception occurs.



If  $IPARM(10+i) = 1$ , the pivot element is replaced with the value in  $RPARAM(10+i)$ , and processing continues normally.

If you are doing a **solve only**, these arguments are not used.

- $IPARM(16)$  through  $IPARM(25)$ , see “On Return” on page 649.

Specified as: a one-dimensional array of (at least) length 25, containing fullword integers, where:

$IPARM(1) = 0$  or  $1$

$IPARM(2) = 0, 1, 2, 10, 11, 100, 101, 102, 110,$  or  $111$

If  $IPARM(2) = 0, 2, 10, 100, 102,$  or  $110$ , then  $IPARM(3) = 0$

If  $IPARM(2) = 1, 11, 101,$  or  $111$ , then  $0 \leq IPARM(3) \leq n$

$IPARM(4), IPARM(5) = 0$  or  $1$

If  $IPARM(2) = 0, 1, 10,$  or  $11$ , then:

$IPARM(10) = 0$  or  $1$

$IPARM(11), IPARM(12) = -1, 0,$  or  $1$

$IPARM(13) = -1$  or  $1$

$IPARM(14), IPARM(15) = -1, 0,$  or  $1$

If  $IPARM(2) = 100, 101, 110,$  or  $111$ , then:

$IPARM(10) = 0$  or  $1$

$IPARM(11), IPARM(12), IPARM(13) = -1$  or  $1$

$IPARM(14), IPARM(15) = -1, 0,$  or  $1$

*rparm*

is an array of parameters,  $RPARAM(i)$ , where:

- $RPARAM(1)$  through  $RPARAM(9)$  are reserved.
- $RPARAM(10)$  has the following meaning, where:

If you are doing a **factor and solve** or a **factor only**,  $RPARAM(10)$  is the tolerance value for small pivots. This sets the bounds for the pivot regions, where pivots are processed according to the options you specify for the five regions in  $IPARM(11)$  through  $IPARM(15)$ , respectively. The suggested value is  $10^{-15} \leq IPARM(10) \leq 1$ .

If you are doing a **solve only**, this argument is not used.

- $RPARAM(11)$  through  $RPARAM(15)$  have the following meaning, where:

If you are doing a **factor and solve** or a **factor only**,  $RPARAM(11)$  through  $RPARAM(15)$  are the fix-up values to use for the pivots in regions 1 through 5, respectively. For each  $RPARAM(10+i)$  for  $i = 1, 5$ , where the pivot occurs in region  $i$ :

If  $IPARM(10+i) = 1$ , the pivot is replaced with  $RPARAM(10+i)$ , where  $|RPARAM(10+i)|$  should be a sufficiently large nonzero value to avoid overflow when calculating the reciprocal of the pivot. For Gaussian elimination, the suggested value is  $10^{-15} \leq |RPARAM(10+i)| \leq 1$ . For Cholesky decomposition, the value must be  $RPARAM(10+i) > 0$ .

If  $IPARM(10+i) \neq 1$ ,  $RPARAM(10+i)$  is not used.

If you are doing a **solve only**, these arguments are not used.

- $RPARAM(16)$  through  $RPARAM(25)$ , see “On Return” on page 649.

Specified as: a one-dimensional array of (at least) length 25, containing long-precision real numbers, where if  $IPARM(2) = 0, 1, 10, 11, 100, 101, 110,$  or  $111$ , then:

$RPARAM(10) \geq 0.0$

If  $IPARM(2) = 0, 1, 10,$  or  $11$ , then  $RPARAM(11)$  through  $RPARAM(15) \neq 0.0$

If  $IPARM(2) = 100, 101, 110,$  or  $111$ , then  $RPARAM(11)$  through  $RPARAM(15) > 0.0$

- aux* has the following meaning:
- If  $n_{aux} = 0$  and error 2015 is unrecoverable, *aux* is ignored.
- Otherwise, it is the storage work area used by this subroutine. Its size is specified by *n<sub>aux</sub>*.
- Specified as: an area of storage, containing long-precision real numbers.
- n<sub>aux</sub>* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.
- Specified as: a fullword integer, where:
- If  $n_{aux} = 0$  and error 2015 is unrecoverable, DSKFS dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.
- Otherwise, If you are doing a **factor only**, you can use  $n_{aux} \geq n$ ; however, for optimal performance, use  $n_{aux} \geq 3n$ .
- If you are doing a **factor and solve** or a **solve only**, use  $n_{aux} \geq 3n+4mbx$ .
- For further details on error handling and the special factor-only case, see “Notes” on page 651.
- bx* has the following meaning, where:
- If you are doing a **factor and solve** or a **solve only**, *bx* is the array, containing the *mbx* right-hand side vectors **b** of the system  $Ax = b$ . Each vector **b** is length *n* and is stored in the corresponding column of the array.
- If you are doing a **factor only**, this argument is not used in the computation.
- Specified as: an *ldb<sub>x</sub>* by (at least) *mbx* array, containing long-precision real numbers.
- ldb<sub>x</sub>* has the following meaning, where:
- If you are doing a **factor and solve** or a **solve only**, *ldb<sub>x</sub>* is the leading dimension of the array specified for *bx*.
- If you are doing a **factor only**, this argument is not used in the computation.
- Specified as: a fullword integer;  $ldb_x \geq n$  and:
- If  $mbx \neq 0$ , then  $ldb_x > 0$ .
- If  $mbx = 0$ , then  $ldb_x \geq 0$ .

*mbx* has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, *mbx* is the number of right-hand side vectors, *b*, in the array specified for *bx*.

If you are doing a **factor only**, this argument is not used in the computation.

Specified as: a fullword integer;  $mbx \geq 0$ .

## On Return

*a* is the array, referred to as *A*, containing the upper triangular part of symmetric sparse matrix *A* in  $LDL^T$  or  $R^T R$  factored form, where:

If  $IPARM(5) = 0$ , diagonal-out skyline storage mode is used for *A*.

If  $IPARM(5) = 1$ , profile-in skyline storage mode is used for *A*.

(If  $mbx = 0$  and you are doing a solve only, then *a* is unchanged on output.) Returned as: a one-dimensional array of (at least) length *na*, containing long-precision real numbers.

*idiag* is the array, referred to as *IDIAG*, containing the relative positions of the diagonal elements of the factored output matrix *A* in array *A*. (If  $mbx = 0$  and you are doing a solve only, then *idiag* is unchanged on output.)

Returned as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.

*iparm* is an array of parameters,  $IPARM(i)$ , where:

- $IPARM(1)$  through  $IPARM(15)$  are unchanged.
- $IPARM(16)$  has the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, and:

If  $IPARM(16) = -1$ , your factorization did not complete successfully, resulting in computational error 2126.

If  $IPARM(16) > 0$ , it is the row number *k*, in which the maximum absolute value of the ratio  $a_{kk}/d_{kk}$  for Gaussian elimination and  $a_{kk}/r_{kk}$  for Cholesky decomposition occurred, where:

If  $IPARM(3) = 0$ , *k* can be any of the rows, 1 through *n*, in the full factorization.

If  $IPARM(3) > 0$ , *k* can be any of the rows,  $IPARM(3)+1$  through *n*, in the partial factorization.

If you are doing a **solve only**, this argument is not used in the computation and is unchanged.

- $IPARM(17)$  through  $IPARM(20)$  are reserved.
- $IPARM(21)$  through  $IPARM(25)$  have the following meaning, where:

If you are doing a **factor and solve** or a **factor only**,  $IPARM(21)$  through  $IPARM(25)$  have the following meanings for each region *i* for  $i = 1, 5$ , respectively:

If  $IPARM(20+i) = -1$ , your factorization did not complete successfully, resulting in computational error 2126.

If  $IPARM(20+i) \geq 0$ , it is the number of pivots in region *i* for the columns that were factored in matrix *A*, where:

If  $\text{IPARM}(3) = 0$ , columns 1 through  $n$  were factored in the full factorization.

If  $\text{IPARM}(3) > 0$ , columns  $\text{IPARM}(3)+1$  through  $n$  were factored in the partial factorization.

If you are doing a **solve only**, these arguments are not used in the computation and are unchanged.

Returned as: a one-dimensional array of (at least) length 25, containing fullword integers.

*rparm*

is an array of parameters,  $\text{RPARAM}(i)$ , where:

- $\text{RPARAM}(1)$  through  $\text{RPARAM}(15)$  are unchanged.
- $\text{RPARAM}(16)$  has the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, and:

If  $\text{RPARAM}(16) = 0.0$ , your factorization did not complete successfully, resulting in computational error 2126.

If  $|\text{RPARAM}(16)| > 0.0$ , it is the ratio for row  $k$ ,  $a_{kk}/d_{kk}$  for Gaussian elimination and  $a_{kk}/r_{kk}$  for Cholesky decomposition, having the maximum absolute value. Row  $k$  is indicated in  $\text{IPARM}(16)$ , and:

If  $\text{IPARM}(3) = 0$ , the ratio corresponds to one of the rows, 1 through  $n$ , in the full factorization.

If  $\text{IPARM}(3) > 0$ , the ratio corresponds to one of the rows,  $\text{IPARM}(3)+1$  through  $n$ , in the partial factorization.

If you are doing a **solve only**, this argument is not used in the computation and is unchanged.

- $\text{RPARAM}(17)$  and  $\text{RPARAM}(18)$  have the following meaning, where:

If you are **computing the determinant** of matrix  $A$ , then  $\text{RPARAM}(17)$  is the mantissa,  $\text{detbas}$ , and  $\text{RPARAM}(18)$  is the power of 10,  $\text{detpow}$ , used to express the value of the determinant:  $\text{detbas}(10^{\text{detpow}})$ , where  $1 \leq \text{detbas} < 10$ . Also:

If  $\text{IPARM}(3) = 0$ , the determinant is computed for columns 1 through  $n$  in the full factorization.

If  $\text{IPARM}(3) > 0$ , the determinant is computed for columns  $\text{IPARM}(3)+1$  through  $n$  in the partial factorization.

If you are **not computing the determinant** of matrix  $A$ , these arguments are not used in the computation and are unchanged.

- $\text{RPARAM}(19)$  through  $\text{RPARAM}(25)$  are reserved.

Returned as: a one-dimensional array of (at least) length 25, containing long-precision real numbers.

*bx*

has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**,  $bx$  is the array, containing the  $mbx$  solution vectors  $x$  of the system  $Ax = b$ . Each vector  $x$  is length  $n$  and is stored in the corresponding column of the array. (If  $mbx = 0$ , then  $bx$  is unchanged on output.)

If you are doing a **factor only**, this argument is not used in the computation and is unchanged.

Returned as: an *ldb*x by (at least) *mb*x array, containing long-precision real numbers.

## Notes

- When doing a **solve only**, you should specify the same factorization method in IPARM(2), Gaussian elimination or Cholesky decomposition, that you specified for your factorization on a previous call to this subroutine.
- If you set either IPARM(1) = 0 or IPARM(10) = 0, indicating you want to use the default values for IPARM(11) through IPARM(15) and RPARAM(10), then:
  - Matrix *A* must be positive definite.
  - No pivots are fixed, using RPARAM(11) through RPARAM(15) values.
  - No small pivots are tolerated; that is, the value should be  $|pivot| > RPARAM(10)$ .
- Many of the input and output parameters for *iparm* and *rparm* are defined for the five pivot regions handled by this subroutine. The limits of the regions are based on RPARAM(10), as shown in Figure 12. The pivot values in each region are:

Region 1:  $pivot < -RPARAM(10)$   
 Region 2:  $-RPARAM(10) \leq pivot < 0$   
 Region 3:  $pivot = 0$   
 Region 4:  $0 < pivot \leq RPARAM(10)$   
 Region 5:  $pivot > RPARAM(10)$

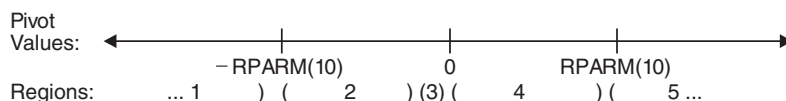


Figure 12. Five Pivot Regions

- The IPARM(4) and IPARM(5) arguments allow you to specify the same or different skyline storage modes for your input and output arrays for matrix *A*. This allows you to change storage modes as needed. However, if you are concerned with performance, you should use diagonal-out skyline storage mode for both input and output, if possible, because there is less overhead. For a description of how sparse matrices are stored in skyline storage mode, see “Profile-In Skyline Storage Mode” on page 104 and “Diagonal-Out Skyline Storage Mode” on page 102. Those descriptions use different array and variable names from the ones used here. To relate the two sets, use the following table:

Name Here	Name in the Storage Description
A	AU
<i>na</i>	<i>nu</i>
IDIAG	IDU

- Following is an illustration of the portion of matrix *A* factored in the partial factorization when IPARM(3) > 0. In this case, the subroutine assumes that rows and columns 1 through IPARM(3) are already factored and that rows and columns IPARM(3)+1 through *n* are to be factored in this computation.

$$\begin{array}{c}
 \overleftarrow{\uparrow} \\
 \text{factored} \\
 \downarrow \\
 \overleftarrow{\uparrow} \\
 \text{to be} \\
 \text{factored} \\
 \downarrow
 \end{array}
 \left[ \begin{array}{ccccccc}
 & & & & \leftarrow \text{factored} \rightarrow & & \leftarrow \text{to be factored} \rightarrow \\
 & a_{11} & \cdot & \cdot & \cdot & a_{1j} & a_{1,j+1} & \cdot & \cdot & \cdot & a_{1n} \\
 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & a_{1j} & \cdot & \cdot & \cdot & a_{jj} & & & & & \cdot \\
 & a_{1,j+1} & & & & & & & & & \cdot \\
 & \cdot & & & & & \cdot & & & & \cdot \\
 & \cdot & & & & & & \cdot & & & \cdot \\
 & \cdot & & & & & & & \cdot & & \cdot \\
 & a_{1n} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a_{mn}
 \end{array} \right]
 \quad \text{where } j = \text{IPARM}(3)$$

You use the partial factorization function when, for design or storage reasons, you must factor the matrix  $A$  in stages. When doing a partial factorization, you must use the same skyline storage mode for all parts of the matrix as it is progressively factored.

6. Your various arrays must have no common elements; otherwise, results are unpredictable.
7. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

### Function

This subroutine can factor, compute the determinant of, and solve symmetric sparse matrix  $A$ , stored in skyline storage mode. It can use either Gaussian elimination or Cholesky decomposition. For all computations, input matrix  $A$  can be stored in either diagonal-out or profile-in skyline storage mode. Output matrix  $A$  can also be stored in either of these modes and can be different from the mode used for input.

For Gaussian elimination, matrix  $A$  is factored into the following form using specified pivot processing:

$$A = LDL^T$$

where:

- $D$  is a diagonal matrix.
- $L$  is a lower triangular matrix.

The transformed matrix  $A$ , factored into its  $LDL^T$  form, is stored in packed format in array  $A$ , such that the inverse of the diagonal matrix  $D$  is stored in the corresponding elements of array  $A$ . The off-diagonal elements of the unit upper triangular matrix  $L^T$  are stored in the corresponding off-diagonal elements of array  $A$ .

For Cholesky decomposition, matrix  $A$  is factored into the following form using specified pivot processing:

$$A = R^T R$$

where  $R$  is an upper triangular matrix

The transformed matrix  $A$ , factored into its  $R^T R$  form, is stored in packed format in array  $A$ , such that the inverse of the diagonal elements of the upper triangular matrix  $R$  is stored in the corresponding elements of array  $A$ . The off-diagonal elements of matrix  $R$  are stored in the corresponding off-diagonal elements of array  $A$ .

The partial factorization of matrix  $A$ , which you can do when you specify the factor-only option, assumes that the first  $\text{IPARM}(3)$  rows and columns are already factored in the input matrix. It factors the remaining  $n - \text{IPARM}(3)$  rows and columns in matrix  $A$ . (See “Notes” on page 651 for an illustration.) It updates only the elements in array  $A$  corresponding to the part of matrix  $A$  that is factored.

The determinant can be computed with any of the factorization computations. With a full factorization, you get the determinant for the whole matrix. With a partial factorization, you get the determinant for only that part of the matrix factored in this computation.

The system  $Ax = b$ , having multiple right-hand sides, is solved for  $x$  using the transformed matrix  $A$  produced by this call or a subsequent call to this subroutine.

See references [11], [14], [27], [49], [74]. If  $n$  is 0, no computation is performed. If  $mbx$  is 0, no solve is performed.

## Error conditions

### Resource Errors

- Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.
- Unable to allocate internal work area.

### Computational Errors

1. If a pivot occurs in region  $i$  for  $i = 1, 5$  and  $\text{IPARM}(10+i) = 1$ , the pivot value is replaced with  $\text{RPARM}(10+i)$ , an attention message is issued, and processing continues.
2. Unacceptable pivot values occurred in the factorization of matrix  $A$ .
  - One or more diagonal elements of  $D$  or  $R$  contains unacceptable pivots and no valid fixup is applicable. The row number  $i$  of the first unacceptable pivot element is identified in the computational error message.
  - The return code is set to 2.
  - $i$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use `ERRSET` to change the number of allowable errors for error code 2126 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $n < 0$
2.  $na < 0$
3.  $\text{IDIAG}(n+1) > na+1$
4.  $\text{IDIAG}(i+1) \leq \text{IDIAG}(i)$  for  $i = 1, n$
5.  $\text{IDIAG}(i+1) > \text{IDIAG}(i)+i$  and  $\text{IPARM}(4) = 0$  for  $i = 1, n$
6.  $\text{IDIAG}(i) > \text{IDIAG}(i-1)+i$  and  $\text{IPARM}(4) = 1$  for  $i = 2, n$
7.  $\text{IPARM}(1) \neq 0$  or 1
8.  $\text{IPARM}(2) \neq 0, 1, 2, 10, 11, 100, 101, 102, 110, \text{ or } 111$

- 9. IPARM(3) < 0
- 10. IPARM(3) > n
- 11. IPARM(3) > 0 and IPARM(2) ≠ 1, 11, 101, or 111
- 12. IPARM(4), IPARM(5) ≠ 0 or 1
- 13. IPARM(2) = 0, 1, 10, or 11 and:

IPARM(10) ≠ 0 or 1  
 IPARM(11), IPARM(12) ≠ -1, 0, or 1  
 IPARM(13) ≠ -1 or 1  
 IPARM(14), IPARM(15) ≠ -1, 0, or 1  
 RPARM(10) < 0.0  
 RPARM(10+i) = 0.0 and IPARM(10+i) = 1 for i = 1,5

- 14. IPARM(2) = 100, 101, 110, or 111 and:

IPARM(10) ≠ 0 or 1  
 IPARM(11), IPARM(12), IPARM(13) ≠ -1 or 1  
 IPARM(14), IPARM(15) ≠ -1, 0, or 1  
 RPARM(10) < 0.0  
 RPARM(10+i) ≤ 0.0 and IPARM(10+i) = 1 for i = 1,5

- 15. IPARM(2) = 0, 2, 10, 100, 102, or 110 and:

$ldb_x \leq 0$  and  $mb_x \neq 0$  and  $n \neq 0$   
 $ldb_x < 0$  and  $mb_x = 0$   
 $ldb_x < n$  and  $mb_x \neq 0$   
 $mb_x < 0$

- 16. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to factor a 9 by 9 symmetric sparse matrix  $A$  and solve the system  $Ax = b$  with three right-hand sides. It uses Gaussian elimination. The default values are used for IPARM and RPARM. Input matrix  $A$ , shown here, is stored in diagonal-out skyline storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 2.0 & 2.0 & 1.0 & 1.0 & 0.0 & 1.0 & 0.0 \\ 1.0 & 2.0 & 3.0 & 3.0 & 2.0 & 2.0 & 0.0 & 2.0 & 0.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 3.0 & 3.0 & 0.0 & 3.0 & 0.0 \\ 0.0 & 1.0 & 2.0 & 3.0 & 4.0 & 4.0 & 1.0 & 4.0 & 0.0 \\ 0.0 & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 2.0 & 5.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 3.0 & 2.0 \\ 0.0 & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 3.0 & 7.0 & 3.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 4.0 \end{bmatrix}$$

Output matrix  $A$ , shown here, is in  $LDL^T$  factored form with  $D^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 1.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 1.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 1.0 & 0.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \end{bmatrix}$$



$$\begin{bmatrix} 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 \end{bmatrix}$$

**Call Statement and Input:**

```

      N  A  NA  IDIAG  IPARM  RPARM  AUX  NAUX  BX  LDBX  MBX
CALL DSKFS( 9, A, 33, IDIAG, IPARM, RPARM, AUX, 39 , BX , 12 , 3 )
A      = (1.0, 2.0, 1.0, 3.0, 2.0, 1.0, 4.0, 3.0, 2.0, 1.0, 4.0,
          3.0, 2.0, 1.0, 5.0, 4.0, 3.0, 2.0, 1.0, 3.0, 2.0, 1.0,
          7.0, 3.0, 5.0, 4.0, 3.0, 2.0, 1.0, 4.0, 3.0, 2.0, 1.0)
IDIAG  = (1, 2, 4, 7, 11, 15, 20, 23, 30, 34)
IPARM  = (0, . , . , . , . , . , . , . , . , . , . , . , . , . , . ,
          . , . , . , . , . , . , . , . , . , . , . , . , . , . , . ,
          . , . , . , . , . , . , . , . , . , . , . , . , . , . , . )

```

RPARM =(not relevant)

```

BX =
  [ 4.00  8.00 12.00
 10.00 20.00 30.00
 15.00 30.00 45.00
 19.00 38.00 57.00
 19.00 38.00 57.00
 23.00 46.00 69.00
 11.00 22.00 33.00
 28.00 56.00 84.00
 10.00 20.00 30.00
  .      .      .
  .      .      .
  .      .      . ]

```

**Output:**

```

A      = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
1.0,
          1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
          1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IDIAG  =(same as input)
IPARM  = (0, . , . , . , . , . , . , . , . , . , . , . , . , . , . ,
          . , 8, . , . , . , . , . , 0, 0, 0, 0, 9)
RPARM  = ( . , . , . , . , . , . , . , . , . , . , . , . , . , . , . ,
          . , 7.0, . , . , . , . , . , . , . , . , . , . , . , . , . )

```

```

BX =
  [ 1.00  2.00  3.00
  1.00  2.00  3.00
  1.00  2.00  3.00
  1.00  2.00  3.00
  1.00  2.00  3.00
  1.00  2.00  3.00
  1.00  2.00  3.00
  1.00  2.00  3.00
  1.00  2.00  3.00
  .      .      .
  .      .      .
  .      .      . ]

```

**Example 2**

This example shows how to factor the 9 by 9 symmetric sparse matrix  $A$  from Example 1, solve the system  $Ax = b$  with three right-hand sides, and compute the determinant of  $A$ . It uses Gaussian elimination. The default values for pivot

processing are used for IPARM. Input matrix  $A$  is stored in profile-in skyline storage mode. Output matrix  $A$  is in  $LDL^T$  factored form with  $D^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. It is the same as output matrix  $A$  in Example 1.

**Call Statement and Input:**

```

          N  A  NA  IDIAG  IPARM  RPARM  AUX  NAUX  BX  LDBX  MBX
          |  |  |  |      |      |      |  |   |   |   |
CALL DSKFS( 9, A, 33, IDIAG, IPARM, RPARM, AUX, 39 , BX , 12 , 3 )
A          = (1.0, 1.0, 2.0, 1.0, 2.0, 3.0, 1.0, 2.0, 3.0, 4.0, 1.0,
              2.0, 3.0, 4.0, 1.0, 2.0, 3.0, 4.0, 5.0, 1.0, 2.0, 3.0,
              1.0, 2.0, 3.0, 4.0, 5.0, 3.0, 7.0, 1.0, 2.0, 3.0, 4.0)
IDIAG      = (1, 3, 6, 10, 14, 19, 22, 29, 33, 34)
IPARM      = (1, 10, 0, 1, 0, ., ., ., ., ., 0, ., ., ., ., ., ., ., ., ., .,
              ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .)

RPARM      =(not relevant)

```

```

BX          =
[
  4.00  8.00 12.00
 10.00 20.00 30.00
 15.00 30.00 45.00
 19.00 38.00 57.00
 19.00 38.00 57.00
 23.00 46.00 69.00
 11.00 22.00 33.00
 28.00 56.00 84.00
 10.00 20.00 30.00
  .      .      .
  .      .      .
  .      .      .
]

```

**Output:**

```

A          =(same as output A in Example 1)
IDIAG      =(same as input IDIAG in Example 1)
IPARM      = (1, 10, 0, 1, 0, ., ., ., ., ., 0, ., ., ., ., ., ., ., ., ., .,
              ., ., ., ., ., 0, 0, 0, 0, 9)
RPARM      = ( ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,
              ., 7.0, 1.0, 0.0, ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .)
BX          =(same as output BX in Example 1)

```

**Example 3**

This example shows how to factor a 9 by 9 negative-definite symmetric sparse matrix  $A$ , solve the system  $Ax = b$  with three right-hand sides, and compute the determinant of  $A$ . It uses Gaussian elimination. (Default values for pivot processing are not used for IPARM because  $A$  is negative-definite.) Input matrix  $A$ , shown here, is stored in diagonal-out skyline storage mode. Matrix  $A$  is:

```

[
-1.0 -1.0 -1.0 -1.0  0.0  0.0  0.0  0.0  0.0
-1.0 -2.0 -2.0 -2.0 -1.0 -1.0  0.0 -1.0  0.0
-1.0 -2.0 -3.0 -3.0 -2.0 -2.0  0.0 -2.0  0.0
-1.0 -2.0 -3.0 -4.0 -3.0 -3.0  0.0 -3.0  0.0
  0.0 -1.0 -2.0 -3.0 -4.0 -4.0 -1.0 -4.0  0.0
  0.0 -1.0 -2.0 -3.0 -4.0 -5.0 -2.0 -5.0 -1.0
  0.0  0.0  0.0  0.0 -1.0 -2.0 -3.0 -3.0 -2.0
  0.0 -1.0 -2.0 -3.0 -4.0 -5.0 -3.0 -7.0 -3.0
  0.0  0.0  0.0  0.0  0.0 -1.0 -2.0 -3.0 -4.0
]

```

Output matrix  $A$ , shown here, is in  $LDL^T$  factored form with  $D^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Matrix  $A$  is:

$$\begin{bmatrix} -1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & -1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 1.0 & 0.0 \\ 1.0 & 1.0 & -1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 1.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & -1.0 & 1.0 & 1.0 & 0.0 & 1.0 & 0.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & -1.0 & 1.0 & 1.0 & 1.0 & 0.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & -1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & -1.0 & 1.0 & 1.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & -1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & -1.0 \end{bmatrix}$$

**Call Statement and Input:**

```

          N  A  NA  IDIAG  IPARM  RPARM  AUX  NAUX  BX  LDBX  MBX
CALL DSKFS(9, A, 33, IDIAG, IPARM, RPARM, AUX, 39, BX, 12, 3)
A       = (-1.0, -2.0, -1.0, -3.0, -2.0, -1.0, -4.0, -3.0, -2.0,
          -1.0, -4.0, -3.0, -2.0, -1.0, -5.0, -4.0, -3.0, -2.0,
          -1.0, -3.0, -2.0, -1.0, -7.0, -3.0, -5.0, -4.0, -3.0,
          -2.0, -1.0, -4.0, -3.0, -2.0, -1.0)
IDIAG   = (1, 2, 4, 7, 11, 15, 20, 23, 30, 34)
IPARM   = (1, 10, 0, 0, 0, ., ., ., ., ., 1, 0, -1, -1, -1, -1, .,
          ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .)
RPARM   = (., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,
          ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .)
BX      =(same as input BX in Example 1)

```

**Output:**

```

A       = (-1.0, -1.0, 1.0, -1.0, 1.0, 1.0, -1.0, 1.0,
          1.0, 1.0,
          -1.0, 1.0, 1.0, 1.0, -1.0, 1.0, 1.0, 1.0, 1.0, -1.0, 1.0,
          1.0, -1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, -1.0, 1.0, 1.0,
          1.0)
IDIAG   =(same as input)
IPARM   = (1, 10, 0, 0, 0, ., ., ., ., ., 1, 0, -1, -1, -1, -1, 8,
          ., ., ., ., ., 9, 0, 0, 0, 0)
RPARM   = (., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,
          ., ., ., ., 7.0, -1.0, 0.0, ., ., ., ., ., ., ., ., ., ., .)

```

$$BX = \begin{bmatrix} -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ -1.00 & -2.00 & -3.00 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Example 4**

This example shows how to factor the first six rows and columns, referred to as matrix  $A1$ , of the 9 by 9 symmetric sparse matrix  $A$  from Example 1 and compute

the determinant of  $A1$ . It uses Gaussian elimination. Input matrix  $A1$ , shown here, is stored in diagonal-out skyline storage mode. Input matrix  $A1$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 2.0 & 2.0 & 1.0 & 1.0 \\ 1.0 & 2.0 & 3.0 & 3.0 & 2.0 & 2.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 3.0 & 3.0 \\ 0.0 & 1.0 & 2.0 & 3.0 & 4.0 & 4.0 \\ 0.0 & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \end{bmatrix}$$

Output matrix  $A1$ , shown here, is in  $LDL^T$  factored form with  $D^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Output matrix  $A1$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \end{bmatrix}$$

**Call Statement and Input:**

```

          N   A   NA   IDIAG   IPARM   RPARM   AUX   NAUX   BX   LDBX   MBX
CALL DSKFS (6 , A , 33 , IDIAG , IPARM , RPARM , AUX , 27 , BX , LDBX , MBX )
    
```

A            =(same as input A in Example 1)  
 IDIAG       = (1, 2, 4, 7, 11, 15, 20)  
 IPARM       = (1, 11, 0, 0, 0, ., ., ., ., ., 0, ., ., ., ., ., .,  
               ., ., ., ., ., ., ., ., ., ., ., .)  
 RPARM       =(not relevant)  
 BX           =(not relevant)  
 LDBX        =(not relevant)  
 MBX         =(not relevant)

**Output:**

A            = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,  
 1.0,  
               1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 3.0, 2.0, 1.0,  
               7.0, 3.0, 5.0, 4.0, 3.0, 2.0, 1.0, 4.0, 3.0, 2.0, 1.0)  
 IDIAG       =(same as input)  
 IPARM       = (1, 11, 0, 0, 0, ., ., ., ., ., 0, ., ., ., ., ., ., 6,  
               ., ., ., ., ., 0, 0, 0, 0, 6)  
 RPARM       = (., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,  
               ., 5.0, 1.0, 0.0, ., ., ., ., ., ., ., .)  
 BX           =(same as input)  
 LDBX        =(same as input)  
 MBX         =(same as input)

**Example 5**

This example shows how to do a partial factorization of the 9 by 9 symmetric sparse matrix  $A$  from Example 1, where the first six rows and columns were factored in Example 4. It factors the remaining three rows and columns and computes the determinant of that part of the matrix. It uses Gaussian elimination.

The input matrix, referred to as  $A2$ , shown here, is made up of the output factored matrix  $A1$  plus the three remaining unfactored rows and columns of matrix  $A$ . Matrix  $A2$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 1.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 2.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 3.0 & 0.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 4.0 & 0.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 2.0 & 5.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 3.0 & 2.0 \\ 0.0 & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 3.0 & 7.0 & 3.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 4.0 \end{bmatrix}$$

Both parts of input matrix  $A2$  are stored in diagonal-out skyline storage mode.

Output matrix  $A2$  is the same as output matrix  $A$  in Example 1 and is stored in diagonal-out skyline storage mode.

**Call Statement and Input:**

```

          N  A  NA  IDIAG  IPARM  RPARAM  AUX  NAUX  BX  LDBX  MBX
CALL DSKFS (9 , A , 33 , IDIAG , IPARM , RPARAM , AUX , 27 , BX , LDBX , MBX )
    
```

- A = (same as output A in Example 4)
- IDIAG = (same as input IDIAG in Example 1)
- IPARM = (1, 11, 6, 0, 0, ., ., ., ., ., 0, ., ., ., ., ., ., ., ., ., .)
- RPARAM = (not relevant)
- BX = (not relevant)
- LDBX = (not relevant)
- MBX = (not relevant)

**Output:**

- A = (same as output A in Example 1)
- IDIAG = (same as output IDIAG in Example 1)
- IPARM = (1, 11, 6, 0, 0, ., ., ., ., ., 0, ., ., ., ., ., ., ., ., ., 8, ., ., ., ., ., 0, 0, 0, 0, 3)
- RPARAM = (., 7.0, 1.0, 0.0, ., ., ., ., ., ., .)
- BX = (same as input)
- LDBX = (same as input)
- MBX = (same as input)

**Example 6**

This example shows how to solve the system  $Ax = b$  with one right-hand side for a symmetric sparse matrix  $A$ . Input matrix  $A$ , used here, is the same as factored output matrix  $A$  from Example 1, stored in profile-in skyline storage mode. It specifies Gaussian elimination, as used in Example 1. Here, output matrix  $A$  is unchanged on output and is stored in profile-in skyline storage mode.

**Call Statement and Input:**

```

          N  A  NA  IDIAG  IPARM  RPARAM  AUX  NAUX  BX  LDBX  MBX
CALL DSKFS (9 , A , 33 , IDIAG , IPARM , RPARAM , AUX , 31 , BX , 9 , 1 )
    
```

## DSKFS

```

A          = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
1.0,
           1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
           1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IDIAG      = (1, 3, 6, 10, 14, 19, 22, 29, 33, 34)
IPARM      = (1, 2, 0, 1, 1, . . . , . . . , . . . , . . . , . . . , . . . , . . . , . . . )
RPARM      =(not relevant)
BX         = (10.0, 38.0, 64.0, 87.0, 103.0, 133.0, 80.0, 174.0, 80.0)

```

### Output:

```

A          =(same as input)
IDIAG      =(same as input)
IPARM      =(same as input)
APARM      =(same as input)
BX         = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0)

```

### Example 7

This example shows how to factor a 9 by 9 symmetric sparse matrix  $A$  and solve the system  $Ax = b$  with four right-hand sides. It uses Cholesky decomposition. Input matrix  $A$ , shown here, is stored in profile-in skyline storage mode Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ 1.0 & 5.0 & 3.0 & 0.0 & 3.0 & 0.0 & 0.0 & 0.0 & 3.0 \\ 1.0 & 3.0 & 11.0 & 3.0 & 5.0 & 3.0 & 3.0 & 0.0 & 5.0 \\ 0.0 & 0.0 & 3.0 & 17.0 & 5.0 & 5.0 & 5.0 & 0.0 & 5.0 \\ 1.0 & 3.0 & 5.0 & 5.0 & 29.0 & 7.0 & 7.0 & 0.0 & 9.0 \\ 0.0 & 0.0 & 3.0 & 5.0 & 7.0 & 39.0 & 9.0 & 6.0 & 9.0 \\ 0.0 & 0.0 & 3.0 & 5.0 & 7.0 & 9.0 & 53.0 & 8.0 & 11.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 6.0 & 8.0 & 66.0 & 10.0 \\ 1.0 & 3.0 & 5.0 & 5.0 & 9.0 & 9.0 & 11.0 & 10.0 & 89.0 \end{bmatrix}$$

Output matrix  $A$ , shown here, is in  $R^T R$  factored form with the inverse of the diagonal of  $R$  on the diagonal, and is stored in profile-in skyline storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ 1.0 & .5 & 1.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 1.0 \\ 1.0 & 1.0 & .333 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 1.0 & .25 & 1.0 & 1.0 & 1.0 & 0.0 & 1.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & .2 & 1.0 & 1.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & .167 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & .143 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & .125 & 1.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & .111 \end{bmatrix}$$

### Call Statement and Input:

```

          N  A  NA  IDIAG  IPARM  RPARM  AUX  NAUX  BX  LDBX  MBX
CALL DSKFS( 9, A, 34, IDIAG, IPARM, RPARM, AUX, 43 , BX , 10 , 4 )
A          = (1.0, 1.0, 5.0, 1.0, 3.0, 11.0, 3.0, 17.0, 1.0, 3.0, 5.0,
           5.0, 29.0, 3.0, 5.0, 7.0, 39.0, 3.0, 5.0, 7.0, 9.0, 53.0,
           6.0, 8.0, 66.0, 1.0, 3.0, 5.0, 5.0, 9.0, 9.0, 11.0, 10.0,
           89.0)

```

```

IDIAG = (1, 3, 6, 8, 13, 17, 22, 25, 34, 35)
IPARM = (1, 110, 0, 1, 1, ., ., ., ., ., ., 0, ., ., ., ., ., .,
        ., ., ., ., ., ., ., ., ., ., ., .)
  
```

RPARM =(not relevant)

```

BX = [ 5.00 10.00 15.00 20.00
      15.00 30.00 45.00 60.00
      34.00 68.00 102.00 136.00
      40.00 80.00 120.00 160.00
      66.00 132.00 198.00 264.00
      78.00 156.00 234.00 312.00
      96.00 192.00 288.00 384.00
      90.00 180.00 270.00 360.00
      142.00 284.00 426.00 568.00
      . . . .
  ]
  
```

**Output:**

```

A = (1.0, 1.0, .5, 1.0, 1.0, .333, 1.0, .25, 1.0, 1.0,
     1.0,
     1.0, .2, 1.0, 1.0, 1.0, .167, 1.0, 1.0, 1.0, 1.0, .143,
     1.0, 1.0, .125, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
     .111)
  
```

IDIAG =(same as input)

```

IPARM = (1, 110, 0, 1, 1, ., ., ., ., ., ., 0, ., ., ., ., ., .,
        9, ., ., ., ., ., 0, 0, 0, 0, 9)
  
```

```

RPARM = (., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., ., .,
        ., 9.89, 1.32, 11.0, ., ., ., ., ., ., ., .)
  
```

```

BX = [ 1.00 2.00 3.00 4.00
      1.00 2.00 3.00 4.00
      1.00 2.00 3.00 4.00
      1.00 2.00 3.00 4.00
      1.00 2.00 3.00 4.00
      1.00 2.00 3.00 4.00
      1.00 2.00 3.00 4.00
      1.00 2.00 3.00 4.00
      1.00 2.00 3.00 4.00
      . . . .
  ]
  
```

## DSRIS — Iterative Linear System Solver for a General or Symmetric Sparse Matrix Stored by Rows

### Purpose

This subroutine solves a general or symmetric sparse linear system of equations, using an iterative algorithm, with or without preconditioning. The methods include conjugate gradient (CG), conjugate gradient squared (CGS), generalized minimum residual (GMRES), more smoothly converging variant of the CGS method (Bi-CGSTAB), or transpose-free quasi-minimal residual method (TFQMR). The preconditioners include an incomplete LU factorization, an incomplete Cholesky factorization (for positive definite symmetric matrices), diagonal scaling, or symmetric successive over-relaxation (SSOR) with two possible choices for the diagonal matrix: one uses the absolute values sum of the input matrix, and the other uses the diagonal obtained from the LU factorization. The sparse matrix is stored using storage-by-rows for general matrices and upper- or lower-storage-by-rows for symmetric matrices. Matrix  $A$  and vectors  $x$  and  $b$  are used:

$$Ax = b$$

where  $A$ ,  $x$ , and  $b$  contain long-precision real numbers.

### Syntax

Fortran	CALL DSRIS ( <i>stor, init, n, ar, ja, ia, b, x, iparm, rparm, aux1, naux1, aux2, naux2</i> )
C and C++	dsris ( <i>stor, init, n, ar, ja, ia, b, x, iparm, rparm, aux1, naux1, aux2, naux2</i> );

### On Entry

*stor* indicates the form of sparse matrix  $A$  and the storage mode used, where:

If *stor* = 'G',  $A$  is a general sparse matrix, stored using storage-by-rows.

If *stor* = 'U',  $A$  is a symmetric sparse matrix, stored using upper-storage-by-rows.

If *stor* = 'L',  $A$  is a symmetric sparse matrix, stored using lower-storage-by-rows.

Specified as: a single character. It must be 'G', 'U', or 'L'.

*init* indicates the type of computation to be performed, where:

If *init* = 'T', the preconditioning matrix is computed, the internal representation of the sparse matrix is generated, and the iteration procedure is performed. The coefficient matrix and preconditioner in internal format are saved in *aux1*.

If *init* = 'S', the iteration procedure is performed using the coefficient matrix and the preconditioner in internal format, stored in *aux1*, created in a preceding call to this subroutine with *init* = 'T'. You use this option to solve the same matrix for different right-hand sides,  $b$ , optimizing your performance. As long as you do not change the coefficient matrix and preconditioner in *aux1*, any number of calls can be made with *init* = 'S'.



- Specified as: a single character. It must be 'I' or 'S'.
- n* is the order of the linear system  $Ax = b$  and the number of rows and columns in sparse matrix  $A$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- ar* is the sparse matrix  $A$  of order  $n$ , stored by rows in an array, referred to as AR. The *stor* argument indicates the storage variation used for storing matrix  $A$ .  
Specified as: a one-dimensional array, containing long-precision real numbers. The number of elements in this array can be determined by subtracting 1 from the value in IA( $n+1$ ).
- ja* is the array, referred to as JA, containing the column numbers of each nonzero element in sparse matrix  $A$ .  
Specified as: a one-dimensional array, containing fullword integers;  $1 \leq (\text{JA elements}) \leq n$ . The number of elements in this array can be determined by subtracting 1 from the value in IA( $n+1$ ).
- ia* is the row pointer array, referred to as IA, containing the starting positions of each row of matrix  $A$  in array AR and one position past the end of array AR. Specified as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers;  $IA(i+1) \geq IA(i)$  for  $i = 1, n+1$ .
- b* is the vector  $b$  of length  $n$ , containing the right-hand side of the matrix problem.  
Specified as: a one-dimensional array of (at least) length  $n$ , containing long-precision real numbers.
- x* is the vector  $x$  of length  $n$ , containing your initial guess of the solution of the linear system.  
Specified as: a one-dimensional array of (at least) length  $n$ , containing long-precision real numbers. The elements can have any value, and if no guess is available, the value can be zero.
- iparm* is an array of parameters, IPARM( $i$ ), where:
- IPARM(1) controls the number of iterations.  
If IPARM(1) > 0, IPARM(1) is the maximum number of iterations allowed.  
If IPARM(1) = 0, the following default values are used:
    - IPARM(1) = 300
    - IPARM(2) = 4
    - IPARM(4) = 4
    - IPARM(5) = 1
    - RPARM(1) =  $10^{-6}$
    - RPARM(2) = 1
  - IPARM(2) is the flag used to select the iterative procedure used in this subroutine.  
If IPARM(2) = 1, the conjugate gradient (CG) method is used.  
Note that this algorithm should only be used with positive definite symmetric matrices.  
If IPARM(2) = 2, the conjugate gradient squared (CGS) method is used.

If IPARM(2) = 3, the generalized minimum residual (GMRES) method, restarted after  $k$  steps, is used.

If IPARM(2) = 4, the more smoothly converging variant of the CGS method (Bi-CGSTAB) is used.

If IPARM(2) = 5, the transpose-free quasi-minimal residual method (TFQMR) is used.

- IPARM(3) has the following meaning, where:

If IPARM(2)  $\neq$  3, then IPARM(3) is not used.

If IPARM(2) = 3, then IPARM(3) =  $k$ , where  $k$  is the number of steps after which the generalized minimum residual method is restarted. A value for  $k$  in the range of 5 to 10 is suitable for most problems.

- IPARM(4) is the flag that determines the type of preconditioning.

If IPARM(4) = 1, the system is not preconditioned.

If IPARM(4) = 2, the system is preconditioned by a diagonal matrix.

If IPARM(4) = 3, the system is preconditioned by SSOR splitting with the diagonal given by the absolute values sum of the input matrix.

If IPARM(4) = 4, the system is preconditioned by an incomplete LU factorization.

If IPARM(4) = 5, the system is preconditioned by SSOR splitting with the diagonal given by the incomplete LU factorization.

**Note:** The multithreaded version of DSRIS only runs on multiple threads when IPARM(4) = 1 or 2.

- IPARM(5) is the flag used to select the stopping criterion used in the computation, where the following items are used in the definitions of the stopping criteria below:

–  $\epsilon$  is the desired relative accuracy and is stored in RPARAM(1).

–  $x_j$  is the solution found at the  $j$ -th iteration.

–  $r_j$  and  $r_0$  are the preconditioned residuals obtained at iterations  $j$  and 0, respectively. (The residual at iteration  $j$  is given by  $b - Ax_j$ .)

If IPARM(5) = 1, the iterative method is stopped when:

$$\|r_j\|_2 / \|x_j\|_2 < \epsilon$$

**Note:** IPARM(5) = 1 is the default value assumed by ESSL if you do not specify one of the values described here; therefore, if you do not update your program to set an IPARM(5) value, you, by default, use the above stopping criterion.

If IPARM(5) = 2, the iterative method is stopped when:

$$\|r_j\|_2 / \|r_0\|_2 < \epsilon$$

If IPARM(5) = 3, the iterative method is stopped when:

$$\|x_j - x_{j-1}\|_2 / \|x_j\|_2 < \epsilon$$

**Note:** Stopping criterion 3 performs poorly with the TFQMR method; therefore, if you specify TFQMR (IPARM(2) = 5), you should not specify stopping criterion 3.

- IPARM(6), see “On Return” on page 666.

Specified as: an array of (at least) length 6, containing fullword integers, where:

IPARM(1)  $\geq 0$   
 IPARM(2) = 1, 2, 3, 4, or 5  
 If IPARM(2) = 3, then IPARM(3)  $> 0$   
 IPARM(4) = 1, 2, 3, 4, or 5  
 IPARM(5) = 1, 2, or 3 (Other values default to stopping criterion 1.)

*rparm*

is an array of parameters, RPARAM(*i*), where:

RPARAM(1) has the following meaning, where:

- if RPARAM(1)  $> 0$ , then RPARAM(1) is the relative accuracy  $\epsilon$  used in the stopping criterion.
- if RPARAM(1) = 0, then the solver is forced to evaluate at most IPARM(1) iterations.

See 5 on page 667.

RPARAM(2), see “On Return” on page 666.

RPARAM(3) has the following meaning, where:

- If IPARM(4)  $\neq 3$ , then RPARAM(3) is not used.
- If IPARM(4) = 3, then RPARAM(3) is the acceleration parameter used in SSOR. (A value in the range 0.5 to 2.0 is suitable for most problems.)

Specified as: a one-dimensional array of (at least) length 3, containing long-precision real numbers, where:

RPARAM(1)  $\geq 0$   
 If IPARM(4) = 3, RPARAM(3)  $> 0$

*aux1*

is working storage for this subroutine, where:

If *init* = 'T', the working storage is computed. It can contain any values.

If *init* = 'S', the working storage is used in solving the linear system. It contains the coefficient matrix and preconditioner in internal format, computed in an earlier call to this subroutine.

Specified as: an area of storage, containing *naux1* long-precision real numbers.

*naux1*

is the number of doublewords in the working storage specified in *aux1*.

Specified as: a fullword integer, where:

In these formulas *nw* has the following value:

If *stor* = 'G', then  $nw = IA(n+1)-1+n$ .

If *stor* = 'U' or 'L', then  $nw = 2(IA(n+1)-1)$ .

If IPARM(4) = 1, use  $naux1 = (3/2)nw + (7/2)n + 40$ .

If IPARM(4) = 2, use  $naux1 = (3/2)nw + (9/2)n + 40$ .

If IPARM(4) = 3, 4, or 5, then:

If IPARM(2)  $\neq$  1, use  $naux1 = 3nw + 10n + 60$ .

If IPARM(2) = 1, use  $naux1 = 3nw + (21/2)n + 60$ .

**Note:** If you receive an attention message, you have not specified sufficient auxiliary storage to achieve optimal performance, but it is enough to perform the computation. To obtain optimal performance, you need to use the amount given by the attention message.

*aux2*

has the following meaning:

If  $naux2 = 0$  and error 2015 is unrecoverable, *aux2* is ignored.

Otherwise, it is working storage used by this subroutine that is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers.

*naux2*

is the number of doublewords in the working storage specified in *aux2*.

Specified as: a fullword integer, where:

If  $naux2 = 0$  and error 2015 is unrecoverable, DSRIS dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,

If IPARM(2) = 1, use  $naux2 \geq 4n$ .

If IPARM(2) = 2, use  $naux2 \geq 7n$ .

If IPARM(2) = 3, use  $naux2 \geq (k+2)n + k(k+4) + 1$ , where  $k = \text{IPARM}(3)$ .

If IPARM(2) = 4, use  $naux2 \geq 7n$ .

If IPARM(2) = 5, use  $naux2 \geq 9n$ .

## On Return

*ar*

is the sparse matrix *A* of order *n*, stored by rows in an array, referred to as AR. The *stor* argument indicates the storage variation used for storing matrix *A*. The order of the elements in each row of *A* in AR may be changed on output.

Returned as: a one-dimensional array, containing long-precision real numbers. The number of elements in this array can be determined by subtracting 1 from the value in IA(*n*+1).

*ja*

is the array, referred to as JA, containing the column numbers of each nonzero element in sparse matrix **A**. These elements correspond to the arrangement of the contents of AR on output.

Returned as: a one-dimensional array, containing fullword integers;  $1 \leq (\text{JA elements}) \leq n$ . The number of elements in this array can be determined by subtracting 1 from the value in IA(*n*+1).

*x*

is the vector *x* of length *n*, containing the solution of the system  $Ax = b$ . Returned as: a one-dimensional array of (at least) length *n*, containing long-precision real numbers.

<i>iparm</i>	<p>is an array of parameters, <math>IPARM(i)</math>, where:  <math>IPARM(1)</math> through <math>IPARM(5)</math> are unchanged.  <math>IPARM(6)</math> contains the number of iterations performed by this subroutine.  Returned as: a one-dimensional array of length 6, containing fullword integers.</p>
<i>rparm</i>	<p>is an array of parameters, <math>RPARAM(i)</math>, where:  <math>RPARAM(1)</math> is unchanged.  <math>RPARAM(2)</math> contains the estimate of the error of the solution. If the process converged, <math>RPARAM(2) \leq \epsilon</math>.  <math>RPARAM(3)</math> is unchanged.  Returned as: a one-dimensional array of length 3, containing long-precision real numbers.</p>
<i>aux1</i>	<p>is working storage for this subroutine, containing the coefficient matrix and preconditioner in internal format, ready to be passed in a subsequent invocation of this subroutine. Returned as: an area of storage, containing <i>naux1</i> long-precision real numbers.</p>

## Notes

1. If you want to solve the same sparse linear system of equations multiple times using a different algorithm with the same preconditioner and using a different right-hand side each time, you get the best performance by using the following technique. Call DSRIS the first time with *init* = 'T'. This solves the system, and then stores the coefficient matrix and preconditioner in internal format in *aux1*. On the subsequent invocations of DSRIS with different right-hand sides, specify *init* = 'S'. This indicates to DSRIS to use the contents of *aux1*, saving the time to convert your coefficient matrix and preconditioner to internal format. If you use this technique, you should not modify the contents of *aux1* between calls to DSRIS.

In some cases, you can specify a different algorithm in  $IPARM(2)$  when making calls with *init* = 'S'. (See "Example 2" on page 670.) However, DSRIS sometimes needs different information in *aux1* for different algorithms. When this occurs, DSRIS issues an attention message, continues processing the computation, and then resets the contents of *aux1*. Your performance is not improved in this case, which is functionally equivalent to calling DSRIS with *init* = 'T'.

2. If you use the CG method with *init* = 'T', you must use the CG method when you specify *init* = 'S'. However, if you use a different method with *init* = 'T', you can use any other method, except CG, when you specify *init* = 'S'.
3. These subroutines accept lowercase letters for the *stor* and *init* arguments.
4. Matrix *A*, vector *x*, and vector *b* must have no common elements; otherwise, results are unpredictable.
5. The algorithm computes a sequence of approximate solution vectors *x* that converge to the solution. The iterative procedure is stopped when the selected stopping criterion is satisfied or when more than the maximum number of iterations (in  $IPARM(1)$ ) is reached.

For the stopping criteria specified in  $IPARM(5)$ , the relative accuracy  $\epsilon$  (in  $RPARAM(1)$ ) must be specified reasonably ( $10^{-4}$  to  $10^{-8}$ ). If you specify a larger  $\epsilon$ , the algorithm takes fewer iterations to converge to a solution. If you specify a

smaller  $\epsilon$ , the algorithm requires more iterations and computer time, but converges to a more precise solution. If the value you specify is unreasonably small, the algorithm may fail to converge within the number of iterations it is allowed to perform.

6. For a description of how sparse matrices are stored by rows, see “Storage-by-Rows” on page 100.
7. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## Function

The linear system:

$$Ax = b$$

is solved using one of the following methods: conjugate gradient (CG), conjugate gradient squared (CGS), generalized minimum residual (GMRES), more smoothly converging variant of the CGS method (Bi-CGSTAB), or transpose-free quasi-minimal residual method (TFQMR), where:

$A$  is a sparse matrix of order  $n$ . The matrix is stored in arrays AR, IA, and JA. If it is general, it is stored by rows. If it is symmetric, it can be stored using upper- or lower-storage-by-rows.

$x$  is a vector of length  $n$ .

$b$  is a vector of length  $n$ .

One of the following preconditioners is used:

- an incomplete LU factorization
- an incomplete Cholesky factorization (for positive definite symmetric matrices)
- diagonal scaling
- symmetric successive over-relaxation (SSOR) with two possible choices for the diagonal matrix:
  - the absolute values sum of the input matrix
  - the diagonal obtained from the LU factorization

See references [38], [58], [85], [90], [93], and [99].

When you call this subroutine to solve a system for the first time, you specify *init* = 'I'. After that, you can solve the same system any number of times by calling this subroutine each time with *init* = 'S'. These subsequent calls use the coefficient matrix and preconditioner, stored in internal format in *aux1*. You optimize performance by doing this, because certain portions of the computation have already been performed.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable, *naux2* = 0, and unable to allocate work area.

## Computational Errors

The following errors, with their corresponding return codes, can occur in this subroutine. For details on error handling, see “What Can You Do about ESSL Computational Errors?” on page 51.

- For error 2110, if  $RPARM(1) >$ , return code 1 indicates that the subroutine exceeded  $IPARM(1)$  iterations without converging. Vector  $x$  contains the approximate solution computed at the last iteration.
- For error 2130, return code 2 indicates that the incomplete LU factorization of  $A$  could not be completed, because one pivot was 0.
- For error 2124, the subroutine has been called with  $init = 'S'$ , but the data contained in  $aux1$  was computed for a different algorithm. An attention message is issued. Processing continues, and the contents of  $aux1$  are reset correctly.
- For error 2134, return code 3 indicates that the data contained in  $aux1$  is not consistent with the input sparse matrix. The subroutine has been called with  $init = 'S'$ , and  $aux1$  contains an incomplete factorization and internal data storage for the input matrix  $A$  that was computed by a previous call to the subroutine when  $init = 'T'$ . This error indicates that  $aux1$  has been modified since the last call to the subroutine, or that the input matrix is not the same as the one that was factored. If the default action has been overridden, the subroutine can be called again with the same parameters, with the exception of  $IPARM(4) = 1$  or 4.
- For error 2131, return code 4 indicates that the matrix is singular, because all elements in one row of the matrix contain zero.
- For error 2129, return code 5 indicates that the matrix is not positive definite.
- For error 2128, return code 8 indicates an internal ESSL error. Please contact your IBM Representative.

## Input-Argument Errors

1.  $n < 0$
2.  $stor \neq 'G', 'U', \text{ or } 'L'$
3.  $init \neq 'T' \text{ or } 'S'$
4.  $IA(n+1) < 1$
5.  $IA(i+1) - IA(i) < 0$ , for any  $i = 1, n$
6.  $IPARM(1) < 0$
7.  $IPARM(2) \neq 1, 2, 3, 4, \text{ or } 5$
8.  $IPARM(3) \leq 0$  and  $IPARM(2) = 3$
9.  $IPARM(4) \neq 1, 2, 3, 4, \text{ or } 5$
10.  $RPARM(1) < 0$
11.  $RPARM(3) \leq 0$  and  $IPARM(4) = 3$
12.  $naux1$  is too small—that is, less than the minimum required value. Return code 6 is returned if error 2015 is recoverable.
13. Error 2015 is recoverable or  $naux2 \neq 0$ , and  $naux2$  is too small—that is, less than the minimum required value. Return code 7 is returned for  $naux2$  if error 2015 is recoverable.

## Examples

### Example 1

This example finds the solution of the linear system  $Ax = b$  for the sparse matrix  $A$ , which is stored by rows in arrays  $AR$ ,  $IA$ , and  $JA$ . The system is solved using the Bi-CGSTAB algorithm. The iteration is stopped when the norm of the residual is less than the given threshold specified in  $RPARM(1)$ . The algorithm is allowed to perform 20 iterations. The process converges after 9 iterations. Matrix  $A$  is:

$$\begin{bmatrix} 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{bmatrix}$$

## DSRIS

$$\begin{bmatrix} 0.0 & 1.0 & 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 \end{bmatrix}$$

### Call Statement and Input:

```

      STOR INIT  N  AR  JA  IA  B  X  IPARM  RPARM  AUX1  NAUX1  AUX2  NAUX2
CALL DSRIS( 'G' , 'I' , 9 , AR , JA , IA , B , X , IPARM , RPARM , AUX1 , 98 , AUX2 , 63 )

```

```

AR      = (2.0, 2.0, -1.0, 1.0, 2.0, 1.0, 2.0, -1.0, 1.0, 2.0, -1.0,
          1.0, 2.0, -1.0, 1.0, 2.0, -1.0, 1.0, 2.0, -1.0, 1.0, 2.0)
JA      = (1, 2, 3, 2, 3, 1, 4, 5, 4, 5, 6, 5, 6, 7, 6, 7, 8, 7, 8,
          9, 8, 9)
IA      = (1, 2, 4, 6, 9, 12, 15, 18, 21, 23)
B       = (2.0, 1.0, 3.0, 2.0, 2.0, 2.0, 2.0, 2.0, 3.0)
X       = (0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0)
IPARM(1) = 20
IPARM(2) = 4
IPARM(3) = 0
IPARM(4) = 1
IPARM(5) = 10
RPARM(1) = 1.D-7
RPARM(3) = 1.0

```

### Output:

```

X       = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IPARM(6) = 9
RPARM(2) = 0.29D-16

```

### Example 2

This example finds the solution of the linear system  $Ax = b$  for the same sparse matrix  $A$  used in Example 1. It also uses the same right-hand side in  $b$  and the same initial guesses in  $x$ . However, the system is solved using a different algorithm, conjugate gradient squared (CGS). Because INIT is 'S', the best performance is achieved. The iteration is stopped when the norm of the residual is less than the given threshold specified in RPARAM(1). The algorithm is allowed to perform 20 iterations. The process converges after 9 iterations.

### Call Statement and Input:

```

      STOR INIT  N  AR  JA  IA  B  X  IPARM  RPARM  AUX1  NAUX1  AUX2  NAUX2
CALL DSRIS( 'G' , 'S' , 9 , AR , JA , IA , B , X , IPARM , RPARM , AUX1 , 98 , AUX2 , 63 )

```

```

AR      =(same as input AR in Example 1)
JA      =(same as input JA in Example 1)
IA      =(same as input IA in Example 1)
B       =(same as input B in Example 1)
X       =(same as input X in Example 1)
IPARM(1) = 20
IPARM(2) = 2
IPARM(3) = 0
IPARM(4) = 1

```



```

IPARM(5) = 10
RPARAM(1) = 1.D-7
RPARAM(3) = 1.0

```

**Output:**

```

X = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IPARM(6) = 9
RPARAM(2) = 0.42D-19

```

**Example 3**

This example finds the solution of the linear system  $Ax = b$  for the sparse matrix  $A$ , which is stored by rows in arrays AR, IA, and JA. The system is solved using the two-term conjugate gradient method (CG), preconditioned by incomplete LU factorization. The iteration is stopped when the norm of the residual is less than the given threshold specified in RPARAM(1). The algorithm is allowed to perform 20 iterations. The process converges after 1 iteration. Matrix  $A$  is:

$$\begin{bmatrix}
 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
 -1.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
 0.0 & -1.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 \\
 0.0 & 0.0 & -1.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 \\
 0.0 & 0.0 & 0.0 & -1.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 \\
 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 0.0 & 2.0 & 0.0 & -1.0 \\
 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 0.0 & 2.0 & 0.0 \\
 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 0.0 & 2.0
 \end{bmatrix}$$

**Call Statement Input:**

```

          STOR INIT  N  AR  JA  IA  B  X  IPARM  RPARAM  AUX1  NAUX1  AUX2  NAUX2
          |      |   |   |   |   |   |   |   |   |   |   |   |   |
CALL DSRIS( 'G' , 'I' , 9 , AR , JA , IA , B , X , IPARM , RPARAM , AUX1 , 223 , AUX2 , 36 )

```

```

AR = (2.0, -1.0, 2.0, -1.0, -1.0, 2.0, -1.0, -1.0, 2.0, -1.0,
      -1.0, 2.0, -1.0, -1.0, 2.0, -1.0, -1.0, 2.0, -1.0, -1.0,
      2.0, -1.0, 2.0)
JA = (1, 3, 2, 4, 1, 3, 5, 2, 4, 6, 3, 5, 7, 4, 6, 8, 5, 7, 9,
      6, 8, 7, 9)
IA = (1, 3, 5, 8, 11, 14, 17, 20, 22, 24)
B = (1.0, 1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0, 1.0)
X = (0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0)
IPARM(1) = 20
IPARM(2) = 1
IPARM(3) = 0
IPARM(4) = 4
IPARM(5) = 1
RPARAM(1) = 1.D-7
RPARAM(3) = 1.0

```

**Output:**

```

X = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IPARM(6) = 1
RPARAM(2) = 0.16D-15

```

**Example 4**

This example finds the solution of the linear system  $Ax = b$  for the same sparse matrix  $A$  used in Example 3. However, matrix  $A$  is stored using upper-storage-by-rows in arrays AR, IA, and JA. The system is solved using the generalized minimum residual (GMRES), restarted after 5 steps and preconditioned with SSOR splitting. The iteration is stopped when the norm of the residual is less

## DSRIS

than the given threshold specified in RPARAM(1). The algorithm is allowed to perform 20 iterations. The process converges after 12 iterations.

### Call Statement Input:

```
          STOR INIT  N  AR  JA  IA  B  X  IPARM  RPARAM  AUX1  NAUX1  AUX2  NAUX2
          |   |     |  |   |   |   |   |   |   |   |   |   |
CALL DSRIS( 'U' , 'I' , 9 , AR , JA , IA , B , X , IPARM , RPARAM , AUX1 , 219 , AUX2 , 109 )
```

```
AR      = (2.0, -1.0, 2.0, -1.0, 2.0, -1.0, 2.0, -1.0, 2.0, -1.0,
           2.0, -1.0, 2.0, -1.0, 2.0, 2.0)
JA      = (1, 3, 2, 4, 3, 5, 4, 6, 5, 7, 6, 8, 7, 9, 8, 9)
IA      = (1, 3, 5, 7, 9, 11, 13, 15, 16, 17)
B       = (1.0, 1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0, 1.0)
X       = (0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0)
IPARM(1) = 20
IPARM(2) = 3
IPARM(3) = 5
IPARM(4) = 3
IPARM(5) = 1
RPARAM(1) = 1.D-7
RPARAM(3) = 2.0
```

### Output:

```
X       = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IPARM(6) = 12
RPARAM(2) = 0.33D-7
```

## DSMCG — Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Matrix Storage Mode

### Purpose

This subroutine solves a symmetric, positive definite or negative definite linear system, using the conjugate gradient method, with or without preconditioning by an incomplete Cholesky factorization, for a sparse matrix stored in compressed-matrix storage mode. Matrix  $A$  and vectors  $x$  and  $b$  are used:

$$Ax = b$$

where  $A$ ,  $x$ , and  $b$  contain long-precision real numbers.

### Notes:

1. These subroutines are provided only for migration purposes. You get better performance and a wider choice of algorithms if you use the DSRIS subroutine.
2. If your sparse matrix is stored by rows, as defined in "Storage-by-Rows" on page 100, you should first use the utility subroutine DSRSM to convert your sparse matrix to compressed-matrix storage mode. See "DSRSM — Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode" on page 1026

### Syntax

Fortran	CALL DSMCG ( <i>m</i> , <i>nz</i> , <i>ac</i> , <i>ka</i> , <i>lda</i> , <i>b</i> , <i>x</i> , <i>iparm</i> , <i>rparm</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
C and C++	dsmcg ( <i>m</i> , <i>nz</i> , <i>ac</i> , <i>ka</i> , <i>lda</i> , <i>b</i> , <i>x</i> , <i>iparm</i> , <i>rparm</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

- m* is the order of the linear system  $Ax = b$  and the number of rows in sparse matrix  $A$ .  
Specified as: a fullword integer;  $m \geq 0$ .
- nz* is the maximum number of nonzero elements in each row of sparse matrix  $A$ .  
Specified as: a fullword integer;  $nz \geq 0$ .
- ac* is the array, referred to as AC, containing the values of the nonzero elements of the sparse matrix, stored in compressed-matrix storage mode.  
Specified as: an *lda* by (at least) *nz* array, containing long-precision real numbers.
- ka* is the array, referred to as KA, containing the column numbers of the matrix  $A$  elements stored in the corresponding positions in array AC.  
Specified as: an *lda* by (at least) *nz* array, containing fullword integers, where  $1 \leq (\text{elements of KA}) \leq m$ .
- lda* is the leading dimension of the arrays specified for *ac* and *ka*.  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq m$ .
- b* is the vector  $b$  of length *m*, containing the right-hand side of the matrix problem.

- Specified as: a one-dimensional array of (at least) length  $m$ , containing long-precision real numbers.
- $x$  is the vector  $x$  of length  $m$ , containing your initial guess of the solution of the linear system.
- Specified as: a one-dimensional array of (at least) length  $m$ , containing long-precision real numbers. The elements can have any value, and if no guess is available, the value can be zero.
- $iparm$  is an array of parameters,  $IPARM(i)$ , where:
- $IPARM(1)$  controls the number of iterations.
    - If  $IPARM(1) > 0$ ,  $IPARM(1)$  is the maximum number of iterations allowed.
    - If  $IPARM(1) = 0$ , the following default values are used:
      - $IPARM(1) = 300$
      - $IPARM(2) = 1$
      - $IPARM(3) = 0$
      - $RPARM(1) = 10^{-6}$
  - $IPARM(2)$  is the flag used to select the stopping criterion.
    - If  $IPARM(2) = 0$ , the conjugate gradient iterative procedure is stopped when:
 
$$\|r\|_2 / \|x\|_2 < \epsilon$$
 where  $r = b - Ax$  is the residual, and  $\epsilon$  is the desired relative accuracy.  $\epsilon$  is stored in  $RPARM(1)$ .
      - If  $IPARM(2) = 1$ , the conjugate gradient iterative procedure is stopped when:
 
$$\|r\|_2 / \lambda \|x\|_2 < \epsilon$$
 where  $\lambda$  is an estimate to the minimum eigenvalue of the iteration matrix.  $\lambda$  is computed adaptively by this program and, on output, is stored in  $RPARM(2)$ .
      - If  $IPARM(2) = 2$ , the conjugate gradient iterative procedure is stopped when:
 
$$\|r\|_2 / \lambda \|x\|_2 < \epsilon$$
 where  $\lambda$  is a predetermined estimate to the minimum eigenvalue of the iteration matrix. This eigenvalue estimate, on input, is stored in  $RPARM(2)$  and may be obtained by an earlier call to this subroutine with the same matrix.
  - $IPARM(3)$  is the flag that determines whether the system is to be solved using the conjugate gradient method, preconditioned by an incomplete Cholesky factorization with no fill-in.
    - If  $IPARM(3) = 0$ , the system is not preconditioned.
    - If  $IPARM(3) = 10$ , the system is preconditioned by an incomplete Cholesky factorization.
    - If  $IPARM(3) = -10$ , the system is preconditioned by an incomplete Cholesky factorization, where the factorization matrix was computed in an earlier call to this subroutine and is stored in  $aux2$ .
  - $IPARM(4)$ , see "On Return" on page 675.

Specified as: an array of (at least) length 4, containing fullword integers, where:

IPARM(1)  $\geq 0$   
 IPARM(2) = 0, 1, or 2  
 IPARM(3) = 0, 10, or -10

*rparm* is an array of parameters, RPARAM(*i*), where  $\epsilon$  is stored in RPARAM(1), and  $\lambda$  is stored in RPARAM(2).

RPARAM(1)  $> 0$ , is the relative accuracy  $\epsilon$  used in the stopping criterion.

RPARAM(2)  $> 0$ , is the estimate of the smallest eigenvalue,  $\lambda$ , of the iteration matrix. It is only used when IPARM(2) = 2.

RPARAM(3), see "On Return."

Specified as: a one-dimensional array of (at least) length 3, containing long-precision real numbers.

*aux1* has the following meaning:

If *naux1* = 0 and error 2015 is unrecoverable, *aux1* is ignored.

Otherwise, it is a storage work area used by this subroutine, which is available for use by the calling program between calls to this subroutine. Its size is specified by *naux1*.

Specified as: an area of storage, containing long-precision real numbers.

*naux1* is the size of the work area specified by *aux1*—that is, the number of elements in *aux1*.

Specified as: a fullword integer, where:

If *naux1* = 0 and error 2015 is unrecoverable, DSMCG dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, *naux1* must have at least the following value, where:

If IPARM(2) = 0 or 2, use  $naux1 \geq 3m$ .

If IPARM(2) = 1 and IPARM(1)  $\neq 0$ , use  $naux1 \geq 3m+2(IPARM(1))$ .

If IPARM(2) = 1 and IPARM(1) = 0, use  $naux1 \geq 3m+600$ .

*aux2* is a storage work area used by this subroutine. If IPARM(3) = -10, *aux2* must contain the incomplete Cholesky factorization of matrix *A*, computed in an earlier call to DSMCG. The size of *aux2* is specified by *naux2*.

Specified as: an area of storage, containing long-precision real numbers.

*naux2* is the size of the work area specified by *aux2*—that is, the number of elements in *aux2*.

Specified as: a fullword integer. When IPARM(3) = 10 or -10, *naux2* must have at least the following value:

$naux2 \geq m(nz-1)1.5+2(m+6)$ .

## On Return

*x* is the vector *x* of length *m*, containing the solution of the system

	$Ax = b$ . Returned as: a one-dimensional array of (at least) length $m$ , containing long-precision real numbers.
<i>iparm</i>	<p>is an array of parameters, <math>IPARM(i)</math>, where:</p> <p><math>IPARM(1)</math> is unchanged.</p> <p><math>IPARM(2)</math> is unchanged.</p> <p><math>IPARM(3)</math> is unchanged.</p> <p><math>IPARM(4)</math> contains the number of iterations performed by this subroutine.</p> <p>Returned as: a one-dimensional array of length 4, containing fullword integers.</p>
<i>rparm</i>	<p>is an array of parameters, <math>RPARAM(i)</math>, where:</p> <p><math>RPARAM(1)</math> is unchanged.</p> <p><math>RPARAM(2)</math> is unchanged if <math>IPARM(2) = 0</math> or <math>2</math>. If <math>IPARM(2) = 1</math>, <math>RPARAM(2)</math> contains <math>\lambda</math>, an estimate of the smallest eigenvalue of the iteration matrix.</p> <p><math>RPARAM(3)</math> contains the estimate of the error of the solution. If the process converged, <math>RPARAM(3) \leq \epsilon</math>.</p> <p>Returned as: a one-dimensional array of length 3, containing long-precision real numbers; <math>\lambda &gt; 0</math>.</p>
<i>aux2</i>	<p>is the storage work area used by this subroutine.</p> <p>If <math>IPARM(3) = 10</math>, <i>aux2</i> contains the incomplete Cholesky factorization of matrix <math>A</math>.</p> <p>If <math>IPARM(3) = -10</math>, <i>aux2</i> is unchanged.</p> <p>See "Notes" for additional information on <i>aux2</i>. Returned as: an area of storage, containing long-precision real numbers.</p>

## Notes

1. When  $IPARM(3) = -10$ , this subroutine uses the incomplete Cholesky factorization in *aux2*, computed in an earlier call to this subroutine. When  $IPARM(3) = 10$ , this subroutine computes the incomplete Cholesky factorization and stores it in *aux2*.
2. If you solve the same sparse linear system of equations several times with different right-hand sides using the preconditioned algorithm, specify  $IPARM(3) = 10$  on the first invocation. The incomplete factorization is stored in *aux2*. You may save computing time on subsequent calls by setting  $IPARM(3) = -10$ . In this way, the algorithm reutilizes the incomplete factorization that was computed the first time. Therefore, you should not modify the contents of *aux2* between calls.
3. Matrix  $A$  must have no common elements with vectors  $x$  and  $b$ ; otherwise, results are unpredictable.
4. In the iterative solvers for sparse matrices, the relative accuracy  $\epsilon$  ( $RPARAM(1)$ ) must be specified "reasonably" ( $10^{-4}$  to  $10^{-8}$ ). The algorithm computes a sequence of approximate solution vectors  $x$  that converge to the solution. The iterative procedure is stopped when the norm of the residual is sufficiently small—that is, when:

$$\|b - Ax\|_2 / \lambda \|x\|_2 < \epsilon$$

where  $\lambda$  is an estimate of the minimum eigenvalue of the iteration matrix, which is either estimated adaptively or given by the user. As a result, if you specify a larger  $\epsilon$ , the algorithm takes fewer iterations to converge to a solution. If you specify a smaller  $\epsilon$ , the algorithm requires more iterations and computer time, but converges to a more precise solution. If the value you specify is unreasonably small, the algorithm may fail to converge within the number of iterations it is allowed to perform.

5. For a description of how sparse matrices are stored in compressed-matrix storage mode, see “Compressed-Matrix Storage Mode” on page 95.
6. On output, array  $AC$  and vector  $b$  are not bitwise identical to what they were on input, because the matrix  $A$  and the right-hand side are scaled before starting the iterative process and are unscaled before returning control to the user. In addition, arrays  $AC$  and  $KA$  may be rearranged on output, but still contain a mathematically equivalent mapping of the elements in matrix  $A$ .
7. You have the option of having the minimum required value for  $naux$  dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## Function

The sparse positive definite or negative definite linear system:

$$Ax = b$$

is solved, where:

$A$  is a symmetric, positive definite or negative definite sparse matrix of order  $m$ , stored in compressed-matrix storage mode in  $AC$  and  $KA$ .

$x$  is a vector of length  $m$ .

$b$  is a vector of length  $m$ .

The system is solved using the two-term conjugate gradient method, with or without preconditioning by an incomplete Cholesky factorization. In both cases, the matrix is scaled by the square root of the diagonal.

See references [64] and [71]. [38].

If your program uses a sparse matrix stored by rows and you want to use this subroutine, first convert your sparse matrix to compressed-matrix storage mode by using the subroutine  $DSRSM$  described on page 1026.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux1 = 0$ , and unable to allocate work area.

### Computational Errors

The following errors, with their corresponding return codes, can occur in this subroutine. Where a value of  $i$  is indicated, it can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use  $ERRSET$  to change the number of allowable errors for that particular error code in the ESSL error option table; otherwise, the default value causes your program to terminate when the error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

- For error 2110, return code 1 indicates that the subroutine exceeded IPARM(1) iterations without converging. Vector  $x$  contains the approximate solution computed at the last iteration.
- For error 2111, return code 2 indicates that  $aux2$  contains an incorrect factorization. The subroutine has been called with IPARM(3) = -10, and  $aux2$  contains an incomplete factorization of the input matrix  $A$  that was computed by a previous call to the subroutine when IPARM(3) = 10. This error indicates that  $aux2$  has been modified since the last call to the subroutine, or that the input matrix is not the same as the one that was factored. If the default action has been overridden, the subroutine can be called again with the same parameters, with the exception of IPARM(3) = 0 or 10.
- For error 2109, return code 3 indicates that the inner product  $(y, Ay)$  is negative in the iterative procedure after iteration  $i$ . This should not occur, because the input matrix is assumed to be positive or negative definite. Vector  $x$  contains the results of the last iteration. The value  $i$  is identified in the computational error message.
- For error 2108, return code 4 indicates that the matrix is not positive definite. AC is partially modified and does not represent the same matrix as on entry.

### Input-Argument Errors

1.  $m < 0$
2.  $lda < 1$
3.  $lda < m$
4.  $nz < 0$
5.  $nz = 0$  and  $m > 0$
6. IPARM(1) < 0
7. IPARM(2)  $\neq$  0, 1, or 2
8. IPARM(3)  $\neq$  0, 10, or -10
9. RPARAM(1) < 0
10. RPARAM(2) < 0
11. Error 2015 is recoverable or  $naux1 \neq 0$ , and  $naux1$  is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.
12.  $naux2$  is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example finds the solution of the linear system  $Ax = b$  for the sparse matrix  $A$ , which is stored in compressed-matrix storage mode in arrays AC and KA. The system is solved using the conjugate gradient method. Matrix  $A$  is:

$$\begin{bmatrix} 2.0 & 0.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & -1.0 & 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ -1.0 & 0.0 & 0.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & -1.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 2.0 & -1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 2.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 2.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 2.0 \end{bmatrix}$$

**Note:** For input matrix KA, ( . ) indicates any value between 1 and 9.

### Call Statement and Input:



```

          M  NZ  AC  KA  LDA  B  X  IPARM  RPARM  AUX1  NAUX1  AUX2  NAUX2
CALL DSMCG( 9 , 3 , AC, KA, 9 , B , X, IPARM, RPARM, AUX1, 27 , AUX2, 0 )
IPARM(1) = 20
IPARM(2) = 0
IPARM(3) = 0
RPARM(1) = 1.D-7

```

$$AC = \begin{bmatrix} 2.0 & -1.0 & 0.0 \\ 2.0 & -1.0 & 0.0 \\ -1.0 & 2.0 & 0.0 \\ -1.0 & 2.0 & -1.0 \\ -1.0 & 2.0 & -1.0 \\ -1.0 & 2.0 & -1.0 \\ -1.0 & 2.0 & -1.0 \\ -1.0 & 2.0 & -1.0 \\ -1.0 & 2.0 & 0.0 \end{bmatrix}$$

$$KA = \begin{bmatrix} 1 & 4 & . \\ 2 & 3 & . \\ 2 & 3 & . \\ 1 & 4 & 5 \\ 4 & 5 & 6 \\ 5 & 6 & 7 \\ 6 & 7 & 8 \\ 7 & 8 & 9 \\ 8 & 9 & . \end{bmatrix}$$

```

B      = (1.0, 1.0, 1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0)
X      = (0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0)

```

**Output:**

```

X      = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IPARM(4) = 5
RPARM(2) = 0
RPARM(3) = 0.351D-15

```

**Example 2**

This example finds the solution of the linear system  $Ax = b$  for the same sparse matrix  $A$  as in Example 1, which is stored in compressed-matrix storage mode in arrays AC and KA. The system is solved using the conjugate gradient method, preconditioned with an incomplete Cholesky factorization. The smallest eigenvalue of the iteration matrix is computed and used in stopping the computation.

**Note:** For input matrix KA, ( . ) indicates any value between 1 and 9.

**Call Statement and Input:**

```

          M  NZ  AC  KA  LDA  B  X  IPARM  RPARM  AUX1  NAUX1  AUX2  NAUX2
CALL DSMCG( 9 , 3 , AC, KA, 9 , B , X, IPARM, RPARM, AUX1, 67 , AUX2, 74 )

IPARM(1) = 20
IPARM(2) = 1
IPARM(3) = 10
RPARM(1) = 1.D-7
AC      =(same as input AC in Example 1)
KA      =(same as input KA in Example 1)
B      = (1.0, 1.0, 1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0)
X      = (0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0)

```

## DSMCG

### Output:

```
X          = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IPARM(4) = 1
RPARAM(2) = 1
RPARAM(3) = 0.100D-15
```

## DSDCG — Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Diagonal Storage Mode

### Purpose

This subroutine solves a symmetric, positive definite or negative definite linear system, using the two-term conjugate gradient method, with or without preconditioning by an incomplete Cholesky factorization, for a sparse matrix stored in compressed-diagonal storage mode. Matrix  $A$  and vectors  $x$  and  $b$  are used:

$$Ax = b$$

where  $A$ ,  $x$ , and  $b$  contain long-precision real numbers.

### Syntax

Fortran	CALL DSDCG ( <i>iopt</i> , <i>m</i> , <i>nd</i> , <i>ad</i> , <i>lda</i> , <i>la</i> , <i>b</i> , <i>x</i> , <i>iparm</i> , <i>rparm</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
C and C++	<code>dsdcg</code> ( <i>iopt</i> , <i>m</i> , <i>nd</i> , <i>ad</i> , <i>lda</i> , <i>la</i> , <i>b</i> , <i>x</i> , <i>iparm</i> , <i>rparm</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

- iopt* indicates the type of storage used, where:
- If *iopt* = 0, all the nonzero diagonals of the sparse matrix are stored in compressed-diagonal storage mode.
- If *iopt* = 1, the sparse matrix, stored in compressed-diagonal storage mode, is symmetric. Only the main diagonal and one of each pair of identical diagonals are stored in array AD.
- Specified as: a fullword integer; *iopt* = 0 or 1.
- m* is the order of the linear system  $Ax = b$  and the number of rows in sparse matrix  $A$ .
- Specified as: a fullword integer;  $m \geq 0$ .
- nd* is the number of nonzero diagonals stored in the columns of array AD, the number of columns in the array AD, and the number of elements in array LA.
- Specified as: a fullword integer; it must have the following value, where:
- If  $m > 0$ , then  $nd > 0$ .
- If  $m = 0$ , then  $nd \geq 0$ .
- ad* is the array, referred to as AD, containing the values of the nonzero elements of the sparse matrix stored in compressed-diagonal storage mode. If *iopt* = 1, the main diagonal and one of each pair of identical diagonals is stored in this array.
- Specified as: an *lda* by (at least) *nd* array, containing long-precision real numbers.
- lda* is the leading dimension of the array specified for *ad*.
- Specified as: a fullword integer;  $lda > 0$  and  $lda \geq m$ .
- la* is the array, referred to as LA, containing the diagonal numbers  $k$  for the diagonals stored in each corresponding column in array AD.

For an explanation of how diagonal numbers are assigned, see “Compressed-Diagonal Storage Mode” on page 96.

Specified as: a one-dimensional array of (at least) length  $nd$ , containing fullword integers, where  $1-m \leq$  (elements of LA)  $\leq m-1$ .

*b* is the vector **b** of length  $m$ , containing the right-hand side of the matrix problem.

Specified as: a one-dimensional array of (at least) length  $m$ , containing long-precision real numbers.

*x* is the vector **x** of length  $m$ , containing your initial guess of the solution of the linear system.

Specified as: a one-dimensional array of (at least) length  $m$ , containing long-precision real numbers. The elements can have any value, and if no guess is available, the value can be zero.

*iparm* is an array of parameters,  $IPARM(i)$ , where:

- $IPARM(1)$  controls the number of iterations.  
If  $IPARM(1) > 0$ ,  $IPARM(1)$  is the maximum number of iterations allowed.

If  $IPARM(1) = 0$ , the following default values are used:

$IPARM(1) = 300$   
 $IPARM(2) = 1$   
 $IPARM(3) = 0$   
 $RPARAM(1) = 10^{-6}$

- $IPARM(2)$  is the flag used to select the stopping criterion.  
If  $IPARM(2) = 0$ , the conjugate gradient iterative procedure is stopped when:

$$\|r\|_2 / \|x\|_2 < \epsilon$$

where  $r = b - Ax$  is the residual and  $\epsilon$  is the desired relative accuracy.  $\epsilon$  is stored in  $RPARAM(1)$ .

If  $IPARM(2) = 1$ , the conjugate gradient iterative procedure is stopped when:

$$\|r\|_2 / \lambda \|x\|_2 < \epsilon$$

where  $\lambda$  is an estimate to the minimum eigenvalue of the iteration matrix.  $\lambda$  is computed adaptively by this program and, on output, is stored in  $RPARAM(2)$ .

If  $IPARM(2) = 2$ , the conjugate gradient iterative procedure is stopped when:

$$\|r\|_2 / \lambda \|x\|_2 < \epsilon$$

where  $\lambda$  is a predetermined estimate to the minimum eigenvalue of the iteration matrix. This eigenvalue estimate, on input, is stored in  $RPARAM(2)$  and may be obtained by an earlier call to this subroutine with the same matrix.

- $IPARM(3)$  is the flag that determines whether the system is to be solved using the conjugate gradient method, preconditioned by an incomplete Cholesky factorization with no fill-in.

If  $IPARM(3) = 0$ , the system is not preconditioned.

If  $IPARM(3) = 10$ , the system is preconditioned by an incomplete Cholesky factorization.

If  $IPARM(3) = -10$ , the system is preconditioned by an incomplete Cholesky factorization, where the factorization matrix was computed in an earlier call to this subroutine and is stored in *aux2*.

- $IPARM(4)$ , see “On Return” on page 684.

Specified as: an array of (at least) length 4, containing fullword integers, where:

$IPARM(1) = 0$   
 $IPARM(2) = 0, 1, \text{ or } 2$   
 $IPARM(3) = 0, 10, \text{ or } -10$

*rparm* is an array of parameters,  $RPARM(i)$ , where  $\epsilon$  is stored in  $RPARM(1)$ , and  $\lambda$  is stored in  $RPARM(2)$ .

$RPARM(1) > 0$ , is the relative accuracy  $\epsilon$  used in the stopping criterion.

$RPARM(2) > 0$ , is the estimate of the smallest eigenvalue,  $\lambda$ , of the iteration matrix. It is only used when  $IPARM(2) = 2$ .

$RPARM(3)$ , see “On Return” on page 684.

Specified as: a one-dimensional array of (at least) length 3, containing long-precision real numbers.

*aux1* has the following meaning:

If  $naux1 = 0$  and error 2015 is unrecoverable, *aux1* is ignored.

Otherwise, it is a storage work area used by this subroutine, which is available for use by the calling program between calls to this subroutine. Its size is specified by *naux1*.

Specified as: an area of storage, containing long-precision real numbers.

*naux1* is the size of the work area specified by *aux1*—that is, the number of elements in *aux1*.

Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, DSDCG dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, it must have at least the following value, where:

If  $IPARM(2) = 0$  or  $2$ , use  $naux1 \geq 3m$ .

If  $IPARM(2) = 1$  and  $IPARM(1) \neq 0$ , use  $naux1 \geq 3m+2(IPARM(1))$ .

If  $IPARM(2) = 1$  and  $IPARM(1) = 0$ , use  $naux1 \geq 3m+600$ .

*aux2* is the storage work area used by this subroutine. If  $IPARM(3) = -10$ , *aux2* must contain the incomplete Cholesky factorization of matrix  $A$ , computed in an earlier call to DSDCG. Its size is specified by *naux2*.

Specified as: an area of storage, containing long-precision real numbers.

*naux2* is the size of the work area specified by *aux2*—that is, the number of elements in *aux2*.

Specified as: a fullword integer. When  $\text{IPARM}(3) = 10$  or  $-10$ , *naux2* must have at least the following value, where:

If  $\text{iopt} = 0$ , use  $\text{naux2} \geq m(1.5nd+2)1.5+2(m+6)$ .

If  $\text{iopt} = 1$ , use  $\text{naux2} \geq m(3nd+2)+8$ .

### On Return

*x* is the vector  $x$  of length  $m$ , containing the solution of the system  $Ax = b$ . Returned as: a one-dimensional array, containing long-precision real numbers.

*iparm* As an array of parameters,  $\text{IPARM}(i)$ , where:

$\text{IPARM}(1)$  is unchanged.

$\text{IPARM}(2)$  is unchanged.

$\text{IPARM}(3)$  is unchanged.

$\text{IPARM}(4)$  contains the number of iterations performed by this subroutine.

Returned as: a one-dimensional array of length 4, containing fullword integers.

*rparm* is an array of parameters,  $\text{RPARAM}(i)$ , where:

$\text{RPARAM}(1)$  is unchanged.

$\text{RPARAM}(2)$  is unchanged if  $\text{IPARM}(2) = 0$  or  $2$ . If  $\text{IPARM}(2) = 1$ ,  $\text{RPARAM}(2)$  contains  $\lambda$ , an estimate of the smallest eigenvalue of the iteration matrix.

$\text{RPARAM}(3)$  contains the estimate of the error of the solution. If the process converged,  $\text{RPARAM}(3) \leq \epsilon$ .

Returned as: a one-dimensional array of length 3, containing long-precision real numbers;  $\lambda > 0$ .

*aux2* is the storage work area used by this subroutine.

If  $\text{IPARM}(3) = 10$ , *aux2* contains the incomplete Cholesky factorization of matrix  $A$ .

If  $\text{IPARM}(3) = -10$ , *aux2* is unchanged.

See “Notes” for additional information on *aux2*. Returned as: an area of storage, containing long-precision real numbers.

### Notes

1. When  $\text{IPARM}(3) = -10$ , this subroutine uses the incomplete Cholesky factorization in *aux2*, computed in an earlier call to this subroutine. When  $\text{IPARM}(3) = 10$ , this subroutine computes the incomplete Cholesky factorization and stores it in *aux2*.
2. If you solve the same sparse linear system of equations several times with different right-hand sides using the preconditioned algorithm, specify  $\text{IPARM}(3) = 10$  on the first invocation. The incomplete factorization is stored in *aux2*. You may save computing time on subsequent calls by setting  $\text{IPARM}(3) = -10$ . In this way, the algorithm reutilizes the incomplete

factorization that was computed the first time. Therefore, you should not modify the contents of *aux2* between calls.

3. Matrix *A* must have no common elements with vectors *x* and *b*; otherwise, results are unpredictable.
4. In the iterative solvers for sparse matrices, the relative accuracy  $\epsilon$  (RPARM(1)) must be specified “reasonably” ( $10^{-4}$  to  $10^{-8}$ ). The algorithm computes a sequence of approximate solution vectors *x* that converge to the solution. The iterative procedure is stopped when the norm of the residual is sufficiently small—that is, when:

$$\|b - Ax\|_2 / \lambda \|x\|_2 < \epsilon$$

where  $\lambda$  is an estimate of the minimum eigenvalue of the iteration matrix, which is either estimated adaptively or given by the user. As a result, if you specify a larger  $\epsilon$ , the algorithm takes fewer iterations to converge to a solution. If you specify a smaller  $\epsilon$ , the algorithm requires more iterations and computer time, but converges to a more precise solution. If the value you specify is unreasonably small, the algorithm may fail to converge within the number of iterations it is allowed to perform.

5. For a description of how sparse matrices are stored in compressed-matrix storage mode, see “Compressed-Matrix Storage Mode” on page 95.
6. On output, array *AD* and vector *b* are not bitwise identical to what they were on input, because the matrix *A* and the right-hand side are scaled before starting the iterative process and are unscaled before returning control to the user. In addition, arrays *AD* and *LA* may be rearranged on output, but still contain a mathematically equivalent mapping of the elements in matrix *A*.
7. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## Function

The sparse positive definite or negative definite linear system:

$$Ax = b$$

is solved, where:

*A* is a symmetric, positive definite or negative definite sparse matrix of order *m*, stored in compressed-diagonal storage mode in arrays *AD* and *LA*.

*x* is a vector of length *m*.

*b* is a vector of length *m*.

The system is solved using the two-term conjugate gradient method, with or without preconditioning by an incomplete Cholesky factorization. In both cases, the matrix is scaled by the square root of the diagonal.

See references [64] and [71]. [38].

## Error conditions

### Resource Errors

Error 2015 is unrecoverable, *naux1* = 0, and unable to allocate work area.

## Computational Errors

The following errors, with their corresponding return codes, can occur in this subroutine. Where a value of  $i$  is indicated, it can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for that particular error code in the ESSL error option table; otherwise, the default value causes your program to terminate when the error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

- For error 2110, return code 1 indicates that the subroutine exceeded IPARM(1) iterations without converging. Vector  $x$  contains the approximate solution computed at the last iteration.
- For error 2111, return code 2 indicates that  $aux2$  contains an incorrect factorization. The subroutine has been called with IPARM(3) = -10, and  $aux2$  contains an incomplete factorization of the input matrix  $A$  that was computed by a previous call to the subroutine when IPARM(3) = 10. This error indicates that  $aux2$  has been modified since the last call to the subroutine, or that the input matrix is not the same as the one that was factored. If the default action has been overridden, the subroutine can be called again with the same parameters, with the exception of IPARM(3) = 0 or 10.
- For error 2109, return code 3 indicates that the inner product  $(y, Ay)$  is negative in the iterative procedure after iteration  $i$ . This should not occur, because the input matrix is assumed to be positive or negative definite. Vector  $x$  contains the results of the last iteration. The value  $i$  is identified in the computational error message.
- For error 2108, return code 4 indicates that the matrix is not positive definite. AC is partially modified and does not represent the same matrix as on entry.

## Input-Argument Errors

1.  $iopt \neq 0$  or 1
2.  $m < 0$
3.  $lda < 1$
4.  $lda < m$
5.  $nd < 0$
6.  $nd = 0$  and  $m > 0$
7.  $|\lambda(i)| > m-1$  for  $i = 1, nd$
8. IPARM(1) < 0
9. IPARM(2)  $\neq 0, 1,$  or 2
10. IPARM(3)  $\neq 0, 10,$  or -10
11. RPARAM(1) < 0
12. RPARAM(2) < 0
13. Error 2015 is recoverable or  $naux1 \neq 0$ , and  $naux1$  is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.
14.  $naux2$  is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example finds the solution of the linear system  $Ax = b$  for sparse matrix  $A$ , which is stored in compressed-diagonal storage mode in arrays AD and LA. The system is solved using the two-term conjugate gradient method. In this example, IOPT = 0.. Matrix  $A$  is:

$$\begin{bmatrix} 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{bmatrix}$$



$$\begin{bmatrix} -1.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & -1.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & -1.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & -1.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 0.0 & 2.0 & 0.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 0.0 & 2.0 \end{bmatrix}$$

**Call Statement and Input:**

```

      IOPT  M   ND  AD  LDA  LA  B  X  IPARM  RPARM  AUX1  NAUX1  AUX2  NAUX2
CALL DSDCG( 0 , 9 , 3 , AD , 9 , LA , B , X , IPARM , RPARM , AUX1 , 283 , AUX2 , 0 )

```

```

IPARM(1) = 20
IPARM(2) = 0
IPARM(3) = 0
RPARM(1) = 1.D-7

```

$$AD = \begin{bmatrix} 2.0 & 0.0 & -1.0 \\ 2.0 & 0.0 & -1.0 \\ 2.0 & -1.0 & -1.0 \\ 2.0 & -1.0 & -1.0 \\ 2.0 & -1.0 & -1.0 \\ 2.0 & -1.0 & -1.0 \\ 2.0 & -1.0 & -1.0 \\ 2.0 & -1.0 & 0.0 \\ 2.0 & -1.0 & 0.0 \end{bmatrix}$$

```

LA = (0, -2, 2)
B = (1.0, 1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0, 1.0)
X = (0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0)

```

**Output:**

```

X = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IPARM(4) = 5
RPARM(2) = 0
RPARM(3) = 0.46D-16

```

**Example 2**

This example finds the solution of the linear system  $Ax = b$  for the same sparse matrix  $A$  as in Example 1, which is stored in compressed-diagonal storage mode in arrays AD and LA. The system is solved using the two-term conjugate gradient method. In this example,  $IOPT = 1$ , indicating that the matrix is symmetric, and only the main diagonal and one of each pair of identical diagonals are stored in array AD.

**Call Statement and Input:**

```

      IOPT  M   ND  AD  LDA  LA  B  X  IPARM  RPARM  AUX1  NAUX1  AUX2  NAUX2
CALL DSDCG( 1 , 9 , 2 , AD , 9 , LA , B , X , IPARM , RPARM , AUX1 , 283 , AUX2 , 80 )

```

```

IPARM(1) = 20
IPARM(2) = 0
IPARM(3) = 10
RPARM(1) = 1.D-7

```

$$\begin{bmatrix} 2.0 & 0.0 \\ 2.0 & 0.0 \\ 2.0 & -1.0 \end{bmatrix}$$

## DSDCG

$$AD = \begin{bmatrix} 2.0 & -1.0 \\ 2.0 & -1.0 \\ 2.0 & -1.0 \\ 2.0 & -1.0 \\ 2.0 & -1.0 \\ 2.0 & -1.0 \end{bmatrix}$$

$$\begin{aligned} LA &= (0, -2) \\ B &= (1.0, 1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0, 1.0) \\ X &= (0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0) \end{aligned}$$

### Output:

$$\begin{aligned} X &= (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0) \\ IPARM(4) &= 1 \\ RPARAM(2) &= 0 \\ RPARAM(3) &= 0.89D-16 \end{aligned}$$

## DSMGCG — General Sparse Matrix Iterative Solve Using Compressed-Matrix Storage Mode

### Purpose

This subroutine solves a general sparse linear system of equations using an iterative algorithm, conjugate gradient squared or generalized minimum residual, with or without preconditioning by an incomplete LU factorization. The subroutine is suitable for positive real matrices—that is, when the symmetric part of the matrix,  $(A+A^T)/2$ , is positive definite. The sparse matrix is stored in compressed-matrix storage mode. Matrix  $A$  and vectors  $x$  and  $b$  are used:

$$Ax = b$$

where  $A$ ,  $x$ , and  $b$  contain long-precision real numbers.

#### Notes:

1. These subroutines are provided only for migration purposes. You get better performance and a wider choice of algorithms if you use the DSRIS subroutine.
2. If your sparse matrix is stored by rows, as defined in “Storage-by-Rows” on page 100, you should first use the utility subroutine DSRSM to convert your sparse matrix to compressed-matrix storage mode. See “DSRSM — Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode” on page 1026.

### Syntax

Fortran	CALL DSMGCG ( <i>m</i> , <i>nz</i> , <i>ac</i> , <i>ka</i> , <i>lda</i> , <i>b</i> , <i>x</i> , <i>iparm</i> , <i>rparm</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
C and C++	dsmgcg ( <i>m</i> , <i>nz</i> , <i>ac</i> , <i>ka</i> , <i>lda</i> , <i>b</i> , <i>x</i> , <i>iparm</i> , <i>rparm</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

- m* is the order of the linear system  $Ax = b$  and the number of rows in sparse matrix  $A$ .  
Specified as: a fullword integer;  $m \geq 0$ .
- nz* is the maximum number of nonzero elements in each row of sparse matrix  $A$ .  
Specified as: a fullword integer;  $nz \geq 0$ .
- ac* is the array, referred to as AC, containing the values of the nonzero elements of the sparse matrix, stored in compressed-matrix storage mode.  
Specified as: an *lda* by (at least) *nz* array, containing long-precision real numbers.
- ka* is the array, referred to as KA, containing the column numbers of the matrix  $A$  elements stored in the corresponding positions in array AC.  
Specified as: an *lda* by (at least) *nz* array, containing fullword integers, where  $1 \leq (\text{elements of KA}) \leq m$ .
- lda* is the leading dimension of the arrays specified for *ac* and *ka*.  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq m$ .

- b* is the vector **b** of length *m*, containing the right-hand side of the matrix problem.  
Specified as: a one-dimensional array of (at least) length *m*, containing long-precision real numbers.
- x* is the vector **x** of length *m*, containing your initial guess of the solution of the linear system.  
Specified as: a one-dimensional array of (at least) length *m*, containing long-precision real numbers. The elements can have any value, and if no guess is available, the value can be zero.
- iparm* is an array of parameters, *IPARM*(*i*), where:
- *IPARM*(1) controls the number of iterations.  
If *IPARM*(1) > 0, *IPARM*(1) is the maximum number of iterations allowed.  
If *IPARM*(1) = 0, the following default values are used:  
  

$$\begin{aligned} \text{IPARM}(1) &= 300 \\ \text{IPARM}(2) &= 0 \\ \text{IPARM}(3) &= 10 \\ \text{RPARAM}(1) &= 10^{-6} \end{aligned}$$
  - *IPARM*(2) is the flag used to select the iterative procedure used in this subroutine.  
If *IPARM*(2) = 0, the conjugate gradient squared method is used.  
If *IPARM*(2) = *k*, the generalized minimum residual method, restarted after *k* steps, is used. Note that the size of the work area *aux1* becomes larger as *k* increases. A value for *k* in the range of 5 to 10 is suitable for most problems.
  - *IPARM*(3) is the flag that determines whether the system is to be preconditioned by an incomplete LU factorization with no fill-in.  
If *IPARM*(3) = 0, the system is not preconditioned.  
If *IPARM*(3) = 10, the system is preconditioned by an incomplete LU factorization.  
If *IPARM*(3) = -10, the system is preconditioned by an incomplete LU factorization, where the factorization matrix was computed in an earlier call to this subroutine and is stored in *aux2*.
  - *IPARM*(4), see "On Return" on page 691.
- Specified as: an array of (at least) length 4, containing fullword integers, where:
- $$\begin{aligned} \text{IPARM}(1) &\geq 0 \\ \text{IPARM}(2) &\geq 0 \\ \text{IPARM}(3) &= 0, 10, \text{ or } -10 \end{aligned}$$
- rparm* is an array of parameters, *RPARAM*(*i*), where:
- RPARAM*(1) > 0, is the relative accuracy  $\epsilon$  used in the stopping criterion. The iterative procedure is stopped when:
- $$\|\mathbf{b} - \mathbf{Ax}\|_2 / \|\mathbf{x}\|_2 < \epsilon$$
- RPARAM*(2) is reserved.

RPARAM(3), see “On Return.”

Specified as: a one-dimensional array of (at least) length 3, containing long-precision real numbers.

*aux1*

has the following meaning:

If  $naux1 = 0$  and error 2015 is unrecoverable, *aux1* is ignored.

Otherwise, it is a storage work area used by this subroutine, which is available for use by the calling program between calls to this subroutine. Its size is specified by *naux1*.

Specified as: an area of storage, containing long-precision real numbers.

*naux1*

is the size of the work area specified by *aux1*—that is, the number of elements in *aux1*.

Specified as: a fullword integer, where:

If  $naux1 = 0$  and error 2015 is unrecoverable, DSMGCG dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, it must have at least the following value, where:

If  $IPARM(2) = 0$ , use  $naux1 \geq 7m$ .

If  $IPARM(2) > 0$ , use  $naux1 \geq (k+2)m+k(k+4)+1$ , where  $k = IPARM(2)$ .

*aux2*

is the storage work area used by this subroutine. If  $IPARM(3) = -10$ , *aux2* must contain the incomplete LU factorization of matrix *A*, computed in an earlier call to DSMGCG. The size of *aux2* is specified by *naux2*.

Specified as: an area of storage, containing long-precision real numbers.

*naux2*

is the size of the work area specified by *aux2*—that is, the number of elements in *aux2*.

Specified as: a fullword integer. When  $IPARM(3) = 10$ , *naux2* must have at least the following value:  $naux2 \geq 3+2m+1.5nz(m)$ .

## On Return

*x*

is the vector *x* of length *m*, containing the solution of the system  $Ax = b$ . Returned as: a one-dimensional array of (at least) length *m*, containing long-precision real numbers.

*iparm*

is an array of parameters,  $IPARM(i)$ , where:

$IPARM(1)$  is unchanged.

$IPARM(2)$  is unchanged.

$IPARM(3)$  is unchanged.

$IPARM(4)$  contains the number of iterations performed by this subroutine.

Returned as: a one-dimensional array of length 4, containing fullword integers.

*rparm*

is an array of parameters,  $RPARAM(i)$ , where:

RPARAM(1) is unchanged.

RPARAM(2) is reserved.

RPARAM(3) contains the estimate of the error of the solution. If the process converged,  $RPARAM(3) \leq RPARAM(1)$

Returned as: a one-dimensional array of length 3, containing long-precision real numbers.

*aux2*

is the storage work area used by this subroutine.

If  $IPARM(3) = 10$ , *aux2* contains the incomplete LU factorization of matrix *A*.

If  $IPARM(3) = -10$ , *aux2* is unchanged.

See "Notes" for additional information on *aux2*. Returned as: an area of storage, containing long-precision real numbers.

## Notes

1. When  $IPARM(3) = -10$ , this subroutine uses the incomplete LU factorization in *aux2*, computed in an earlier call to this subroutine. When  $IPARM(3) = 10$ , this subroutine computes the incomplete LU factorization and stores it in *aux2*.
2. If you solve the same sparse linear system of equations several times with different right-hand sides using the preconditioned algorithm, specify  $IPARM(2) = 10$  on the first invocation. The incomplete factorization is stored in *aux2*. You may save computing time on subsequent calls by setting  $IPARM(3)$  equal to  $-10$ . In this way, the algorithm reutilizes the incomplete factorization that was computed the first time. Therefore, you should not modify the contents of *aux2* between calls.
3. Matrix *A* must have no common elements with vectors *x* and *b*; otherwise, results are unpredictable.
4. In the iterative solvers for sparse matrices, the relative accuracy  $\epsilon$  ( $RPARAM(1)$ ) must be specified "reasonably" ( $10^{-4}$  to  $10^{-8}$ ). The algorithm computes a sequence of approximate solution vectors *x* that converge to the solution. The iterative procedure is stopped when the norm of the residual is sufficiently small—that is, when:

$$\|b - Ax\|_2 / \|x\|_2 < \epsilon$$

As a result, if you specify a larger  $\epsilon$ , the algorithm takes fewer iterations to converge to a solution. If you specify a smaller  $\epsilon$ , the algorithm requires more iterations and computer time, but converges to a more precise solution. If the value you specify is unreasonably small, the algorithm may fail to converge within the number of iterations it is allowed to perform.

5. For a description of how sparse matrices are stored in compressed-matrix storage mode, see "Compressed-Matrix Storage Mode" on page 95.
6. On output, array *AC* is not bitwise identical to what it was on input because the matrix *A* is scaled before starting the iterative process and is unscaled before returning control to the user.
7. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

## Function

The linear system:

$$Ax = b$$

is solved using either the conjugate gradient squared method or the generalized minimum residual method, with or without preconditioning by an incomplete LU factorization, where:

$A$  is a sparse matrix of order  $m$ , stored in compressed-matrix storage mode in arrays AC and KA.

$x$  is a vector of length  $m$ .

$b$  is a vector of length  $m$ .

See references [90] and [92]. [38].

If your program uses a sparse matrix stored by rows and you want to use this subroutine, first convert your sparse matrix to compressed-matrix storage mode by using the subroutine DSRSM described on page 1026.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux1 = 0$ , and unable to allocate work area.

### Computational Errors

The following errors, with their corresponding return codes, can occur in this subroutine. For details on error handling, see “What Can You Do about ESSL Computational Errors?” on page 51.

- For error 2110, return code 1 indicates that the subroutine exceeded IPARM(1) iterations without converging. Vector  $x$  contains the approximate solution computed at the last iteration.
- For error 2111, return code 2 indicates that  $aux2$  contains an incorrect factorization. The subroutine has been called with IPARM(3) = -10, and  $aux2$  contains an incomplete factorization of the input matrix  $A$  that was computed by a previous call to the subroutine when IPARM(3) = 10. This error indicates that  $aux2$  has been modified since the last call to the subroutine, or that the input matrix is not the same as the one that was factored. If the default action has been overridden, the subroutine can be called again with the same parameters, with the exception of IPARM(3) = 0 or 10.
- For error 2112, return code 3 indicates that the incomplete LU factorization of  $A$  could not be completed, because one pivot was 0.
- For error 2116, return code 4 indicates that the matrix is singular, because all elements in one row of the matrix contain 0. Array AC is partially modified and does not represent the same matrix as on entry.

### Input-Argument Errors

1.  $m < 0$
2.  $lda < 1$
3.  $lda < m$
4.  $nz < 0$
5.  $nz = 0$  and  $m > 0$

## DSMGCG

6. IPARM(1) < 0
7. IPARM(2) < 0
8. IPARM(3) ≠ 0, 10, or -10
9. RPARAM(1) < 0
10. RPARAM(2) < 0
11. Error 2015 is recoverable or *naux1* ≠ 0, and *naux1* is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.
12. *naux2* is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example finds the solution of the linear system  $Ax = b$  for the sparse matrix  $A$ , which is stored in compressed-matrix storage mode in arrays AC and KA. The system is solved using the conjugate gradient squared method. Matrix  $A$  is:

$$\begin{bmatrix} 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 \end{bmatrix}$$

**Note:** For input matrix KA, ( . ) indicates any value between 1 and 9.

### Call Statement and Input:

```
CALL DSMGCG( M , NZ , AC , KA , LDA , B , X , IPARM , RPARAM , AUX1 , NAUX1 , AUX2 , NAUX2 )
```

```
IPARM(1) = 20
IPARM(2) = 0
IPARM(3) = 0
RPARAM(1) = 1.D-7
```

$$AC = \begin{bmatrix} 2.0 & 0.0 & 0.0 \\ 2.0 & -1.0 & 0.0 \\ 1.0 & 2.0 & 0.0 \\ 1.0 & 2.0 & -1.0 \\ 1.0 & 2.0 & -1.0 \\ 1.0 & 2.0 & -1.0 \\ 1.0 & 2.0 & -1.0 \\ 1.0 & 2.0 & -1.0 \\ 1.0 & 2.0 & 0.0 \end{bmatrix}$$

$$KA = \begin{bmatrix} 1 & . & . \\ 2 & 3 & . \\ 2 & 3 & . \\ 1 & 4 & 5 \\ 4 & 5 & 6 \\ 5 & 6 & 7 \end{bmatrix}$$



$$\begin{bmatrix} 6 & 7 & 8 \\ 7 & 8 & 9 \\ 8 & 9 & . \end{bmatrix}$$

$$\begin{aligned} B &= (2.0, 1.0, 3.0, 2.0, 2.0, 2.0, 2.0, 2.0, 3.0) \\ X &= (0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0) \end{aligned}$$

**Output:**

$$\begin{aligned} X &= (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0) \\ \text{IPARM}(4) &= 9 \\ \text{RPARAM}(3) &= 0.1500-19 \end{aligned}$$

**Example 2**

This example finds the solution of the linear system  $Ax = b$  for the same sparse matrix  $A$  as in Example 1, which is stored in compressed-matrix storage mode in arrays AC and KA. The system is solved using the generalized minimum residual method, restarted after 5 steps and preconditioned with an incomplete LU factorization. Most of the input is the same as in Example 1.

**Note:** For input matrix KA, ( . ) indicates any value between 1 and 9.

**Call Statement and Input:**

```

      M  NZ  AC  KA  LDA  B  X  IPARM  RPARAM  AUX1  NAUX1  AUX2  NAUX2
      |  |  |  |  |  |  |  |  |  |  |  |  |
CALL DSMGCG( 9 , 3 , AC , KA , 9 , B , X , IPARM , RPARAM , AUX1 , 109 , AUX2 , 46 )

```

$$\begin{aligned} \text{IPARM}(1) &= 20 \\ \text{IPARM}(2) &= 5 \\ \text{IPARM}(3) &= 10 \\ \text{RPARAM}(1) &= 1.D-7 \\ \text{AC} &= (\text{same as input AC in Example 1}) \\ \text{KA} &= (\text{same as input KA in Example 1}) \\ B &= (2.0, 1.0, 3.0, 2.0, 2.0, 2.0, 2.0, 2.0, 3.0) \\ X &= (0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0) \end{aligned}$$

**Output:**

$$\begin{aligned} X &= (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0) \\ \text{IPARM}(4) &= 2 \\ \text{RPARAM}(3) &= 0.2900-15 \end{aligned}$$

## DSDGCG — General Sparse Matrix Iterative Solve Using Compressed-Diagonal Storage Mode

### Purpose

This subroutine solves a general sparse linear system of equations using an iterative algorithm, conjugate gradient squared or generalized minimum residual, with or without preconditioning by an incomplete LU factorization. The subroutine is suitable for positive real matrices—that is, when the symmetric part of the matrix,  $(A+A^T)/2$ , is positive definite. The sparse matrix is stored in compressed-diagonal storage mode. Matrix  $A$  and vectors  $x$  and  $b$  are used:

$$Ax = b$$

where  $A$ ,  $x$ , and  $b$  contain long-precision real numbers.

### Syntax

Fortran	CALL DSDGCG ( <i>m</i> , <i>nd</i> , <i>ad</i> , <i>lda</i> , <i>la</i> , <i>b</i> , <i>x</i> , <i>iparm</i> , <i>rparm</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
C and C++	dsdgcg ( <i>m</i> , <i>nd</i> , <i>ad</i> , <i>lda</i> , <i>la</i> , <i>b</i> , <i>x</i> , <i>iparm</i> , <i>rparm</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

- m* is the order of the linear system  $Ax = b$  and the number of rows in sparse matrix  $A$ .  
Specified as: a fullword integer;  $m \geq 0$ .
- nd* is the number of nonzero diagonals stored in the columns of array AD, the number of columns in array AD, and the number of elements in array LA.  
Specified as: a fullword integer; it must have the following value, where:  
If  $m > 0$ , then  $nd > 0$ .  
If  $m = 0$ , then  $nd \geq 0$ .
- ad* is the array, referred to as AD, containing the values of the nonzero elements of the sparse matrix, stored in compressed-matrix storage mode.  
Specified as: an *lda* by (at least) *nd* array, containing long-precision real numbers.
- lda* is the leading dimension of the arrays specified for *ad*.  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq m$ .
- la* is the array, referred to as LA, containing the diagonal numbers  $k$  for the diagonals stored in each corresponding column in array AD. For an explanation of how diagonal numbers are stored, see "Compressed-Diagonal Storage Mode" on page 96.  
Specified as: a one-dimensional array of (at least) length *nd*, containing fullword integers, where  $1-m \leq$  (elements of LA)  $\leq (m-1)$ .
- b* is the vector  $b$  of length *m*, containing the right-hand side of the matrix problem.

Specified as: a one-dimensional array of (at least) length  $m$ , containing long-precision real numbers.

$x$  is the vector  $x$  of length  $m$ , containing your initial guess of the solution of the linear system.

Specified as: a one-dimensional array of (at least) length  $m$ , containing long-precision real numbers. The elements can have any value, and if no guess is available, the value can be zero.

$iparm$  is an array of parameters,  $IPARM(i)$ , where:

- $IPARM(1)$  controls the number of iterations.  
If  $IPARM(1) > 0$ ,  $IPARM(1)$  is the maximum number of iterations allowed.

If  $IPARM(1) = 0$ , the following default values are used:

$IPARM(1) = 300$   
 $IPARM(2) = 0$   
 $IPARM(3) = 10$   
 $RPARM(1) = 10^{-6}$

- $IPARM(2)$  is the flag used to select the iterative procedure used in this subroutine.

If  $IPARM(2) = 0$ , the conjugate gradient squared method is used.

If  $IPARM(2) = k$ , the generalized minimum residual method, restarted after  $k$  steps, is used. Note that the size of the work area *aux1* becomes larger as  $k$  increases. A value for  $k$  in the range of 5 to 10 is suitable for most problems.

- $IPARM(3)$  is the flag that determines whether the system is to be preconditioned by an incomplete LU factorization with no fill-in. If  $IPARM(3) = 0$ , the system is not preconditioned.

If  $IPARM(3) = 10$ , the system is preconditioned by an incomplete LU factorization.

If  $IPARM(3) = -10$ , the system is preconditioned by an incomplete LU factorization, where the factorization matrix was computed in an earlier call to this subroutine and is stored in *aux2*.

- $IPARM(4)$ , see “On Return” on page 698.

Specified as: an array of (at least) length 4, containing fullword integers, where:

$IPARM(1) \geq 0$   
 $IPARM(2) \geq 0$   
 $IPARM(3) = 0, 10, \text{ or } -10$

$rparm$  is an array of parameters,  $RPARM(i)$ , where:

If  $RPARM(1) > 0$ , is the relative accuracy  $\epsilon$  used in the stopping criterion. The iterative procedure is stopped when:

$$\|b - Ax\|_2 / \|x\|_2 < \epsilon$$

$RPARM(2)$  is reserved.

$RPARM(3)$ , see “On Return” on page 698.

Specified as: a one-dimensional array of (at least) length 3, containing long-precision real numbers.

*aux1*

has the following meaning:

If  $naux1 = 0$  and error 2015 is unrecoverable, *aux1* is ignored.

Otherwise, it is a storage work area used by this subroutine, which is available for use by the calling program between calls to this subroutine. Its size is specified by *naux1*.

Specified as: an area of storage, containing long-precision real numbers.

*naux1*

is the size of the work area specified by *aux1*—that is, the number of elements in *aux1*.

Specified as: a fullword integer, where:

If  $naux1 = 0$  and error 2015 is unrecoverable, DSDGCG dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux1 > 0$  and must have at least the following value, where:

If  $IPARM(2) = 0$ , use  $naux1 \geq 7m$ .

If  $IPARM(2) > 0$ , use  $naux1 \geq (k+2)m+k(k+4)+1$ , where  $k = PARM(2)$ .

*aux2*

is a storage work area used by this subroutine. If  $IPARM(3) = -10$ , *aux2* must contain the incomplete LU factorization of matrix *A*, computed in an earlier call to DSDGCG. The size of *aux2* is specified by *naux2*.

Specified as: an area of storage, containing long-precision real numbers.

*naux2*

is the size of the work area specified by *aux2*—that is, the number of elements in *aux2*.

Specified as: a fullword integer. When  $IPARM(3) = 10$  or  $-10$ , *naux2* must have at least the following value:  $naux2 \geq 3+2m+1.5nd(m)$ .

## On Return

*x*

is the vector *x* of length *m*, containing the solution of the system  $Ax = b$ . Returned as: a one-dimensional array of (at least) length *m*, containing long-precision real numbers.

*iparm*

is an array of parameters,  $IPARM(i)$ , where:

$IPARM(1)$  is unchanged.

$IPARM(2)$  is unchanged.

$IPARM(3)$  is unchanged.

$IPARM(4)$  contains the number of iterations performed by this subroutine.

Returned as: a one-dimensional array of length 4, containing fullword integers.

*rparm*

is an array of parameters,  $RPARAM(i)$ , where:

$RPARAM(1)$  is unchanged.

RPARAM(2) is reserved.

RPARAM(3) contains the estimate of the error of the solution. If the process converged,  $\text{RPARAM}(3) \leq \text{RPARAM}(1)$ .

Returned as: a one-dimensional array of length 3, containing long-precision real numbers.

*aux2* is the storage work area used by this subroutine.

If  $\text{IPARM}(3) = 10$ , *aux2* contains the incomplete LU factorization of matrix *A*.

If  $\text{IPARM}(3) = -10$ , *aux2* is unchanged.

See “Notes” for additional information on *aux2*. Returned as: an area of storage, containing long-precision real numbers.

## Notes

1. When  $\text{IPARM}(3) = -10$ , this subroutine uses the incomplete LU factorization in *aux2*, computed in an earlier call to this subroutine. When  $\text{IPARM}(3) = 10$ , this subroutine computes the incomplete LU factorization and stores it in *aux2*.
2. If you solve the same sparse linear system of equations several times with different right-hand sides, using the preconditioned algorithm, specify  $\text{IPARM}(3) = 10$  on the first invocation. The incomplete factorization is stored in *aux2*. You may save computing time on subsequent calls by setting  $\text{IPARM}(3) = -10$ . In this way, the algorithm reutilizes the incomplete factorization that was computed the first time. Therefore, you should not modify the contents of *aux2* between calls.
3. Matrix *A* must have no common elements with vectors *x* and *b*; otherwise, results are unpredictable.
4. In the iterative solvers for sparse matrices, the relative accuracy  $\epsilon$  ( $\text{RPARAM}(1)$ ) must be specified “reasonably” ( $10^{-4}$  to  $10^{-8}$ ). The algorithm computes a sequence of approximate solution vectors *x* that converge to the solution. The iterative procedure is stopped when the norm of the residual is sufficiently small—that is, when:

$$\|b - Ax\|_2 / \|x\|_2 < \epsilon$$

As a result, if you specify a larger  $\epsilon$ , the algorithm takes fewer iterations to converge to a solution. If you specify a smaller  $\epsilon$ , the algorithm requires more iterations and computer time, but converges to a more precise solution. If the value you specify is unreasonably small, the algorithm may fail to converge within the number of iterations it is allowed to perform.

5. For a description of how sparse matrices are stored in compressed-diagonal storage mode, see “Compressed-Diagonal Storage Mode” on page 96.
6. On output, array *AD* is not bitwise identical to what it was on input, because matrix *A* is scaled before starting the iterative process and is unscaled before returning control to the user.
7. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## Function

The linear system:

$$Ax = b$$

is solved using either the conjugate gradient squared method or the generalized minimum residual method, with or without preconditioning by an incomplete LU factorization, where:

$A$  is a sparse matrix of order  $m$ , stored in compressed-diagonal storage mode in arrays AD and LA.

$x$  is a vector of length  $m$ .

$b$  is a vector of length  $m$ .

See references [90] and [92]. [38].

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux1 = 0$ , and unable to allocate work area.

### Computational Errors

The following errors, with their corresponding return codes, can occur in this subroutine. For details on error handling, see “What Can You Do about ESSL Computational Errors?” on page 51.

- For error 2110, return code 1 indicates that the subroutine exceeded IPARM(1) iterations without converging. Vector  $x$  contains the approximate solution computed at the last iteration.
- For error 2111, return code 2 indicates that  $aux2$  contains an incorrect factorization. The subroutine has been called with IPARM(3) = -10, and  $aux2$  contains an incomplete factorization of the input matrix  $A$  that was computed by a previous call to the subroutine when IPARM(3) = 10. This error indicates that  $aux2$  has been modified since the last call to the subroutine, or that the input matrix is not the same as the one that was factored. If the default action has been overridden, the subroutine can be called again with the same parameters, with the exception of IPARM(3) = 0 or 10.
- For error 2112, return code 3 indicates that the incomplete LU factorization of  $A$  could not be completed, because one pivot was 0.
- For error 2116, return code 4 indicates that the matrix is singular, because all elements in one row of the matrix contain 0. Array AC is partially modified and does not represent the same matrix as on entry.

### Input-Argument Errors

1.  $m < 0$
2.  $lda < 1$
3.  $lda < m$
4.  $nd < 0$
5.  $nd = 0$  and  $m > 0$
6. IPARM(1) < 0
7. IPARM(2) < 0
8. IPARM(3)  $\neq$  0, 10, or -10
9. RPARAM(1) < 1.D0

10. Error 2015 is recoverable or  $naux1 \neq 0$ , and  $naux1$  is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.
11.  $naux2$  is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example finds the solution of the linear system  $Ax = b$  for the sparse matrix  $A$ , which is stored in compressed-diagonal storage mode in arrays AD and LA. The system is solved using the conjugate gradient squared method. Matrix  $A$  is:

$$\begin{bmatrix} 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 2.0 & 0.0 & -1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 2.0 & 0.0 & 0.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 2.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 2.0 \end{bmatrix}$$

#### Call Statement and Input:

```
CALL DSDGCG( M , ND , AD , LDA , LA , B , X , IPARM , RPARAM , AUX1 , NAUX1 , AUX2 , NAUX2 )
```

```
IPARM(1) = 20
IPARM(2) = 0
IPARM(3) = 0
RPARAM(1) = 1.D-7
```

$$AD = \begin{bmatrix} 2.0 & -1.0 & 0.0 \\ 2.0 & -1.0 & 0.0 \\ 2.0 & -1.0 & 0.0 \\ 2.0 & -1.0 & 0.0 \\ 2.0 & -1.0 & 1.0 \\ 2.0 & -1.0 & 1.0 \\ 2.0 & -1.0 & 1.0 \\ 2.0 & 0.0 & 1.0 \\ 2.0 & 0.0 & 1.0 \end{bmatrix}$$

```
LA = (0, 2, -4)
B = (1, 1, 1, 1, 2, 2, 2, 3, 3)
X = (0, 0, 0, 0, 0, 0, 0, 0, 0)
```

#### Output:

```
X = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IPARM(4) = 8
RPARAM(3) = 0.308D-17
```

### Example 2

This example finds the solution of the linear system  $Ax = b$  for the same sparse matrix  $A$  as in Example 1, which is stored in compressed-diagonal storage mode in arrays AD and LA. The system is solved using the generalized minimum residual method, restarted after 5 steps and preconditioned with an incomplete LU factorization. Most of the input is the same as in Example 1.

## DSDGCG

### Call Statement and Input:

```
          M  ND  AD  LDA  LA  B  X  IPARM  RPARM  AUX1  NAUX1  AUX2  NAUX2
          |  |  |  |  |  |  |  |  |  |  |  |  |
CALL DSDGCG( 9 , 3 , AD , 9 , LA , B , X , IPARM , RPARM , AUX1 , 109 , AUX2 , 46 )
```

IPARM(1) = 20

IPARM(2) = 5

IPARM(3) = 10

RPARM(1) = 1.D-7

AD =(same as input AD in Example 1)

LA =(same as input LA in Example 1)

B = (1, 1, 1, 1, 2, 2, 2, 3, 3)

X = (0, 0, 0, 0, 0, 0, 0, 0, 0)

### Output:

X = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)

IPARM(4) = 6

RPARM(3) = 0.250D-15



---

## Linear Least Squares Subroutines

This section contains the linear least squares subroutine descriptions.

## SGESVF and DGESVF — Singular Value Decomposition for a General Matrix

### Purpose

These subroutines compute the singular value decomposition of general matrix  $A$  in preparation for solving linear least squares problems. To compute the minimal norm linear least squares solution of  $AX \cong B$ , follow the call to these subroutines with a call to SGESVS or DGESVS, respectively.

Table 127. Data Types

$A, B, s, aux$	Subroutine
Short-precision real	SGESVF
Long-precision real	DGESVF

### Syntax

Fortran	CALL SGESVF   DGESVF ( <i>iopt, a, lda, b, ldb, nb, s, m, n, aux, nauX</i> )
C and C++	sgesvf   dgesvf ( <i>iopt, a, lda, b, ldb, nb, s, m, n, aux, nauX</i> );

### On Entry

- iopt* indicates the type of computation to be performed, where:
- If *iopt* = 0 or 10, singular values are computed.
  - If *iopt* = 1 or 11, singular values and  $V$  are computed.
  - If *iopt* = 2 or 12, singular values,  $V$ , and  $U^T B$  are computed.
- Specified as: a fullword integer; *iopt* = 0, 1, 2, 10, 11, or 12.
- If *iopt* < 10, singular values are unordered.
- If *iopt* ≥ 10, singular values are sorted in descending order and, if applicable, the columns of  $V$  and the rows of  $U^T B$  are swapped to correspond to the sorted singular values.
- a* is the  $m$  by  $n$  general matrix  $A$ , whose singular value decomposition is to be computed.
- Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 127.
- lda* is the leading dimension of the array specified for *a*.
- Specified as: a fullword integer; *lda* > 0 and *lda* ≥ max( $m, n$ ).
- b* has the following meaning, where:
- If *iopt* = 0, 1, 10, or 11, this argument is not used in the computation.
  - If *iopt* = 2 or 12, it is the  $m$  by  $nb$  matrix  $B$ .
- Specified as: an *ldb* by (at least)  $nb$  array, containing numbers of the data type indicated in Table 127.
- If this subroutine is followed by a call to SGESVS or DGESVS,  $B$  should contain the right-hand side of the linear least squares problem,  $AX \cong B$ . (The  $nb$  column vectors of  $B$  contain right-hand

sides for  $nb$  distinct linear least squares problems.) However, if the matrix  $U^T$  is desired on output,  $B$  should be equal to the identity matrix of order  $m$ .

*ldb*

has the following meaning, where:

If  $iopt = 0, 1, 10,$  or  $11$ , this argument is not used in the computation.

If  $iopt = 2$  or  $12$ , it is the leading dimension of the array specified for  $b$ .

Specified as: a fullword integer. It must have the following values, where:

If  $iopt = 0, 1, 10,$  or  $11$ ,  $ldb > 0$ .

If  $iopt = 2$  or  $12$ ,  $ldb > 0$  and  $ldb \geq \max(m, n)$ .

*nb*

has the following meaning, where:

If  $iopt = 0, 1, 10,$  or  $11$ , this argument is not used in the computation.

If  $iopt = 2$  or  $12$ , it is the number of columns in matrix  $B$ .

Specified as: a fullword integer; if  $iopt = 2$  or  $12$ ,  $nb > 0$ .

*s*

See "On Return."

*m*

is the number of rows in matrices  $A$  and  $B$ .

Specified as: a fullword integer;  $m \geq 0$ .

*n*

is the number of columns in matrix  $A$  and the number of elements in vector  $s$ .

Specified as: a fullword integer;  $n \geq 0$ .

*aux*

has the following meaning:

If  $naux = 0$  and error 2015 is unrecoverable,  $aux$  is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by  $naux$ .

Specified as: an area of storage, containing numbers of the data type indicated in Table 127 on page 704.

*naux*

is the size of the work area specified by  $aux$ —that is, the number of elements in  $aux$ .

Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, SGESVF and DGESVF dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, It must have the following value, where:

If  $iopt = 0$  or  $10$ ,  $naux \geq n + \max(m, n)$ .

If  $iopt = 1$  or  $11$ ,  $naux \geq 2n + \max(m, n)$ .

If  $iopt = 2$  or  $12$ ,  $naux \geq 2n + \max(m, n, nb)$ .

## On Return

*a*

has the following meaning, where:

If  $iopt = 0$ , or 10,  $A$  is overwritten; that is, the original input is not preserved.

If  $iopt = 1, 2, 11$ , or 12,  $A$  contains the real orthogonal matrix  $V$ , of order  $n$ , in its first  $n$  rows and  $n$  columns. If  $iopt = 11$  or 12, the columns of  $V$  are swapped to correspond to the sorted singular values. If  $m > n$ , rows  $n+1, n+2, \dots, m$  of array  $A$  are overwritten; that is, the original input is not preserved.

Returned as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 127 on page 704.

$b$  has the following meaning, where:

If  $iopt = 0, 1, 10$ , or 11,  $B$  is not used in the computation.

If  $iopt = 2$  or 12,  $B$  is overwritten by the  $n$  by  $nb$  matrix  $U^T B$ .

If  $iopt = 12$ , the rows of  $U^T B$  are swapped to correspond to the sorted singular values. If  $m > n$ , rows  $n+1, n+2, \dots, m$  of array  $B$  are overwritten; that is, the original input is not preserved.

Returned as: an  $ldb$  by (at least)  $nb$  array, containing numbers of the data type indicated in Table 127 on page 704.

$s$  is the vector  $s$  of length  $n$ , containing the singular values of matrix  $A$ . Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 127 on page 704;  $s_i \geq 0$ , where:

If  $iopt < 10$ , the singular values are unordered in  $s$ .

If  $iopt \geq 10$ , the singular values are sorted in descending order in  $s$ ; that is,  $s_1 \geq s_2 \geq \dots \geq s_n \geq 0$ . If applicable, the columns of  $V$  and the rows of  $U^T B$  are swapped to correspond to the sorted singular values.

## Notes

1. The following items must have no common elements; otherwise, results are unpredictable: matrices  $A$  and  $B$ , vector  $s$ , and the data area specified for  $aux$ .
2. When you specify  $iopt = 0, 1, 10$ , or 11, you must also specify:
  - A dummy argument for  $b$
  - A positive value for  $ldb$
 See "Example" on page 594.
3. You have the option of having the minimum required value for  $naux$  dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

## Function

The singular value decomposition of a real general matrix is computed as follows:

$$A = U \Sigma V^T$$

where:

$$U^T U = V^T V = V V^T = I$$

$A$  is an  $m$  by  $n$  real general matrix.

$V$  is a real general orthogonal matrix of order  $n$ . On output,  $V$  overwrites the first  $n$  rows and  $n$  columns of  $A$ .

$U^T B$  is an  $n$  by  $nb$  real general matrix. On output,  $U^T B$  overwrites the first  $n$  rows and  $nb$  columns of  $B$ .

$\Sigma$  is an  $n$  by  $n$  real diagonal matrix. The diagonal elements of  $\Sigma$  are the singular values of  $A$ , returned in the vector  $s$ .

If  $m$  or  $n$  is equal to 0, no computation is performed.

One of the following algorithms is used:

1. Golub-Reinsch Algorithm (See pages 134 to 151 in reference [103].)
  - a. Reduce the real general matrix  $A$  to bidiagonal form using Householder transformations.
  - b. Iteratively reduce the bidiagonal form to diagonal form using a variant of the QR algorithm.
2. Chan Algorithm (See reference [15].)
  - a. Compute the QR decomposition of matrix  $A$  using Householder transformations; that is,  $A = QR$ .
  - b. Apply the Golub-Reinsch Algorithm to the matrix  $R$ .  
 If  $R = XWY^T$  is the singular value decomposition of  $R$ , the singular value decomposition of matrix  $A$  is given by:

$$A = Q \begin{bmatrix} X \\ 0 \end{bmatrix} WY^T$$

where:

$$U = Q \begin{bmatrix} X \\ 0 \end{bmatrix}$$

$$\Sigma = W$$

$$V = Y$$

Also, see references [15], [60], [81], and pages 134 to 151 in reference [103]. These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

Singular value ( $i$ ) failed to converge after ( $x$ ) iterations.

## SGESVF and DGESVF

- The singular values ( $s_j, j = n, n-1, \dots, i+1$ ) are correct. If  $iopt < 10$ , they are unordered. Otherwise, they are ordered.
- $a$  has been modified.
- If  $iopt = 2$  or  $12$ , then  $b$  has been modified.
- The return code is set to 1.
- $i$  and  $x$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2107 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $iopt \neq 0, 1, 2, 10, 11, \text{ or } 12$
2.  $lda \leq 0$
3.  $\max(m, n) > lda$
4.  $ldb \leq 0$  and  $iopt = 2, 12$
5.  $\max(m, n) > ldb$  and  $iopt = 2, 12$
6.  $nb \leq 0$  and  $iopt = 2, 12$
7.  $m < 0$
8.  $n < 0$
9. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 2 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to find only the singular values,  $s$ , of a real long-precision general matrix  $A$ , where:

- $M$  is greater than  $N$ .
- $NAUX$  is greater than or equal to  $N + \max(M, N) = 7$ .
- $LDB$  has been set to 1 to avoid a Fortran error message.
- $DUMMY$  is a placeholder for argument  $b$ , which is not used in the computation.
- The singular values are returned in  $S$ .
- On output, matrix  $A$  is overwritten; that is, the original input is not preserved.

#### Call Statement and Input:

```
          IOPT  A  LDA  B   LDB  NB  S  M  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |    |
CALL DGESVF( 0 , A , 4 , DUMMY , 1 , 0 , S , 4 , 3 , AUX , 7 )
```

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 4.0 & 5.0 & 6.0 \\ 7.0 & 8.0 & 9.0 \\ 10.0 & 11.0 & 12.0 \end{bmatrix}$$

#### Output:

```
S          = (25.462, 1.291, 0.000)
```

### Example 2

This example computes the singular values,  $s$ , of a real long-precision general matrix  $A$  and the matrix  $V$ , where:

- $M$  is equal to  $N$ .
- $NAUX$  is greater than or equal to  $2N + \max(M, N) = 9$ .
- $LDB$  has been set to 1 to avoid a Fortran error message.
- $DUMMY$  is a placeholder for argument  $b$ , which is not used in the computation.

- The singular values are returned in S.
- The matrix  $V$  is returned in A.

**Call Statement and Input:**

```

          IOPT  A  LDA  B  LDB  NB  S  M  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |    |
CALL DGESVF( 1 , A , 3 , DUMMY , 1 , 0 , S , 3 , 3 , AUX , 9 )
    
```

$$A = \begin{bmatrix} 2.0 & 1.0 & 1.0 \\ 4.0 & 1.0 & 0.0 \\ -2.0 & 2.0 & 1.0 \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} -0.994 & 0.105 & -0.041 \\ -0.112 & -0.870 & 0.480 \\ -0.015 & -0.482 & -0.876 \end{bmatrix}$$

$$S = (4.922, 2.724, 0.597)$$

**Example 3**

This example computes the singular values,  $s$ , and computes matrices  $V$  and  $U^T B$  in preparation for solving the underdetermined system  $AX \cong B$ , where:

- M is less than N.
- NAUX is greater than or equal to  $2N + \max(M, N, NB) = 9$ .
- The singular values are returned in S.
- The matrix  $V$  is returned in A.
- The matrix  $U^T B$  is returned in B.

**Call Statement and Input:**

```

          IOPT  A  LDA  B  LDB  NB  S  M  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |    |
CALL DGESVF( 2 , A , 3 , B , 3 , 1 , S , 2 , 3 , AUX , 9 )
    
```

$$A = \begin{bmatrix} 1.0 & 2.0 & 2.0 \\ 2.0 & 4.0 & 5.0 \\ \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 \\ 4.0 \\ \cdot \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} -0.304 & -0.894 & 0.328 \\ -0.608 & 0.447 & 0.656 \\ -0.733 & 0.000 & -0.680 \end{bmatrix}$$

$$B = \begin{bmatrix} -4.061 \\ 0.000 \\ -0.714 \end{bmatrix}$$

$$S = (7.342, 0.000, 0.305)$$

### Example 4

This example computes the singular values,  $s$ , and matrices  $V$  and  $U^T B$  in preparation for solving the overdetermined system  $AX \cong B$ , where:

- $M$  is greater than  $N$ .
- $NAUX$  is greater than or equal to  $2N + \max(M, N, NB) = 7$ .
- The singular values are returned in  $S$ .
- The matrix  $V$  is returned in  $A$ .
- The matrix  $U^T B$  is returned in  $B$ .

#### Call Statement and Input:

```

          IOPT  A  LDA  B  LDB  NB  S  M  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |    |
CALL DGESVF( 2 , A , 3 , B , 3 , 2 , S , 3 , 2 , AUX , 7 )
    
```

$$A = \begin{bmatrix} 1.0 & 4.0 \\ 2.0 & 5.0 \\ 3.0 & 6.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 7.0 & 10.0 \\ 8.0 & 11.0 \\ 9.0 & 12.0 \end{bmatrix}$$

#### Output:

$$A = \begin{bmatrix} 0.922 & -0.386 \\ -0.386 & -0.922 \\ . & . \end{bmatrix}$$

$$B = \begin{bmatrix} -1.310 & -2.321 \\ -13.867 & -18.963 \\ . & . \end{bmatrix}$$

$$X = (0.773, 9.508)$$

### Example 5

This example computes the singular values,  $s$ , and matrices  $V$  and  $U^T B$  in preparation for solving the overdetermined system  $AX \cong B$ . The singular values are sorted in descending order, and the columns of  $V$  and the rows of  $U^T B$  are swapped to correspond to the sorted singular values.

- $M$  is greater than  $N$ .
- $NAUX$  is greater than or equal to  $2N + \max(M, N, NB) = 7$ .
- The singular values are returned in  $S$ .
- The matrix  $V$  is returned in  $A$ .
- The matrix  $U^T B$  is returned in  $B$ .

#### Call Statement and Input:

```

          IOPT  A  LDA  B  LDB  NB  S  M  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |    |
CALL DGESVF( 12 , A , 3 , B , 3 , 2 , S , 3 , 2 , AUX , 7 )
    
```

$$A = \begin{bmatrix} 1.0 & 4.0 \\ 2.0 & 5.0 \\ 3.0 & 6.0 \end{bmatrix}$$



$$B = \begin{bmatrix} 7.0 & 10.0 \\ 8.0 & 11.0 \\ 9.0 & 12.0 \end{bmatrix}$$

**Output:**

$$A = \begin{bmatrix} -0.386 & 0.922 \\ -0.922 & -0.386 \\ \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} -13.867 & -18.963 \\ -1.310 & -2.321 \\ \cdot & \cdot \end{bmatrix}$$

$$S = (9.508, 0.773)$$

## SGESVS and DGESVS — Linear Least Squares Solution for a General Matrix Using the Singular Value Decomposition

### Purpose

These subroutines compute the minimal norm linear least squares solution of  $AX \cong B$ , where  $A$  is a general matrix, using the singular value decomposition computed by SGESVF or DGESVF.

Table 128. Data Types

$V, UB, X, s, \tau$	Subroutine
Short-precision real	SGESVS
Long-precision real	DGESVS

### Syntax

Fortran	CALL SGESVS   DGESVS ( $v, ldv, ub, ldub, nb, s, x, ldx, m, n, tau$ )
C and C++	sgesvs   dgesvs ( $v, ldv, ub, ldub, nb, s, x, ldx, m, n, tau$ );

### On Entry

- $v$  is the orthogonal matrix  $V$  of order  $n$  in the singular value decomposition of matrix  $A$ . It is produced by a preceding call to SGESVF or DGESVF, where it corresponds to output argument  $a$ .  
Specified as: an  $ldv$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 128.
- $ldv$  is the leading dimension of the array specified for  $v$ .  
Specified as: a fullword integer;  $ldv > 0$  and  $ldv \geq n$ .
- $ub$  is an  $n$  by  $nb$  matrix, containing  $U^T B$ . It is produced by a preceding call to SGESVF or DGESVF, where it corresponds to output argument  $b$ . On output,  $U^T B$  is overwritten; that is, the original input is not preserved.  
Specified as: an  $ldub$  by (at least)  $nb$  array, containing numbers of the data type indicated in Table 128.
- $ldub$  is the leading dimension of the array specified for  $ub$ .  
Specified as: a fullword integer;  $ldub > 0$  and  $ldub \geq n$ .
- $nb$  is the number of columns in matrices  $X$  and  $U^T B$ .  
Specified as: a fullword integer;  $nb > 0$ .
- $s$  is the vector  $s$  of length  $n$ , containing the singular values of matrix  $A$ . It is produced by a preceding call to SGESVF or DGESVF, where it corresponds to output argument  $s$ .  
Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 128;  $s_i \geq 0$ .
- $x$  See "On Return" on page 713.
- $ldx$  is the leading dimension of the array specified for  $x$ .  
Specified as: a fullword integer;  $ldx > 0$  and  $ldx \geq n$ .

- m* is the number of rows in matrix *A*.  
Specified as: a fullword integer;  $m \geq 0$ .
- n* is the number of columns in matrix *A*, the order of matrix *V*, the number of elements in vector *s*, the number of rows in matrix *UB*, and the number of rows in matrix *X*. Specified as: a fullword integer;  $n \geq 0$ .
- tau* is the error tolerance  $\tau$ . Any singular values in vector *s* that are less than  $\tau$  are treated as zeros when computing matrix *X*.  
Specified as: a number of the data type indicated in Table 128 on page 712;  $\tau \geq 0$ . For more information on the values for  $\tau$ , see "Notes."

**On Return**

- x* is an *n* by *nb* matrix, containing the minimal norm linear least solutions of  $AX \cong B$ . The *nb* column vectors of *X* contain minimal norm solution vectors for *nb* distinct linear least squares problems.  
Returned as: an *ldx* by (at least) *nb* array, containing numbers of the data type indicated in Table 128 on page 712.

**Notes**

- V*, *X*, *s*, and  $U^T B$  can have no common elements; otherwise the results are unpredictable.
- In problems involving experimental data,  $\tau$  should reflect the absolute accuracy of the matrix elements:

$$\tau \geq \max(|\Delta_{ij}|)$$

where  $\Delta_{ij}$  are the errors in  $a_{ij}$ . In problems where the matrix elements are known exactly or are only affected by roundoff errors:

$$\left[ \tau \geq \epsilon \left( \sqrt{mn} \right) \right] \max(s_j) \quad \text{for } j = (1, \dots, n)$$

where:

$\epsilon$  is equal to 0.11920E-06 for SGESVS and 0.22204D-15 for DGESVS. *s* is a vector containing the singular values of matrix *A*.

For more information, see references [15], [60], [81], and pages 134 to 151 in reference [103].

**Function**

The minimal norm linear least squares solution of  $AX \cong B$ , where *A* is a real general matrix, is computed using the singular value decomposition, produced by a preceding call to SGESVF or DGESVF. From SGESVF or DGESVF, the singular value decomposition of *A* is given by the following:

$$A = U \Sigma V^T$$

The linear least squares of solution *X*, for  $AX \cong B$ , is given by the following formula:

$$X = V \Sigma^+ U^T B$$

## SGESVS and DGESVS

where:

$\Sigma^+$  is the diagonal matrix with elements  $\sigma_j^+$ , where:

$$\begin{aligned}\sigma_j^+ &= 1.0/\sigma_j \quad \text{if } \sigma_j \geq \tau \text{ and } \sigma_j \neq 0 \\ \sigma_j^+ &= 0 \quad \text{for all other cases}\end{aligned}$$

If  $m$  or  $n$  is equal to 0, no computation is performed. See references [15], [60], [81], and pages 134 to 151 in reference [103]. These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $ldv \leq 0$
2.  $n > ldv$
3.  $ldub \leq 0$
4.  $n > ldub$
5.  $ldx \leq 0$
6.  $n > ldx$
7.  $nb \leq 0$
8.  $m < 0$
9.  $n < 0$
10.  $\tau < 0$

## Examples

### Example 1

This example finds the linear least squares solution for the underdetermined system  $AX \cong B$ , using the singular value decomposition computed by DGESVF. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 2.0 & 2.0 \\ 2.0 & 4.0 & 5.0 \end{bmatrix}$$

and matrix  $B$  is:

$$\begin{bmatrix} 1.0 \\ 4.0 \end{bmatrix}$$

On output, matrix  $U^T B$  is overwritten.

**Note:** This example corresponds to Example 3 of DGESVF on page 709.

### Call Statement and Input:

```
          V  LDV  UB  LDUB  NB  S  X  LDX  M  N  TAU
          |  |   |  |   |  |  |   |  |  |
CALL DGESVS( V , 3 , UB , 3 , 1 , S , X , 3 , 2 , 3 , TAU )
```

$$V = \begin{bmatrix} -0.304 & -0.894 & 0.328 \\ -0.608 & 0.447 & 0.656 \\ -0.733 & 0.000 & -0.680 \end{bmatrix}$$

$$UB = \begin{bmatrix} -4.061 \\ 0.000 \\ -0.714 \end{bmatrix}$$

$$S = (7.342, 0.000, 0.305)$$

$$TAU = 0.3993D-14$$

**Output:**

$$X = \begin{bmatrix} -0.600 \\ -1.200 \\ 2.000 \end{bmatrix}$$

**Example 2**

This example finds the linear least squares solution for the overdetermined system  $AX \cong B$ , using the singular value decomposition computed by DGESVF. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & 4.0 \\ 2.0 & 5.0 \\ 3.0 & 6.0 \end{bmatrix}$$

and where  $B$  is:

$$\begin{bmatrix} 7.0 & 10.0 \\ 8.0 & 11.0 \\ 9.0 & 12.0 \end{bmatrix}$$

On output, matrix  $U^T B$  is overwritten.

**Note:** This example corresponds to Example 4 of DGESVF on page 710.

**Call Statement:**

```

          V  LDV  UB  LDUB  NB  S  X  LDX  M  N  TAU
CALL DGESVS( V , 3 , UB , 3 , 2 , S , X , 2 , 3 , 2 , TAU )

```

**Input:**

$$V = \begin{bmatrix} 0.922 & -0.386 \\ -0.386 & -0.922 \\ . & . \end{bmatrix}$$

$$UB = \begin{bmatrix} -1.310 & -2.321 \\ -13.867 & -18.963 \\ . & . \end{bmatrix}$$

$$S = (0.773, 9.508)$$

$$TAU = 0.5171D-14$$

## SGESVS and DGESVS

Output:

$$X = \begin{bmatrix} -1.000 & -2.000 \\ 2.000 & 3.000 \end{bmatrix}$$

## DGEQRF — General Matrix QR Factorization

### Purpose

This subroutine computes the  $QR$  factorization of a real general matrix

$$A = QR$$

where:

$Q$  is an orthogonal matrix.

For  $m \geq n$ ,  $R$  is an upper triangular matrix.

For  $m < n$ ,  $R$  is an upper trapezoidal matrix.

Table 129. Data Types

$A, \tau, work$	Subroutine
Long-precision real	DGEQRF <sup>△</sup>
△LAPACK	

### Syntax

Fortran	CALL DGEQRF( $m, n, a, lda, tau, work, lwork, info$ )
C and C++	dgeqrf ( $m, n, a, lda, tau, work, lwork, info$ );

### On Entry

- $m$  is the number of rows in matrix  $A$  used in the computation.  
Specified as: a fullword integer;  $m \geq 0$ .
- $n$  is the number of columns in matrix  $A$  used in the computation.  
Specified as: a fullword integer;  $n \geq 0$ .
- $a$  is the  $m$  by  $n$  general matrix  $A$  whose  $QR$  factorization is to be computed.  
Specified as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 129.
- $lda$  is the leading dimension of the array specified for  $a$ .  
Specified as: a fullword integer;  $lda > 0$  and  $lda \geq m$ .
- $tau$  See On Return.
- $work$  has the following meaning:  
If  $lwork = 0$ ,  $work$  is ignored.  
If  $lwork \neq 0$ ,  $work$  is the work area used by this subroutine, where:
- If  $lwork \neq -1$ , its size is (at least) of length  $lwork$ .
  - If  $lwork = -1$ , its size is (at least) of length 1.
- Specified as: an area of storage containing numbers of data type indicated in Table 129.
- $lwork$  is the number of elements in array WORK.  
Specified as: a fullword integer; where:

- If  $lwork = 0$ , DGEQRF dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program. This option is an extension to the LAPACK standard.
- If  $lwork = -1$ , DGEQRF performs a work area query and returns the optimal size of  $work$  in  $work_1$ . No computation is performed and the subroutine returns after error checking is complete.
- Otherwise, it must be:  

$$lwork \geq \max(1, n)$$

*info* See On Return.

### On Return

*a* is the updated general matrix  $A$ , containing the results of the computation.

The elements on and above the diagonal of the array contain the  $\min(m, n) \times n$  upper trapezoidal matrix  $R$  ( $R$  is upper triangular if  $m \geq n$ ). The elements below the diagonal with  $\tau$  represent the orthogonal matrix  $Q$  as a product of  $\min(m, n)$  elementary reflectors.

Returned as: an  $lda$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 129 on page 717.

*tau* is the vector  $\tau$ , of length  $\min(m, n)$ , containing the scalar factors of the elementary reflectors.

Returned as: a one-dimensional array of (at least) length  $\min(m, n)$ , containing numbers of the data type indicated in Table 129 on page 717.

*work* is the work area used by this subroutine if  $lwork \neq 0$ , where:

If  $lwork \neq 0$  and  $lwork \neq -1$ , its size is (at least) of length  $lwork$ .

If  $lwork = -1$ , its size is (at least) of length 1.

Returned as: an area of storage, where:

If  $lwork \geq 1$  or  $lwork = -1$ , then  $work_1$  is set to the optimal  $lwork$  value and contains numbers of the data type indicated in Table 129 on page 717. Except for  $work_1$ , the contents of  $work$  are overwritten on return.

*info* indicates that a successful computation occurred.

Returned as: a fullword integer;  $info = 0$ .

## Notes and Coding Rules

1. In your C program, argument *info* must be passed by reference.
2. The vectors and matrices used in the computation must have no common elements; otherwise, results are unpredictable.
3. For best performance specify  $lwork = 0$ .

## Function

Compute the  $QR$  factorization of a real general matrix  $A$

$$A = QR$$



where:

The orthogonal matrix  $Q$  is represented as a product of elementary reflectors:

$$Q = H_1 H_2 \dots H_k$$

where:

$$k = \min(m, n)$$

$$\text{For each } i: H_i = I - \tau v v^T$$

$\tau$  is a real scalar, stored on return in  $\tau_i$

$v$  is a real vector with  $v_{1:i-1} = 0$ ,  $v_i = 1$ .

$v_{i+1:m}$  is stored on return in  $A_{i+1:m, i}$

$I$  is the identity matrix

For  $m \geq n$ ,  $R$  is an upper triangular matrix.

For  $m < n$ ,  $R$  is an upper trapezoidal matrix.

If  $m = 0$  or  $n = 0$ , no computation is performed and the subroutine returns after doing some parameter checking.

See references [54,8,67,52,53].

## Error conditions

### Resource Errors

$lwork = 0$  and unable to allocate work space.

### Computational Errors

None.

### Input-Argument Errors

1.  $m < 0$
2.  $n < 0$
3.  $lda \leq 0$
4.  $lda < m$
5.  $lwork \neq 0$ ,  $lwork \neq -1$ , and  $lwork < \max(1, n)$

## Examples

### Example 1

This example shows the  $QR$  factorization of a general matrix  $A$  of size  $6 \times 2$ .

**Note:** Because  $lwork = 0$ , DGEQRF dynamically allocates the work area used by this subroutine.

### Call Statements and Input:

	M	N	A	LDA	TAU	WORK	LWORK	INFO
CALL DGEQRF (	6	2	A	6	TAU	WORK	0	INFO)

General matrix  $A$  of size  $6 \times 2$ :

$$A = \begin{bmatrix} .000000 & 2.000000 \\ 2.000000 & -1.000000 \\ 2.000000 & -1.000000 \end{bmatrix}$$

## DGEQRF

$$\begin{bmatrix} .000000 & 1.500000 \\ 2.000000 & -1.000000 \\ 2.000000 & -1.000000 \end{bmatrix}$$

### Output:

General matrix  $A$  of size  $6 \times 2$ .

$$A = \begin{bmatrix} -4.000000 & 2.000000 \\ .500000 & 2.500000 \\ .500000 & .285714 \\ .000000 & -.428571 \\ .500000 & .285714 \\ .500000 & .285714 \end{bmatrix}$$

Vector  $\tau$  of length 2:

$$\text{TAU} = \begin{bmatrix} 1.000000 & 1.400000 \end{bmatrix}$$

INFO = 0

### Example 2

This example shows the  $QR$  factorization of a general matrix  $A$  of size  $4 \times 5$ .

**Note:** Because  $lwork = 0$ , DGEQRF dynamically allocates the work area used by this subroutine.

### Call Statements and Input:

```
          M   N   A   LDA   TAU   WORK   LWORK   INFO
          |   |   |   |   |   |   |   |
CALL DGEQRF ( 4 , 5 , A , 4 , TAU , WORK , 0 , INFO)
```

General matrix  $A$  of size  $4 \times 5$ :

$$A = \begin{bmatrix} .500000 & .500000 & 1.207107 & .000000 & 1.707107 \\ .500000 & -1.500000 & -.500000 & 2.414214 & .707107 \\ .500000 & .500000 & .207107 & .000000 & .292893 \\ .500000 & -1.500000 & -.500000 & -.414214 & -.707107 \end{bmatrix}$$

### Output:

General matrix  $A$  of size  $4 \times 5$ :

$$A = \begin{bmatrix} -1.000000 & 1.000000 & -.207107 & -1.000000 & -1.000000 \\ .333333 & 2.000000 & 1.207107 & -1.000000 & 1.000000 \\ .333333 & -.200000 & .707107 & .000000 & 1.000000 \\ .333333 & .400000 & .071068 & -2.000000 & -1.000000 \end{bmatrix}$$

Vector  $\tau$  of length 4:

$$\text{TAU} = \begin{bmatrix} 1.500000 & 1.666667 & 1.989949 & .000000 \end{bmatrix}$$

INFO = 0

## DGELS — Linear Least Squares Solution for a General Matrix

### Purpose

This subroutine computes the linear least squares solution for a general matrix  $A$  or its transpose using a  $QR$  factorization without column pivoting, where  $A$  is assumed to have full rank.

The following options are provided:

- If  $transa = 'N'$  and  $m \geq n$ : find the least squares solution of an overdetermined system; that is, solve the least squares problem: minimize  $\|B - AX\|$
- If  $transa = 'N'$  and  $m < n$ : find the minimum norm solution of an underdetermined system; that is, the problem is:  $AX = B$
- If  $transa = 'T'$  and  $m \geq n$ : find the minimum norm solution of an underdetermined system; that is, the problem is  $A^T X = B$
- If  $transa = 'T'$  and  $m < n$ : find the least squares solution of an overdetermined system; that is, solve the least squares problem: minimize  $\|B - A^T X\|$

Table 130. Data Types

$A, B, work$	Subroutine
Long-precision real	DGELS <sup>△</sup>
△LAPACK	

### Syntax

Fortran	CALL DGELS ( <i>transa, m, n, nrhs, a, lda, b, ldb, work, lwork, info</i> )
C and C++	dgels ( <i>transa,m, n, nrhs, a, lda, b ,ldb, work, lwork, info</i> );

### On Entry

*transa* indicate the form of matrix  $A$  to use in the computation, where:

If  $transa = 'N'$ , matrix  $A$  is used.

If  $transa = 'T'$ , matrix  $A^T$  is used.

Specified as: a single character;  $transa = 'N'$  or  $'T'$ .

*m* is the number of rows in matrix  $A$  used in the computation.

Specified as: a fullword integer;  $m \geq 0$ .

*n* is the number of columns in matrix  $A$  used in the computation.

Specified as: a fullword integer;  $n \geq 0$ .

*nrhs* is the number of right-hand sides; that is, the number of columns in matrix  $B$  used in the computation.

Specified as: a fullword integer;  $nrhs \geq 0$ .

*a* is the  $m$  by  $n$  coefficient matrix  $A$ .

**Note:** No data should be moved to form  $A^T$ ; that is, the matrix  $A$  should always be stored in its untransposed form.

Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 130.

<i>lda</i>	<p>is the leading dimension of the array specified for <i>a</i>. Specified as: a fullword integer; <math>lda &gt; 0</math> and <math>lda \geq m</math>.</p>
<i>b</i>	<p>is the matrix <i>B</i> of right-hand side vectors. If <i>transa</i> = 'N', matrix <i>B</i> has <i>m</i> rows and <i>nrhs</i> columns. If <i>transa</i> = 'T', matrix <i>B</i> has <i>n</i> rows and <i>nrhs</i> columns. Specified as: the <i>ldb</i> by (at least) <i>nrhs</i> array, containing numbers of the data type indicated in Table 130 on page 721.</p>
<i>ldb</i>	<p>is the leading dimension of the array specified for <i>b</i>. Specified as: a fullword integer; <math>ldb &gt; 0</math> and <math>ldb \geq \max(m,n)</math>.</p>
<i>work</i>	<p>has the following meaning: If <i>lwork</i> = 0, <i>work</i> is ignored. If <i>lwork</i> <math>\neq</math> 0, <i>work</i> is the work area used by this subroutine, where:</p> <ul style="list-style-type: none"> <li>• If <i>lwork</i> <math>\neq</math> -1, its size is (at least) of length <i>lwork</i>.</li> <li>• If <i>lwork</i> = -1, its size is (at least) of length 1.</li> </ul> <p>Specified as: an area of storage containing numbers of data type indicated in Table 130 on page 721.</p>
<i>lwork</i>	<p>is the number of elements in array <i>work</i>. Specified as: a fullword integer; where:</p> <ul style="list-style-type: none"> <li>• If <i>lwork</i> = 0, DGELS dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program. This option is an extension to the LAPACK standard.</li> <li>• If <i>lwork</i> = -1, DGELS performs a work area query and returns the optimal size of <i>work</i> in <i>work</i><sub>1</sub>. No computation is performed, and the subroutine returns after error checking is complete.</li> <li>• Otherwise, it must be: <math>lwork \geq \max(1, mn + \max(mn, nrhs))</math> where <math>mn = \min(m, n)</math>.</li> </ul>
<i>info</i>	<p>See "On Return."</p>

### On Return

<i>a</i>	<p>is the updated general matrix <i>A</i>. The matrix <i>A</i> is overwritten; that is, the original input is not preserved. Returned as: an <i>lda</i> by (at least) <i>n</i> array, containing numbers of the data type indicated in Table 130 on page 721.</p>
<i>b</i>	<p>is the updated general matrix <i>B</i>, containing the results of the computation. <i>B</i> is overwritten by the solution vectors, stored columnwise:</p> <ul style="list-style-type: none"> <li>• If <i>transa</i> = 'N' and <math>m \geq n</math>, rows 1 to <i>n</i> of <i>B</i> contain the least squares solution vectors; the residual sum of squares for the solution in each column is given by the sum of squares of elements <i>n</i>+1 to <i>m</i> in that column.</li> <li>• If <i>transa</i> = 'N' and <math>m &lt; n</math>, rows 1 to <i>n</i> of <i>B</i> contain the minimum norm solution vectors.</li> <li>• If <i>transa</i> = 'T' and <math>m \geq n</math>, rows 1 to <i>m</i> of <i>B</i> contain the minimum norm solution vectors.</li> </ul>

- If  $transa = 'T'$  and  $m < n$ , rows 1 to  $m$  of  $B$  contain the least squares solution vectors; the residual sum of squares for the solution in each column is given by the sum of squares of elements  $m+1$  to  $n$  in that column.

Returned as: an  $ldb$  by (at least)  $nrhs$  array, containing numbers of the data type indicated in Table 130 on page 721.

$work$  is the work area used by this subroutine if  $lwork \neq 0$ , where:

If  $lwork \neq 0$  and  $lwork \neq -1$ , its size is (at least) of length  $lwork$ .

If  $lwork = -1$ , its size is (at least) of length 1.

Returned as: an area of storage, where:

If  $lwork \geq 1$  or  $lwork = -1$ , then  $work_1$  is set to the optimal  $lwork$  value and contains numbers of the data type indicated in Table 130 on page 721.

Except for  $work_1$ , the contents of  $work$  are overwritten on return.

$info$  indicates that a successful computation occurred.

Returned as: a fullword integer;  $info = 0$ .

## Notes and Coding Rules

1. In your C program, argument  $info$  must be passed by reference.
2. All subroutines accept lowercase letters for the  $transa$  argument.
3. The vectors and matrices used in the computation must have no common elements; otherwise, results are unpredictable.
4. For best performance specify  $lwork = 0$ .

## Function

This subroutine computes the linear least squares solution for a general matrix  $A$  or its transpose using a  $QR$  factorization without column pivoting, where  $A$  is assumed to have full rank.

The following options are provided:

- If  $transa = 'N'$  and  $m \geq n$ : find the least squares solution of an overdetermined system; that is, solve the least squares problem: minimize  $\|B - AX\|$
- If  $transa = 'N'$  and  $m < n$ : find the minimum norm solution of an underdetermined system; that is, the problem is:  $AX = B$
- If  $transa = 'T'$  and  $m \geq n$ : find the minimum norm solution of an underdetermined system; that is, the problem is  $A^T X = B$
- If  $transa = 'T'$  and  $m < n$ : find the least squares solution of an overdetermined system; that is, solve the least squares problem: minimize  $\|B - A^T X\|$

If ( $m = 0$  and  $n = 0$ ) or  $nrhs = 0$ , then no computation is performed and the subroutine returns after doing some parameter checking.

See reference [64].

## Error conditions

### Resource Errors

$lwork = 0$  and unable to allocate work space.

### Computational Errors

None.

### Input-Argument Errors

1. *transa* ≠ 'N' or 'T'
2. *m* < 0
3. *n* < 0
4. *nrhs* < 0
5. *lda* < *m*
6. *lda* ≤ 0
7. *ldb* < max(*m*, *n*)
8. *ldb* ≤ 0
9. *lwork* ≠ 0, *lwork* ≠ -1, and *lwork* < max(1, *mn* + max(*mn*, *nrhs*)) where *mn* = min(*m*, *n*)

## Examples

### Example 1

This example finds the least squares solution of an overdetermined system; that is, it solves the least squares problem: minimize  $\|B-AX\|$ . Matrix *A* is size 6 × 2 and matrix *B* is size 6 × 3.

**Note:** Because *lwork* = 0, DGELS dynamically allocates the work area used by this subroutine.

#### Call Statements and Input:

```

          TRANSA  M  N  NRHS  A  LDA  B  LDB  WORK  LWORK  INFO
CALL DGELS ( 'N' , 6 , 2 , 3 , A , 6 , B , 6 , WORK , 0 , INFO )
    
```

General matrix *A* of size 6 × 2:

$$A = \begin{bmatrix} .000000000 & 2.000000000 \\ 2.000000000 & -1.000000000 \\ 2.000000000 & -1.000000000 \\ .000000000 & 1.500000000 \\ 2.000000000 & -1.000000000 \\ 2.000000000 & -1.000000000 \end{bmatrix}$$

General matrix *B* of size 6 × 3:

$$B = \begin{bmatrix} 1.000000000 & 4.000000000 & 1.000000000 \\ 1.000000000 & 1.000000000 & 2.000000000 \\ 1.000000000 & -1.000000000 & 1.000000000 \\ 1.000000000 & 3.000000000 & 2.000000000 \\ 1.000000000 & 1.000000000 & 1.000000000 \\ 1.000000000 & -1.000000000 & 1.000000000 \end{bmatrix}$$

#### Output:

General matrix *A* is overwritten.

Solution matrix *X* overwrites *B*:

$$B = \begin{bmatrix} .780000000 & 1.000000000 & 1.025000000 \\ .560000000 & 2.000000000 & .800000000 \\ .042857143 & -1.285714286 & -.250000000 \\ .185714286 & .428571429 & 1.250000000 \\ .042857143 & .714285714 & -.250000000 \\ .042857143 & -1.285714286 & -.250000000 \end{bmatrix}$$

INFO = 0

### Example 2

This example finds the minimum norm solution of an underdetermined system  $A^T X = B$ . Matrix  $A$  is size  $6 \times 2$ . On input, matrix  $B$  is size  $2 \times 1$ , stored in array  $b$  with leading dimension 6.

**Note:** Because  $lwork = 0$ , DGELS dynamically allocates the work area used by this subroutine.

#### Call Statements and Input:

```

          TRANSA  M  N  NRHS  A  LDA  B  LDB  WORK  LWORK  INFO
          |      |  |  |      |  |   |   |   |   |   |
CALL DGELS ( 'T' , 6 , 2 , 1 , A , 6 , B , 6 , WORK , 0 , INFO )
    
```

General matrix  $A$  of size  $6 \times 2$ :

$$A = \begin{bmatrix} .000000000 & 2.000000000 \\ 2.000000000 & -1.000000000 \\ 2.000000000 & -1.000000000 \\ .000000000 & 1.500000000 \\ 2.000000000 & -1.000000000 \\ 2.000000000 & -1.000000000 \end{bmatrix}$$

General matrix  $B$  of size  $2 \times 1$ :

$$B = \begin{bmatrix} 1.000000000 \\ 1.000000000 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

#### Output:

General matrix  $A$  is overwritten.

Solution matrix  $X$  overwrites  $B$ :

$$B = \begin{bmatrix} .480000000 \\ .125000000 \\ .125000000 \\ .360000000 \\ .125000000 \\ .125000000 \end{bmatrix}$$

INFO = 0

### Example 3

This example finds the minimum norm solution of an underdetermined system  $AX = B$ . Matrix  $A$  is size  $3 \times 4$ . On input, matrix  $B$  is size  $3 \times 4$ , stored in array  $b$  with leading dimension 4.

**Note:** Because  $lwork = 0$ , DGELS dynamically allocates the work area used by this subroutine.

#### Call Statements and Input:

```

          TRANSA  M  N  NRHS  A  LDA  B  LDB  WORK  LWORK  INFO
          |      |  |  |      |  |  |  |  |      |
CALL DGELS ( 'N' , 3 , 4 , 4 , A , 3 , B , 4 , WORK , 0 , INFO )
    
```

General matrix  $A$  of size  $3 \times 4$ :

$$A = \begin{bmatrix} .500000000 & .500000000 & .500000000 & .500000000 \\ .500000000 & -1.500000000 & .500000000 & -1.500000000 \\ 1.000000000 & 1.000000000 & .000000000 & 1.000000000 \end{bmatrix}$$

General matrix  $B$  of size  $3 \times 4$ :

$$B = \begin{bmatrix} 1.000000000 & 1.000000000 & 1.000000000 & .000000000 \\ 1.000000000 & -1.000000000 & 2.500000000 & 1.000000000 \\ 1.000000000 & 1.000000000 & 3.000000000 & .000000000 \\ . & . & . & . \end{bmatrix}$$

#### Output:

General matrix  $A$  is overwritten.

Solution matrix  $X$  overwrites  $B$ :

$$B = \begin{bmatrix} 1.000000000 & .000000000 & 3.500000000 & .500000000 \\ .000000000 & .500000000 & -.250000000 & -.250000000 \\ 1.000000000 & 1.000000000 & -1.000000000 & .000000000 \\ .000000000 & .500000000 & -.250000000 & -.250000000 \end{bmatrix}$$

INFO = 0

### Example 4

This example finds the least squares solution of an overdetermined system; that is, it solves the least squares problem: minimize  $\|B - A^T X\|$ . Matrix  $A$  is size  $3 \times 4$ . On input, matrix  $B$  is size  $4 \times 4$ .

**Note:** Because  $lwork = 0$ , DGELS dynamically allocates the work area used by this subroutine.

#### Call Statements and Input:

```

          TRANSA  M  N  NRHS  A  LDA  B  LDB  WORK  LWORK  INFO
          |      |  |  |      |  |  |  |  |      |
CALL DGELS ( 'T' , 3 , 4 , 4 , A , 3 , B , 4 , WORK , 0 , INFO )
    
```

General matrix  $A$  of size  $3 \times 4$ :



$$A = \begin{bmatrix} .500000000 & .500000000 & .500000000 & .500000000 \\ .500000000 & -1.500000000 & .500000000 & -1.500000000 \\ 1.207106781 & -.500000000 & .207106781 & -.500000000 \end{bmatrix}$$

General matrix  $B$  of size  $4 \times 4$ :

$$B = \begin{bmatrix} 1.000000000 & 1.000000000 & 1.000000000 & .000000000 \\ 1.000000000 & -1.000000000 & 2.000000000 & 2.414213562 \\ 1.000000000 & 1.000000000 & 3.000000000 & .000000000 \\ 1.000000000 & -1.000000000 & 4.000000000 & -.414213562 \end{bmatrix}$$

**Output:**

General matrix  $A$  is overwritten.

Solution matrix  $X$  overwrites  $B$ :

$$B = \begin{bmatrix} 2.000000000 & 1.000000000 & 6.121320344 & .500000000 \\ .000000000 & 1.000000000 & .707106781 & -.500000000 \\ .000000000 & .000000000 & -2.000000000 & .000000000 \\ .000000000 & .000000000 & 1.414213562 & -2.000000000 \end{bmatrix}$$

INFO = 0

## SGELLS and DGELLS — Linear Least Squares Solution for a General Matrix with Column Pivoting

### Purpose

These subroutines compute the minimal norm linear least squares solution of  $AX \cong B$ , using a QR decomposition with column pivoting.

Table 131. Data Types

<i>A, B, X, rn, τ, aux</i>	Subroutine
Short-precision real	SGELLS
Long-precision real	DGELLS

### Syntax

Fortran	CALL SGELLS   DGELLS ( <i>iopt, a, lda, b, ldb, x, ldx, rn, tau, m, n, nb, k, aux, naux</i> )
C and C++	sgells   dgells ( <i>iopt, a, lda, b, ldb, x, ldx, rn, tau, m, n, nb, k, aux, naux</i> );

### On Entry

- iopt* indicates the type of computation to be performed, where:
- If *iopt* = 0, **X** is computed.
  - If *iopt* = 1, **X** and the Euclidean Norm of the residual vectors are computed.
- Specified as: a fullword integer; *iopt* = 0 or 1.
- a* is the *m* by *n* coefficient matrix **A**. On output, **A** is overwritten; that is, the original input is not preserved.
- Specified as: an *lda* by (at least) *n* array, containing numbers of the data type indicated in Table 131.
- lda* is the leading dimension of the array specified for *a*.
- Specified as: a fullword integer; *lda* > 0 and *lda* ≥ *m*.
- b* is the *m* by *nb* matrix **B**, containing the right-hand sides of the linear systems. The *nb* column vectors of **B** contain right-hand sides for *nb* distinct linear least squares problems. On output, **B** is overwritten; that is, the original input is not preserved.
- Specified as: an *ldb* by (at least) *nb* array, containing numbers of the data type indicated in Table 131.
- ldb* is the leading dimension of the array specified for *b*.
- Specified as: a fullword integer; *ldb* > 0 and *ldb* ≥ *m*.
- x* See “On Return” on page 729.
- ldx* is the leading dimension of the array specified for *x*.
- Specified as: a fullword integer; *ldx* > 0 and *ldx* ≥ *n*.
- rn* See “On Return” on page 729.
- tau* is the tolerance  $\tau$ , used to determine the subset of the columns of **A** used in the solution.

Specified as: a number of the data type indicated in Table 131 on page 728;  $\tau \geq 0$ . For more information on how to select a value for  $\tau$ , see “Notes” on page 730.

- m* is the number of rows in matrices *A* and *B*.  
Specified as: a fullword integer;  $m \geq 0$ .
- n* is the number of columns in matrix *A* and the number of rows in matrix *X*.  
Specified as: a fullword integer;  $n \geq 0$ .
- nb* is the number of columns in matrices *B* and *X* and the number of elements in vector *rn*.  
Specified as: a fullword integer;  $nb > 0$ .
- k* See “On Return.”
- aux* has the following meaning:  
If  $naux = 0$  and error 2015 is unrecoverable, *aux* is ignored.  
Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*.  
Specified as: an area of storage, containing numbers of the data type indicated in Table 131 on page 728. On output, the contents of *aux* are overwritten.
- naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.  
Specified as: a fullword integer, where:  
If  $naux = 0$  and error 2015 is unrecoverable, SGELLS and DGELLS dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.  
Otherwise, It must have the following values:  
 $naux \geq 3n + \max(n, nb)$  for SGELLS  
 $naux \geq [\text{ceiling}(2.5n) + \max(n, nb)]$  for DGELLS

### On Return

- x* is the solution matrix *X*, with *n* rows and *nb* columns, where:  
If  $k \neq 0$ , the *nb* column vectors of *X* contain minimal norm least squares solutions for *nb* distinct linear least squares problems. The elements in each solution vector correspond to the original columns of *A*.  
If  $k = 0$ , the *nb* column vectors of *X* are set to 0.  
Returned as: an *ldx* by (at least) *nb* array, containing numbers of the data type indicated in Table 131 on page 728.
- rn* is the vector *rn* of length *nb*, where:  
If  $iopt = 0$  or  $k = 0$ , *rn* is not used in the computation.  
If  $iopt = 1$ ,  $rn_i$  is the Euclidean Norm of the residual vector for the linear least squares problem defined by the *i*-th column vector of *B*.

Returned as: a one-dimensional array of (at least)  $nb$ , containing numbers of the data type indicated in Table 131 on page 728.

$k$  is the number of columns of matrix  $A$  used in the solution.  
Returned as: a fullword integer;  $k =$  (the number of diagonal elements of matrix  $R$  exceeding  $\tau$  in magnitude).

## Notes

1. In your C program, argument  $k$  must be passed by reference.
2. If  $ldb \geq \max(m, n)$ , matrix  $X$  and matrix  $B$  can be the same; otherwise, matrix  $X$  and matrix  $B$  can have no common elements, or the results are unpredictable.
3. The following items must have no common elements; otherwise, results are unpredictable:
  - Matrices  $A$  and  $X$ , vector  $rn$ , and the data area specified for  $aux$
  - Matrices  $A$  and  $B$ , vector  $rn$ , and the data area specified for  $aux$ .
4. If the relative uncertainty in the matrix  $B$  is  $\rho$ , then:

$$\tau \geq \rho \|A\|_F$$

See references [46], [64], and [81] for additional guidance on determining suitable values for  $\tau$ .

5. When you specify  $iopt = 0$ , you must also specify a dummy argument for  $rn$ . For more details, see "Example 1" on page 731.
6. You have the option of having the minimum required value for  $naux$  dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

## Function

The minimal norm linear least squares solution of  $AX \cong B$  is computed using a QR decomposition with column pivoting, where:

$A$  is an  $m$  by  $n$  real general matrix.

$B$  is an  $m$  by  $nb$  real general matrix.

$X$  is an  $n$  by  $nb$  real general matrix.

Optionally, the Euclidean Norms of the residual vectors can be computed. Following are the steps involved in finding the minimal norm linear least squares solution of  $AX \cong B$ .  $A$  is decomposed, using Householder transformations and column pivoting, into the following form:

$$AP = QR$$

where:

$P$  is a permutation matrix.

$Q$  is an orthogonal matrix.

$R$  is an upper triangular matrix.

$k$  is the first index, where:

$$|r_{k+1,k+1}| \leq \tau$$

If  $k = n$ , the minimal norm linear least squares solution is obtained by solving  $RX = Q^T B$  and reordering  $X$  to correspond to the original columns of  $A$ .

If  $k < n$ ,  $R$  has the following form:

$$R = \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix}$$

To find the minimal norm linear least squares solution, it is necessary to zero the submatrix  $R_{12}$  using Householder transformations. See references [46], [64], and [81]. If  $m$  or  $n$  is equal to 0, no computation is performed. These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $iopt \neq 0$  or 1
2.  $lda \leq 0$
3.  $m > lda$
4.  $ldb \leq 0$
5.  $m > ldb$
6.  $ldx \leq 0$
7.  $n > ldx$
8.  $m < 0$
9.  $n < 0$
10.  $nb \leq 0$
11.  $\tau < 0$
12. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example solves the underdetermined system  $AX \cong B$ . On output,  $A$  and  $B$  are overwritten. DUMMY is used as a placeholder for argument  $m$ , which is not used in the computation.

## SGELLS and DGELLS

### Call Statement and Input:

```
          IOPT  A  LDA  B  LDB  X  LDX  RN  TAU  M  N  NB  K  AUX  NAUX
CALL DGELLS( 0 , A , 2 , B , 2 , X , 3 , DUMMY , TAU , 2 , 3 , 1 , K , AUX , 11 )
```

$$A = \begin{bmatrix} 1.0 & 2.0 & 2.0 \\ 2.0 & 4.0 & 5.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 \\ 4.0 \end{bmatrix}$$

$$\text{TAU} = 0.0$$

### Output:

$$X = \begin{bmatrix} -0.6000 \\ -1.2000 \\ 2.0000 \end{bmatrix}$$

$$K = 2$$

### Example 2

This example solves the overdetermined system  $AX \cong B$ . On output,  $A$  and  $B$  are overwritten. DUMMY is used as a placeholder for argument  $m$ , which is not used in the computation.

### Call Statement and Input:

```
          IOPT  A  LDA  B  LDB  X  LDX  RN  TAU  M  N  NB  K  AUX  NAUX
CALL DGELLS( 0 , A , 3 , B , 3 , X , 2 , DUMMY , TAU , 3 , 2 , 2 , K , AUX , 7 )
```

$$A = \begin{bmatrix} 1.0 & 4.0 \\ 2.0 & 5.0 \\ 3.0 & 6.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 7.0 & 10.0 \\ 8.0 & 11.0 \\ 9.0 & 12.0 \end{bmatrix}$$

$$\text{TAU} = 0.0$$

### Output:

$$X = \begin{bmatrix} -1.0000 & -2.0000 \\ 2.0000 & 3.0000 \end{bmatrix}$$

$$K = 2$$

### Example 3

This example solves the overdetermined system  $AX \cong B$  and computes the Euclidean Norms of the residual vectors. On output,  $A$  and  $B$  are overwritten.

**Call Statement and Input:**

```

          IOPT  A  LDA  B  LDB  X  LDX  RN  TAU  M  N  NB  K  AUX  NAUX
CALL DGELLS( 1 , A , 3 , B , 3 , X , 2 , RN , TAU , 3 , 2 , 2 , K , AUX , 7 )

```

$$A = \begin{bmatrix} 1.1 & -4.3 \\ 2.0 & -5.0 \\ 3.0 & -6.0 \end{bmatrix}$$

$$B = \begin{bmatrix} -7.0 & 10.0 \\ -8.0 & 11.0 \\ -9.0 & 12.0 \end{bmatrix}$$

$$TAU = 0.0$$

**Output:**

$$X = \begin{bmatrix} 0.543 & -1.360 \\ 1.785 & -2.699 \end{bmatrix}$$

$$RN = \begin{bmatrix} 0.196 \\ 0.275 \end{bmatrix}$$

$$K = 2$$

## SGELLS and DGELLS



---

## Chapter 11. Eigensystem Analysis

The eigensystem analysis subroutines are described in this chapter.

---

### Overview of the Eigensystem Analysis Subroutines

The eigensystem analysis subroutines provide solutions to the algebraic eigensystem analysis problem  $Az = wz$  and the generalized eigensystem analysis problem  $Az = wBz$  ( Table 132). Many of the eigensystem analysis subroutines use the algorithms presented in *Linear Algebra* by Wilkinson and Reinsch [103] or use adaptations of EISPACK routines, as described in the *EISPACK Guide Lecture Notes in Computer Science* in reference [91] or in the *EISPACK Guide Extension Lecture Notes in Computer Science* in reference [60]. (EISPACK is available from the sources listed in reference [51].)

Table 132. List of Eigensystem Analysis Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Eigenvalues and, Optionally, All or Selected Eigenvectors of a General Matrix	SGEEV <sup>‡</sup> CGEEV <sup>‡</sup>	DGEEV <sup>‡</sup> ZGEEV <sup>‡</sup>	737
Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix	SSPEV <sup>‡</sup> CHPEV <sup>‡</sup>	DSPEV <sup>‡</sup> ZHPEV <sup>‡</sup>	748
Extreme Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix	SSPSV <sup>‡</sup> CHPSV <sup>‡</sup>	DSPSV <sup>‡</sup> ZHPSV <sup>‡</sup>	757
Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Eigensystem, $Az=wBz$ , where A and B Are Real General Matrices	SGEGV <sup>‡</sup>	DGEGV <sup>‡</sup>	764
Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Symmetric Eigensystem, $Az=wBz$ , where A Is Real Symmetric and B Is Real Symmetric Positive Definite	SSYGV <sup>‡</sup>	DSYGV <sup>‡</sup>	770

<sup>‡</sup>Not LAPACK. Although this subroutine has the same name as an existing LAPACK subroutine, its calling-sequence arguments and functionality are different from that LAPACK subroutine.

---

### Performance and Accuracy Considerations

1. The accuracy of the resulting eigenvalues and eigenvectors varies between the short- and long-precision versions of each subroutine. The degree of difference depends on the size and conditioning of the matrix computation. Some of the subroutines have examples illustrating this difference.
2. The short precision subroutines provide increased accuracy by accumulating intermediate results in long precision. Occasionally, for performance reasons, these intermediate results are stored.
3. If you want to compute 10% or fewer eigenvalues only, or you want to compute 30% or fewer eigenvalues and eigenvectors, you get better performance if you use `_SPSV` and `_HPSV` instead of `_SPEV` and `_HPEV`, respectively. For all other uses, you should use `_SPEV` and `_HPEV`.
4. There are some ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 48.

---

## **Eigensystem Analysis Subroutines**

This section contains the eigensystem analysis subroutine descriptions.

## SGEEV, DGEEV, CGEEV, and ZGEEV — Eigenvalues and, Optionally, All or Selected Eigenvectors of a General Matrix

### Purpose

SGEEV and DGEEV compute the eigenvalues and, optionally, all or selected eigenvectors of real general matrix  $A$ . CGEEV and ZGEEV compute the eigenvalues and, optionally, all or selected eigenvectors of complex general matrix  $A$ . Eigenvalues are returned in complex vector  $w$ , and eigenvectors are returned in complex matrix  $Z$ :

$$Az = wz$$

Table 133. Data Types

$A$	$w, Z$	$aux$	Subroutine
Short-precision real	Short-precision complex	Short-precision real	SGEEV <sup>‡</sup>
Long-precision real	Long-precision complex	Long-precision real	DGEEV <sup>‡</sup>
Short-precision complex	Short-precision complex	Short-precision real	CGEEV <sup>‡</sup>
Long-precision complex	Long-precision complex	Long-precision real	ZGEEV <sup>‡</sup>

<sup>‡</sup>Not LAPACK. Although this subroutine has the same name as an existing LAPACK subroutine, its calling-sequence arguments and functionality are different from that LAPACK subroutine.

### Syntax

Fortran	CALL SGEEV   DGEEV   CGEEV   ZGEEV ( <i>iopt, a, lda, w, z, ldz, select, n, aux, naux</i> )
C and C++	sgeev   dgeev   cgeev   zgeev ( <i>iopt, a, lda, w, z, ldz, select, n, aux, naux</i> );

### On Entry

- iopt* indicates the type of computation to be performed, where:
- If *iopt* = 0, eigenvalues only are computed.
  - If *iopt* = 1, eigenvalues and eigenvectors are computed.
  - If *iopt* = 2, eigenvalues and eigenvectors corresponding to selected eigenvalues are computed.
- Specified as: a fullword integer; *iopt* = 0, 1, or 2.
- a* is the real or complex general matrix  $A$  of order  $n$ , whose eigenvalues and, optionally, eigenvectors are computed. Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 133. On output,  $A$  is overwritten; that is, the original input is not preserved.
- lda* is the leading dimension of the array specified for *a*. Specified as: a fullword integer;  $lda > 0$  and  $lda \geq n$ .
- w* See “On Return” on page 738.
- z* See “On Return” on page 738.
- ldz* has the following meaning, where:
- If *iopt* = 0, it is not used in the computation.

## SGEEV, DGEEV, CGEEV, and ZGEEV

If  $iopt = 1$  or  $2$ , it is the leading dimension of the output array specified for  $z$ .

Specified as: a fullword integer. It must have the following values, where:

If  $iopt = 0$ ,  $ldz > 0$ .

If  $iopt = 1$  or  $2$ ,  $ldz > 0$  and  $ldz \geq n$ .

*select* has the following meaning, where:

If  $iopt = 0$  or  $1$ , it is not used in the computation.

If  $iopt = 2$ , it is the logical vector *select* of length  $n$  whose true elements indicate those eigenvalues whose corresponding eigenvectors are to be computed.

Specified as: a one-dimensional array of (at least) length  $n$ , containing logical data items. Element values can be true (.TRUE.) or false (.FALSE.).

$n$  is the order of matrix  $A$ .

Specified as: a fullword integer;  $n \geq 0$ .

*aux* has the following meaning:

If  $naux = 0$  and error 2015 is unrecoverable, *aux* is ignored.

Otherwise, it is a storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing numbers of the data type indicated in Table 133 on page 737. On output, the contents are overwritten.

*naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.

Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, SGEEV, DGEEV, CGEEV, and ZGEEV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, it must have the following value, where:

For SGEEV and DGEEV:

If  $iopt = 0$ ,  $naux \geq n$ .

If  $iopt = 1$ ,  $naux \geq 2n$ .

If  $iopt = 2$ ,  $naux \geq n^2 + 4n$ .

For CGEEV and ZGEEV:

If  $iopt = 0$ ,  $naux \geq 2n$ .

If  $iopt = 1$ ,  $naux \geq 3n$ .

If  $iopt = 2$ ,  $naux \geq 2n^2 + 5n$ .

### On Return

$w$  is the vector  $w$  of length  $n$ , containing the eigenvalues of  $A$ . The

eigenvalues are unordered. For SGEEV and DGEEV, complex conjugate pairs appear consecutively with the eigenvalue having the positive imaginary part first.

Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 133 on page 737.

$z$  has the following meaning, where:

If  $iopt = 0$ , it is not used in the computation.

If  $iopt = 1$ , it is the matrix  $Z$  of order  $n$ , containing the eigenvectors of matrix  $A$ . The eigenvector in column  $i$  of matrix  $Z$  corresponds to the eigenvalue  $w_i$ .

If  $iopt = 2$ , it is the  $n$  by  $m$  matrix  $Z$ , containing the  $m$  eigenvectors of matrix  $A$ , which correspond to the  $m$  selected eigenvalues in  $w_i$ , where  $m$  is the number of true elements in the logical vector *select*. The eigenvector in column  $i$  of matrix  $Z$  corresponds to the  $i$ -th selected eigenvalue. Any eigenvector that does not converge is set to 0.

Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 133 on page 737, where:

If  $iopt = 1$ , the array must be  $ldz$  by (at least)  $n$ .

If  $iopt = 2$ , the array must be  $ldz$  by (at least)  $m$ .

## Notes

- When you specify  $iopt = 0$ , you must also specify:
  - A positive value for  $ldz$
  - A dummy argument for  $z$  (see "Example 1" on page 742)
  - A dummy argument for *select*.
- When you specify  $iopt = 1$ , you must also specify a dummy argument for *select*.
- The following items must have no common elements: matrix  $A$ , matrix  $Z$ , vector  $w$ , vector *select*, and the data area specified for *aux*; otherwise, results are unpredictable. See "Concepts" on page 59.
- You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

## Function

The next two sections describe the methods used to compute the eigenvectors and eigenvalues for either a real general matrix or a complex general matrix. For more information on these methods, see references [41], [45], [47], [65], [91], [101], and [103]. If  $n$  is 0, no computation is performed. The results of the computations using short- and long-precision data can vary in accuracy. See the examples for an illustration of the difference in the results.

These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

### Real General Matrix

The eigenvalues and, optionally, all or selected eigenvectors of a real general matrix  $A$  are computed as follows.

- For  $iopt = 0$ , the eigenvalues are computed as follows:
  1. Balance the real general matrix  $A$ .
  2. Reduce the balanced matrix to a real upper Hessenberg matrix using orthogonal similarity transformations.
  3. Compute the eigenvalues of the real upper Hessenberg matrix using the QR algorithm.
  4. The eigenvalues are returned in vector  $w$ .
- For  $iopt = 1$ , the eigenvalues and eigenvectors are computed as follows:
  1. Balance the real general matrix  $A$ .
  2. Reduce the balanced matrix to a real upper Hessenberg matrix using orthogonal similarity transformations.
  3. Accumulate the orthogonal similarity transformations used in the reduction of the real balanced matrix to upper Hessenberg form.
  4. Compute the eigenvalues of the real upper Hessenberg matrix and the eigenvectors of the corresponding real balanced matrix using the QR algorithm.
  5. Back transform the eigenvectors of the balanced matrix to the eigenvectors of the original matrix.
  6. The eigenvalues are returned in vector  $w$ , and the eigenvectors are returned in matrix  $Z$ .
- For  $iopt = 2$ , the eigenvalues and selected eigenvectors are computed as follows:
  1. Balance the real general matrix  $A$ .
  2. Reduce the balanced matrix to a real upper Hessenberg matrix using orthogonal similarity transformations.
  3. Compute the eigenvalues of the real upper Hessenberg matrix using the QR algorithm.
  4. Compute the eigenvectors of the real upper Hessenberg matrix corresponding to selected eigenvalues, indicated in the logical vector *select*, using inverse iteration.
  5. Back transform the eigenvectors of the real upper Hessenberg matrix to the eigenvectors of the balanced matrix.
  6. Back transform the eigenvectors of the balanced matrix to the eigenvectors of the original matrix.
  7. The eigenvalues are returned in vector  $w$ , and the eigenvectors are returned in matrix  $Z$ .

### Complex General Matrix

The eigenvalues and, optionally, all or selected eigenvectors of a complex general matrix  $A$  are computed as follows.

- For  $iopt = 0$ , the eigenvalues are computed as follows:
  1. Balance the complex general matrix  $A$ .
  2. Reduce the complex balanced matrix to a complex upper Hessenberg matrix using unitary similarity transformations.
  3. Compute the eigenvalues of the complex upper Hessenberg matrix using a QR algorithm with implicit shift.
  4. The eigenvalues are returned in vector  $w$ .
- For  $iopt = 1$ , the eigenvalues and eigenvectors are computed as follows:
  1. Balance the complex general matrix  $A$ .
  2. Reduce the complex balanced matrix to a complex upper Hessenberg matrix using unitary similarity transformations.
  3. Accumulate the unitary similarity transformations used in the reduction of the complex balanced matrix to complex upper Hessenberg form.

4. Compute the eigenvalues of the complex upper Hessenberg matrix and the eigenvectors of the complex balanced matrix using a QR algorithm with implicit shift.
  5. Back transform the eigenvectors of the complex balanced matrix to the eigenvectors of the original matrix.
  6. The eigenvalues are returned in vector  $w$ , and the eigenvectors are returned in matrix  $Z$ .
- For  $iopt = 2$ , the eigenvalues and selected eigenvectors are computed as follows:
    1. Balance the complex general matrix  $A$ .
    2. Reduce the complex balanced matrix to a complex upper Hessenberg matrix using unitary similarity transformations.
    3. Compute the eigenvalues of the complex upper Hessenberg matrix using a QR algorithm with implicit shift.
    4. Compute the eigenvectors of the complex upper Hessenberg matrix corresponding to selected eigenvalues, indicated in the logical vector *select*, using inverse iteration.
    5. Back transform the eigenvectors of the complex upper Hessenberg matrix to the eigenvectors of the complex balanced matrix.
    6. Back transform the eigenvectors of the complex balanced matrix to the eigenvectors of the original matrix.
    7. The eigenvalues are returned in vector  $w$ , and the eigenvectors are returned in matrix  $Z$ .

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

1. Eigenvalue ( $i$ ) failed to converge after ( $xxx$ ) iterations.
  - The eigenvalues ( $w_j$ ,  $j = n, n-1, \dots, i+1$ ) are correct.
  - If  $iopt = 1$ , then  $z$  is modified, but no eigenvectors are correct.
  - $a$  is modified.
  - The return code is set to 1.
  - $i$  and  $xxx$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2101 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See “What Can You Do about ESSL Computational Errors?” on page 51.
2. Eigenvector ( $yyy$ ) failed to converge after ( $zzz$ ) iterations. (The computational error message may occur multiple times with processing continuing after each error, because the number of allowable errors for error code 2102 is set to be unlimited in the ESSL error option table.)
  - All eigenvalues are correct.
  - The eigenvector that failed to converge is set to 0.
  - Any selected eigenvectors for which this message has not been issued are correct.
  - $a$  is modified.
  - The return code is set to 2.
  - $yyy$  and  $zzz$  for the last eigenvector that failed to converge can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error 2199 in the ESSL error option table. See “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $iopt \neq 0, 1, \text{ or } 2$
2.  $n < 0$
3.  $lda \leq 0$
4.  $n > lda$
5.  $ldz \leq 0$  and  $iopt \neq 0$
6.  $n > ldz$  and  $iopt \neq 0$
7. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 3 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to find the eigenvalues only of a real short-precision general matrix  $A$  of order 4, where:

- NAUX is equal to N.
- AUX contains N elements.
- LDZ is set to avoid an error condition.
- DUMMY1 and DUMMY2 are used as placeholders for arguments  $z$  and  $select$ , which are not used in the computation.
- On output,  $A$  has been overwritten.

**Note:** This matrix is used in Example 5.5 in referenced text [65].

#### Call Statement and Input:

```

          IOPT  A  LDA  W  Z  LDZ  SELECT  N  AUX  NAUX
CALL SGEEV( 0 , A , 4 , W , DUMMY1 , 1 , DUMMY2 , 4 , AUX , 4 )
    
```

$$A = \begin{bmatrix} -2.0 & 2.0 & 2.0 & 2.0 \\ -3.0 & 3.0 & 2.0 & 2.0 \\ -2.0 & 0.0 & 4.0 & 2.0 \\ -1.0 & 0.0 & 0.0 & 5.0 \end{bmatrix}$$

#### Output:

$$W = \begin{bmatrix} (0.999999, & 0.000000) \\ (2.000001, & 0.000000) \\ (2.999996, & 0.000000) \\ (3.999999, & 0.000000) \end{bmatrix}$$

### Example 2

This example shows how to find the eigenvalues and eigenvectors of a real short-precision general matrix  $A$  of order 3, where:

- NAUX is equal to 2N.
- AUX contains 2N elements.
- DUMMY is used as a placeholder for argument  $select$ , which is not used in the computation.
- On output,  $A$  has been overwritten.

**Note:** This matrix is used in Example 5.1 in referenced text [65].

#### Call Statement and Input:



```

          IOPT  A  LDA  W  Z  LDZ  SELECT  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |    |
CALL SGEEV( 1 , A , 3 , W , Z , 3 , DUMMY , 3 , AUX , 6 )

```

$$A = \begin{bmatrix} 33.0 & 16.0 & 72.0 \\ -24.0 & -10.0 & -57.0 \\ -8.0 & -4.0 & -17.0 \end{bmatrix}$$

**Output:**

$$W = \begin{bmatrix} (3.000022, 0.000000) \\ (1.000019, 0.000000) \\ (1.999961, 0.000000) \end{bmatrix}$$

$$Z = \begin{bmatrix} (2.498781, 0.000000) & (76.837608, 0.000000) & (79.999451, 0.000000) \\ (-1.874081, 0.000000) & (-61.470169, 0.000000) & (-64.999649, 0.000000) \\ (-0.624695, 0.000000) & (-20.489990, 0.000000) & (-19.999886, 0.000000) \end{bmatrix}$$

### Example 3

This example shows how to find the eigenvalues and eigenvectors of a real short-precision general matrix  $A$  of order 3, where:

- NAUX is equal to 2N.
- AUX contains 2N elements.
- DUMMY is used as a placeholder for argument *select*, which is not used in the computation.
- On output, A has been overwritten.

**Note:** This matrix is used in Example 5.4 in referenced text [65].

**Call Statement and Input:**

```

          IOPT  A  LDA  W  Z  LDZ  SELECT  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |    |
CALL SGEEV( 1 , A , 3 , W , Z , 3 , DUMMY , 3 , AUX , 6 )

```

$$A = \begin{bmatrix} 8.0 & -1.0 & -5.0 \\ -4.0 & 4.0 & -2.0 \\ 18.0 & -5.0 & -7.0 \end{bmatrix}$$

**Output:**

$$W = \begin{bmatrix} (1.999999, 3.999998) \\ (1.999999, -3.999998) \\ (0.999997, 0.000000) \end{bmatrix}$$

$$Z = \begin{bmatrix} (0.044710, 0.410578) & (0.044710, -0.410578) & (1.732048, 0.000000) \\ (-0.365868, 0.455287) & (-0.365868, -0.455287) & (3.464096, 0.000000) \\ (0.455287, 0.365868) & (0.455287, -0.365868) & (1.732049, 0.000000) \end{bmatrix}$$

### Example 4

This example shows how to find the eigenvalues and selected eigenvectors of a real short-precision general matrix  $A$  of order 4, where:

- NAUX is equal to  $N^2+4N$ .

## SGEEV, DGEEV, CGEEV, and ZGEEV

- AUX contains NAUX elements.
- The first, third, and fourth eigenvectors are selected and appear in the first, second, and third columns of matrix Z, respectively.
- On output, A has been overwritten.

**Note:** This matrix is used in Example 5.5 in referenced text [65].

### Call Statement and Input:

```

          IOPT  A  LDA  W  Z  LDZ  SELECT  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |
CALL SGEEV( 2 , A , 4 , W , Z , 4 , SELECT , 4 , AUX , 32 )

```

$$A = \begin{bmatrix} -2.0 & 2.0 & 2.0 & 2.0 \\ -3.0 & 3.0 & 2.0 & 2.0 \\ -2.0 & 0.0 & 4.0 & 2.0 \\ -1.0 & 0.0 & 0.0 & 5.0 \end{bmatrix}$$

$$\text{SELECT} = \begin{bmatrix} \text{.TRUE.} \\ \text{.FALSE.} \\ \text{.TRUE.} \\ \text{.TRUE.} \end{bmatrix}$$

### Output:

$$W = \begin{bmatrix} (0.999999, 0.000000) \\ (2.000001, 0.000000) \\ (2.999996, 0.000000) \\ (3.999999, 0.000000) \end{bmatrix}$$

$$Z = \begin{bmatrix} (1.000000, 0.000000) & (-0.674014, 0.000000) & (-0.474306, 0.000000) \\ (0.750000, 0.000000) & (-0.674014, 0.000000) & (-0.474306, 0.000000) \\ (0.500000, 0.000000) & (-0.674013, 0.000000) & (-0.474306, 0.000000) \\ (0.250000, 0.000000) & (-0.337006, 0.000000) & (-0.474305, 0.000000) \end{bmatrix}$$

### Example 5

This example shows how to find the eigenvalues and selected eigenvectors of a real short-precision general matrix  $A$  of order 3, where:

- NAUX is equal to  $N^2+4N$ .
- AUX contains NAUX elements.
- The first and second eigenvectors are selected and appear in the first and second columns of matrix Z, respectively.
- On output, A has been overwritten.

**Note:** This matrix is used in Example 5.4 in referenced text [65].

### Call Statement and Input:

```

          IOPT  A  LDA  W  Z  LDZ  SELECT  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |
CALL SGEEV( 2 , A , 3 , W , Z , 3 , SELECT , 3 , AUX , 21 )

```

$$A = \begin{bmatrix} 8.0 & -1.0 & -5.0 \\ -4.0 & 4.0 & -2.0 \\ 18.0 & -5.0 & -7.0 \end{bmatrix}$$

$$\text{SELECT} = \begin{bmatrix} \text{.TRUE.} \\ \text{.TRUE.} \\ \text{.FALSE.} \end{bmatrix}$$

**Output:**

$$W = \begin{bmatrix} (1.999999, 3.999998) \\ (1.999999, -3.999998) \\ (0.999997, 0.000000) \end{bmatrix}$$

$$Z = \begin{bmatrix} (0.500000, 0.000000) & (0.500000, 0.000000) \\ (0.500000, 0.500000) & (0.500000, -0.500000) \\ (0.500000, -0.500000) & (0.500000, 0.500000) \end{bmatrix}$$

### Example 6

This example shows how the results of Example 5 would differ if matrix *A* was a real long-precision general matrix. On output, *A* has been overwritten.

**Call Statement and Input:**

```

          IOPT  A  LDA  W  Z  LDZ  SELECT  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |
CALL DGEEV( 2 , A , 3 , W , Z , 3 , SELECT , 3 , AUX , 21 )
    
```

**Output:**

$$W = \begin{bmatrix} (2.000000, 4.000000) \\ (2.000000, -4.000000) \\ (1.000000, 0.000000) \end{bmatrix}$$

$$Z = \begin{bmatrix} (0.500000, 0.000000) & (0.500000, 0.000000) \\ (0.500000, 0.500000) & (0.500000, -0.500000) \\ (0.500000, -0.500000) & (0.500000, 0.500000) \end{bmatrix}$$

### Example 7

This example shows how to find the eigenvalues only of a complex long-precision general matrix *A* of order 3, where:

- NAUX is equal to 2N.
- AUX contains 2N elements.
- LDZ is set to avoid an error condition.
- DUMMY1 and DUMMY2 are used as placeholders for arguments *z* and *select*, which are not used in the computation.
- On output, *A* has been overwritten.

**Note:** This matrix is used in Example 6.4 in referenced text [65].

**Call Statement and Input:**

```

          IOPT  A  LDA  W  Z  LDZ  SELECT  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |
CALL ZGEEV( 0 , A , 3 , W , DUMMY1 , 1 , DUMMY2 , 3 , AUX , 6 )
    
```

$$A = \begin{bmatrix} (1.0, 2.0) & (3.0, 4.0) & (21.0, 22.0) \\ (43.0, 44.0) & (13.0, 14.0) & (15.0, 16.0) \\ (5.0, 6.0) & (7.0, 8.0) & (25.0, 26.0) \end{bmatrix}$$

## SGEEV, DGEEV, CGEEV, and ZGEEV

**Output:**

$$W = \begin{bmatrix} (39.776655, 42.995668) \\ (-7.477530, 6.880321) \\ (6.700876, -7.875989) \end{bmatrix}$$

### Example 8

This example shows how to find the eigenvalues and eigenvectors of a complex long-precision general matrix  $A$  of order 4, where:

- NAUX is equal to 3N.
- AUX contains 3N elements.
- DUMMY is used as a placeholder for argument *select*, which is not used in the computation.
- On output,  $A$  has been overwritten.

**Note:** This matrix is used in Example 6.5 in referenced text [65].

**Call Statement and Input:**

```

          IOPT  A  LDA  W  Z  LDZ  SELECT  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |
CALL ZGEEV( 1 , A , 4 , W , Z , 4 , DUMMY , 4 , AUX , 12 )

```

$$A = \begin{bmatrix} (5.0, 9.0) & (5.0, 5.0) & (-6.0, -6.0) & (-7.0, -7.0) \\ (3.0, 3.0) & (6.0, 10.0) & (-5.0, -5.0) & (-6.0, -6.0) \\ (2.0, 2.0) & (3.0, 3.0) & (-1.0, 3.0) & (-5.0, -5.0) \\ (1.0, 1.0) & (2.0, 2.0) & (-3.0, -3.0) & (0.0, 4.0) \end{bmatrix}$$

**Output:**

$$W = \begin{bmatrix} (4.000000, 8.000000) \\ (2.000000, 6.000000) \\ (3.000000, 7.000000) \\ (1.000000, 5.000000) \end{bmatrix}$$

$$Z = \begin{bmatrix} (0.625817, 0.229776) & (0.333009, -0.729358) & (-1.535458, 1.519551) & (0.000000, 3.464102) \\ (0.625817, 0.229776) & (0.666017, -1.458715) & (-1.535458, 1.519551) & (0.000000, 1.732051) \\ (0.625817, 0.229776) & (0.333009, -0.729358) & (0.000000, 0.000000) & (0.000000, 1.732051) \\ (0.000000, 0.000000) & (0.333009, -0.729358) & (-1.535458, 1.519551) & (0.000000, 1.732051) \end{bmatrix}$$

### Example 9

This example shows how to find the eigenvalues and selected eigenvectors of a complex long-precision general matrix  $A$  of order 4, where:

- NAUX is equal to  $2N^2+5N$ .
- AUX contains NAUX elements.
- The first, third, and fourth eigenvectors are selected and appear in the first, second, and third columns of matrix  $Z$ , respectively.
- On output,  $A$  has been overwritten.

**Note:** This matrix is used in Example 6.5 in referenced text [65].

**Call Statement and Input:**

```

          IOPT  A  LDA  W  Z  LDZ  SELECT  N  AUX  NAUX
          |    |    |    |    |    |    |    |    |
CALL ZGEEV( 2 , A , 4 , W , Z , 4 , SELECT , 4 , AUX , 52 )
    
```

$$A = \begin{bmatrix} (5.0, 9.0) & (5.0, 5.0) & (-6.0, -6.0) & (-7.0, -7.0) \\ (3.0, 3.0) & (6.0, 10.0) & (-5.0, -5.0) & (-6.0, -6.0) \\ (2.0, 2.0) & (3.0, 3.0) & (-1.0, 3.0) & (-5.0, -5.0) \\ (1.0, 1.0) & (2.0, 2.0) & (-3.0, -3.0) & (0.0, 4.0) \end{bmatrix}$$

$$SELECT = \begin{bmatrix} .TRUE. \\ .FALSE. \\ .TRUE. \\ .TRUE. \end{bmatrix}$$

**Output:**

$$W = \begin{bmatrix} (4.000000, 8.000000) \\ (2.000000, 6.000000) \\ (3.000000, 7.000000) \\ (1.000000, 5.000000) \end{bmatrix}$$

$$Z = \begin{bmatrix} (-0.748331, 0.000000) & (-0.935414, 0.000000) & (-1.247219, 0.000000) \\ (-0.748331, 0.000000) & (-0.935414, 0.000000) & (-0.623610, 0.000000) \\ (-0.748331, 0.000000) & (0.000000, 0.000000) & (-0.623610, 0.000000) \\ (0.000000, 0.000000) & (-0.935414, 0.000000) & (-0.623610, 0.000000) \end{bmatrix}$$

## SSPEV, DSPEV, CHPEV, and ZHPEV — Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix

### Purpose

SSPEV and DSPEV compute the eigenvalues and, optionally, the eigenvectors of real symmetric matrix  $A$ , stored in lower- or upper-packed storage mode. CHPEV and ZHPEV compute the eigenvalues and, optionally, the eigenvectors of complex Hermitian matrix  $A$ , stored in lower- or upper-packed storage mode. Eigenvalues are returned in vector  $w$ , and eigenvectors are returned in matrix  $Z$ :

$$Az = wz$$

where  $A = A^T$  or  $A = A^H$ .

Table 134. Data Types

$A, z$	$w, aux$	Subroutine
Short-precision real	Short-precision real	SSPEV <sup>‡</sup>
Long-precision real	Long-precision real	DSPEV <sup>‡</sup>
Short-precision complex	Short-precision real	CHPEV <sup>‡</sup>
Long-precision complex	Long-precision real	ZHPEV <sup>‡</sup>

<sup>‡</sup>Not LAPACK. Although this subroutine has the same name as an existing LAPACK subroutine, its calling-sequence arguments and functionality are different from that LAPACK subroutine.

**Note:** For compatibility with earlier releases of ESSL, you can use the names SSLEV, DSLEV, CHLEV, and ZHLEV for SSPEV, DSPEV, CHPEV, and ZHPEV, respectively.

### Syntax

<b>Fortran</b>	CALL SSPEV   DSPEV   CHPEV   ZHPEV ( <i>iopt, ap, w, z, ldz, n, aux, naux</i> )
<b>C and C++</b>	sspev   dspev   chpev   zhpev ( <i>iopt, ap, w, z, ldz, n, aux, naux</i> );

### On Entry

*iopt* indicates the type of computation to be performed, where:

If *iopt* = 0 or 20, eigenvalues only are computed.

If *iopt* = 1 or 21, eigenvalues and eigenvectors are computed.

Specified as: a fullword integer; *iopt* = 0, 1, 20, or 21.

*ap* is the real symmetric or complex Hermitian matrix  $A$  of order  $n$ , whose eigenvalues and, optionally, eigenvectors are computed. It is stored in an array, referred to as  $AP$ , where:

If *iopt* = 0 or 1, it is stored in lower-packed storage mode.

If *iopt* = 20 or 21, it is stored in upper-packed storage mode.

Specified as: a one-dimensional array of (at least) length  $n(n+1)/2$ , containing numbers of the data type indicated in Table 134. On

output, for SSPEV and DSPEV if  $iopt = 0$  or  $20$ , and for CHPEV and ZHPEV,  $AP$  is overwritten; that is, the original input is not preserved.

$w$  See "On Return."

$z$  See "On Return."

$ldz$  has the following meaning, where:

If  $iopt = 0$  or  $20$ , it is not used in the computation.

If  $iopt = 1$  or  $21$ , it is the leading dimension of the output array specified for  $z$ .

Specified as: a fullword integer. It must have the following value, where:

If  $iopt = 0$  or  $20$ ,  $ldz > 0$ .

If  $iopt = 1$  or  $21$ ,  $ldz > 0$  and  $ldz \geq n$ .

$n$  is the order of matrix  $A$ .

Specified as: a fullword integer;  $n \geq 0$ .

$aux$  has the following meaning:

If  $naux = 0$  and error 2015 is unrecoverable,  $aux$  is ignored.

Otherwise, it is a storage work area used by this subroutine. Its size is specified by  $naux$ .

Specified as: an area of storage, containing numbers of the data type indicated in Table 134 on page 748. On output, the contents are overwritten.

$naux$  is the size of the work area specified by  $aux$ —that is, the number of elements in  $aux$ .

Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, SSPEV, DSPEV, CHPEV, and ZHPEV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, It must have the following value, where:

For SSPEV and DSPEV:

If  $iopt = 0$  or  $20$ ,  $naux \geq n$ .

If  $iopt = 1$  or  $21$ ,  $naux \geq 2n$ .

For CHPEV and ZHPEV:

If  $iopt = 0$  or  $20$ ,  $naux \geq 3n$ .

If  $iopt = 1$  or  $21$ ,  $naux \geq 4n$ .

### On Return

$w$  is the vector  $w$  of length  $n$ , containing the eigenvalues of  $A$  in ascending order. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 134 on page 748.

$z$  has the following meaning, where:

## SSPEV, DSPEV, CHPEV, and ZHPEV

If  $iopt = 0$  or  $20$ , it is not used in the computation.

If  $iopt = 1$  or  $21$ , it is the matrix  $Z$  of order  $n$ , containing the orthonormal eigenvectors of matrix  $A$ . The eigenvector in column  $i$  of matrix  $Z$  corresponds to the eigenvalue  $w_i$ .

Returned as: an  $ldz$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 134 on page 748.

### Notes

1. When you specify  $iopt = 0$  or  $20$ , you must specify:
  - A positive value for  $ldz$
  - A dummy argument for  $z$  (see “Example 1” on page 752)
2. The following items must have no common elements: matrix  $A$ , matrix  $Z$ , vector  $w$ , and the data area specified for  $aux$ ; otherwise, results are unpredictable. See “Concepts” on page 59.
3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values.
4. For a description of how real symmetric matrices are stored in lower- or upper-packed storage mode, see “Lower-Packed Storage Mode” on page 69 or “Upper-Packed Storage Mode” on page 71, respectively.  
For a description of how complex Hermitian matrices are stored in lower- or upper-packed storage mode, see “Complex Hermitian Matrix” on page 73.
5. You have the option of having the minimum required value for  $naux$  dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

### Function

The next two sections describe the methods used to compute the eigenvalues and, optionally, the eigenvectors for either a real symmetric matrix or a complex Hermitian matrix. For more information on these methods, see references [41], [45], [65], [91], [101], and [103]. If  $n$  is 0, no computation is performed. The results of the computations using short- and long-precision data can vary in accuracy. See “Example 3” on page 753 and “Example 4” on page 753 for an illustration of the difference in results. Eigenvalues computed using equivalent  $iopt$  values are mathematically equivalent, but are not guaranteed to be bitwise identical. For example, the results computed using  $iopt = 0$  and  $iopt = 20$  are mathematically equivalent, but are not necessarily bitwise identical.

These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

#### Real Symmetric Matrix

The eigenvalues and, optionally, the eigenvectors of a real symmetric matrix  $A$  are computed as follows:

- For  $iopt = 0$  or  $20$ , the eigenvalues are computed as follows:
  1. Reduce the real symmetric matrix  $A$  to a real symmetric tridiagonal matrix using orthogonal similarity transformations.
  2. Compute the eigenvalues of the real symmetric tridiagonal matrix using the implicit QL algorithm.
  3. The eigenvalues are ordered and returned in vector  $w$ .
- For  $iopt = 1$  or  $21$ , the eigenvalues and eigenvectors are computed as follows:



1. Reduce the real symmetric matrix  $A$  to a real symmetric tridiagonal matrix using and accumulating orthogonal similarity transformations.
2. Compute the eigenvalues of the real symmetric tridiagonal matrix and the eigenvectors of the real symmetric matrix using the implicit QL algorithm.
3. The eigenvalues are ordered and returned in vector  $w$ , and the corresponding eigenvectors are returned in matrix  $Z$ .

### Complex Hermitian Matrix

The eigenvalues and, optionally, the eigenvectors of a complex Hermitian matrix  $A$  are computed as follows:

- For  $iopt = 0$  or  $20$ , the eigenvalues are computed as follows:
  1. Reduce the complex Hermitian matrix  $A$  to a real symmetric tridiagonal matrix using unitary similarity transformations.
  2. Compute the eigenvalues of the real symmetric tridiagonal matrix using the implicit QL algorithm.
  3. The eigenvalues are ordered and returned in vector  $w$ .
- For  $iopt = 1$  or  $21$ , the eigenvalues and eigenvectors are computed as follows:
  1. Reduce the complex Hermitian matrix  $A$  to a real symmetric tridiagonal matrix using unitary similarity transformations.
  2. Compute the eigenvalues and eigenvectors of the real symmetric tridiagonal matrix using the implicit QL algorithm.
  3. Back transform the eigenvectors of the real symmetric tridiagonal matrix to those of the original complex Hermitian matrix.
  4. The eigenvalues are ordered and returned in vector  $w$ , and the corresponding eigenvectors are returned in matrix  $Z$ .

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

Eigenvalue ( $i$ ) failed to converge after ( $xxx$ ) iterations:

- The eigenvalues ( $w_j$ ,  $j = 1, 2, \dots, i-1$ ) are correct, but are unordered.
- If  $iopt = 1$  or  $21$ , then  $z$  is modified, but no eigenvectors are correct.
- If  $iopt = 0$  or  $20$  for SSPEV and DSPEV,  $ap$  is modified.
- For CHPEV and ZHPEV,  $ap$  is modified.
- The return code is set to 1.
- $i$  and  $xxx$  can be determined at run time by use of the ESSL error-handling-facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2101 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See "What Can You Do about ESSL Computational Errors?" on page 51.

### Input-Argument Errors

1.  $iopt \neq 0, 1, 20, \text{ or } 21$
2.  $n < 0$
3.  $ldz \leq 0$  and  $iopt = 1$  or  $21$
4.  $n > ldz$  and  $iopt = 1$  or  $21$
5. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 2 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to find the eigenvalues only of a real short-precision symmetric matrix  $A$  of order 3, stored in lower-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 1.0 & -1.0 & 0.0 \\ -1.0 & 2.0 & -1.0 \\ 0.0 & -1.0 & 1.0 \end{bmatrix}$$

where:

- NAUX is equal to N.
- AUX contains N elements.
- LDZ is set to 1 to avoid an error condition.
- DUMMY is used as a placeholder for argument  $z$ , which is not used in the computation.
- On output, AP has been overwritten.

#### Call Statement and Input:

```

          IOPT  AP  W  Z  LDZ  N  AUZ  NAUX
          |    |  |  |  |    |  |    |
CALL SSPEV( 0 , AP , W , DUMMY , 1 , 3 , AUX , 3 )
    
```

AP = (1.0, -1.0, 0.0, 2.0, -1.0, 1.0)

#### Output:

$$W = \begin{bmatrix} 0.000000 \\ 1.000000 \\ 3.000000 \end{bmatrix}$$

### Example 2

This example shows how to find the eigenvalues and eigenvectors of a real short-precision symmetric matrix  $A$  of order 4, stored in upper-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 5.0 & 4.0 & 1.0 & 1.0 \\ 4.0 & 5.0 & 1.0 & 1.0 \\ 1.0 & 1.0 & 4.0 & 2.0 \\ 1.0 & 1.0 & 2.0 & 4.0 \end{bmatrix}$$

where:

- NAUX is equal to 2N.
- AUX contains 2N elements.

**Note:** This matrix is used in Example 4.1 in referenced text [65].

#### Call Statement and Input:

```

          IOPT  AP  W  Z  LDZ  N  AUZ  NAUX
          |    |  |  |  |    |  |    |
CALL SSPEV( 21 , AP , W , Z , 4 , 4 , AUX , 8 )
    
```

AP = (5.0, 4.0, 5.0, 1.0, 1.0, 4.0, 1.0, 1.0, 2.0, 4.0)

#### Output:

$$W = \begin{bmatrix} 1.000000 \\ 2.000000 \\ 5.000000 \\ 9.999999 \end{bmatrix}$$

$$Z = \begin{bmatrix} 0.707107 & 0.000000 & 0.316227 & 0.632455 \\ -0.707107 & 0.000000 & 0.316228 & 0.632455 \\ 0.000000 & -0.707106 & -0.632455 & 0.316227 \\ 0.000000 & 0.707107 & -0.632455 & 0.316228 \end{bmatrix}$$

### Example 3

This example shows how to find the eigenvalues and eigenvectors of a real short-precision symmetric matrix  $A$ , stored in lower-packed storage mode, which has an eigenvalue of multiplicity 2. Matrix  $A$  is:

$$\begin{bmatrix} 6.0 & 4.0 & 4.0 & 1.0 \\ 4.0 & 6.0 & 1.0 & 4.0 \\ 4.0 & 1.0 & 6.0 & 4.0 \\ 1.0 & 4.0 & 4.0 & 6.0 \end{bmatrix}$$

where:

- NAUX is equal to 2N.
- AUX contains 2N elements.

**Note:** This matrix is used in Example 4.2 in referenced text [65].

#### Call Statement and Input:

```

          IOPT  AP   W   Z  LDZ  N   AUZ  NAUX
          |    |   |   |   |   |   |   |
CALL SSPEV( 1 , AP , W , Z , 7 , 4 , AUX , 8 )
    
```

AP = (6.0, 4.0, 4.0, 1.0, 6.0, 1.0, 4.0, 6.0, 4.0, 6.0)

#### Output:

$$W = \begin{bmatrix} -1.000000 \\ 4.999999 \\ 5.000000 \\ 15.000000 \end{bmatrix}$$

$$Z = \begin{bmatrix} -0.500000 & 0.000000 & 0.707107 & 0.500000 \\ 0.500000 & 0.707107 & 0.000000 & 0.500000 \\ 0.500000 & -0.707107 & 0.000000 & 0.500000 \\ -0.500000 & 0.000000 & -0.707107 & 0.500000 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 4

This example shows how the results of Example 3 differ if matrix  $A$  is a real long-precision symmetric matrix.

#### Call Statement and Input:

## SSPEV, DSPEV, CHPEV, and ZHPEV

```

          IOPT  AP   W   Z   LDZ  N   AUZ  NAUX
          |    |   |   |   |   |   |   |
CALL DSPEV( 1 , AP , W , Z , 7 , 4 , AUX , 8 )

```

### Output:

$$W = \begin{bmatrix} -1.000000 \\ 5.000000 \\ 5.000000 \\ 15.000000 \end{bmatrix}$$

$$Z = \begin{bmatrix} -0.500000 & -0.216773 & -0.673060 & 0.500000 \\ 0.500000 & 0.673060 & -0.216773 & 0.500000 \\ 0.500000 & -0.673060 & 0.216773 & 0.500000 \\ -0.500000 & 0.216773 & 0.673060 & 0.500000 \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

### Example 5

This example shows how to find the eigenvalues and eigenvectors of a complex Hermitian matrix  $A$  of order 2, stored in lower-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} (1.0, 0.0) & (0.0, -1.0) \\ (0.0, 1.0) & (1.0, 0.0) \end{bmatrix}$$

where:

- NAUX is equal to 4N.
- AUX contains 4N elements.
- On output, AP has been overwritten.

**Note:** This matrix is used in Example 6.1 in referenced text [65].

### Call Statement and Input:

```

          IOPT  AP   W   Z   LDZ  N   AUZ  NAUX
          |    |   |   |   |   |   |   |
CALL ZHPEV( 1 , AP , W , Z , 2 , 2 , AUX , 8 )

```

```
AP = ((1.0, . ), (0.0, 1.0), (1.0, . ))
```

### Output:

$$W = \begin{bmatrix} 0.000000 \\ 2.000000 \end{bmatrix}$$

$$Z = \begin{bmatrix} (0.000000, -0.707107) & (0.000000, -0.707107) \\ (-0.707107, 0.000000) & (0.707107, 0.000000) \end{bmatrix}$$

### Example 6

This example shows how to find the eigenvalues only of a complex Hermitian matrix  $A$  of order 4, stored in upper-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} (3.0, 0.0) & (1.0, 0.0) & (0.0, 0.0) & (0.0, 2.0) \\ (1.0, 0.0) & (3.0, 0.0) & (0.0, -2.0) & (0.0, 0.0) \end{bmatrix}$$

$$\begin{bmatrix} (0.0, 0.0) & (0.0, 2.0) & (1.0, 0.0) & (1.0, 0.0) \\ (0.0, -2.0) & (0.0, 0.0) & (1.0, 0.0) & (1.0, 0.0) \end{bmatrix}$$

where:

- NAUX is equal to 3N.
- AUX contains 3N elements.
- LDZ is set to 1 to avoid an error condition.
- DUMMY is used as a placeholder for argument  $z$ , which is not used in the computation.
- On output, AP has been overwritten.

**Note:** This matrix is used in Example 6.6 in referenced text [65].

**Call Statement and Input:**

```

          IOPT  AP  W  Z  LDZ  N  AUZ  NAUX
CALL ZHPEV( 20 , AP , W , DUMMY , 1 , 4 , AUX , 12 )

```

$$AP = \begin{pmatrix} (3.0, .) & (1.0, 0.0) & (3.0, .) & (0.0, 0.0) \\ (0.0, -2.0) & (1.0, .) & (0.0, 2.0) & (0.0, 0.0) \\ (1.0, 0.0) & (1.0, .) & & \end{pmatrix}$$

**Output:**

$$W = \begin{bmatrix} -0.828427 \\ 0.000000 \\ 4.000000 \\ 4.828427 \end{bmatrix}$$

**Example 7**

This example shows how to find the eigenvalues and eigenvectors of a complex Hermitian matrix  $A$  of order 2, stored in lower-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} (1.0, 0.0) & (1.0, -1.0) \\ (1.0, 1.0) & (1.0, 0.0) \end{bmatrix}$$

where:

- NAUX is equal to 4N.
- AUX contains 4N elements.
- On output, AP has been overwritten.

**Note:** This matrix is used in Example 6.2 in referenced text [65].

**Call Statement and Input:**

```

          IOPT  AP  W  Z  LDZ  N  AUZ  NAUX
CALL ZHPEV( 1 , AP , W , Z , 2 , 2 , AUX , 8 )

```

$$AP = \begin{pmatrix} (1.0, .) & (1.0, 1.0) & (1.0, .) \end{pmatrix}$$

**Output:**

$$W = \begin{bmatrix} -0.414214 \\ 2.414214 \end{bmatrix}$$

## SSPEV, DSPEV, CHPEV, and ZHPEV

$$Z = \begin{bmatrix} (0.500000, -0.500000) & (0.500000, -0.500000) \\ (-0.707107, 0.000000) & (0.707107, 0.000000) \end{bmatrix}$$

## SSPSV, DSPSV, CHPSV, and ZHPSV — Extreme Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix

### Purpose

SSPSV and DSPSV compute the extreme eigenvalues and, optionally, the eigenvectors of real symmetric matrix  $A$ , stored in lower- or upper-packed storage mode. CHPSV and ZHPSV compute the extreme eigenvalues and, optionally, the eigenvectors of complex Hermitian matrix  $A$ , stored in lower- or upper-packed storage mode. The extreme eigenvalues are returned in vector  $w$ , and the corresponding eigenvectors are returned in matrix  $Z$ :

$$Az = wz$$

where  $A = A^T$  or  $A = A^H$ .

Table 135. Data Types

$A, z$	$w, aux$	Subroutine
Short-precision real	Short-precision real	SSPSV <sup>‡</sup>
Long-precision real	Long-precision real	DSPSV <sup>‡</sup>
Short-precision complex	Short-precision real	CHPSV <sup>‡</sup>
Long-precision complex	Long-precision real	ZHPSV <sup>‡</sup>

<sup>‡</sup>Not LAPACK. Although this subroutine has the same name as an existing LAPACK subroutine, its calling-sequence arguments and functionality are different from that LAPACK subroutine.

**Note:** If you want to compute 10% or fewer eigenvalues only, or you want to compute 30% or fewer eigenvalues and eigenvectors, you get better performance if you use `_SPSV` and `_HPSV` instead of `_SPEV` and `_HPEV`, respectively. For all other uses, you should use `_SPEV` and `_HPEV`.

### Syntax

<b>Fortran</b>	CALL SSPSV   DSPSV   CHPSV   ZHPSV ( <i>iopt</i> , <i>ap</i> , <i>w</i> , <i>z</i> , <i>ldz</i> , <i>n</i> , <i>m</i> , <i>aux</i> , <i>naux</i> )
<b>C and C++</b>	sspsv   dspsv   chpsv   zhpsv ( <i>iopt</i> , <i>ap</i> , <i>w</i> , <i>z</i> , <i>ldz</i> , <i>n</i> , <i>m</i> , <i>aux</i> , <i>naux</i> );

### On Entry

*iopt* indicates the type of computation to be performed, where:

- If *iopt* = 0 or 20, the *m* smallest eigenvalues only are computed.
- If *iopt* = 1 or 21, the *m* smallest eigenvalues and the eigenvectors are computed.
- If *iopt* = 10 or 30, the *m* largest eigenvalues only are computed.
- If *iopt* = 11 or 31, the *m* largest eigenvalues and the eigenvectors are computed.

Specified as: a fullword integer; *iopt* = 0, 1, 10, 11, 20, 21, 30, or 31.

*ap* is the real symmetric or complex Hermitian matrix  $A$  of order  $n$ ,

## SSPSV, DSPSV, CHPSV, and ZHPSV

whose  $m$  smallest or largest eigenvalues and, optionally, the corresponding eigenvectors are computed. It is stored in an array, referred to as  $AP$ , where:

If  $iopt = 0, 1, 10,$  or  $11$ , it is stored in lower-packed storage mode.

If  $iopt = 20, 21, 30,$  or  $31$ , it is stored in upper-packed storage mode.

Specified as: a one-dimensional array of (at least) length  $n(n+1)/2$ , containing numbers of the data type indicated in Table 135 on page 757. On output,  $AP$  is overwritten; that is, the original input is not preserved.

$w$  See "On Return" on page 759.

$z$  See "On Return" on page 759.

$ldz$  has the following meaning, where:

If  $iopt = 0, 10, 20,$  or  $30$ , it is not used in the computation.

If  $iopt = 1, 11, 21,$  or  $31$ , it is the leading dimension of the output array specified for  $z$ .

Specified as: a fullword integer. It must have the following value, where:

If  $iopt = 0, 10, 20,$  or  $30$ ,  $ldz > 0$ .

If  $iopt = 1, 11, 21,$  or  $31$ ,  $ldz > 0$  and  $ldz \geq n$ .

$n$  is the order of matrix  $A$ .

Specified as: a fullword integer;  $n \geq 0$ .

$m$  is the number of eigenvalues and, optionally, eigenvectors to be computed. Specified as: a fullword integer;  $0 \leq m \leq n$ .

$aux$  has the following meaning:

If  $naux = 0$  and error 2015 is unrecoverable,  $aux$  is ignored.

Otherwise, it is a storage work area used by this subroutine. Its size is specified by  $naux$ .

Specified as: an area of storage, containing numbers of the data type indicated in Table 135 on page 757. On output, the contents are overwritten.

$naux$  is the size of the work area specified by  $aux$ —that is, the number of elements in  $aux$ .

Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, SSPSV, DSPSV, CHPSV, and ZHPSV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, It must have the following value, where:

For SSPSV and DSPSV:

If  $iopt = 0, 10, 20,$  or  $30$ ,  $naux \geq 3n$ .

If  $iopt = 1, 11, 21,$  or  $31$ ,  $naux \geq 9n$ .



For CHPSV and ZHPSV:

If  $iopt = 0, 10, 20,$  or  $30$ ,  $naux \geq 5n$ .

If  $iopt = 1, 11, 21,$  or  $31$ ,  $naux \geq 11n$ .

## On Return

$w$  is the vector  $w$  of length  $n$ , containing in the first  $m$  positions of either the  $m$  smallest eigenvalues of  $A$  in ascending order or the  $m$  largest eigenvalues of  $A$  in descending order.

Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 135 on page 757.

$z$  has the following meaning, where:

If  $iopt = 0, 10, 20,$  or  $30$ , it is not used in the computation.

If  $iopt = 1, 11, 21,$  or  $31$ , it is the  $n$  by  $m$  matrix  $Z$ , containing  $m$  orthonormal eigenvectors of matrix  $A$ . The eigenvector in column  $i$  of matrix  $Z$  corresponds to the eigenvalue  $w_i$ .

Returned as: an  $ldz$  by (at least)  $m$  array, containing numbers of the data type indicated in Table 135 on page 757.

## Notes

- When you specify  $iopt = 0, 10, 20,$  or  $30$ , you must specify:
  - A positive value for  $ldz$
  - A dummy argument for  $z$  (see "Example 4" on page 763)
- The following items must have no common elements: matrix  $A$ , matrix  $Z$ , vector  $w$ , and the data area specified for  $aux$ ; otherwise, results are unpredictable. See "Concepts" on page 59.
- On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $A$  are assumed to be zero, so you do not have to set these values.
- For a description of how real symmetric matrices are stored in lower- or upper-packed storage mode, see "Lower-Packed Storage Mode" on page 69 or "Upper-Packed Storage Mode" on page 71, respectively.  
For a description of how complex Hermitian matrices are stored in lower- or upper-packed storage mode, see "Complex Hermitian Matrix" on page 73.
- You have the option of having the minimum required value for  $naux$  dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

## Function

The methods used to compute the extreme eigenvalues and, optionally, the eigenvectors for either a real symmetric matrix or a complex Hermitian matrix are described in the steps below. For more information on these methods, see references [41], [45], [65], [91], [101], and [103]. If  $n$  or  $m$  is 0, no computation is performed. The results of the computations using short- and long-precision data can vary in accuracy. Eigenvalues computed using equivalent  $iopt$  values are mathematically equivalent, but are not guaranteed to be bitwise identical. For example, the results computed using  $iopt = 0$  and  $iopt = 20$  are mathematically equivalent, but are not necessarily bitwise identical.

## SSPSV, DSPSV, CHPSV, and ZHPSV

These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

The extreme eigenvalues and, optionally, the eigenvectors of a real symmetric matrix  $A$  or complex Hermitian matrix  $A$  are computed as follows:

- For  $iopt = 0, 10, 20,$  or  $30$ , the eigenvalues are computed as follows:
  1. Reduce the real symmetric matrix  $A$  (for SSPSV and DSPSV) or complex Hermitian matrix  $A$  (for CHPSV and ZHPSV) to a real symmetric tridiagonal matrix using orthogonal similarity transformations (for SSPSV and DSPSV) or unitary similarity transforms (for CHPSV and ZHPSV).
  2. Compute the  $m$  smallest eigenvalues or  $m$  largest eigenvalues of the real symmetric tridiagonal matrix using a rational variant of the QR method with Newton corrections.
  3. The eigenvalues are returned in vector  $w$  in the first  $m$  positions, where the  $m$  smallest are placed in ascending order, or the  $m$  largest are placed in descending order.
- For  $iopt = 1, 11, 21,$  or  $31$ , the eigenvalues and eigenvectors are computed as follows:
  1. Reduce the real symmetric matrix  $A$  (for SSPSV and DSPSV) or complex Hermitian matrix  $A$  (for CHPSV and ZHPSV) to a real symmetric tridiagonal matrix using orthogonal similarity transformations (for SSPSV and DSPSV) or unitary similarity transforms (for CHPSV and ZHPSV).
  2. Compute the  $m$  smallest eigenvalues or  $m$  largest eigenvalues of the real symmetric tridiagonal matrix using a rational variant of the QR method with Newton corrections.
  3. Compute the corresponding eigenvectors of the real symmetric tridiagonal matrix using inverse iteration.
  4. Back transform the eigenvectors of the real symmetric tridiagonal matrix to those of the original matrix.
  5. The eigenvalues are returned in vector  $w$  in the first  $m$  positions, where the  $m$  smallest are placed in ascending order, or the  $m$  largest are placed in descending order. The corresponding eigenvectors are returned in matrix  $Z$ .

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

1. Eigenvalue ( $i$ ) failed to converge after ( $xxx$ ) iterations. (The computational error message may occur multiple times with processing continuing after each error, because the number of allowable errors for error code 2114 is set to be unlimited in the ESSL error option table.)
  - The eigenvalue,  $w_i$ , is the best estimate obtained. Any eigenvalues for which this message has not been issued are correct.
  - $ap$  is modified.
  - The return code is set to 1.
  - $i$  and  $xxx$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error 2199 in the ESSL error option table. See “What Can You Do about ESSL Computational Errors?” on page 51.
2. Eigenvector ( $i$ ) failed to converge after ( $xxx$ ) iterations. (The computational error message may occur multiple times with processing continuing after each error,

because the number of allowable errors for error code 2102 is set to be unlimited in the ESSL error option table.)

- All eigenvalues are correct.
- The eigenvector that failed to converge is set to zero; however, any selected eigenvectors for which this message is not issued are correct.
- $ap$  is modified.
- The return code is set to 2.
- $i$  and  $xxx$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error 2199 in the ESSL error option table. See “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $iopt \neq 0, 1, 10, 11, 20, 21, 30,$  or  $31$
2.  $n < 0$
3.  $m < 0$
4.  $m > n$
5.  $ldz \leq 0$  and  $iopt = 1, 11, 21,$  or  $31$
6.  $n > ldz$  and  $iopt = 1, 11, 21,$  or  $31$
7. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 3 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to find the two smallest eigenvalues and corresponding eigenvectors of a real long-precision symmetric matrix  $A$  of order 4, stored in upper-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 5.0 & 4.0 & 1.0 & 1.0 \\ 4.0 & 5.0 & 1.0 & 1.0 \\ 1.0 & 1.0 & 4.0 & 2.0 \\ 1.0 & 1.0 & 2.0 & 4.0 \end{bmatrix}$$

where:

- NAUX is equal to 9N.
- AUX contains 9N elements.
- On output, AP has been overwritten.

**Note:** This matrix is used in Example 4.1 in referenced text [65].

### Call Statement and Input:

```

          IOPT  AP   W   Z  LDZ  N   M   AUX  NAUX
          |    |   |   |   |   |   |   |
CALL DSPSV( 21 , AP , W , Z , 4 , 4 , 2 , AUX , 36 )

AP      = (5.0, 4.0, 5.0, 1.0, 1.0, 4.0, 1.0, 1.0, 2.0, 4.0)

```

### Output:

$$W = \begin{bmatrix} 1.000000 \\ 2.000000 \\ \cdot \\ \cdot \end{bmatrix}$$

## SSPSV, DSPSV, CHPSV, and ZHPSV

$$Z = \begin{bmatrix} -0.707107 & 0.000000 \\ 0.707107 & 0.000000 \\ 0.000000 & -0.707107 \\ 0.000000 & 0.707107 \end{bmatrix}$$

### Example 2

This example shows how to find the three largest eigenvalues and corresponding eigenvectors of a real long-precision symmetric matrix  $A$  of order 4, stored in lower-packed storage mode, having an eigenvalue of multiplicity two. Matrix  $A$  is:

$$\begin{bmatrix} 6.0 & 4.0 & 4.0 & 1.0 \\ 4.0 & 6.0 & 1.0 & 4.0 \\ 4.0 & 1.0 & 6.0 & 4.0 \\ 1.0 & 4.0 & 4.0 & 6.0 \end{bmatrix}$$

where:

- NAUX is equal to 9N.
- AUX contains 9N elements.
- On output, AP has been overwritten.

**Note:** This matrix is used in Example 4.2 in referenced text [65].

### Call Statement and Input:

```
          IOPT  AP  W  Z  LDZ  N  M  AUX  NAUX
          |    |  |  |  |    |  |  |    |
CALL DSPSV( 11 , AP , W , Z , 8 , 4 , 3 , AUX , 36 )
```

```
AP      = (6.0, 4.0, 4.0, 1.0, 6.0, 1.0, 4.0, 6.0, 4.0, 6.0)
```

### Output:

$$W = \begin{bmatrix} 15.000000 \\ 5.000000 \\ 5.000000 \\ \cdot \end{bmatrix}$$

$$Z = \begin{bmatrix} 0.500000 & 0.707107 & 0.000000 \\ 0.500000 & 0.000000 & -0.707107 \\ 0.500000 & 0.000000 & 0.707107 \\ 0.500000 & -0.707107 & 0.000000 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

### Example 3

This example shows how to find the largest eigenvalue and the corresponding eigenvector of a complex Hermitian matrix  $A$  of order 2, stored in lower-packed storage mode. Matrix  $A$  is:

$$\begin{bmatrix} (1.0, 0.0) & (0.0, -1.0) \\ (0.0, 1.0) & (1.0, 0.0) \end{bmatrix}$$

where:

- NAUX is equal to 11N.

- AUX contains 11N elements.
- On output, AP has been overwritten.

**Note:** This matrix is used in Example 6.1 in referenced text [65].

**Call Statement and Input:**

```

          IOPT  AP   W   Z   LDZ  N   M   AUX  NAUX
          |    |   |   |   |    |   |   |    |
CALL ZHPSV( 11 , AP , W , Z , 2 , 2 , 1 , AUX , 22 )

AP      = ((1.0, . ), (0.0, 1.0), (1.0, . ))

```

**Output:**

$$W = \begin{bmatrix} 2.000000 \\ \cdot \end{bmatrix}$$

$$Z = \begin{bmatrix} (0.000000, -0.707107) \\ (0.707107, 0.000000) \end{bmatrix}$$

**Example 4**

This example shows how to find the two smallest eigenvalues only of a complex Hermitian matrix *A* of order 4, stored in upper-packed storage mode. Matrix *A* is:

$$\begin{bmatrix} (3.0, 0.0) & (1.0, 0.0) & (0.0, 0.0) & (0.0, 2.0) \\ (1.0, 0.0) & (3.0, 0.0) & (0.0, -2.0) & (0.0, 0.0) \\ (0.0, 0.0) & (0.0, 2.0) & (1.0, 0.0) & (1.0, 0.0) \\ (0.0, -2.0) & (0.0, 0.0) & (1.0, 0.0) & (1.0, 0.0) \end{bmatrix}$$

where:

- NAUX is equal to 5N.
- AUX contains 5N elements.
- LDZ is set to 1 to avoid an error condition.
- DUMMY is used as a placeholder for argument *z*, which is not used in the computation.
- On output, AP has been overwritten.

**Note:** This matrix is used in Example 6.6 in referenced text [65].

**Call Statement and Input:**

```

          IOPT  AP   W   Z   LDZ  N   M   AUX  NAUX
          |    |   |   |   |    |   |   |    |
CALL ZHPSV( 20 , AP , W , DUMMY , 1 , 4 , 2 , AUX , 20 )

AP      = ((3.0, . ), (1.0, 0.0), (3.0, . ), (0.0, 0.0),
          (0.0, -2.0), (1.0, . ), (0.0, 2.0), (0.0, 0.0),
          (1.0, 0.0), (1.0, . ))

```

**Output:**

$$W = \begin{bmatrix} -0.828427 \\ 0.000000 \\ \cdot \\ \cdot \end{bmatrix}$$

## SGEGV and DGEV — Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Eigensystem, $Az=wBz$ , where $A$ and $B$ Are Real General Matrices

### Purpose

These subroutines compute the eigenvalues and, optionally, the eigenvectors of a generalized real eigensystem, where  $A$  and  $B$  are real general matrices. Eigenvalues  $w$  are based on the two parts returned in vectors  $\alpha$  and  $\beta$ , such that  $w_i = \alpha_i / \beta_i$  for  $\beta_i \neq 0$ , and  $w_i = \infty$  for  $\beta_i = 0$ . Eigenvectors are returned in matrix  $Z$ :

$$Az = wBz$$

Table 136. Data Types

$A, B, \beta, aux$	$\alpha, Z$	Subroutine
Short-precision real	Short-precision complex	SGEGV <sup>z</sup>
Long-precision real	Long-precision complex	DGEV <sup>z</sup>

<sup>z</sup>Not LAPACK. Although this subroutine has the same name as an existing LAPACK subroutine, its calling-sequence arguments and functionality are different from that LAPACK subroutine.

### Syntax

<b>Fortran</b>	CALL SGEGV   DGEV ( <i>iopt, a, lda, b, ldb, alpha, beta, z, ldz, n, aux, naux</i> )
<b>C and C++</b>	sgegv   dgegv ( <i>iopt, a, lda, b, ldb, alpha, beta, z, ldz, n, aux, naux</i> );

### On Entry

- iopt* indicates the type of computation to be performed, where:  
 If *iopt* = 0, eigenvalues only are computed.  
 If *iopt* = 1, eigenvalues and eigenvectors are computed.  
 Specified as: a fullword integer; *iopt* = 0 or 1.
- a* is the real general matrix  $A$  of order  $n$ .  
 Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 136. On output,  $A$  is overwritten; that is, the original input is not preserved.
- lda* is the leading dimension of the array specified for *a*.  
 Specified as: a fullword integer; *lda* > 0 and *lda* ≥  $n$ .
- b* is the real general matrix  $B$  of order  $n$ .  
 Specified as: an *ldb* by (at least)  $n$  array, containing numbers of the data type indicated in Table 136. On output,  $B$  is overwritten; that is, the original input is not preserved.
- ldb* is the leading dimension of the array specified for *b*.  
 Specified as: a fullword integer; *ldb* > 0 and *ldb* ≥  $n$ .
- alpha* See “On Return” on page 765.
- beta* See “On Return” on page 765.
- z* See “On Return” on page 765.

- ldz* has the following meaning, where:  
 If  $iopt = 0$ , it is not used in the computation.  
 If  $iopt = 1$ , it is the leading dimension of the output array specified for  $z$ .  
 Specified as: a fullword integer. It must have the following value, where:  
 If  $iopt = 0$ ,  $ldz > 0$ .  
 If  $iopt = 1$ ,  $ldz > 0$  and  $ldz \geq n$ .
- n* is the order of matrices  $A$  and  $B$ .  
 Specified as: a fullword integer;  $n \geq 0$ .
- aux* has the following meaning:  
 If  $naux = 0$  and error 2015 is unrecoverable, *aux* is ignored.  
 Otherwise, it is a storage work area used by this subroutine. Its size is specified by *naux*.  
 Specified as: an area of storage, containing numbers of the data type indicated in Table 136 on page 764. On output, the contents are overwritten.
- naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.  
 Specified as: a fullword integer, where:  
 If  $naux = 0$  and error 2015 is unrecoverable, SGEGV and DGEGV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.  
 Otherwise,  $naux \geq 3n$ .

### On Return

- alpha* is the vector  $\alpha$  of length  $n$ , containing the numerators of the eigenvalues of the generalized real eigensystem  $Az = wBz$ .  
 Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 136 on page 764.
- beta* is the vector  $\beta$  of length  $n$ , containing the denominators of the eigenvalues of the generalized real eigensystem  $Az = wBz$ .  
 Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 136 on page 764.
- z* has the following meaning, where:  
 If  $iopt = 0$ , it is not used in the computation.  
 If  $iopt = 1$ , it is the matrix  $Z$  of order  $n$ , containing the eigenvectors of the generalized real eigensystem,  $Az = wBz$ . The eigenvector in column  $i$  of matrix  $Z$  corresponds to the eigenvalue  $w_i$ , computed using the  $\alpha_i$  and  $\beta_i$  values. Each eigenvector is normalized so that the modulus of its largest element is 1.  
 Returned as: an  $ldz$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 136 on page 764.

## Notes

- When you specify  $iopt = 0$ , you must specify:
  - A positive value for  $ldz$
  - A dummy argument for  $z$  (see “Example 1” on page 767)
- Matrices  $A$ ,  $B$ , and  $Z$ , vectors  $\alpha$  and  $\beta$ , and the work area specified for  $aux$  must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
- You have the option of having the minimum required value for  $naux$  dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## Function

The following steps describe the methods used to compute the eigenvalues and, optionally, the eigenvectors of a generalized real eigensystem,  $Az = wBz$ , where  $A$  and  $B$  are real general matrices. The methods are based upon Moler and Stewart’s QZ algorithm. You must calculate the resulting eigenvalues  $w$  based on the two parts returned in vectors  $\alpha$  and  $\beta$ . Each eigenvalue is calculated as follows:  $w_i = \alpha_i/\beta_i$  for  $\beta_i \neq 0$  and  $w_i = \infty$  for  $\beta_i = 0$ . Eigenvalues are unordered, except that complex conjugate pairs appear consecutively with the eigenvalue having the positive imaginary part first.

- For  $iopt = 0$ , the eigenvalues are computed as follows:
  - Simultaneously reduce  $A$  to upper Hessenberg form and  $B$  to upper triangular form using orthogonal transformations.
  - Reduce  $A$  from upper Hessenberg form to quasi-upper triangular form while maintaining the upper triangular form of  $B$  using orthogonal transformations.
  - Compute the eigenvalues of the generalized real eigensystem with  $A$  in quasi-upper triangular form and  $B$  in upper triangular form using orthogonal transformations.
  - The numerators and denominators of the eigenvalues are returned in vectors  $\alpha$  and  $\beta$ , respectively.
- For  $iopt = 1$ , the eigenvalues and eigenvectors are computed as follows:
  - Simultaneously reduce  $A$  to upper Hessenberg form and  $B$  to upper triangular form using and accumulating orthogonal transformations.
  - Reduce  $A$  from upper Hessenberg form to quasi-upper triangular form while maintaining the upper triangular form of  $B$  using and accumulating orthogonal transformations.
  - Compute the eigenvalues of the generalized real eigensystem with  $A$  in quasi-upper triangular form and  $B$  in upper triangular form using and accumulating orthogonal transformations.
  - Compute the eigenvectors of the generalized real eigensystem with  $A$  in quasi-upper triangular form and  $B$  in upper triangular form using back substitution.
  - The numerators and denominators of the eigenvalues are returned in vectors  $\alpha$  and  $\beta$ , respectively, and the eigenvectors are returned in matrix  $Z$ .

For more information on these methods, see references [41], [45], [60], [86], [65], [64], [91], [101], and [103]. If  $n$  is 0, no computation is performed. The results of the computations using short- and long-precision data can vary in accuracy.

These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.



## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

Eigenvalue ( $i$ ) failed to converge after ( $xxx$ ) iterations:

- The eigenvalues ( $w_j$ ,  $j = i+1, i+2, \dots, n$ ) are correct.
- If  $iopt = 1$ , then  $Z$  is modified, but no eigenvectors are correct.
- $A$  and  $B$  have been modified.
- The return code is set to 1.
- $i$  and  $xxx$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2101 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $iopt \neq 0$  or 1
2.  $n < 0$
3.  $lda \leq 0$
4.  $n > lda$
5.  $ldb \leq 0$
6.  $n > ldb$
7.  $ldz \leq 0$  and  $iopt = 1$
8.  $n > ldz$  and  $iopt = 1$
9. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 2 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to find the eigenvalues only of a real generalized eigensystem problem,  $AZ = wBZ$ , where:

- $NAUX$  is equal to  $3N$ .
- $AUX$  contains  $3N$  elements.
- $LDZ$  is set to 1 to avoid an error condition.
- $DUMMY$  is used as a placeholder for argument  $z$ , which is not used in the computation.
- On output, matrices  $A$  and  $B$  are overwritten.

**Note:** These matrices are from page 257 in referenced text [64].

### Call Statement and Input:

```

          IOPT  A  LDA  B  LDB  ALPHA  BETA  Z  LDZ  N  AUX  NAUX
CALL DGEV( 0 , A , 3 , B , 3 , ALPHA , BETA , DUMMY , 1 , 3 , AUX , 9 )

```

$$A = \begin{bmatrix} 10.0 & 1.0 & 2.0 \\ 1.0 & 3.0 & -1.0 \\ 1.0 & 1.0 & 2.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 4.0 & 5.0 & 6.0 \\ 7.0 & 8.0 & 9.0 \end{bmatrix}$$

## SGEGV and DGEGV

### Output:

$$\text{ALPHA} = \begin{bmatrix} (4.778424, 0.000000) \\ (-4.760580, 0.000000) \\ (2.769466, 0.000000) \end{bmatrix}$$

$$\text{BETA} = \begin{bmatrix} 0.000000 \\ 0.934851 \\ 15.446215 \end{bmatrix}$$

### Example 2

This example shows how to find the eigenvalues and eigenvectors of a real generalized eigensystem problem,  $AZ = wBZ$ , where:

- NAUX is equal to 3N.
- AUX contains 3N elements.
- On output, matrices A and B are overwritten.

**Note:** These matrices are from page 263 in referenced text [64].

### Call Statement and Input:

```

          IOPT  A  LDA  B  LDB  ALPHA  BETA  Z  LDZ  N  AUX  NAUX
CALL DGEGV( 1 , A , 5 , B , 5 , ALPHA , BETA , Z , 5 , 5 , AUX , 15 )

```

$$A = \begin{bmatrix} 2.0 & 3.0 & 4.0 & 5.0 & 6.0 \\ 4.0 & 4.0 & 5.0 & 6.0 & 7.0 \\ 0.0 & 3.0 & 6.0 & 7.0 & 8.0 \\ 0.0 & 0.0 & 2.0 & 8.0 & 9.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 10.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -1.0 & -1.0 & -1.0 & -1.0 \\ 0.0 & 1.0 & -1.0 & -1.0 & -1.0 \\ 0.0 & 0.0 & 1.0 & -1.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{bmatrix}$$

### Output:

$$\text{ALPHA} = \begin{bmatrix} (7.950050, 0.000000) \\ (-0.277338, 0.000000) \\ (2.149669, 0.000000) \\ (6.720718, 0.000000) \\ (10.987556, 0.000000) \end{bmatrix}$$

$$\text{BETA} = \begin{bmatrix} 0.374183 \\ 1.480299 \\ 1.636872 \\ 1.213574 \\ 0.908837 \end{bmatrix}$$

$$Z = \begin{bmatrix} (1.000000, 0.000000) & (-0.483408, 0.000000) & (0.540696, 0.000000) \\ (0.565497, 0.000000) & (1.000000, 0.000000) & (0.684441, 0.000000) \\ (0.180429, 0.000000) & (-0.661372, 0.000000) & (-1.000000, 0.000000) \\ (0.034182, 0.000000) & (0.180646, 0.000000) & (0.363671, 0.000000) \\ (0.003039, 0.000000) & (-0.017732, 0.000000) & (-0.041865, 0.000000) \end{bmatrix}$$

(1.000000, 0.000000)	(-1.000000, 0.000000)
(0.722065, 0.000000)	(-0.610415, 0.000000)
(-0.089003, 0.000000)	(-0.116987, 0.000000)
(-0.223599, 0.000000)	(0.038979, 0.000000)
(0.050111, 0.000000)	(0.018653, 0.000000)

## SSYGV and DSYGV — Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Symmetric Eigensystem, $Az=wBz$ , where $A$ Is Real Symmetric and $B$ Is Real Symmetric Positive Definite

### Purpose

These subroutines compute the eigenvalues and, optionally, the eigenvectors of a generalized real symmetric eigensystem, where  $A$  is a real symmetric matrix, and  $B$  is a real positive definite symmetric matrix. Both  $A$  and  $B$  are stored in lower storage mode in two-dimensional arrays. Eigenvalues are returned in vector  $w$ , and eigenvectors are returned in matrix  $Z$ :

$$Az = wBz$$

where  $A = A^T$ ,  $B = B^T$ , and  $x^T B x > 0$ .

Table 137. Data Types

$A, B, w, Z, aux$	Subroutine
Short-precision real	SSYGV <sup>‡</sup>
Long-precision real	DSYGV <sup>‡</sup>
<sup>‡</sup> Not LAPACK. Although this subroutine has the same name as an existing LAPACK subroutine, its calling-sequence arguments and functionality are different from that LAPACK subroutine.	

### Syntax

Fortran	CALL SSYGV   DSYGV ( <i>iopt</i> , <i>a</i> , <i>lda</i> , <i>b</i> , <i>ldb</i> , <i>w</i> , <i>z</i> , <i>ldz</i> , <i>n</i> , <i>aux</i> , <i>naux</i> )
C and C++	ssygv   dsygv ( <i>iopt</i> , <i>a</i> , <i>lda</i> , <i>b</i> , <i>ldb</i> , <i>w</i> , <i>z</i> , <i>ldz</i> , <i>n</i> , <i>aux</i> , <i>naux</i> );

### On Entry

- iopt* indicates the type of computation to be performed, where:
- If *iopt* = 0, eigenvalues only are computed.
  - If *iopt* = 1, eigenvalues and eigenvectors are computed.
- Specified as: a fullword integer; *iopt* = 0 or 1.
- a* is the real symmetric matrix  $A$  of order  $n$ . It is stored in lower storage mode.
- Specified as: an *lda* by (at least)  $n$  array, containing numbers of the data type indicated in Table 137. On output, the data in the lower triangle of  $A$  is overwritten; that is, the original input is not preserved.
- lda* is the leading dimension of the array specified for *a*.
- Specified as: a fullword integer; *lda* > 0 and *lda* ≥  $n$ .
- b* is the real positive definite symmetric matrix  $B$  of order  $n$ . It is stored in lower storage mode.

Specified as: an  $ldb$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 137 on page 770. On output, the data in the lower triangle of  $B$  is overwritten; that is, the original input is not preserved.

*ldb* is the leading dimension of the array specified for  $b$ .  
Specified as: a fullword integer;  $ldb > 0$  and  $ldb \geq n$ .

*w* See "On Return."

*z* See "On Return."

*ldz* has the following meaning, where:  
If  $iopt = 0$ , it is not used in the computation.  
If  $iopt = 1$ , it is the leading dimension of the output array specified for  $z$ .  
Specified as: a fullword integer. It must have the following value, where:  
If  $iopt = 0$ ,  $ldz > 0$ .  
If  $iopt = 1$ ,  $ldz > 0$  and  $ldz \geq n$ .

*n* is the order of matrices  $A$  and  $B$ .  
Specified as: a fullword integer;  $n \geq 0$ .

*aux* has the following meaning:  
If  $naux = 0$  and error 2015 is unrecoverable, *aux* is ignored.  
Otherwise, it is a storage work area used by this subroutine. Its size is specified by *naux*.  
Specified as: an area of storage, containing numbers of the data type indicated in Table 137 on page 770. On output, the contents are overwritten.

*naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.  
Specified as: a fullword integer, where:  
If  $naux = 0$  and error 2015 is unrecoverable, SSYGV and DSYGV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.  
Otherwise, It must have the following value, where:  
If  $iopt = 0$ ,  $naux \geq n$ .  
If  $iopt = 1$ ,  $naux \geq 2n$ .

### On Return

*w* is the vector  $w$  of length  $n$ , containing the eigenvalues of the generalized real symmetric eigensystem  $Az = wBz$  in ascending order. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 137 on page 770.

*z* has the following meaning, where:  
If  $iopt = 0$ , it is not used in the computation.

If  $iopt = 1$ , it is the matrix  $Z$  of order  $n$ , containing the eigenvectors of the generalized real symmetric eigensystem,  $Az = wBz$ . The eigenvectors are normalized so that  $Z^T B Z = I$ . The eigenvector in column  $i$  of matrix  $Z$  corresponds to the eigenvalue  $w_i$ .

Returned as: an  $ldz$  by (at least)  $n$  array, containing numbers of the data type indicated in Table 137 on page 770.

## Notes

- When you specify  $iopt = 0$ , you must specify:
  - A positive value for  $ldz$
  - A dummy argument for  $z$  (see "Example 1" on page 773)
- Matrices  $A$  and  $Z$  may coincide. Matrices  $A$  and  $B$ , vector  $w$ , and the data area specified for  $aux$  must have no common elements; otherwise, results are unpredictable. Matrices  $Z$  and  $B$ , vector  $w$ , and the data area specified for  $aux$  must also have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.
- For a description of how real symmetric matrices are stored in lower storage mode, see "Lower Storage Mode" on page 72.
- You have the option of having the minimum required value for  $naux$  dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

## Function

The following steps describe the methods used to compute the eigenvalues and, optionally, the eigenvectors of a generalized real symmetric eigensystem,  $Az = wBz$ , where  $A$  is a real symmetric matrix, and  $B$  is a real positive definite symmetric matrix. Both  $A$  and  $B$  are stored in lower storage mode in two-dimensional arrays.

- Compute the Cholesky Decomposition of  $B$ :

$$B = LL^T$$

For a description of methods used in this computation, see "SPOTRF, DPOTRF, CPOTRF, ZPOTRF, SPOF, DPOF, CPOF, ZPOF, SPPTRF, DPPTRF, CPPTRF, ZPPTRF, SPPF, and DPPF — Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization" on page 495.

- Compute  $C$ :

$$C = L^{-1}AL^{-T}$$

In this computation,  $C$  overwrites  $A$ .

- Solve the real symmetric eigensystems analysis problem, computing the eigenvalues  $w$  and, optionally, the eigenvectors  $Y$ :

$$CY = wY$$

where:

$$Y = L^T Z$$

For a description of the methods used for this computation, see "Real Symmetric Matrix" on page 750. In this computation,  $Y$  overwrites  $Z$ .

- If eigenvectors are requested (with  $iopt = 1$ ), transform the eigenvectors  $Y$  into the eigenvectors  $Z$  of the original system,  $Az = wBz$ , by solving  $L^T Z = Y$  for  $Z$ :

$$Z = L^{-T}Y$$

For more information on these methods, see references [41], [45], [60], [65], [64], [91], [101], and [103]. If  $n$  is 0, no computation is performed. The results of the computations using short- and long-precision data can vary in accuracy.

These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

1. The  $B$  matrix is not positive definite. The leading minor of order  $i$  has a nonpositive determinant.
  - $B$  is modified, but no eigenvalues or eigenvectors are correct.
  - The return code is set to 1.
  - $i$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2115 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See “What Can You Do about ESSL Computational Errors?” on page 51.
2. Eigenvalue ( $i$ ) failed to converge after ( $xxx$ ) iterations:
  - The eigenvalues ( $w_j, j = 1, 2, \dots, i-1$ ) are correct, but are unordered.
  - If  $iopt = 1$ , then  $z$  is modified, but no eigenvectors are correct.
  - $A$  and  $B$  have been modified.
  - The return code is set to 2.
  - $i$  and  $xxx$  can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2101 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $iopt \neq 0$  or 1
2.  $n < 0$
3.  $lda \leq 0$
4.  $n > lda$
5.  $ldb \leq 0$
6.  $n > ldb$
7.  $ldz \leq 0$  and  $iopt = 1$
8.  $n > ldz$  and  $iopt = 1$
9. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 3 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to find the eigenvalues only of a real symmetric generalized eigensystem problem,  $AZ = wBZ$ , where:

- NAUX is equal to N.
- AUX contains N elements.

## SSYGV and DSYGV

- LDZ is set to 1 to avoid an error condition.
- DUMMY is used as a placeholder for argument  $z$ , which is not used in the computation.
- On output, the lower triangle of A and B is overwritten.

**Note:** These matrices are used in Example 8.6.2 in referenced text [64].

### Call Statement and Input:

```

          IOPT  A  LDA  B  LDB  W    Z    LDZ  N  AUX  NAUX
CALL DSYGV( 0 , A , 2 , B , 2 , W , DUMMY , 1 , 2 , AUX , 2 )

```

$$A = \begin{bmatrix} 229.0 & . \\ 163.0 & 116.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 81.0 & . \\ 59.0 & 43.0 \end{bmatrix}$$

### Output:

$$W = \begin{bmatrix} -0.500000 \\ 5.000000 \end{bmatrix}$$

### Example 2

This example shows how to find the eigenvalues and eigenvectors of a real symmetric generalized eigensystem problem,  $AZ = \omega BZ$ , where:

- NAUX is equal to 2N.
- AUX contains 2N elements.
- On output, the lower triangle of A and B is overwritten.

**Note:** These matrices are from page 67 in referenced text [60].

### Call Statement and Input:

```

          IOPT  A  LDA  B  LDB  W    Z    LDZ  N  AUX  NAUX
CALL DSYGV( 1 , A , 3 , B , 3 , W , Z , 3 , N , AUX , 6 )

```

$$A = \begin{bmatrix} -1.0 & . & . \\ 1.0 & 1.0 & . \\ -1.0 & -1.0 & 1.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 2.0 & . & . \\ 1.0 & 2.0 & . \\ 0.0 & 1.0 & 2.0 \end{bmatrix}$$

### Output:

$$W = \begin{bmatrix} -1.500000 \\ 0.000000 \\ 2.000000 \end{bmatrix}$$



$$Z = \begin{bmatrix} 0.866025 & 0.000000 & 0.000000 \\ -0.577350 & -0.408248 & -0.707107 \\ 0.288675 & -0.408248 & 0.707107 \end{bmatrix}$$

## SSYGV and DSYGV

---

## Chapter 12. Fourier Transforms, Convolutions and Correlations, and Related Computations

The signal processing subroutines, provided in three areas, are described in this chapter.

---

### Overview of the Signal Processing Subroutines

This section describes the subroutines in each of the three signal processing areas:

- Fourier transform subroutines (Table 138)
- Convolution and correlation subroutines (Table 139)
- Related-computation subroutines (Table 140)

### Fourier Transforms Subroutines

The Fourier transform subroutines perform mixed-radix transforms in one, two, and three dimensions.

Table 138. List of Fourier Transform Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Complex Fourier Transform	SCFT SCFTP <sup>§</sup>	DCFT	787
Real-to-Complex Fourier Transform	SRCFT	DRCFT	796
Complex-to-Real Fourier Transform	SCRFT	DCRFT	804
Cosine Transform	SCOSF SCOSFT <sup>§</sup>	DCOSF	812
Sine Transform	SSINF	DSINF	820
Complex Fourier Transform in Two Dimensions	SCFT2 SCFT2P <sup>§</sup>	DCFT2	828
Real-to-Complex Fourier Transform in Two Dimensions	SRCFT2	DRCFT2	835
Complex-to-Real Fourier Transform in Two Dimensions	SCRFT2	DCRFT2	842
Complex Fourier Transform in Three Dimensions	SCFT3 SCFT3P <sup>§</sup>	DCFT3	850
Real-to-Complex Fourier Transform in Three Dimensions	SRCFT3	DRCFT3	856
Complex-to-Real Fourier Transform in Three Dimensions	SCRFT3	DCRFT3	862

<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.

### Convolution and Correlation Subroutines

The convolution and correlation subroutines provide the choice of using Fourier methods or direct methods. The Fourier-method subroutines contain a high-performance mixed-radix capability. There are also several direct-method subroutines that provide decimated output.

Table 139. List of Convolution and Correlation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Convolution or Correlation of One Sequence with One or More Sequences	SCON <sup>§</sup> SCOR <sup>§</sup>		869
Convolution or Correlation of One Sequence with Another Sequence Using a Direct Method	SCOND SCORD		875
Convolution or Correlation of One Sequence with One or More Sequences Using the Mixed-Radix Fourier Method	SCONF SCORF		881
Convolution or Correlation with Decimated Output Using a Direct Method	SDCON SDCOR	DDCON DDCOR	891
Autocorrelation of One or More Sequences	SACOR <sup>§</sup>		896
Autocorrelation of One or More Sequences Using the Mixed-Radix Fourier Method	SACORF		900

<sup>§</sup> These subroutines are provided only for migration from earlier releases of ESSL and are not intended for use in new programs.

## Related-Computation Subroutines

The related-computation subroutines consist of a group of computations that can be used in general signal processing applications. They are similar to those provided on the IBM 3838 Array Processor; however, the ESSL subroutines generally solve a wider range of problems.

Table 140. List of Related-Computation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Polynomial Evaluation	SPOLY	DPOLY	907
I-th Zero Crossing	SIZC	DIZC	910
Time-Varying Recursive Filter	STREC	DTREC	913
Quadratic Interpolation	SQINT	DQINT	916
Wiener-Levinson Filter Coefficients	SWLEV CWLEV	DWLEV ZWLEV	920

## Fourier Transforms, Convolutions, and Correlations Considerations

This section describes some global information applying to the Fourier transform, convolution, and correlation subroutines.

### Use Considerations

This section provides some key points about using the Fourier transform, convolution, and correlation subroutines.

#### Understanding the Terminology and Conventions Used for Your Array Data

These subroutines use the term “sequences,” rather than vectors and matrices, to describe the data that is stored in the arrays. The conventions used for representing sequences are defined in “Sequences” on page xvi.

Some of the sequences used in these computations use a zero origin rather than a one-origin. For example,  $x_j$  can be expressed with  $j = 0, 1, \dots, n-1$  rather than

$j = 1, 2, \dots, n$ . When using the formulas provided in this book to calculate array sizes or offsets into arrays, you need to be careful that you substitute the correct values. For example, the number of  $x_j$  elements in the sequence is  $n$ , not  $n-1$ .

### Concerns about Lengths of Transforms

The length of the transform you can use in your program depends on the limits of the addressability of your processor.

### Determining an Acceptable Length of a Transform

To determine acceptable lengths of the transforms in the Fourier transform subroutines, you have several choices. First, you can use the formula or table of values in "Acceptable Lengths for the Transforms" to choose a value. Second, ESSL's input-argument error recovery provides a means of determining an acceptable length of the transform. It uses the optionally-recoverable error 2030. For details, see "Providing a Correct Transform Length to ESSL" on page 42.

### Acceptable Lengths for the Transforms

Use the following formula to determine acceptable transform lengths:

$$n = (2^h) (3^i) (5^j) (7^k) (11^m) \quad \text{for } n \leq 37748736$$

where:

$$h = 1, 2, \dots, 25$$

$$i = 0, 1, 2$$

$$j, k, m = 0, 1$$

Figure 13 on page 780 lists all the acceptable values for transform lengths in the Fourier transform subroutines.

2	4	6	8	10	12	14	16	18
20	22	24	28	30	32	36	40	42
44	48	56	60	64	66	70	72	80
84	88	90	96	110	112	120	126	128
132	140	144	154	160	168	176	180	192
198	210	220	224	240	252	256	264	280
288	308	320	330	336	352	360	384	396
420	440	448	462	480	504	512	528	560
576	616	630	640	660	672	704	720	768
770	792	840	880	896	924	960	990	1008
1024	1056	1120	1152	1232	1260	1280	1320	1344
1386	1408	1440	1536	1540	1584	1680	1760	1792
1848	1920	1980	2016	2048	2112	2240	2304	2310
2464	2520	2560	2640	2688	2772	2816	2880	3072
3080	3168	3360	3520	3584	3696	3840	3960	4032
4096	4224	4480	4608	4620	4928	5040	5120	5280
5376	5544	5632	5760	6144	6160	6336	6720	6930
7040	7168	7392	7680	7920	8064	8192	8448	8960
9216	9240	9856	10080	10240	10560	10752	11088	11264
11520	12288	12320	12672	13440	13860	14080	14336	14784
15360	15840	16128	16384	16896	17920	18432	18480	19712
20160	20480	21120	21504	22176	22528	23040	24576	24640
25344	26880	27720	28160	28672	29568	30720	31680	32256
32768	33792	35840	36864	36960	39424	40320	40960	42240
43008	44352	45056	46080	49152	49280	50688	53760	55440
56320	57344	59136	61440	63360	64512	65536	67584	71680
73728	73920	78848	80640	81920	84480	86016	88704	90112
92160	98304	98560	101376	107520	110880	112640	114688	118272
122880	126720	129024	131072	135168	143360	147456	147840	157696
161280	163840	168960	172032	177408	180224	184320	196608	197120
202752	215040	221760	225280	229376	236544	245760	253440	258048
262144	270336	286720	294912	295680	315392	322560	327680	337920
344064	354816	360448	368640	393216	394240	405504	430080	443520
450560	458752	473088	491520	506880	516096	524288	540672	573440
589824	591360	630784	645120	655360	675840	688128	709632	720896
737280	786432	788480	811008	860160	887040	901120	917504	946176
983040	1013760	1032192	1048576	1081344	1146880	1179648	1182720	1261568
1290240	1310720	1351680	1376256	1419264	1441792	1474560	1572864	1576960
1622016	1720320	1774080	1802240	1835008	1892352	1966080	2027520	2064384
2097152	2162688	2293760	2359296	2365440	2523136	2580480	2621440	2703360
2752512	2838528	2883584	2949120	3145728	3153920	3244032	3440640	3548160
3604480	3670016	3784704	3932160	4055040	4128768	4194304	4325376	4587520
4718592	4730880	5046272	5160960	5242880	5406720	5505024	5677056	5767168
5898240	6291456	6307840	6488064	6881280	7096320	7208960	7340032	7569408
7864320	8110080	8257536	8388608	8650752	9175040	9437184	9461760	10092544
10321920	10485760	10813440	11010048	11354112	11534336	11796480	12582912	12615680
12976128	13762560	14192640	14417920	14680064	15138816	15728640	16220160	16515072
16777216	17301504	18350080	18874368	18923520	20185088	20643840	20971520	21626880
22020096	22708224	23068672	23592960	25165824	25231360	25952256	27525120	28385280
28835840	29360128	30277632	31457280	32440320	33030144	33554432	34603008	36700160
37748736								

Figure 13. Table of Acceptable Lengths for the Transforms

## Understanding Auxiliary Working Storage Requirements

Auxiliary working storage is required by the Fourier transform subroutines and by the SCONE, SCORE, and SACORF subroutines. This storage is provided through the calling sequence arguments *aux*, *aux1*, and *aux2*. The sizes of these storage areas are specified by the calling sequence arguments *naux*, *naux1*, and *naux2*, respectively.

**AUX1:** The *aux1* array is used for storing tables and other parameters when you call a Fourier transform, convolution, or correlation subroutine for initialization

with *init* = 1. The initialized *aux1* array is then used on succeeding calls with *init* = 0, when the computation is actually done. You should not use this array between the initialization and the computation.

**AUX and AUX2:** The *aux* and *aux2* arrays are used for temporary storage during the running of the subroutine and are available for use by your program between calls to the subroutine.

**AUX3:** The *aux3* argument is provided for migration purposes only and is ignored.

## Initializing Auxiliary Working Storage

In many of those subroutines requiring *aux1* auxiliary working storage, two invocations of the subroutines are necessary. The first invocation initializes the working storage in *aux1* for the subroutine, and the second performs the computations. (For an explanation of auxiliary working storage, see Understanding Auxiliary Working Storage Requirements.) As a result, the working storage in *aux1* should not be used by the calling program between the two calls to the subroutine. However, it can be reused after intervening calls to the subroutine with different arguments.

If you plan to repeat a computation many times using the same set of arguments, you only need to do one initialization of the *aux1* array; that is, the initialized *aux1* array can be saved and reused as many times as needed for the computation.

If you plan to perform different computations, with different sets of arguments (except for input argument *x*), you need to do an initialization for each different computation; that is, you initialize the various *aux1* arrays for use with the different computations, saving and reusing them until they are not needed any more.

## Determining the Amount of Auxiliary Working Storage That You Need

To determine the size of auxiliary storage, you have several choices. First, you can use the formulas provided in each subroutine description. Second, ESSL's input-argument error recovery provides a means of determining the minimum size you need for auxiliary storage. It uses the optionally-recoverable error 2015. For details, see "Using Auxiliary Storage in ESSL" on page 36. Third, you can have ESSL dynamically allocate *aux* and *aux2*. For details, see "Dynamic Allocation of Auxiliary Storage" on page 37.

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## Performance and Accuracy Considerations

The following sections explain the performance and accuracy considerations for the Fourier transforms, convolution, and correlation subroutines. For further details about performance and accuracy, see Chapter 2, "Planning Your Program," on page 25.

## When Running on the Workstation Processors

There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 48.

## Defining Arrays

The stride arguments, *inc1h*, *inc1x*, *inc1y*, *inc2x*, *inc2y*, *inc3x*, and *inc3y*, provide great flexibility in defining the input and output data arrays. The arrangement of data in storage, however, can have an effect upon cache performance. By using strides, you can have data scattered in storage. Best performance is obtained with data closely spaced in storage and with elements of the sequence in contiguous locations. The optimum values for *inc1h*, *inc1x*, and *inc1y* are 1.

In writing the calling program, you may find it convenient to declare *X* or *Y* as a two-dimensional array. For example, you can declare *X* in a DIMENSION statement as *X(INC2X,M)*.

## Fourier Transform Considerations

This section describes some ways to optimize performance in the Fourier transform subroutines.

### Setting Up Your Data

Many of the Fourier transform, convolution, and correlation subroutines provide the facility for processing many sequences in one call. For short sequences, for example 1024 elements or less, this facility should be used as much as possible. This provides improved performance compared to processing only one sequence at a time.

If possible, you should use the same array for input and output. In addition, the requirements for the strides of the input and output arrays are explained in the Notes for each subroutine.

For improved performance, small values of *inc1x* and *inc1y* should be used, where applicable, preferably *inc1x* = 1 and *inc1y* = 1. A stride of 1 means the sequence elements are stored contiguously. Also, if possible, the sequences should be stored close to each other. For all the Fourier transform subroutines except *\_RCFT* and *\_CRFT*, you should use the STRIDE subroutine to determine the optimal stride(s) for your input or output data. Complete instructions on how to use STRIDE for each of these subroutines is included in "STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on page 1017.

To obtain the best performance in the three-dimensional Fourier transform subroutines, you should use strides, *inc2* and *inc3*, provided by the STRIDE subroutine and declare your three-dimensional data structure as a one-dimensional array. The three-dimensional Fourier transform subroutines assume that *inc1* for the array is 1. Therefore, each element  $x_{ijk}$  for  $i = 0, 1, \dots, n1-1$ ,  $j = 0, 1, \dots, n2-1$ , and  $k = 0, 1, \dots, n3-1$  of the three-dimensional data structure of dimensions  $n1$  by  $n2$  by  $n3$  is stored in a one-dimensional array  $X(0:L)$  at location  $X(l)$ , where  $l = i+inc2(j)+inc3(k)$ . The minimum required value of  $L$  is calculated by inserting the maximum values for  $i$ ,  $j$ , and  $k$  in the above equation, giving  $L = (n1-1)+inc2(n2-1)+inc3(n3-1)$ . The minimum total size of array  $X$  is  $L+1$ . To ensure that this mapping is unique so no two elements  $x_{ijk}$  occupy the same array element,  $X(l)$ , the subroutines have the following restriction:  $inc2 \geq n1$  and  $inc3 \geq (inc2)(n2)$ . This arrangement of array data in storage leaves some blank space between successive planes of the array  $X$ . By determining the best size for this space, specifying an optimum *inc3* stride, the third dimension of the array does not create conflicts in the 3090™ storage hierarchy.

If the *inc3* stride value returned by the STRIDE subroutine turns out to be a multiple of *inc2*, the array  $X$  can be declared as a three-dimensional array as



$X(\text{inc2}, \text{inc3}/\text{inc2}, n3)$ ; otherwise, it can be declared as either a one-dimensional array,  $X(0:L)$ , as described above, or a two-dimensional array  $X(0:\text{inc3}-1, 0:n3-1)$ , where  $x_{ijk}$  is stored in  $X(l,k)$  where  $l = i+(\text{inc2})(j)$ .

### Using the Scale Argument

If you must multiply either the input or the output sequences by a common factor, you can avoid the multiplication by letting the *scale* argument contain the factor. The subroutines multiply the sine and cosine values by the scale factor during the initialization. Thus, scaling takes no time after the initialization of the Fourier transform calculations.

## How the Fourier Transform Subroutines Achieve High Performance

There are two levels of optimization for the fast Fourier transforms (FFTs) in the ESSL library:

- For sequences with a large power of 2 length, we provide efficient implementations by factoring the transform length as follows:

$$N=N_1N_2N_3\dots N_p$$

where each  $N_i$  is a power of 2; the power of 2 used depends on the machine model.

The cache optimization includes ordering of operations to maximize stride-1 data access and prefetching cache lines.

Similar optimization techniques are used for sequence lengths which are not a power of 2 and mixed-radix FFT's are performed. Many short sequence FFT's have sequence size specific optimizations. Some of these optimizations were originally developed for a vector machine and have been adapted for cache based RISC machines (see references [1], [5], and [7])

- The other optimization in the FFT routine is to treat multiple sequences as efficiently as possible. Techniques here include blocking sequences to fit into available CPU cache and transposing sequences to ensure stride-1 access. Whenever possible, the highest performance can be obtained when multiple sequences are transformed in a single call.

## Convolution and Correlation Considerations

This section describes some ways to optimize performance in the convolution and correlation subroutines.

### Performance Tradeoffs between Subroutines

The subroutines *SCON*, *SCOR*, *SACOR*, *SCOND*, *SCORD*, *SDCON*, *SDCOR*, *DDCON*, and *DDCOR* compute convolutions, correlations, and autocorrelations using essentially the same methods. They make a decision, based on estimated timings, to use one of two methods:

- A direct method that is most efficient when one or both of the input sequences are short
- A direct method that is most efficient when the output sequence is short

Using this approach has the following advantages:

- In most cases, improved performance can be achieved for direct methods because:
  - No initialization is required.
  - No working storage or padding of sequences is necessary.
- In some cases, greater accuracy may be available.

- Negative strides can be used.

In general, using SCONF, SCOREF, and SACORF provides the best performance, because the mixed-radix Fourier transform subroutines are used. However, if you can determine from your arguments that a direct method is preferred, you should use SCOND and SCORD instead. These give you better performance for the direct methods, and also give you additional capabilities.

In cases where there is doubt as to the best choice of a subroutine, perform timing experiments.

### Special Uses of SCORD

The subroutine SCORD can perform the functions of SCON and SACOR; that is, it can compute convolutions and autocorrelations. To compute a convolution, you must specify a negative stride for  $h$  (see Example 4 in SCORD). To compute the autocorrelation, you must specify the two input sequences to be the same (see Example 5 in SCORD).

### Special Uses of \_DCON and \_DCOR

The \_DCON and \_DCOR subroutines compute convolutions and correlations, respectively, by the direct method with decimated output. Setting the decimation interval  $id = 1$  in SDCON and SDCOR provides the same function as SCOND and SCORD, respectively. Doing the same in DDCON and DDCOR provides long-precision versions of SCOND and SCORD, respectively, which are not otherwise available.

### Accuracy When Direct Methods Are Used

The direct methods used by the convolution and correlation subroutines use vector operations to accumulate sums of products. The products are computed and accumulated in long precision. As a result, higher accuracy can be obtained in the final results for some types of data. For example, if input data consists only of integers, and if no intermediate and final numbers become too large (larger than  $2^{24}-1$  for short-precision computations and larger than  $2^{56}-1$  for long-precision computations), the results are exact.

### Accuracy When Fourier Methods Are Used

The Fourier methods used by the convolution and correlation subroutines compute Fourier transforms of input data that is multiplied element-by-element in short-precision arithmetic. The inverse Fourier transform is then computed. There are internally generated rounding errors in the Fourier transforms. It has been shown in references [ 100] and [ 89] that, in the case of white noise data, the relative root mean square (RMS) error of the Fourier transform is proportional to  $\log_2 n$  with a very small proportionality factor. In general, with random, evenly distributed data, this is better than the RMS error of the direct method. However, one must keep in mind the fact that, while the Fourier method may yield a smaller root mean square error, there can be points with large relative errors. Thus, it can happen that some points, usually at the ends of the output sequence, can be obtained with greater relative accuracy with direct methods.

### Convolutions and Correlations by Fourier Methods

The convolution and correlation subroutines that use the Fourier methods determine a sequence length  $n$ , whose Fourier transform is computed using ESSL subroutines. In the simple case where  $iy0 = 0$  for convolution or  $iy0 = -nh+1$  for correlation,  $n$  is chosen as a value greater than or equal to the following, which is also acceptable to the Fourier transform subroutines:

$nt = \min(nh+nx-1, ny)$  for convolution and correlation  
 $nt = \min(nx+nx-1, ny)$  for autocorrelation

which is also acceptable to the Fourier subroutines.

---

## Related Computation Considerations

This section describes some key points about using the related-computation subroutines.

### Accuracy Considerations

- Many of the subroutines performing short-precision computations provide increased accuracy by accumulating results in long precision. This is noted in the functional description for each subroutine.
- There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see “What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?” on page 48.

---

## Fourier Transform Subroutines

This section contains the Fourier transform subroutine descriptions.

## SCFT and DCFT — Complex Fourier Transform

### Purpose

These subroutines compute a set of  $m$  complex discrete  $n$ -point Fourier transforms of complex data.

Table 141. Data Types

$X, Y$	<i>scale</i>	Subroutine
Short-precision complex	Short-precision real	SCFT
Long-precision complex	Long-precision real	DCFT

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

<b>Fortran</b>	CALL SCFT   DCFT ( <i>init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2</i> )
<b>C and C++</b>	scft   dcft ( <i>init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2</i> );

### On Entry

<i>init</i>	is a flag, where:  If $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than $x$ , are computed and saved in $aux1$ . The contents of $x$ and $y$ are not used or changed.  If $init = 0$ , the discrete Fourier transforms of the given sequences are computed. The only arguments that may change after initialization are $x, y$ , and $aux2$ . All scalar arguments must be the same as when the subroutine was called for initialization with $init \neq 0$ .  Specified as: a fullword integer. It can have any value.
$x$	is the array $X$ , consisting of $m$ sequences of length $n$ .  Specified as: an array of (at least) length $1+(n-1)inc1x+(m-1)inc2x$ , containing numbers of the data type indicated in Table 141.
<i>inc1x</i>	is the stride between the elements within each sequence in array $X$ .  Specified as: a fullword integer; $inc1x > 0$ .
<i>inc2x</i>	is the stride between the first elements of the sequences in array $X$ . (If $m = 1$ , this argument is ignored.) Specified as: a fullword integer; $inc2x > 0$ .
$y$	See "On Return" on page 789.
<i>inc1y</i>	is the stride between the elements within each sequence in array $Y$ .  Specified as: a fullword integer; $inc1y > 0$ .
<i>inc2y</i>	is the stride between the first elements of each sequence in array $Y$ . (If $m = 1$ , this argument is ignored.) Specified as: a fullword integer; $inc2y > 0$ .

## SCFT and DCFT

- n* is the length of each sequence to be transformed.  
Specified as: a fullword integer;  $n \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument, as well as in the optionally-recoverable error 2030. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- m* is the number of sequences to be transformed.  
Specified as: a fullword integer;  $m > 0$ .
- isign* controls the direction of the transform, determining the sign *Isign* of the exponent of  $W_n$ , where:  
If *isign* = positive value, *Isign* = + (transforming time to frequency).  
If *isign* = negative value, *Isign* = - (transforming frequency to time).  
Specified as: a fullword integer;  $isign > 0$  or  $isign < 0$ .
- scale* is the scaling constant *scale*. See “Function” on page 790 for its usage.  
Specified as: a number of the data type indicated in Table 141 on page 787, where  $scale > 0.0$  or  $scale < 0.0$
- aux1* is the working storage for this subroutine, where:  
If *init*  $\neq 0$ , the working storage is computed.  
If *init* = 0, the working storage is used in the computation of the Fourier transforms.  
Specified as: an area of storage, containing *naux1* long-precision real numbers.
- naux1* is the number of doublewords in the working storage specified in *aux1*.  
Specified as: a fullword integer;  $naux1 > 7$  and  $naux1 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For values between 7 and the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.
- aux2* has the following meaning:  
If *naux2* = 0 and error 2015 is unrecoverable, *aux2* is ignored.  
Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.  
Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.
- naux2* is the number of doublewords in the working storage specified in *aux2*.  
Specified as: a fullword integer, where:

If  $naux2 = 0$  and error 2015 is unrecoverable, SCFT and DCFT dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## On Return

$y$  has the following meaning, where:

If  $init \neq 0$ , this argument is not used, and its contents remain unchanged.

If  $init = 0$ , this is array  $Y$ , consisting of the results of the  $m$  discrete Fourier transforms, each of length  $n$ .

Returned as: an array of (at least) length  $1+(n-1)inc1y+(m-1)inc2y$ , containing numbers of the data type indicated in Table 141 on page 787. This array must be aligned on a doubleword boundary.

$aux1$  is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If  $init = 0$ , its contents are unchanged.

Returned as: the contents are not relevant.

## Notes

1.  $aux1$  should **not** be used by the calling program between calls to this subroutine with  $init \neq 0$  and  $init = 0$ . However, it can be reused after intervening calls to this subroutine with different arguments.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for  $init \neq 0$  and  $init = 0$ .
3. For optimal performance, the preferred value for  $inc1x$  and  $inc1y$  is 1. This implies that the sequences are stored with stride 1. The preferred value for  $inc2x$  and  $inc2y$  is  $n$ . This implies that sequences are stored one after another without any gap.

It is possible to specify sequences in the transposed form—that is, as rows of a two-dimensional array. In this case,  $inc2x$  (or  $inc2y$ ) = 1 and  $inc1x$  (or  $inc1y$ ) is equal to the leading dimension of the array. One can specify either input, output, or both in the transposed form by specifying appropriate values for the stride parameters. For selecting optimal values of  $inc1x$  and  $inc1y$  for  $\_CFT$ , you should use “STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines” on page 1017. Example 1 in the STRIDE subroutine description explains how it is used for  $\_CFT$ .

If you specify the same array for  $X$  and  $Y$ , then  $inc1x$  and  $inc1y$  must be equal, and  $inc2x$  and  $inc2y$  must be equal. In this case, output overwrites input. If  $m = 1$ , the  $inc2x$  and  $inc2y$  values are not used by the subroutine. If you specify different arrays for  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.

## Formulas

### Processor-Independent Formulas for SCFT for NAUX1 and NAUX2

#### NAUX1 Formulas::

If  $n \leq 8192$ , use  $naux1 = 20000$ .  
 If  $n > 8192$ , use  $naux1 = 20000 + 1.14n$ .

#### NAUX2 Formulas::

If  $n \leq 8192$ , use  $naux2 = 20000$ .  
 If  $n > 8192$ , use  $naux2 = 20000 + 1.14n$ .

For the transposed case, where  $inc2x = 1$  or  $inc2y = 1$ , and where  $n \geq 252$ , add the following to the above storage requirements:

$$(n+256)(\min(64, m))$$

### Processor-Independent Formulas for DCFT for NAUX1 and NAUX2

#### NAUX1 Formulas::

If  $n \leq 2048$ , use  $naux1 = 20000$ .  
 If  $n > 2048$ , use  $naux1 = 20000 + 2.28n$ .

#### NAUX2 Formulas::

If  $n \leq 2048$ , use  $naux2 = 20000$ .  
 If  $n > 2048$ , use  $naux2 = 20000 + 2.28n$ .

For the transposed case, where  $inc2x = 1$  or  $inc2y = 1$ , and where  $n \geq 252$ , add the following to the above storage requirements:

$$(2n+256)(\min(64, m))$$

## Function

The set of  $m$  complex discrete  $n$ -point Fourier transforms of complex data in array  $X$ , with results going into array  $Y$ , is expressed as follows:

$$y_{ki} = scale \sum_{j=0}^{n-1} x_{ji} W_n^{(I\text{sign})jk}$$

for:

$$k = 0, 1, \dots, n-1$$

$$i = 1, 2, \dots, m$$

where:



$$W_n = e^{-2\pi(\sqrt{-1})/n}$$

and where:

$x_{ji}$  are elements of the sequences in array  $X$ .

$y_{ki}$  are elements of the sequences in array  $Y$ .

$isign$  is + or - (determined by argument  $isign$ ).

$scale$  is a scalar value.

For  $scale = 1.0$  and  $isign$  being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with  $scale = 1.0/n$  and  $isign$  being negative. See references [1], [3], [4], [21], and [22].

Two invocations of this subroutine are necessary:

1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the  $aux1$  working storage.
2. With  $init = 0$ , the subroutine checks that the initialization arguments in the  $aux1$  working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transforms.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux2 = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n > 37748736$
2.  $inc1x$ ,  $inc2x$ ,  $inc1y$ , or  $inc2y \leq 0$
3.  $m \leq 0$
4.  $isign = 0$
5.  $scale = 0.0$
6. The subroutine has not been initialized with the present arguments.
7. The length of the transform in  $n$  is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
8.  $naux1 \leq 7$
9.  $naux1$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
10. Error 2015 is recoverable or  $naux2 \neq 0$ , and  $naux2$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows an input array  $X$  with a set of four short-precision complex sequences:

$$e^{2\pi(\sqrt{-1})jk/n}$$

## SCFT and DCFT

for  $j = 0, 1, \dots, n-1$  with  $n = 8$ , and the single frequencies  $k = 0, 1, 2$ , and 3. The arrays are declared as follows:

```
COMPLEX*8  X(0:1023),Y(0:1023)
REAL*8     AUX1(1693),AUX2(1)
```

First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```

      INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  N  M  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2
      |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SCFT(INIT, X , 1 , 8 , Y , 1 , 8 , 8 , 4 , 1 , SCALE, AUX1 , 1693 , AUX2 , 0)
```

```
INIT      = 1 (for initialization)
INIT      = 0 (for computation)
SCALE     = 1.0
```

X contains the following four sequences:

```
(1.0000, 0.0000) ( 1.0000, 0.0000) ( 1.0000, 0.0000) ( 1.0000, 0.0000)
(1.0000, 0.0000) ( 0.7071, 0.7071) ( 0.0000, 1.0000) (-0.7071, 0.7071)
(1.0000, 0.0000) ( 0.0000, 1.0000) (-1.0000, 0.0000) ( 0.0000, -1.0000)
(1.0000, 0.0000) (-0.7071, 0.7071) ( 0.0000, -1.0000) ( 0.7071, 0.7071)
(1.0000, 0.0000) (-1.0000, 0.0000) ( 1.0000, 0.0000) (-1.0000, 0.0000)
(1.0000, 0.0000) (-0.7071, -0.7071) ( 0.0000, 1.0000) ( 0.7071, -0.7071)
(1.0000, 0.0000) ( 0.0000, -1.0000) (-1.0000, 0.0000) ( 0.0000, 1.0000)
(1.0000, 0.0000) ( 0.7071, -0.7071) ( 0.0000, -1.0000) (-0.7071, -0.7071)
```

**Output:** Y contains the following four sequences:

```
(8.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (8.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (8.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (8.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
```

### Example 2

This example shows an input array X with a set of four input spike sequences equal to the output of Example 1. This shows how you can compute the inverse of the transform in Example 1 by using a negative *isign*, giving as output the four sequences listed in the input for Example 1. First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```

      INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  N  M  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2
      |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SCFT(INIT, X , 1 , 8 , Y , 1 , 8 , 8 , 4 , -1 , SCALE, AUX1 , 1693 , AUX2 , 0)
```

INIT = 1 (for initialization)  
 INIT = 0 (for computation)  
 SCALE = 0.125  
 X = (same as output Y in Example 1)

**Output:**

Y =(same as input X in Example 1)

**Example 3**

This example shows an input array X with a set of four short-precision complex sequences

$$e^{2\pi(\sqrt{-1})jk/n}$$

for  $j = 0, 1, \dots, n-1$  with  $n = 12$ , and the single frequencies  $k = 0, 1, 2$ , and 3. Also,  $inc1x = inc1y = m$  and  $inc2x = inc2y = 1$  to show how the input and output arrays can be stored in the transposed form. The arrays are declared as follows:

```
COMPLEX*8 X (4,0:11),Y(4,0:11)
REAL*8 AUX1(10000),AUX2(1)
```

First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

**Call Statement and Input:**

```
INIT X INC1X INC2X Y INC1Y INC2Y N M ISIGN SCALE AUX1 NAUX1 AUX2 NAUX2
| | | | | | | | | | | | | | |
CALL SCFT(INIT, X , 4 , 1 , Y , 4 , 1 , 12 , 4 , 1 , SCALE, AUX1 , 10000 , AUX2 , 0)
```

INIT = 1 (for initialization)  
 INIT = 0 (for computation)  
 SCALE = 1.0

X contains the following four sequences:

```
(1.0000, 0.0000) ( 1.0000, 0.0000) ( 1.0000, 0.0000) ( 1.0000, 0.0000)
(1.0000, 0.0000) ( 0.8660, 0.5000) ( 0.5000, 0.8660) ( 0.0000, 1.0000)
(1.0000, 0.0000) ( 0.5000, 0.8660) (-0.5000, 0.8660) (-1.0000, 0.0000)
(1.0000, 0.0000) ( 0.0000, 1.0000) (-1.0000, 0.0000) ( 0.0000, -1.0000)
(1.0000, 0.0000) (-0.5000, 0.8660) (-0.5000, -0.8660) ( 1.0000, 0.0000)
(1.0000, 0.0000) (-0.8660, 0.5000) ( 0.5000, -0.8660) ( 0.0000, 1.0000)
(1.0000, 0.0000) (-1.0000, 0.0000) ( 1.0000, 0.0000) (-1.0000, 0.0000)
(1.0000, 0.0000) (-0.8660, -0.5000) ( 0.5000, 0.8660) ( 0.0000, -1.0000)
(1.0000, 0.0000) (-0.5000, -0.8660) (-0.5000, 0.8660) ( 1.0000, 0.0000)
(1.0000, 0.0000) ( 0.0000, -1.0000) (-1.0000, 0.0000) ( 0.0000, 1.0000)
(1.0000, 0.0000) ( 0.5000, -0.8660) (-0.5000, -0.8660) (-1.0000, 0.0000)
(1.0000, 0.0000) ( 0.8660, -0.5000) ( 0.5000, -0.8660) ( 0.0000, -1.0000)
```

**Output:** Y contains the following four sequences:

```
(12.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000)
( 0.0000, 0.0000) (12.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000)
( 0.0000, 0.0000) ( 0.0000, 0.0000) (12.0000, 0.0000) ( 0.0000, 0.0000)
( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000) (12.0000, 0.0000)
( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000)
( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000)
```

## SCFT and DCFT

```
( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000)
( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000)
( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000)
( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000)
( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000)
( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000) ( 0.0000, 0.0000)
```

### Example 4

This example shows an input array  $X$  with a set of four input spike sequences exactly equal to the output of Example 3. This shows how you can compute the inverse of the transform in Example 3 by using a negative *isign*, giving as output the four sequences listed in the input for Example 3. First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

#### Call Statement and Input:

```
INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  N  M  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2
CALL SCFT(INIT, X, 4, 1, Y, 4, 1, 12, 4, -1, SCALE, AUX1, 10000, AUX2, 0)
```

```
INIT      = 1 (for initialization)
INIT      = 0 (for computation)
SCALE     = 1.0/12.0
X         = (same as output Y in Example 3)
```

#### Output:

Y = (same as input X in Example 3)

### Example 5

This example shows how to compute a transform of a single long-precision complex sequence. It uses  $isign = 1$  and  $scale = 1.0$ . The arrays are declared as follows:

```
COMPLEX*16  X(0:7),Y(0:7)
REAL*8      AUX1(26),AUX2(1)
```

The input in  $X$  is an impulse at zero, and the output in  $Y$  is constant for all frequencies. First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

#### Call Statement and Input:

```
INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  N  M  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2
CALL DCFT(INIT, X, 1, 0, Y, 1, 0, 8, 1, 1, SCALE, AUX1, 26, AUX2, 0)
```

```
INIT      = 1 (for initialization)
INIT      = 0 (for computation)
SCALE     = 1.0
```

$X$  contains the following sequence:

```
(1.0000, 0.0000)
(0.0000, 0.0000)
(0.0000, 0.0000)
(0.0000, 0.0000)
(0.0000, 0.0000)
(0.0000, 0.0000)
(0.0000, 0.0000)
(0.0000, 0.0000)
```

**Output:**

```
(1.0000, 0.0000)
(1.0000, 0.0000)
(1.0000, 0.0000)
(1.0000, 0.0000)
(1.0000, 0.0000)
(1.0000, 0.0000)
(1.0000, 0.0000)
(1.0000, 0.0000)
```

---

## SRCFT and DRCFT — Real-to-Complex Fourier Transform

### Purpose

These subroutines compute a set of  $m$  complex discrete  $n$ -point Fourier transforms of real data.

Table 142. Data Types

$\chi$ , <i>scale</i>	Y	Subroutine
Short-precision real	Short-precision complex	SRCFT
Long-precision real	Long-precision complex	DRCFT

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

<b>Fortran</b>	CALL SRCFT ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> , <i>aux3</i> , <i>naux3</i> )
	CALL DRCFT ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
<b>C and C++</b>	srcft ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> , <i>aux3</i> , <i>naux3</i> ); drcft ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

<i>init</i>	is a flag, where:  If <i>init</i> $\neq$ 0, trigonometric functions and other parameters, depending on arguments other than <i>x</i> , are computed and saved in <i>aux1</i> . The contents of <i>x</i> and <i>y</i> are not used or changed.  If <i>init</i> = 0, the discrete Fourier transforms of the given sequences are computed. The only arguments that may change after initialization are <i>x</i> , <i>y</i> , and <i>aux2</i> . All scalar arguments must be the same as when the subroutine was called for initialization with <i>init</i> $\neq$ 0.  Specified as: a fullword integer. It can have any value.
<i>x</i>	is the array $\chi$ , consisting of $m$ sequences of length $n$ , which are to be transformed. The sequences are assumed to be stored with stride 1.  Specified as: an array of (at least) length $n+(m-1)inc2x$ , containing numbers of the data type indicated in Table 142. See "Notes" on page 798 for more details. (It can be declared as $\chi(inc2x,m)$ .)
<i>inc2x</i>	is the stride between the first elements of the sequences in array $\chi$ . (If $m = 1$ , this argument is ignored.) Specified as: a fullword integer; $inc2x \geq n$ .
<i>y</i>	See "On Return" on page 798.
<i>inc2y</i>	is the stride between the first elements of the sequences in array Y. (If $m = 1$ , this argument is ignored.) Specified as: a fullword integer; $inc2y \geq (n/2)+1$ .

- n* is the length of each sequence to be transformed.  
Specified as: a fullword integer;  $n \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- m* is the number of sequences to be transformed.  
Specified as: a fullword integer;  $m > 0$ .
- isign* controls the direction of the transform, determining the sign *Isign* of the exponent of  $W_n$ , where:  
If *isign* = positive value, *Isign* = + (transforming time to frequency).  
If *isign* = negative value, *Isign* = - (transforming frequency to time).  
Specified as: a fullword integer;  $isign > 0$  or  $isign < 0$ .
- scale* is the scaling constant *scale*. See “Function” on page 799 for its usage.  
Specified as: a number of the data type indicated in Table 142 on page 796, where  $scale > 0.0$  or  $scale < 0.0$ .
- aux1* is the working storage for this subroutine, where:  
If *init*  $\neq 0$ , the working storage is computed.  
If *init* = 0, the working storage is used in the computation of the Fourier transforms.  
Specified as: an area of storage, containing *naux1* long-precision real numbers.
- naux1* is the number of doublewords in the working storage specified in *aux1*.  
Specified as: a fullword integer;  $naux1 > 14$  and  $naux1 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For values between 14 and the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.
- aux2* has the following meaning:  
If *naux2* = 0 and error 2015 is unrecoverable, *aux2* is ignored.  
Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.  
Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.
- naux2* is the number of doublewords in the working storage specified in *aux2*.  
Specified as: a fullword integer, where:

If  $naux2 = 0$  and error 2015 is unrecoverable, SRCFT and DRCFT dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.

<i>aux3</i>	<p>this argument is provided for migration purposes only and is ignored.</p> <p>Specified as: an area of storage, containing <i>naux3</i> long-precision real numbers.</p>
<i>naux3</i>	<p>this argument is provided for migration purposes only and is ignored.</p> <p>Specified as: a fullword integer.</p>

### On Return

<i>y</i>	<p>has the following meaning, where:</p> <p>If <math>init \neq 0</math>, this argument is not used, and its contents remain unchanged.</p> <p>If <math>init = 0</math>, this is array <math>Y</math>, consisting of the results of the <math>m</math> complex discrete Fourier transforms, each of length <math>n</math>. The sequences are stored with the stride 1. Due to complex conjugate symmetry, only the first <math>(n/2) + 1</math> elements of each sequence are given in the output—that is, <math>y_{ki}</math>, <math>k = 0, 1, \dots, n/2</math>, <math>i = 1, 2, \dots, m</math>.</p> <p>Returned as: an array of (at least) length <math>n/2+1+(m-1)inc2y</math>, containing numbers of the data type indicated in Table 142 on page 796. This array must be aligned on a doubleword boundary. (It can be declared as <math>Y(inc2y,m)</math>.)</p>
<i>aux1</i>	<p>is the working storage for this subroutine, where:</p> <p>If <math>init \neq 0</math>, it contains information ready to be passed in a subsequent invocation of this subroutine.</p> <p>If <math>init = 0</math>, its contents are unchanged.</p> <p>Returned as: the contents are not relevant.</p>

### Notes

1. *aux1* should **not** be used by the calling program between calls to this subroutine with  $init \neq 0$  and  $init = 0$ . However, it can be reused after intervening calls to this subroutine with different arguments.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for  $init \neq 0$  and  $init = 0$ .
3. In these subroutines, the elements in each sequence in  $x$  and  $y$  are assumed to be stored in contiguous storage locations, using a stride of 1; therefore, *inc1x* and *inc1y* values are not a part of the argument list. For optimal performance, the *inc2x* and *inc2y* values should be close to their respective minimum values, which are given below:



$$\begin{aligned}\min(\text{inc}2x) &= n \\ \min(\text{inc}2y) &= n/2+1\end{aligned}$$

If you specify the same array for  $X$  and  $Y$ , then  $\text{inc}2x$  must equal  $2(\text{inc}2y)$ . In this case, output overwrites input. If  $m = 1$ , the  $\text{inc}2x$  and  $\text{inc}2y$  values are not used by the subroutine. If you specify different arrays for  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.

4. Be sure to align array  $X$  on a doubleword boundary, and specify an even number for  $\text{inc}2x$ , if possible.

## Formulas

### Processor-Independent Formulas for SRCFT for NAUX1 and NAUX2

#### NAUX1 Formulas:

If  $n \leq 16384$ , use  $\text{naux}1 = 25000$ .  
If  $n > 16384$ , use  $\text{naux}1 = 20000+0.82n$ .

#### NAUX2 Formulas:

If  $n \leq 16384$ , use  $\text{naux}2 = 20000$ .  
If  $n > 16384$ , use  $\text{naux}2 = 20000+0.57n$ .

### Processor-Independent Formulas for DRCFT for NAUX1 and NAUX2

#### NAUX1 Formulas:

If  $n \leq 4096$ , use  $\text{naux}1 = 22000$ .  
If  $n > 4096$ , use  $\text{naux}1 = 20000+1.64n$ .

#### NAUX2 Formulas:

If  $n \leq 4096$ , use  $\text{naux}2 = 20000$ .  
If  $n > 4096$ , use  $\text{naux}2 = 20000+1.14n$ .

## Function

The set of  $m$  complex conjugate even discrete  $n$ -point Fourier transforms of real data in array  $X$ , with results going into array  $Y$ , is expressed as follows:

$$y_{ki} = \text{scale} \sum_{j=0}^{n-1} x_{ji} W_n^{(I\text{sign})jk}$$

for:

$$\begin{aligned}k &= 0, 1, \dots, n-1 \\ i &= 1, 2, \dots, m\end{aligned}$$

where:

$$W_n = e^{-2\pi(\sqrt{-1})/n}$$

and where:

$x_{ji}$  are elements of the sequences in array  $X$ .

$y_{ki}$  are elements of the sequences in array  $Y$ .

$isign$  is + or - (determined by argument  $isign$ ).

$scale$  is a scalar value.

The output in array  $Y$  is complex. For  $scale = 1.0$  and  $isign$  being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with  $scale = 1.0/n$  and  $isign$  being negative. See references [1], [4], [21], and [22].

Two invocations of this subroutine are necessary:

1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.
2. With  $init = 0$ , the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transforms.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux2 = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n > 37748736$
2.  $m \leq 0$
3.  $inc2x < n$
4.  $inc2y < n/2+1$
5.  $isign = 0$
6.  $scale = 0.0$
7. The subroutine has not been initialized with the present arguments.
8. The length of the transform in  $n$  is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
9.  $naux1 \leq 14$
10.  $naux1$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
11. Error 2015 is recoverable or  $naux2 \neq 0$ , and  $naux2$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows an input array  $X$  with a set of  $m$  cosine sequences  $\cos(2\pi jk/n)$ ,  $j = 0, 1, \dots, 15$  with the single frequencies  $k = 0, 1, 2, 3$ . The Fourier transform of the cosine sequence with frequency  $k = 0$  or  $n/2$  has 1.0 in the 0 or  $n/2$  position, respectively, and zeros elsewhere. For all other  $k$ , the Fourier transform has 0.5 in the  $k$  position and zeros elsewhere. The arrays are declared as follows:

```

REAL*4    X(0:65535)
COMPLEX*8 Y(0:32768)
REAL*8    AUX1(41928), AUX2(1), AUX3(1)

```

First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

**Call Statement and Input:**

```

          INIT  X  INC2X Y  INC2Y  N  M  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
CALL SRCFT( INIT, X , 16 , Y , 9 , 16 , 4 , 1 , SCALE, AUX1 , 41928 , AUX2 , 0 , AUX3 , 0 )

```

```

INIT      = 1 (for initialization)
INIT      = 0 (for computation)
SCALE     = 1.0/16

```

X contains the following four sequences:

```

1.0000  1.0000  1.0000  1.0000
1.0000  0.9239  0.7071  0.3827
1.0000  0.7071  0.0000 -0.7071
1.0000  0.3827 -0.7071 -0.9239
1.0000  0.0000 -1.0000  0.0000
1.0000 -0.3827 -0.7071  0.9239
1.0000 -0.7071  0.0000  0.7071
1.0000 -0.9239  0.7071 -0.3827
1.0000 -1.0000  1.0000 -1.0000
1.0000 -0.9239  0.7071 -0.3827
1.0000 -0.7071  0.0000  0.7071
1.0000 -0.3827 -0.7071  0.9239
1.0000  0.0000 -1.0000  0.0000
1.0000  0.3827 -0.7071 -0.9239
1.0000  0.7071  0.0000 -0.7071
1.0000  0.9239  0.7071  0.3827

```

**Output:** Y contains the following four sequences:

```

(1.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.5000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.5000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.5000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)

```

**Example 2**

This example shows another transform computation with different data using the same initialized array AUX1 as in Example 1. The input is also a set of four cosine sequences  $\cos(2\pi jk/n)$ ,  $j = 0, 1, \dots, 15$  with the single frequencies  $k = 8, 9, 10, 11$ , thus including the middle frequency  $k = 8$ . The middle frequency has the value 1.0. For other frequencies, the transform has zeros, except for frequencies  $k$  and  $n-k$ . Only the values for  $j = n-k$  are given in the output.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

## SRCFT and DRCFT

### Call Statement and Input:

```

      INIT X  INC2X Y  INC2Y  N  M  ISIGN SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
      |   |   |   |   |   |   |   |   |   |   |   |   |   |
CALL SRCFT( 0 , X , 16 , Y , 9 , 16 , 4 , 1 , SCALE, AUX1 , 41928 , AUX2 , 0 , AUX3 , 0 )

```

SCALE = 1.0/16

X contains the following four sequences:

```

 1.0000  1.0000  1.0000  1.0000
-1.0000 -0.9239 -0.7071 -0.3827
 1.0000  0.7071  0.0000 -0.7071
-1.0000 -0.3827  0.7071  0.9239
 1.0000  0.0000 -1.0000  0.0000
-1.0000  0.3827  0.7071 -0.9239
 1.0000 -0.7071  0.0000  0.7071
-1.0000  0.9239 -0.7071  0.3827
 1.0000 -1.0000  1.0000 -1.0000
-1.0000  0.9239 -0.7071  0.3827
 1.0000 -0.7071  0.0000  0.7071
-1.0000  0.3827  0.7071 -0.9239
 1.0000  0.0000 -1.0000  0.0000
-1.0000 -0.3827  0.7071  0.9239
 1.0000  0.7071  0.0000 -0.7071
-1.0000 -0.9239 -0.7071 -0.3827

```

Output: Y contains the following four sequences:

```

(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.5000, 0.0000)
(0.0000, 0.0000) (0.0000, 0.0000) (0.5000, 0.0000) (0.0000, 0.0000)
(0.0000, 0.0000) (0.5000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)
(1.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000) (0.0000, 0.0000)

```

### Example 3

This example uses the mixed-radix capability. The arrays are declared as follows:

```

REAL*8      X(0:11)
COMPLEX*16  Y(0:6)
REAL*8      AUX1(50),AUX2(1)

```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage:

```
EQUIVALENCE (X,Y)
```

First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```

      INIT X  INC2X Y  INC2Y  N  M  ISIGN SCALE  AUX1  NAUX1  AUX2  NAUX2
      |   |   |   |   |   |   |   |   |   |   |   |
CALL DRCFT(INIT, X , 0 , Y , 0 , 12 , 1 , 1 , SCALE , AUX1 , 50 , AUX2 , 0)

```

INIT = 1 (for initialization)

INIT = 0 (for computation)

```
SCALE = 1.0
X      = (1.0000 , 1.0000 , 1.0000 , 1.0000 , 1.0000 , 1.0000 ,
          1.0000 , 1.0000 , 1.0000 , 1.0000 , 1.0000 , 1.0000)
```

**Output:** Y contains the following sequence:

```
(12.0000 , 0.0000)
(0.0000 , 0.0000)
(0.0000 , 0.0000)
(0.0000 , 0.0000)
(0.0000 , 0.0000)
(0.0000 , 0.0000)
(0.0000 , 0.0000)
```

---

## SCRFT and DCRFT — Complex-to-Real Fourier Transform

### Purpose

These subroutines compute a set of  $m$  real discrete  $n$ -point Fourier transforms of complex conjugate even data.

Table 143. Data Types

$X$	$Y, scale$	Subroutine
Short-precision complex	Short-precision real	SCRFT
Long-precision complex	Long-precision real	DCRFT

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

<b>Fortran</b>	CALL SCRFT ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> , <i>aux3</i> , <i>naux3</i> ) CALL DCRFT ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
<b>C and C++</b>	scrft ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> , <i>aux3</i> , <i>naux3</i> ); dcrft ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

- init* is a flag, where:
- If  $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than  $x$ , are computed and saved in  $aux1$ . The contents of  $x$  and  $y$  are not used or changed.
- If  $init = 0$ , the discrete Fourier transforms of the given sequences are computed. The only arguments that may change after initialization are  $x$ ,  $y$ , and  $aux2$ . All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .
- Specified as: a fullword integer. It can have any value.
- $x$  is the array  $X$ , consisting of  $m$  sequences. Due to complex conjugate symmetry, the input consists of only the first  $(n/2)+1$  elements of each sequence; that is,  $x_{ji}$ ,  $j = 0, 1, \dots, n/2$ ,  $i = 1, 2, \dots, m$ . The sequences are assumed to be stored with stride 1.
- Specified as: an array of (at least) length  $n/2+1+(m-1)inc2x$ , containing numbers of the data type indicated in Table 143. This array must be aligned on a doubleword boundary. (It can be declared as  $X(inc2x,m)$ .)
- $inc2x$  is the stride between the first elements of the sequences in array  $X$ . (If  $m = 1$ , this argument is ignored.) Specified as: a fullword integer;  $inc2x \geq (n/2)+1$ .
- $y$  See "On Return" on page 806.

- inc2y* is the stride between the first elements of the sequences in array *Y*. (If  $m = 1$ , this argument is ignored.) Specified as: a fullword integer;  $inc2y \geq n$ .
- n* is the length of each sequence to be transformed.  
Specified as: a fullword integer;  $n \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- m* is the number of sequences to be transformed.  
Specified as: a fullword integer;  $m > 0$ .
- isign* controls the direction of the transform, determining the sign *Isign* of the exponent of  $W_n$ , where:  
If *isign* = positive value, *Isign* = + (transforming time to frequency).  
If *isign* = negative value, *Isign* = - (transforming frequency to time).  
Specified as: a fullword integer;  $isign > 0$  or  $isign < 0$ .
- scale* is the scaling constant *scale*. See “Function” on page 807 for its usage.  
Specified as: a number of the data type indicated in Table 143 on page 804, where  $scale > 0.0$  or  $scale < 0.0$ .
- aux1* is the working storage for this subroutine, where:  
If *init*  $\neq 0$ , the working storage is computed.  
If *init* = 0, the working storage is used in the computation of the Fourier transforms.  
Specified as: an area of storage, containing *naux1* long-precision real numbers.
- naux1* is the number of doublewords in the working storage specified in *aux1*.  
Specified as: a fullword integer;  $naux1 > 13$  and  $naux1 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For values between 13 and the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.
- aux2* has the following meaning:  
If *naux2* = 0 and error 2015 is unrecoverable, *aux2* is ignored.  
Otherwise, it is the working storage used by this subroutine that is available for use by the calling program between calls to this subroutine.  
Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

## SCRFT and DCRFT

<i>naux2</i>	<p>is the number of doublewords in the working storage specified in <i>aux2</i>.</p> <p>Specified as: a fullword integer, where:</p> <p>If <i>naux2</i> = 0 and error 2015 is unrecoverable, SCRFT and DCRFT dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.</p> <p>Otherwise, <math>naux2 \geq</math> (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.</p>
<i>aux3</i>	<p>this argument is provided for migration purposes only and is ignored.</p> <p>Specified as: an area of storage, containing <i>naux3</i> long-precision real numbers.</p>
<i>naux3</i>	<p>this argument is provided for migration purposes only and is ignored.</p> <p>Specified as: a fullword integer.</p>

### On Return

<i>y</i>	<p>has the following meaning, where:</p> <p>If <i>init</i> <math>\neq</math> 0, this argument is not used, and its contents remain unchanged.</p> <p>If <i>init</i> = 0, this is array <i>Y</i>, consisting of the results of the <i>m</i> discrete Fourier transforms of the complex conjugate even data, each of length <i>n</i>. The sequences are stored with stride 1.</p> <p>Returned as: an array of (at least) length <math>n+(m-1)inc2y</math>, containing numbers of the data type indicated in Table 143 on page 804. See “Notes” for more details. (It can be declared as <math>Y(inc2y,m)</math>.)</p>
<i>aux1</i>	<p>is the working storage for this subroutine, where:</p> <p>If <i>init</i> <math>\neq</math> 0, it contains information ready to be passed in a subsequent invocation of this subroutine.</p> <p>If <i>init</i> = 0, its contents are unchanged.</p> <p>Returned as: the contents are not relevant.</p>

### Notes

1. *aux1* should **not** be used by the calling program between calls to this subroutine with *init*  $\neq$  0 and *init* = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for *init*  $\neq$  0 and *init* = 0.
3. The elements in each sequence in *x* and *y* are assumed to be stored in contiguous storage locations—that is, with a stride of 1. Therefore, *inc1x* and *inc1y* values are not a part of the argument list. For optimal performance, the *inc2x* and *inc2y* values should be close to their respective minimum values, which are given below:



$$\begin{aligned}\min(\text{inc}2y) &= n \\ \min(\text{inc}2x) &= n/2+1\end{aligned}$$

If you specify the same array for  $X$  and  $Y$ , then  $\text{inc}2y$  must equal  $2(\text{inc}2x)$ . In this case, output overwrites input. If  $m = 1$ , the  $\text{inc}2x$  and  $\text{inc}2y$  values are not used by the subroutine. If you specify different arrays for  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.

4. Be sure to align array  $Y$  on a doubleword boundary, and specify an even number for  $\text{inc}2y$ , if possible.

## Formulas

### Processor-Independent Formulas for SCRFT for NAUX1 and NAUX2

#### NAUX1 Formulas:

If  $n \leq 16384$ , use  $\text{naux}1 = 25000$ .  
If  $n > 16384$ , use  $\text{naux}1 = 20000+0.82n$ .

#### NAUX2 Formulas:

If  $n \leq 16384$ , use  $\text{naux}2 = 20000$ .  
If  $n > 16384$ , use  $\text{naux}2 = 20000+0.57n$ .

### Processor-Independent Formulas for DCRFT for NAUX1 and NAUX2

#### NAUX1 Formulas:

If  $n \leq 4096$ , use  $\text{naux}1 = 22000$ .  
If  $n > 4096$ , use  $\text{naux}1 = 20000+1.64n$ .

#### NAUX2 Formulas:

If  $n \leq 4096$ , use  $\text{naux}2 = 20000$ .  
If  $n > 4096$ , use  $\text{naux}2 = 20000+1.14n$ .

## Function

The set of  $m$  real discrete  $n$ -point Fourier transforms of complex conjugate even data in array  $X$ , with results going into array  $Y$ , is expressed as follows:

$$y_{ki} = \text{scale} \sum_{j=0}^{n-1} x_{ji} W_n^{(I\text{sign})jk}$$

for:

$$\begin{aligned}k &= 0, 1, \dots, n-1 \\ i &= 1, 2, \dots, m\end{aligned}$$

where:

$$W_n = e^{-2\pi(\sqrt{-1})/n}$$

and where:

$x_{ji}$  are elements of the sequences in array  $X$ .

$y_{ki}$  are elements of the sequences in array  $Y$ .

$isign$  is + or - (determined by argument  $isign$ ).

$scale$  is a scalar value.

Because of the symmetry,  $Y$  has real data. For  $scale = 1.0$  and  $isign$  being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with  $scale = 1.0/n$  and  $isign$  being negative. See references [1], [4], [21], and [22].

Two invocations of this subroutine are necessary:

1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.
2. With  $init = 0$ , the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transforms.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux2 = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n > 37748736$
2.  $m \leq 0$
3.  $inc2x < n/2+1$
4.  $inc2y < n$
5.  $scale = 0.0$
6.  $isign = 0$
7. The subroutine has not been initialized with the present arguments.
8. The length of the transform in  $n$  is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
9.  $naux1 \leq 13$
10.  $naux1$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
11. Error 2015 is recoverable or  $naux2 \neq 0$ , and  $naux2$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example uses the mixed-radix capability and shows how to compute a single transform. The arrays are declared as follows:

```
COMPLEX*8  X(0:6)
REAL*8     AUX1(50), AUX2(1), AUX3(1)
REAL*4     Y(0:11)
```

First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Notes:**

1. X shows the  $n/2+1 = 7$  elements used in the computation.
2. Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

**Call Statement and Input:**

```

      INIT  X  INC2X  Y  INC2Y  N  M  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
      |    |    |    |    |    |  |  |    |    |    |    |    |    |
CALL SCRFT( INIT, X , 0 , Y , 0 , 12 , 1 , 1 , SCALE, AUX1 , 50 , AUX2 , 0 , AUX3 , 0 )
    
```

INIT = 1 (for initialization)  
 INIT = 0 (for computation)  
 SCALE = 1.0

X contains the following sequence:

```

(1.0, 0.0)
(0.0, 0.0)
(0.0, 0.0)
(0.0, 0.0)
(0.0, 0.0)
(0.0, 0.0)
(0.0, 0.0)
    
```

**Output:**

Y = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)

**Example 2**

This example shows another transform computation with different data using the same initialized array AUX1 as in Example 1.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

**Call Statement and Input:**

```

      INIT  X  INC2X  Y  INC2Y  N  M  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
      |    |    |    |    |    |  |  |    |    |    |    |    |    |
CALL SCRFT( 0 , X , 0 , Y , 0 , 12 , 1 , 1 , SCALE, AUX1 , 50 , AUX2 , 0 , AUX3 , 0 )
    
```

SCALE = 1.0

X contains the following sequence:

```

(1.0, 0.0)
(1.0, 0.0)
(1.0, 0.0)
(1.0, 0.0)
(1.0, 0.0)
(1.0, 0.0)
(1.0, 0.0)
    
```

**Output:**

Y = (12.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0)

## SCRFT and DCRFT

### Example 3

This example shows how to compute many transforms simultaneously. The arrays are declared as follows:

```
COMPLEX*8 X(0:8,2)
REAL*8    AUX1(50), AUX2(1), AUX3(1)
REAL*4    Y(0:15,2)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

#### Call Statement and Input:

```
          INIT  X  INC2X  Y  INC2Y  N  M  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
CALL SCRFT( |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | )
          |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
```

```
INIT      = 1 (for initialization)
INIT      = 0 (for computation)
SCALE     = 1.0
```

X contains the following two sequences:

```
(1.0, 0.0) (0.0, 0.0)
(1.0, 0.0) (0.0, 0.0)
(1.0, 0.0) (0.0, 0.0)
(1.0, 0.0) (0.0, 0.0)
(1.0, 0.0) (0.0, 0.0)
(1.0, 0.0) (0.0, 0.0)
(1.0, 0.0) (0.0, 0.0)
(1.0, 0.0) (0.0, 0.0)
(1.0, 0.0) (0.0, 0.0)
(1.0, 0.0) (1.0, 0.0)
```

**Output:** Y contains the following two sequences:

```
16.0  1.0
0.0  -1.0
0.0  1.0
0.0  -1.0
0.0  1.0
0.0  -1.0
0.0  1.0
0.0  -1.0
0.0  1.0
0.0  -1.0
0.0  1.0
0.0  -1.0
0.0  1.0
0.0  -1.0
0.0  1.0
0.0  -1.0
```

### Example 4

This example shows the same array being used for input and output. The arrays are declared as follows:

```
COMPLEX*16 X(0:8,2)
REAL*8     AUX1(50), AUX2(1)
REAL*8     Y(0:17,2)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage:

```
EQUIVALENCE (X,Y)
```

This requires  $INC2Y = 2(INC2X)$ . First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

**Call Statement and Input:**

```

                INIT  X  INC2X  Y  INC2Y  N  M  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2
                |   |   |   |   |   |   |   |   |   |   |   |
CALL DCRFT(INIT, X , 9 , Y , 18 , 16 , 2 , -1 , SCALE, AUX1 , 50 , AUX2 , 0)

```

```

INIT      = 1 (for initialization)
INIT      = 0 (for computation)
SCALE     = 0.0625

```

X contains the following two sequences:

```

( 1.0,  0.0) ( 1.0,  0.0)
( 0.0,  1.0) ( 0.0, -1.0)
(-1.0,  0.0) (-1.0,  0.0)
( 0.0, -1.0) ( 0.0,  1.0)
( 1.0,  0.0) ( 1.0,  0.0)
( 0.0,  1.0) ( 0.0, -1.0)
(-1.0,  0.0) (-1.0,  0.0)
( 0.0, -1.0) ( 0.0,  1.0)
( 1.0,  0.0) ( 1.0,  0.0)

```

**Output:** Y contains the following two sequences:

```

0.0  0.0
0.0  0.0
0.0  0.0
0.0  0.0
0.0  1.0
0.0  0.0
0.0  0.0
0.0  0.0
0.0  0.0
0.0  0.0
0.0  0.0
0.0  0.0
0.0  0.0
1.0  0.0
0.0  0.0
0.0  0.0
0.0  0.0

```

## SCOSF and DCOSF — Cosine Transform

### Purpose

These subroutines compute a set of  $m$  real even discrete  $n$ -point Fourier transforms of cosine sequences of real even data.

Table 144. Data Types

$X, Y, scale$	Subroutine
Short-precision real	SCOSF
Long-precision real	DCOSF

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

Fortran	CALL SCOSF   DCOSF ( <i>init</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
C and C++	scosf   dcosf ( <i>init</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

<i>init</i>	is a flag, where:  If $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than $x$ , are computed and saved in $aux1$ . The contents of $x$ and $y$ are not used or changed.  If $init = 0$ , the discrete Fourier transforms of the given sequences are computed. The only arguments that may change after initialization are $x$ , $y$ , and $aux2$ . All scalar arguments must be the same as when the subroutine was called for initialization with $init \neq 0$ .  Specified as: a fullword integer. It can have any value.
$x$	is the array $X$ , consisting of $m$ sequences of length $n/2+1$ .  Specified as: an array of (at least) length $1+(n/2)inc1x+(m-1)inc2x$ , containing numbers of the data type indicated in Table 144.
<i>inc1x</i>	is the stride between the elements within each sequence in array $X$ .  Specified as: a fullword integer; $inc1x > 0$ .
<i>inc2x</i>	is the stride between the first elements of the sequences in array $X$ . (If $m = 1$ , this argument is ignored.) Specified as: a fullword integer; $inc2x > 0$ .
$y$	See "On Return" on page 814.
<i>inc1y</i>	is the stride between the elements within each sequence in array $Y$ .  Specified as: a fullword integer; $inc1y > 0$ .
<i>inc2y</i>	is the stride between the first elements of the sequences in array $Y$ . (If $m = 1$ , this argument is ignored.) Specified as: a fullword integer; $inc2y > 0$ .

- n* is the transform length. However, due to symmetry, only the first  $n/2+1$  values are given in the input and output.  
Specified as: a fullword integer;  $n \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- m* is the number of sequences to be transformed.  
Specified as: a fullword integer;  $m > 0$ .
- scale* is the scaling constant *scale*. See “Function” on page 815 for its usage.  
Specified as: a number of the data type indicated in Table 144 on page 812, where  $scale > 0.0$  or  $scale < 0.0$ .
- aux1* is the working storage for this subroutine, where:  
If  $init \neq 0$ , the working storage is computed.  
If  $init = 0$ , the working storage is used in the computation of the Fourier transforms.  
Specified as: an area of storage, containing *naux1* long-precision real numbers.
- naux1* is the number of doublewords in the working storage specified in *aux1*.  
Specified as: a fullword integer;  $naux1 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.
- aux2* has the following meaning:  
If  $naux2 = 0$  and error 2015 is unrecoverable, *aux2* is ignored.  
Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.  
Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.
- naux2* is the number of doublewords in the working storage specified in *aux2*.  
Specified as: a fullword integer, where:  
If  $naux2 = 0$  and error 2015 is unrecoverable, SCOSF and DCOSF dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.  
Otherwise,  $naux2 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the

minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.

### On Return

*y*

has the following meaning, where:

If *init*  $\neq$  0, this argument is not used, and its contents remain unchanged.

If *init* = 0, this is array *Y*, consisting of the results of the *m* discrete Fourier transforms, where each Fourier transform is real and of length *n*. However, due to symmetry, only the first  $n/2+1$  values are given in the output—that is,  $y_{ki}$ ,  $k = 0, 1, \dots, n/2$  for each  $i = 1, 2, \dots, m$ .

Returned as: an array of (at least) length  $1+(n/2)inc1y+(m-1)inc2y$ , containing numbers of the data type indicated in Table 144 on page 812.

*aux1*

is the working storage for this subroutine, where:

If *init*  $\neq$  0, it contains information ready to be passed in a subsequent invocation of this subroutine.

If *init* = 0, its contents are unchanged.

Returned as: the contents are not relevant.

## Notes

1. *aux1* should **not** be used by the calling program between calls to this subroutine with *init*  $\neq$  0 and *init* = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for *init*  $\neq$  0 and *init* = 0.
3. For optimal performance, the preferred value for *inc1x* and *inc1y* is 1. This implies that the sequences are stored with stride 1. In addition, *inc2x* and *inc2y* should be close to  $n/2+1$ .

It is possible to specify sequences in the transposed form—that is, as rows of a two-dimensional array. In this case, *inc2x* (or *inc2y*) = 1 and *inc1x* (or *inc1y*) is equal to the leading dimension of the array. One can specify either input, output, or both in the transposed form by specifying appropriate values for the stride parameters. For selecting optimal values of *inc1x* and *inc1y* for *\_COSF*, you should use “STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines” on page 1017. Example 2 in the STRIDE subroutine description explains how it is used for *\_COSF*.

If you specify the same array for *X* and *Y*, then *inc1x* and *inc1y* must be equal, and *inc2x* and *inc2y* must be equal. In this case, output overwrites input. If  $m = 1$ , the *inc2x* and *inc2y* values are not used by the subroutine. If you specify different arrays for *X* and *Y*, they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.

## Formulas

### Processor-Independent Formulas for SCOSF for NAUX1 and NAUX2

#### NAUX1 Formulas::



If  $n \leq 16384$ , use  $naux1 = 40000$ .  
 If  $n > 16384$ , use  $naux1 = 20000+.30n$ .

#### NAUX2 Formulas::

If  $n \leq 16384$ , use  $naux2 = 25000$ .  
 If  $n > 16384$ , use  $naux2 = 20000+.32n$ .

For the transposed case, where  $inc2x = 1$  or  $inc2y = 1$ , and where  $n \geq 252$ , add the following to the above storage requirements:

$$(n/4+257)(\min(128, m))$$

### Processor-Independent Formulas for DCOSF for NAUX1 and NAUX2

#### NAUX1 Formulas::

If  $n \leq 16384$ , use  $naux1 = 35000$ .  
 If  $n > 16384$ , use  $naux1 = 20000+.60n$ .

#### NAUX2 Formulas::

If  $n \leq 16384$ , use  $naux2 = 20000$ .  
 If  $n > 16384$ , use  $naux2 = 20000+.64n$ .

For the transposed case, where  $inc2x = 1$  or  $inc2y = 1$ , and where  $n \geq 252$ , add the following to the above storage requirements:

$$(n/2+257)(\min(128, m))$$

## Function

The set of  $m$  real even discrete  $n$ -point Fourier transforms of the cosine sequences of real data in array  $X$ , with results going into array  $Y$ , is expressed as follows:

$$y_{ki} = scale \left( .5x_{0,i} + .5(-1)^k x_{n/2,i} + \sum_{j=1}^{n/2-1} x_{ji} \cos(jk(2\pi/n)) \right)$$

for:

$$k = 0, 1, \dots, n/2$$

$$i = 1, 2, \dots, m$$

where:

$x_{ji}$  are elements of the sequences in array  $X$ , where each sequence contains the  $n/2+1$  real nonredundant data  $x_{jv}$   $j = 0, 1, \dots, n/2$ .

$y_{ki}$  are elements of the sequences in array  $Y$ , where each sequence contains the  $n/2+1$  real nonredundant data  $y_{ki}$   $k = 0, 1, \dots, n/2$ .

$scale$  is a scalar value.

You can obtain the inverse cosine transform by specifying  $scale = 4.0/n$ . Thus, if an  $X$  input is used with  $scale = 1.0$ , and its output is used as input on a subsequent call with  $scale = 4.0/n$ , the original  $X$  is obtained. See references [1], [4], [21], and [22].

Two invocations of this subroutine are necessary:

1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.
2. With  $init = 0$ , the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transforms.

These subroutines use a Fourier transform method with a mixed-radix capability. This provides maximum performance for your application.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux2 = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n > 37748736$
2.  $inc1x$  or  $inc1y \leq 0$
3.  $inc2x$  or  $inc2y \leq 0$
4.  $m \leq 0$
5.  $scale = 0.0$
6. The subroutine has not been initialized with the present arguments.
7. The length of the transform in  $n$  is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
8.  $naux1$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
9. Error 2015 is recoverable or  $naux2 \neq 0$ , and  $naux2$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows an input array  $X$  with a set of  $m$  cosine sequences of length  $n/2+1$ ,  $\cos(jk(2\pi/n))$ ,  $j = 0, 1, \dots, n/2$ , with the single frequencies  $k = 0, 1, 2, 3$ . The Fourier transform of the cosine sequence with frequency  $k = 0$  or  $n/2$  has  $n/2$  in the 0-th or  $n/2$ -th position, respectively, and zeros elsewhere. For all other  $k$ , the Fourier transform has  $n/4$  in position  $k$  and zeros elsewhere. The arrays are declared as follows:

```
REAL*4    X(0:71),Y(0:71)
REAL*8    AUX1(414),AUX2(1)
```

First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the  $AUX2$  working storage.

**Call Statement and Input:**

```

      INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  N  M  SCALE  AUX1  NAUX1  AUX2  NAUX2
CALL SCOSF( INIT, X, 1, 18, Y, 1, 18, 32, 4, SCALE, AUX1, 414, AUX2, 0)

```

INIT = 1 (for initialization)  
 INIT = 0 (for computation)  
 SCALE = 1.0

X contains the following four sequences:

```

1.0000  1.0000  1.0000  1.0000
1.0000  0.9808  0.9239  0.8315
1.0000  0.9239  0.7071  0.3827
1.0000  0.8315  0.3827 -0.1951
1.0000  0.7071  0.0000 -0.7071
1.0000  0.5556 -0.3827 -0.9808
1.0000  0.3827 -0.7071 -0.9239
1.0000  0.1951 -0.9239 -0.5556
1.0000  0.0000 -1.0000  0.0000
1.0000 -0.1951 -0.9239  0.5556
1.0000 -0.3827 -0.7071  0.9239
1.0000 -0.5556 -0.3827  0.9808
1.0000 -0.7071  0.0000  0.7071
1.0000 -0.8315  0.3827  0.1951
1.0000 -0.9239  0.7071 -0.3827
1.0000 -0.9808  0.9239 -0.8315
1.0000 -1.0000  1.0000 -1.0000
.       .       .       .

```

**Output:** Y contains the following four sequences:

```

16.0000  0.0000  0.0000  0.0000
 0.0000  8.0000  0.0000  0.0000
 0.0000  0.0000  8.0000  0.0000
 0.0000  0.0000  0.0000  8.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
 0.0000  0.0000  0.0000  0.0000
.       .       .       .

```

**Example 2**

This example shows an input array X with a set of four input spike sequences equal to the output of Example 1. This shows how you can compute the inverse of the transform in Example 1 by using  $scale = 4.0/n$ , giving as output the four sequences listed in the input for Example 1. First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

## SCOSF and DCOSF

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```

      INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  N  M  SCALE  AUX1  NAUX1  AUX2  NAUX2
      |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SCOSF( INIT, X, 1, 18, Y, 1, 18, 32, 4, SCALE, AUX1, 414, AUX2, 0)

```

INIT = 1 (for initialization)  
 INIT = 0 (for computation)  
 SCALE = 4.0/32  
 X = (same sequences as in output Y in Example 1)

### Output:

Y = (same sequences as in output X in Example 1)

### Example 3

This example shows another computation using the same arguments initialized in Example 1 and using different input sequence data. The data for this example has frequencies  $k = 14, 15, 16, 17$ . Because only the sequence data has changed, initialization does not have to be done again.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```

      INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  N  M  SCALE  AUX1  NAUX1  AUX2  NAUX2
      |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SCOSF( 0, X, 1, 18, Y, 1, 18, 32, 4, SCALE, AUX1, 414, AUX2, 0)

```

SCALE = 1.0

X contains the following four sequences:

```

  1.0000  1.0000  1.0000  1.0000
 -0.9239 -0.9808 -1.0000 -0.9808
  0.7071  0.9239  1.0000  0.9239
 -0.3827 -0.8315 -1.0000 -0.8315
  0.0000  0.7071  1.0000  0.7071
  0.3827 -0.5556 -1.0000 -0.5556
 -0.7071  0.3827  1.0000  0.3827
  0.9239 -0.1951 -1.0000 -0.1951
 -1.0000  0.0000  1.0000  0.0000
  0.9239  0.1951 -1.0000  0.1951
 -0.7071 -0.3827  1.0000 -0.3827
  0.3827  0.5556 -1.0000  0.5556
  0.0000 -0.7071  1.0000 -0.7071
 -0.3827  0.8315 -1.0000  0.8315
  0.7071 -0.9239  1.0000 -0.9239
 -0.9239  0.9808 -1.0000  0.9808
  1.0000 -1.0000  1.0000 -1.0000
  .      .      .      .

```

**Output:** Y contains the following four sequences:

```

  0.0000  0.0000  0.0000  0.0000
  0.0000  0.0000  0.0000  0.0000
  0.0000  0.0000  0.0000  0.0000
  0.0000  0.0000  0.0000  0.0000
  0.0000  0.0000  0.0000  0.0000

```

0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000
8.0000	0.0000	0.0000	0.0000
0.0000	8.0000	0.0000	8.0000
0.0000	0.0000	16.0000	0.0000
.	.	.	.

---

## SSINF and DSINF — Sine Transform

### Purpose

These subroutines compute a set of  $m$  real even discrete  $n$ -point Fourier transforms of sine sequences of real even data.

Table 145. Data Types

$X, Y, scale$	Subroutine
Short-precision real	SSINF
Long-precision real	DSINF

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

<b>Fortran</b>	CALL SSINF   DSINF ( <i>init</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
<b>C and C++</b>	ssinf   dsinf ( <i>init</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>n</i> , <i>m</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

<i>init</i>	is a flag, where:  If $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than $x$ , are computed and saved in $aux1$ . The contents of $x$ and $y$ are not used or changed.  If $init = 0$ , the discrete Fourier transforms of the given sequences are computed. The only arguments that may change after initialization are $x$ , $y$ , and $aux2$ . All scalar arguments must be the same as when the subroutine was called for initialization with $init \neq 0$ .  Specified as: a fullword integer. It can have any value.
<i>x</i>	is the array $X$ , consisting of $m$ sequences of length $n/2$ .  Specified as: an array of (at least) length $1+(n / 2-1)inc1x+(m-1)inc2x$ , containing numbers of the data type indicated in Table 145. The first element in $X$ must have a value of 0.0 (otherwise, incorrect results may occur).
<i>inc1x</i>	is the stride between the elements within each sequence in array $X$ .  Specified as: a fullword integer; $inc1x > 0$ .
<i>inc2x</i>	is the stride between the first elements of the sequences in array $X$ . (If $m = 1$ , this argument is ignored.) Specified as: a fullword integer; $inc2x > 0$ .
<i>y</i>	See "On Return" on page 822.
<i>inc1y</i>	is the stride between the elements within each sequence in array $Y$ .  Specified as: a fullword integer; $inc1y > 0$ .

- inc2y* is the stride between the first elements of the sequences in array Y. (If  $m = 1$ , this argument is ignored.) Specified as: a fullword integer;  $inc2y > 0$ .
- n* is the transform length. However, due to symmetry, only the first  $n/2$  values are given in the input and output.  
Specified as: a fullword integer;  $n \leq 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 42.
- m* is the number of sequences to be transformed.  
Specified as: a fullword integer;  $m > 0$ .
- scale* is the scaling constant *scale*. See "Function" on page 823 for its usage.  
Specified as: a number of the data type indicated in Table 145 on page 820, where  $scale > 0.0$  or  $scale < 0.0$ .
- aux1* is the working storage for this subroutine, where:  
If  $init \neq 0$ , the working storage is computed.  
If  $init = 0$ , the working storage is used in the computation of the Fourier transforms.  
Specified as: an area of storage, containing *naux1* long-precision real numbers.
- naux1* is the number of doublewords in the working storage specified in *aux1*.  
Specified as: a fullword integer;  $naux1 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 36.
- aux2* has the following meaning:  
If  $naux2 = 0$  and error 2015 is unrecoverable, *aux2* is ignored.  
Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.  
Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.
- naux2* is the number of doublewords in the working storage specified in *aux2*.  
Specified as: a fullword integer, where:  
If  $naux2 = 0$  and error 2015 is unrecoverable, SSINF and DSINF dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.

### On Return

*y*

has the following meaning, where:

If  $init \neq 0$ , this argument is not used, and its contents remain unchanged.

If  $init = 0$ , this is array  $Y$ , consisting of the results of the  $m$  discrete Fourier transforms, where each Fourier transform is real and of length  $n$ . However, due to symmetry, only the first  $n/2$  values are given in the output—that is,  $y_{ki}$ ,  $k = 0, 1, \dots, n/2-1$  for each  $i = 1, 2, \dots, m$ .

Returned as: an array of (at least) length  $1+(n/2-1)inc1y+(m-1)inc2y$ , containing numbers of the data type indicated in Table 145 on page 820.

*aux1*

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If  $init = 0$ , its contents are unchanged.

Returned as: the contents are not relevant.

### Notes

1. *aux1* should **not** be used by the calling program between calls to this subroutine with  $init \neq 0$  and  $init = 0$ . However, it can be reused after intervening calls to this subroutine with different arguments.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for  $init \neq 0$  and  $init = 0$ .
3. For optimal performance, the preferred value for  $inc1x$  and  $inc1y$  is 1. This implies that the sequences are stored with stride 1. In addition,  $inc2x$  and  $inc2y$  should be close to  $n/2$ .

It is possible to specify sequences in the transposed form—that is, as rows of a two-dimensional array. In this case,  $inc2x$  (or  $inc2y$ ) = 1 and  $inc1x$  (or  $inc1y$ ) is equal to the leading dimension of the array. One can specify either input, output, or both in the transposed form by specifying appropriate values for the stride parameters. For selecting optimal values of  $inc1x$  and  $inc1y$  for  $\_SINF$ , you should use “STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines” on page 1017. Example 3 in the STRIDE subroutine description explains how it is used for  $\_SINF$ .

If you specify the same array for  $X$  and  $Y$ , then  $inc1x$  and  $inc1y$  must be equal, and  $inc2x$  and  $inc2y$  must be equal. In this case, output overwrites input. If  $m = 1$ , the  $inc2x$  and  $inc2y$  values are not used by the subroutine. If you specify different arrays for  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.



## Formulas

### Processor-Independent Formulas for SSINF for NAUX1 and NAUX2

#### NAUX1 Formulas::

If  $n \leq 16384$ , use  $naux1 = 60000$ .  
 If  $n > 16384$ , use  $naux1 = 20000 + .30n$ .

#### NAUX2 Formulas::

If  $n \leq 16384$ , use  $naux2 = 25000$ .  
 If  $n > 16384$ , use  $naux2 = 20000 + .32n$ .

For the transposed case, where  $inc2x = 1$  or  $inc2y = 1$ , and where  $n \geq 252$ , add the following to the above storage requirements:

$$(n/4 + 257)(\min(128, m)).$$

### Processor-Independent Formulas for DSINF for NAUX1 and NAUX2

#### NAUX1 Formulas::

If  $n \leq 16384$ , use  $naux1 = 50000$ .  
 If  $n > 16384$ , use  $naux1 = 20000 + .60n$ .

#### NAUX2 Formulas::

If  $n \leq 16384$ , use  $naux2 = 20000$ .  
 If  $n > 16384$ , use  $naux2 = 20000 + .64n$ .

For the transposed case, where  $inc2x = 1$  or  $inc2y = 1$ , and where  $n \geq 252$ , add the following to the above storage requirements:

$$(n/2 + 257)(\min(128, m))$$

## Function

The set of  $m$  real even discrete  $n$ -point Fourier transforms of the sine sequences of real data in array  $X$ , with results going into array  $Y$ , is expressed as follows:

$$y_{ki} = scale \sum_{j=0}^{n/2-1} x_{ji} \sin(jk(2\pi/n))$$

for:

$$k = 0, 1, \dots, n/2-1$$

$$i = 1, 2, \dots, m$$

where:

$$x_{0i} = 0.0$$

## SSINF and DSINF

$x_{ji}$  are elements of the sequences in array  $X$ , where each sequence contains the  $n/2$  real nonredundant data  $x_{ji}$ ,  $j = 0, 1, \dots, n/2-1$ .

$y_{ki}$  are elements of the sequences in array  $Y$ , where each sequence contains the  $n/2$  real nonredundant data  $y_{ki}$ ,  $k = 0, 1, \dots, n/2-1$ .

$scale$  is a scalar value.

You can obtain the inverse sine transform by specifying  $scale = 4.0/n$ . Thus, if an  $X$  input is used with  $scale = 1.0$ , and its output is used as input on a subsequent call with  $scale = 4.0/n$ , the original  $X$  is obtained. See references [1], [4], [21], and [22].

Two invocations of this subroutine are necessary:

1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the  $aux1$  working storage.
2. With  $init = 0$ , the subroutine checks that the initialization arguments in the  $aux1$  working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transforms.

These subroutines use a Fourier transform method with a mixed-radix capability. This provides maximum performance for your application.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux2 = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n > 37748736$
2.  $inc1x$  or  $inc1y \leq 0$
3.  $inc2x$  or  $inc2y \leq 0$
4.  $m \leq 0$
5.  $scale = 0.0$
6. The subroutine has not been initialized with the present arguments.
7. The length of the transform in  $n$  is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
8.  $naux1$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
9. Error 2015 is recoverable or  $naux2 \neq 0$ , and  $naux2$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows an input array  $X$  with a set of  $m$  sine sequences of length  $n/2$ ,  $\sin(jk(2\pi/n))$ ,  $j = 0, 1, \dots, n/2-1$ , with the single frequencies  $k = 1, 2, 3$ . The Fourier transform of the sine sequence has  $n/4$  in position  $k$  and zeros elsewhere. The arrays are declared as follows:

```

REAL*4    X(0:53),Y(0:53)
REAL*8    AUX1(414),AUX2(1)

```

First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```

          INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  N  M  SCALE  AUX1  NAUX1  AUX2  NAUX2
          |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SSINF(INIT, X , 1 , 18 , Y , 1 , 18 , 32 , 3 , SCALE, AUX1 , 414 , AUX2 , 0)

```

```

INIT      = 1 (for initialization)
INIT      = 0 (for computation)
SCALE     = 1.0

```

X contains the following three sequences:

```

0.0000  0.0000  0.0000
0.1951  0.3827  0.5556
0.3827  0.7071  0.9239
0.5556  0.9239  0.9808
0.7071  1.0000  0.7071
0.8315  0.9239  0.1951
0.9239  0.7071 -0.3827
0.9808  0.3827 -0.8315
1.0000  0.0000 -1.0000
0.9808 -0.3827 -0.8315
0.9239 -0.7071 -0.3827
0.8315 -0.9239  0.1951
0.7071 -1.0000  0.7071
0.5556 -0.9239  0.9808
0.3827 -0.7071  0.9239
0.1951 -0.3827  0.5556
:      :      :
:      :      :

```

**Output:** Y contains the following three sequences:

```

0.0000  0.0000  0.0000
8.0000  0.0000  0.0000
0.0000  8.0000  0.0000
0.0000  0.0000  8.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
0.0000  0.0000  0.0000
:      :      :
:      :      :

```

### Example 2

This example shows an input array X with a set of three input spike sequences equal to the output of Example 1. This shows how you can compute the inverse of

## SSINF and DSINF

the transform in Example 1 by using  $scale = 4.0/n$ , giving as output the three sequences listed in the input for Example 1. First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```

      INIT X INC1X INC2X Y INC1Y INC2Y N M SCALE AUX1 NAUX1 AUX2 NAUX2
      |   |   |   |   |   |   |   |   |   |   |   |   |
CALL SSINF( INIT, X, 1, 18, Y, 1, 18, 32, 3, SCALE, AUX1, 414, AUX2, 0)

```

INIT = 1 (for initialization)  
 INIT = 0 (for computation)  
 SCALE =  $4.0/32$   
 X = (same sequences as in output Y in Example 1)

### Output:

Y = (same sequences as in output X in Example 1)

### Example 3

This example shows another computation using the same arguments initialized in Example 1 and using different input sequence data. The data for this example has frequencies  $k = 14, 15, 17$ . Because only the sequence data has changed, initialization does not have to be done again.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```

      INIT X INC1X INC2X Y INC1Y INC2Y N M SCALE AUX1 NAUX1 AUX2 NAUX2
      |   |   |   |   |   |   |   |   |   |   |   |   |
CALL SSINF( 0, X, 1, 18, Y, 1, 18, 32, 3, SCALE, AUX1, 414, AUX2, 0)

```

SCALE = 1.0

X contains the following three sequences:

```

0.0000  0.0000  0.0000
0.3827  0.1951 -0.1951
-0.7071 -0.3827  0.3827
0.9239  0.5556 -0.5556
-1.0000 -0.7071  0.7071
0.9239  0.8315 -0.8315
-0.7071 -0.9239  0.9239
0.3827  0.9808 -0.9808
0.8573 -1.0000  1.0000
-0.3827  0.9808 -0.9808
0.7071 -0.9239  0.9239
-0.9239  0.8315 -0.8315
1.0000 -0.7071  0.7071
-0.9239  0.5556 -0.5556
0.7071 -0.3827  0.3827
-0.3827  0.1951 -0.1951
.
.
.
```

**Output:** Y contains the following three sequences:

0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
0.0000	0.0000	0.0000
8.0000	0.0000	0.0000
0.0000	8.0000	-8.0000
0.0000	0.0000	0.0000
.	.	.
.	.	.

## SCFT2 and DCFT2 — Complex Fourier Transform in Two Dimensions

### Purpose

These subroutines compute the two-dimensional discrete Fourier transform of complex data.

Table 146. Data Types

X, Y	scale	Subroutine
Short-precision complex	Short-precision real	SCFT2
Long-precision complex	Long-precision real	DCFT2

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

<b>Fortran</b>	CALL SCFT2   DCFT2 ( <i>init</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>n1</i> , <i>n2</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
<b>C and C++</b>	scft2   dcft2 ( <i>init</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>n1</i> , <i>n2</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

*init*

is a flag, where:

If *init*  $\neq$  0, trigonometric functions and other parameters, depending on arguments other than *x*, are computed and saved in *aux1*. The contents of *x* and *y* are not used or changed.

If *init* = 0, the discrete Fourier transform of the given array is computed. The only arguments that may change after initialization are *x*, *y*, and *aux2*. All scalar arguments must be the same as when the subroutine was called for initialization with *init*  $\neq$  0.

Specified as: a fullword integer. It can have any value.

*x*

is the array *X*, containing the two-dimensional data to be transformed, where each element  $x_{j1,j2}$ , using zero-based indexing, is stored in  $X(j1(inc1x)+j2(inc2x))$  for  $j1 = 0, 1, \dots, n1-1$  and  $j2 = 0, 1, \dots, n2-1$ .

Specified as: an array of (at least) length  $1+(n1-1)inc1x+(n2-1)inc2x$ , containing numbers of the data type indicated in Table 146. This array must be aligned on a doubleword boundary, and:

If *inc1x* = 1, the input array is stored in normal form, and *inc2x*  $\geq$  *n1*.

If *inc2x* = 1, the input array is stored in transposed form, and *inc1x*  $\geq$  *n2*.

See "Notes" on page 831 for more details.

*inc1x*

is the stride between the elements in array *X* for the first dimension.

If the array is stored in the normal form, *inc1x* = 1.

- If the array is stored in the transposed form,  $inc1x$  is the leading dimension of the array and  $inc1x \geq n2$ .
- Specified as: a fullword integer;  $inc1x > 0$ . If  $inc2x = 1$ , then  $inc1x \geq n2$ .
- $inc2x$  is the stride between the elements in array X for the second dimension.
- If the array is stored in the transposed form,  $inc2x = 1$ .
- If the array is stored in the normal form,  $inc2x$  is the leading dimension of the array and  $inc2x \geq n1$ .
- Specified as: a fullword integer;  $inc2x > 0$ . If  $inc1x = 1$ , then  $inc2x \geq n1$ .
- $y$  See "On Return" on page 830.
- $inc1y$  is the stride between the elements in array Y for the first dimension.
- If the array is stored in the normal form,  $inc1y = 1$ .
- If the array is stored in the transposed form,  $inc1y$  is the leading dimension of the array and  $inc1y \geq n2$ .
- Specified as: a fullword integer;  $inc1y > 0$ . If  $inc2y = 1$ , then  $inc1y \geq n2$ .
- $inc2y$  is the stride between the elements in array Y for the second dimension.
- If the array is stored in the transposed form,  $inc2y = 1$ .
- If the array is stored in the normal form,  $inc2y$  is the leading dimension of the array and  $inc2y \geq n1$ .
- Specified as: a fullword integer;  $inc2y > 0$ . If  $inc1y = 1$ , then  $inc2y \geq n1$ .
- $n1$  is the length of the first dimension of the two-dimensional data in the array to be transformed.
- Specified as: a fullword integer;  $n1 \leq 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 42.
- $n2$  is the length of the second dimension of the two-dimensional data in the array to be transformed.
- Specified as: a fullword integer;  $n2 \leq 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 42.
- $isign$  controls the direction of the transform, determining the sign  $Isign$  of the exponents of  $W_{n1}$  and  $W_{n2}$ , where:
- If  $isign =$  positive value,  $Isign = +$  (transforming time to frequency).

If *isign* = negative value, *Isign* = - (transforming frequency to time).

Specified as: a fullword integer; *isign* > 0 or *isign* < 0.

*scale* is the scaling constant *scale*. See "Function" on page 832 for its usage.

Specified as: a number of the data type indicated in Table 146 on page 828, where *scale* > 0.0 or *scale* < 0.0.

*aux1* is the working storage for this subroutine, where:

If *init* ≠ 0, the working storage is computed.

If *init* = 0, the working storage is used in the computation of the Fourier transforms.

Specified as: an area of storage, containing *naux1* long-precision real numbers.

*naux1* is the number of doublewords in the working storage specified in *aux1*.

Specified as: a fullword integer; *naux1* ≥ (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 36.

*aux2* has the following meaning:

If *naux2* = 0 and error 2015 is unrecoverable, *aux2* is ignored.

Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

*naux2* is the number of doublewords in the working storage specified in *aux2*.

Specified as: a fullword integer, where:

If *naux2* = 0 and error 2015 is unrecoverable, SCFT2 and DCFT2 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, *naux2* ≥ (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 36.

### On Return

*y* has the following meaning, where:

If *init* ≠ 0, this argument is not used, and its contents remain unchanged.



If  $init = 0$ , this is array  $Y$ , containing the elements resulting from the two-dimensional discrete Fourier transform of the data in  $X$ . Each element  $y_{k_1, k_2}$ , using zero-based indexing, is stored in  $Y(k_1(inc1y)+k_2(inc2y))$  for  $k_1 = 0, 1, \dots, n1-1$  and  $k_2 = 0, 1, \dots, n2-1$ .

Returned as: an array of (at least) length  $1+(n1-1)inc1y+(n2-1)inc2y$ , containing numbers of the data type indicated in Table 146 on page 828. This array must be aligned on a doubleword boundary, and:

If  $inc1y = 1$ , the output array is stored in normal form, and  $inc2y \geq n1$ .

If  $inc2y = 1$ , the output array is stored in transposed form, and  $inc1y \geq n2$ .

See "Notes" for more details.

*aux1* is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If  $init = 0$ , its contents are unchanged.

Returned as: the contents are not relevant.

## Notes

1. *aux1* should **not** be used by the calling program between program calls to this subroutine with  $init \neq 0$  and  $init = 0$ . However, it can be reused after intervening calls to this subroutine with different arguments.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for  $init \neq 0$  and  $init = 0$ .
3. If you specify the same array for  $X$  and  $Y$ , then  $inc1x$  must equal  $inc1y$ , and  $inc2x$  must equal  $inc2y$ . In this case, output overwrites input. If you specify different arrays  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.
4. By appropriately specifying the *inc* arguments, this subroutine allows you to specify that it should use one of two forms of its arrays, the normal untransposed form or the transposed form. As a result, you **do not have to move any data**. Instead, the subroutine performs the adjustments for you. Also, either the input array or the output array can be in transposed form. The FFT computation is symmetrical with respect to  $n1$  and  $n2$ . They can be interchanged without the loss of generality. If they are interchanged, an array that is stored in the normal form appears as an array stored in the transposed form and vice versa. If, for performance reasons, the forms of the input and output arrays are different, then the input array should be specified in the normal form, and the output array should be specified in the transposed form. This can always be done by interchanging  $n1$  and  $n2$ .
5. Although the *inc* arguments for each array can be arbitrary, in most cases, one of the *inc* arguments is 1 for each array. If  $inc1 = 1$ , the array is stored in normal form; that is, the first dimension of the array is along the columns. In this case,  $inc2$  is the leading dimension of the array and must be at least  $n1$ . Conversely, if  $inc2 = 1$ , the array is stored in the transposed form; that is, the first dimension of the array is along the rows. In this case,  $inc1$  is the leading dimension of the array and must be at least  $n2$ . The rows of the arrays are accessed with a stride that equals the leading dimension of the array. To minimize cache interference in accessing a row, an optimal value should be

used for the leading dimension of the array. You should use “STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines” on page 1017 to determine this optimal value. Example 4 in the STRIDE subroutine description explains how it is used to find either *inc1* or *inc2*.

## Formulas

### Processor-Independent Formulas for SCFT2 for NAUX1 and NAUX2

The required values of *naux1* and *naux2* depend on *n1* and *n2*.

**NAUX1 Formulas:** If  $\max(n1, n2) \leq 8192$ , use  $naux1 = 40000$ .

If  $\max(n1, n2) > 8192$ , use  $naux1 = 40000 + 1.14(n1 + n2)$ .

**NAUX2 Formulas:** If  $\max(n1, n2) < 252$ , use  $naux2 = 20000$ .

If  $\max(n1, n2) \geq 252$ , use  $naux2 = 20000 + (r + 256)(s + 1.14)$ , where  $r = \max(n1, n2)$  and  $s = \min(64, n1, n2)$ .

### Processor-Independent Formulas for DCFT2 for NAUX1 and NAUX2

The required values of *naux1* and *naux2* depend on *n1* and *n2*.

**NAUX1 Formulas:** If  $\max(n1, n2) \leq 2048$ , use  $naux1 = 40000$ .

If  $\max(n1, n2) > 2048$ , use  $naux1 = 40000 + 2.28(n1 + n2)$ .

**NAUX2 Formulas:** If  $\max(n1, n2) < 252$ , use  $naux2 = 20000$ .

If  $\max(n1, n2) \geq 252$ , use  $naux2 = 20000 + (2r + 256)(s + 2.28)$ , where  $r = \max(n1, n2)$  and  $s = \min(64, n1, n2)$ .

## Function

The two-dimensional discrete Fourier transform of complex data in array *X*, with results going into array *Y*, is expressed as follows:

$$y_{k1,k2} = scale \sum_{j1=0}^{n1-1} \sum_{j2=0}^{n2-1} x_{j1,j2} W_{n1}^{(Isign)j1k1} W_{n2}^{(Isign)j2k2}$$

for:

$$k1 = 0, 1, \dots, n1-1$$

$$k2 = 0, 1, \dots, n2-1$$

where:

$$W_{n1} = e^{-2\pi(\sqrt{-1})/n1}$$

$$W_{n2} = e^{-2\pi(\sqrt{-1})/n2}$$

and where:

$x_{j1,j2}$  are elements of array X.  
 $y_{k1,k2}$  are elements of array Y.  
 $isign$  is + or - (determined by argument  $isign$ ).  
 $scale$  is a scalar value.

For  $scale = 1.0$  and  $isign$  being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with  $scale = 1.0/((n1)(n2))$  and  $isign$  being negative. See references [1], [4], and [22].

Two invocations of this subroutine are necessary:

1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the  $aux1$  working storage.
2. With  $init = 0$ , the subroutine checks that the initialization arguments in the  $aux1$  working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transform.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux2 = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n1 > 37748736$
2.  $n2 > 37748736$
3.  $inc1x | inc2x | inc1y | inc2y \leq 0$
4.  $scale = 0.0$
5.  $isign = 0$
6. The subroutine has not been initialized with the present arguments.
7. The length of one of the transforms in  $n1$  or  $n2$  is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
8.  $naux1$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
9. Error 2015 is recoverable or  $naux2 \neq 0$ , and  $naux2$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to compute a two-dimensional transform where both input and output are stored in normal form ( $inc1x = inc1y = 1$ ). Also,  $inc2x = inc2y$  so the same array can be used for both input and output. The arrays are declared as follows:

```
COMPLEX*8  X(6,8),Y(6,8)
REAL*8     AUX1(20000),AUX2(1)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage: EQUIVALENCE (X,Y). First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

## SCFT2 and DCFT2

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```
      INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  N1  N2  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2
      |    |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SCFT2(INIT, X , 1 , 6 , Y , 1 , 6 , 6 , 8 , 1 , SCALE, AUX1, 20000 , AUX2, 0)
```

INIT = 1 (for initialization)

INIT = 0 (for computation)

SCALE = 1.0

X is an array with 6 rows and 8 columns with (1.0, 0.0) in all locations.

**Output:** Y is an array with 6 rows and 8 columns having (48.0, 0.0) in location Y(1,1) and (0.0, 0.0) in all others.

### Example 2

This example shows how to compute a two-dimensional inverse Fourier transform. For this example, X is stored in normal untransposed form ( $inc1x = 1$ ), and Y is stored in transposed form ( $inc2y = 1$ ). The arrays are declared as follows:

```
      COMPLEX*16  X(6,8),Y(8,6)
      REAL*8      AUX1(20000), AUX2(1)
```

First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```
      INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  N1  N2  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2
      |    |    |    |    |    |    |    |    |    |    |    |    |    |
CALL DCFT2(INIT, X , 1 , 6 , Y , 8 , 1 , 6 , 8 , -1 , SCALE, AUX1 , 20000 , AUX2 , 0)
```

INIT = 1 (for initialization)

INIT = 0 (for computation)

SCALE = 1.0/48.0

X = (same as output Y in Example 1)

**Output:** Y is an array with 8 rows and 6 columns with (1.0, 0.0) in all locations.

## SRCFT2 and DRCFT2 — Real-to-Complex Fourier Transform in Two Dimensions

### Purpose

These subroutines compute the two-dimensional discrete Fourier transform of real data in a two-dimensional array.

Table 147. Data Types

<i>X, scale</i>	<i>Y</i>	Subroutine
Short-precision real	Short-precision complex	SRCFT2
Long-precision real	Long-precision complex	DRCFT2

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

<b>Fortran</b>	CALL SRCFT2 ( <i>init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3</i> ) CALL DRCFT2 ( <i>init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2</i> )
<b>C and C++</b>	srcft2 ( <i>init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3</i> ); drcft2 ( <i>init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2</i> );

### On Entry

<i>init</i>	is a flag, where:  If <i>init</i> $\neq$ 0, trigonometric functions and other parameters, depending on arguments other than <i>x</i> , are computed and saved in <i>aux1</i> . The contents of <i>x</i> and <i>y</i> are not used or changed.  If <i>init</i> = 0, the discrete Fourier transform of the given array is computed. The only arguments that may change after initialization are <i>x</i> , <i>y</i> , and <i>aux2</i> . All scalar arguments must be the same as when the subroutine was called for initialization with <i>init</i> $\neq$ 0.  Specified as: a fullword integer. It can have any value.
<i>x</i>	is the array <i>X</i> , containing <i>n1</i> rows and <i>n2</i> columns of data to be transformed. The data in each column is stored with stride 1. Specified as: an <i>inc2x</i> by (at least) <i>n2</i> array, containing numbers of the data type indicated in Table 147. See “Notes” on page 837 for more details.
<i>inc2x</i>	is the leading dimension (stride between columns) of array <i>X</i> . Specified as: a fullword integer; <i>inc2x</i> $\geq$ <i>n1</i> .
<i>y</i>	See “On Return” on page 837.
<i>inc2y</i>	is the leading dimension (stride between columns) of array <i>Y</i> . Specified as: a fullword integer; <i>inc2y</i> $\geq$ $((n1)/2)+1$ .
<i>n1</i>	is the number of rows of data—that is, the length of the columns in array <i>X</i> involved in the computation. The length of the columns in array <i>Y</i> are $(n1)/2+1$ .

- Specified as: a fullword integer;  $n1 \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- n2* is the number of columns of data—that is, the length of the rows in arrays *X* and *Y* involved in the computation.
- Specified as: a fullword integer;  $n2 \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- isign* controls the direction of the transform, determining the sign *Isign* of the exponents of  $W_{n1}$  and  $W_{n2}$ , where:
- If *isign* = positive value, *Isign* = + (transforming time to frequency).
- If *isign* = negative value, *Isign* = - (transforming frequency to time).
- Specified as: a fullword integer;  $isign > 0$  or  $isign < 0$ .
- scale* is the scaling constant *scale*. See “Function” on page 838 for its usage.
- Specified as: a number of the data type indicated in Table 147 on page 835, where  $scale > 0.0$  or  $scale < 0.0$ .
- aux1* is the working storage for this subroutine, where:
- If *init*  $\neq$  0, the working storage is computed.
- If *init* = 0, the working storage is used in the computation of the Fourier transforms.
- Specified as: an area of storage, containing *naux1* long-precision real numbers.
- naux1* is the number of doublewords in the working storage specified in *aux1*.
- Specified as: a fullword integer;  $naux1 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.
- aux2* has the following meaning:
- If  $naux2 = 0$  and error 2015 is unrecoverable, *aux2* is ignored.
- Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.
- Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

- naux2* is the number of doublewords in the working storage specified in *aux2*.  
Specified as: a fullword integer, where:  
If *naux2* = 0 and error 2015 is unrecoverable, SRCFT2 and DRCFT2 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.  
Otherwise,  $naux2 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.
- aux3* this argument is provided for migration purposes only and is ignored.  
Specified as: an area of storage containing *naux3* long-precision real numbers.
- naux3* this argument is provided for migration purposes only and is ignored.  
Specified as: a fullword integer.

### On Return

- y* has the following meaning, where:  
If *init*  $\neq$  0, this argument is not used, and its contents remain unchanged.  
If *init* = 0, this is array Y, containing the results of the complex discrete Fourier transform of X. The output consists of *n2* columns of data. The data in each column is stored with stride 1. Due to complex conjugate symmetry, the output consists of only the first  $((n1)/2)+1$  rows of the array—that is,  $y_{k1,k2}$ , where  $k1 = 0, 1, \dots, (n1)/2$  and  $k2 = 0, 1, \dots, n2-1$ .  
Returned as: an *inc2y* by (at least) *n2* array, containing numbers of the data type indicated in Table 147 on page 835. This array must be aligned on a doubleword boundary.
- aux1* is the working storage for this subroutine, where:  
If *init*  $\neq$  0, it contains information ready to be passed in a subsequent invocation of this subroutine.  
If *init* = 0, its contents are unchanged.  
Returned as: the contents are not relevant.

### Notes

1. *aux1* should **not** be used by the calling program between calls to this subroutine with *init*  $\neq$  0 and *init* = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for *init*  $\neq$  0 and *init* = 0.

## SRCFT2 and DRCFT2

3. If you specify the same array for  $X$  and  $Y$ , then  $inc2x$  must equal  $(2)(inc2y)$ . In this case, output overwrites input. If you specify different arrays  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
4. For selecting optimal strides (or leading dimensions  $inc2x$  and  $inc2y$ ) for your input and output arrays, you should use “STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines” on page 1017. Example 5 in the STRIDE subroutine description explains how it is used for these subroutines.
5. Be sure to align array  $X$  on a doubleword boundary, and specify an even number for  $inc2x$ , if possible.

## Formulas

### Processor-Independent Formulas for SRCFT2 for NAUX1 and NAUX2

The required values of  $naux1$  and  $naux2$  depend on  $n1$  and  $n2$ .

#### NAUX1 Formulas:

If  $\max(n1/2, n2) \leq 8192$ , use  $naux1 = 45000$ .

If  $\max(n1/2, n2) > 8192$ , use  $naux1 = 40000 + 0.82n1 + 1.14n2$ .

#### NAUX2 Formulas:

If  $n1 \leq 16384$  and  $n2 < 252$ , use  $naux2 = 20000$ .

If  $n1 > 16384$  and  $n2 < 252$ , use  $naux2 = 20000 + 0.57n1$ .

If  $n2 \geq 252$ , add the following to the above storage requirements:

$$(n2+256)(1.14+s)$$

where  $s = \min(64, 1+n1/2)$ .

### Processor-Independent Formulas for DRCFT2 for NAUX1 and NAUX2

The required values of  $naux1$  and  $naux2$  depend on  $n1$  and  $n2$ .

#### NAUX1 Formulas:

If  $n \leq 2048$ , use  $naux1 = 42000$ .

If  $n > 2048$ , use  $naux1 = 40000 + 1.64n1 + 2.28n2$ ,

where  $n = \max(n1/2, n2)$ .

#### NAUX2 Formulas:

If  $n1 \leq 4096$  and  $n2 < 252$ , use  $naux2 = 20000$ .

If  $n1 > 4096$  and  $n2 < 252$ , use  $naux2 = 20000 + 1.14n1$ .

If  $n2 \geq 252$ , add the following to the above storage requirements:

$$((2)n2+256) (2.28+s)$$

where  $s = \min(64, 1+n1/2)$ .

## Function

The two-dimensional complex conjugate even discrete Fourier transform of real data in array  $X$ , with results going into array  $Y$ , is expressed as follows:



$$y_{k1,k2} = scale \sum_{j1=0}^{n1-1} \sum_{j2=0}^{n2-1} x_{j1,j2} W_{n1}^{(Isign)j1k1} W_{n2}^{(Isign)j2k2}$$

for:

$$k1 = 0, 1, \dots, n1-1$$

$$k2 = 0, 1, \dots, n2-1$$

where:

$$W_{n1} = e^{-2\pi(\sqrt{-1})/n1}$$

$$W_{n2} = e^{-2\pi(\sqrt{-1})/n2}$$

and where:

$x_{j1,j2}$  are elements of array  $X$ .

$y_{k1,k2}$  are elements of array  $Y$ .

$Isign$  is + or - (determined by argument  $isign$ ).

$scale$  is a scalar value.

The output in array  $Y$  is complex. For  $scale = 1.0$  and  $isign$  being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with  $scale = 1.0/((n1)(n2))$  and  $isign$  being negative. See references [1], [4], [21], and [22].

Two invocations of this subroutine are necessary:

1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the  $aux1$  working storage.
2. With  $init = 0$ , the subroutine checks that the initialization arguments in the  $aux1$  working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transform.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux2 = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n1 > 37748736$
2.  $n2 > 37748736$
3.  $inc2x < n1$
4.  $inc2y < (n1)/2+1$
5.  $scale = 0.0$
6.  $isign = 0$
7. The subroutine has not been initialized with the present arguments.
8. The length of one of the transforms in  $n1$  or  $n2$  is not an allowable value. Return code 1 is returned if error 2030 is recoverable.

## SRCFT2 and DRCFT2

9. *naux1* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
10. Error 2015 is recoverable or *naux2* ≠ 0, and *naux2* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to compute a two-dimensional transform. The arrays are declared as follows:

```
COMPLEX*8  Y(0:6,0:7)
REAL*4     X(0:11,0:7)
REAL*8     AUX1(1000), AUX2(1), AUX3(1)
```

First, initialize AUX1 using the calling sequence shown below with *INIT* ≠ 0. Then use the same calling sequence with *INIT* = 0 to do the calculation.

**Note:** Because *NAUX2* = 0, this subroutine dynamically allocates the AUX2 working storage.

#### Call Statement and Input:

```
      INIT  X  INC2X Y  INC2Y N1  N2 ISIGN SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
      |    |  |    |  |    |  |    |    |    |    |    |    |    |
CALL SRCFT2(INIT, X , 12 , Y , 7 , 12 , 8 , 1 , SCALE, AUX1 , 1000 , AUX2 , 0 , AUX3 , 0 )
```

```
INIT      = 1 (for initialization)
INIT      = 0 (for computation)
SCALE     = 1.0
```

X is an array with 12 rows and 8 columns having 1.0 in location X(0,0) and 0.0 in all others.

**Output:** Y is an array with 7 rows and 8 columns with (1.0, 0.0) in all locations.

### Example 2

This example shows another transform computation with different data using the same initialized array AUX1 in Example 1.

**Note:** Because *NAUX2* = 0, this subroutine dynamically allocates the AUX2 working storage.

#### Call Statement and Input:

```
      INIT X  INC2X Y  INC2Y N1  N2 ISIGN SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
      |    |  |    |  |    |  |    |    |    |    |    |    |    |
CALL SRCFT2( 0 , X , 12 , Y , 7 , 12 , 8 , 1 , SCALE, AUX1, 1000 , AUX2, 0 , AUX3 , 0 )
```

```
SCALE     = 1.0
X is an array with 12 rows and 8 columns with 1.0 in all locations.
```

**Output:** Y is an array with 7 rows and 8 columns having (96.0, 0.0) in location Y(0,0) and (0.0, 0.0) in all others.

**Example 3**

This example shows the same array being used for input and output, where  $isign = -1$  and  $scale = 1/((N1)(N2))$ . The arrays are declared as follows:

```
COMPLEX*16  Y(0:8,0:7)
REAL*8      X(0:19,0:7)
REAL*8      AUX1(1000), AUX2(1), AUX3(1)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage.

```
EQUIVALENCE (X,Y)
```

This requires  $inc2x \geq 2(inc2y)$ . First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

**Call Statement and Input:**

```
INIT  X  INC2X Y  INC2Y N1  N2  ISIGN SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
|    |  |    |  |    |  |    |  |    |  |    |  |    |  |    |
CALL DRCFT2(INIT, X , 20 , Y , 9 , 16 , 8 , -1 , SCALE, AUX1 , 1000 , AUX2 , 0 , AUX3 , 0 )
```

```
INIT      = 1 (for initialization)
INIT      = 0 (for computation)
SCALE     = 1.0/128.0
```

X =

2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0
2.0	-2.0	-2.0	2.0	2.0	2.0	-2.0	-2.0
-2.0	-2.0	2.0	2.0	2.0	-2.0	2.0	2.0
-2.0	2.0	2.0	-2.0	-2.0	-2.0	2.0	2.0
2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0
2.0	-2.0	-2.0	2.0	2.0	2.0	-2.0	2.0
-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0
-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0
2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0
2.0	-2.0	-2.0	2.0	2.0	2.0	-2.0	2.0
-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0
-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0
2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0
2.0	-2.0	-2.0	2.0	2.0	2.0	-2.0	2.0
-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0
-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.

**Output:** Y is an array with 9 rows and 8 columns having (1.0, 1.0) in location Y(4,2) and (0.0, 0.0) in all others.

## SCRFT2 and DCRFT2 — Complex-to-Real Fourier Transform in Two Dimensions

### Purpose

These subroutines compute the two-dimensional discrete Fourier transform of complex conjugate even data in a two-dimensional array.

Table 148. Data Types

X	Y, scale	Subroutine
Short-precision complex	Short-precision real	SCRFT2
Long-precision complex	Long-precision real	DCRFT2

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

<b>Fortran</b>	CALL SCRFT2 ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n1</i> , <i>n2</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> , <i>aux3</i> , <i>naux3</i> ) CALL DCRFT2 ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n1</i> , <i>n2</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
<b>C and C++</b>	scrft2 ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n1</i> , <i>n2</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> , <i>aux3</i> , <i>naux3</i> ); dcrft2 ( <i>init</i> , <i>x</i> , <i>inc2x</i> , <i>y</i> , <i>inc2y</i> , <i>n1</i> , <i>n2</i> , <i>isign</i> , <i>scale</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

<i>init</i>	is a flag, where:  If <i>init</i> $\neq$ 0, trigonometric functions and other parameters, depending on arguments other than <i>x</i> , are computed and saved in <i>aux1</i> . The contents of <i>x</i> and <i>y</i> are not used or changed.  If <i>init</i> = 0, the discrete Fourier transform of the given array is computed. The only arguments that may change after initialization are <i>x</i> , <i>y</i> , and <i>aux2</i> . All scalar arguments must be the same as when the subroutine was called for initialization with <i>init</i> $\neq$ 0.  Specified as: a fullword integer. It can have any value.
<i>x</i>	is the array X, containing <i>n2</i> columns of data to be transformed. Due to complex conjugate symmetry, the input consists of only the first $((n1)/2)+1$ rows of the array—that is, $x_{j1,j2}$ , $j1 = 0, 1, \dots, (n1)/2$ , $j2 = 0, 1, \dots, n2-1$ . The data in each column is stored with stride 1.  Specified as: an <i>inc2x</i> by (at least) <i>n2</i> array, containing numbers of the data type indicated in Table 148. This array must be aligned on a doubleword boundary.
<i>inc2x</i>	is the leading dimension (stride between columns) of array X. Specified as: a fullword integer; $inc2x \geq ((n1)/2)+1$ .
<i>y</i>	See “On Return” on page 844.
<i>inc2y</i>	is the leading dimension (stride between the columns) of array Y. Specified as: a fullword integer; $inc2y \geq n1+2$ .

- n1* is the number of rows of data—that is, the length of the columns in array *Y* involved in the computation. The length of the columns in array *X* are  $(n1)/2+1$ .
- Specified as: a fullword integer;  $n1 \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- n2* is the number of columns of data—that is, the length of the rows in arrays *X* and *Y* involved in the computation.
- Specified as: a fullword integer;  $n2 \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- isign* controls the direction of the transform, determining the sign *Isign* of the exponents of  $W_{n1}$  and  $W_{n2}$ , where:
- If *isign* = positive value, *Isign* = + (transforming time to frequency).
- If *isign* = negative value, *Isign* = - (transforming frequency to time).
- Specified as: a fullword integer;  $isign > 0$  or  $isign < 0$ .
- scale* is the scaling constant *scale*. See “Function” on page 845 for its usage.
- Specified as: a number of the data type indicated in Table 148 on page 842, where  $scale > 0.0$  or  $scale < 0.0$ .
- aux1* is the working storage for this subroutine, where:
- If *init*  $\neq$  0, the working storage is computed.
- If *init* = 0, the working storage is used in the computation of the Fourier transforms.
- Specified as: an area of storage, containing *naux1* long-precision real numbers.
- naux1* is the number of doublewords in the working storage specified in *aux*.
- Specified as: a fullword integer;  $naux1 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.
- aux2* has the following meaning:
- If *naux2* = 0 and error 2015 is unrecoverable, *aux2* is ignored.
- Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

## SCRFT2 and DCRFT2

	Specified as: an area of storage, containing <i>naux2</i> long-precision real numbers. On output, the contents are overwritten.
<i>naux2</i>	is the number of doublewords in the working storage specified in <i>aux2</i> .  Specified as: a fullword integer, where:  If <i>naux2</i> = 0 and error 2015 is unrecoverable, SCRFT2 and DCRFT2 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.  Otherwise, <i>naux2</i> ≥ (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.
<i>aux3</i>	this argument is provided for migration purposes only and is ignored.  Specified as: an area of storage, containing <i>naux3</i> long-precision real numbers.
<i>naux3</i>	this argument is provided for migration purposes only and is ignored.  Specified as: a fullword integer.

### On Return

<i>y</i>	has the following meaning, where:  If <i>init</i> ≠ 0, this argument is not used, and its contents remain unchanged.  If <i>init</i> = 0, this is the array <i>Y</i> , containing <i>n1</i> rows and <i>n2</i> columns of results of the real discrete Fourier transform of <i>X</i> . The data in each column of <i>Y</i> is stored with stride 1.  Returned as: an <i>inc2y</i> by (at least) <i>n2</i> array, containing numbers of the data type indicated in Table 148 on page 842. See “Notes” for more details.
<i>aux1</i>	is the working storage for this subroutine, where:  If <i>init</i> ≠ 0, it contains information ready to be passed in a subsequent invocation of this subroutine.  If <i>init</i> = 0, its contents are unchanged.  Returned as: the contents are not relevant.

### Notes

1. *aux1* should **not** be used by the calling program between program calls to this subroutine with *init* ≠ 0 and *init* = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for *init* ≠ 0 and *init* = 0.

3. If you specify the same array for  $X$  and  $Y$ , then  $(2)(inc2x)$  must equal  $inc2y$ . In this case, output overwrites input. If you specify different arrays  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
4. For selecting optimal strides (or leading dimensions  $inc2x$  and  $inc2y$ ) for your input and output arrays, you should use “STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines” on page 1017. Example 6 in the STRIDE subroutine description explains how it is used for these subroutines.
5. Be sure to align array  $Y$  on a doubleword boundary, and specify an even number for  $inc2y$ , if possible.

## Formulas

### Processor-Independent Formulas for SCRFT2 for NAUX1 and NAUX2

The required values of  $naux1$  and  $naux2$  depend on  $n1$  and  $n2$ .

#### NAUX1 Formulas:

If  $\max(n1/2, n2) \leq 8192$ , use  $naux1 = 45000$ .

If  $\max(n1/2, n2) > 8192$ , use  $naux1 = 40000 + 0.82n1 + 1.14n2$ .

#### NAUX2 Formulas:

If  $n1 \leq 16384$  and  $n2 < 252$ , use  $naux2 = 20000$ .

If  $n1 > 16384$  and  $n2 < 252$ , use  $naux2 = 20000 + 0.57n1$ .

If  $n2 \geq 252$ , add the following to the above storage requirements:

$$(n2+256)(1.14+s)$$

where  $s = \min(64, 1+n1/2)$ .

### Processor-Independent Formulas for DCRFT2 for NAUX1 and NAUX2

The required values of  $naux1$  and  $naux2$  depend on  $n1$  and  $n2$ .

#### NAUX1 Formulas:

If  $n \leq 2048$ , use  $naux1 = 42000$ .

If  $n > 2048$ , use  $naux1 = 40000 + 1.64n1 + 2.28n2$ ,

where  $n = \max(n1/2, n2)$ .

#### NAUX2 Formulas:

If  $n1 \leq 4096$  and  $n2 < 252$ , use  $naux2 = 20000$ .

If  $n1 > 4096$  and  $n2 < 252$ , use  $naux2 = 20000 + 1.14n1$ .

If  $n2 \geq 252$ , add the following to the above storage requirements:

$$((2)n2+256) (2.28+s)$$

where  $s = \min(64, 1+n1/2)$ .

## Function

The two-dimensional discrete Fourier transform of complex conjugate even data in array  $X$ , with results going into array  $Y$ , is expressed as follows:

## SCRFT2 and DCRFT2

$$y_{k1,k2} = scale \sum_{j1=0}^{n1-1} \sum_{j2=0}^{n2-1} x_{j1,j2} W_{n1}^{(Isign)j1k1} W_{n2}^{(Isign)j2k2}$$

for:

$$k1 = 0, 1, \dots, n1-1$$

$$k2 = 0, 1, \dots, n2-1$$

where:

$$W_{n1} = e^{-2\pi(\sqrt{-1})/n1}$$

$$W_{n2} = e^{-2\pi(\sqrt{-1})/n2}$$

and where:

$x_{j1,j2}$  are elements of array  $X$ .

$y_{k1,k2}$  are elements of array  $Y$ .

$Isign$  is + or - (determined by argument  $isign$ ).

$scale$  is a scalar value.

Because of the complex conjugate symmetry, the output in array  $Y$  is real. For  $scale = 1.0$  and  $isign$  being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with  $scale = 1.0/((n1)(n2))$  and  $isign$  being negative. See references [1], [4], and [22].

Two invocations of this subroutine are necessary:

1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the  $aux1$  working storage.
2. With  $init = 0$ , the subroutine checks that the initialization arguments in the  $aux1$  working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transform.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux2 = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n1 > 37748736$
2.  $n2 > 37748736$
3.  $inc2x < (n1)/2+1$
4.  $inc2y < n1+2$
5.  $scale = 0.0$
6.  $isign = 0$
7. The subroutine has not been initialized with the present arguments.
8. The length of one of the transforms in  $n1$  or  $n2$  is not an allowable value.  
Return code 1 is returned if error 2030 is recoverable.



9. *naux1* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
10. Error 2015 is recoverable or *naux2* ≠ 0, and *naux2* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to compute a two-dimensional transform. The arrays are declared as follows:

```
REAL*4    Y(0:13,0:7)
COMPLEX*8 X(0:6,0:7)
REAL*8    AUX1(1000), AUX2(1), AUX3(1)
```

First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

#### Call Statement and Input:

```
INIT  X  INC2X  Y  INC2Y  N1  N2  ISIGN  SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
|    |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SCRFT2(INIT, X , 7 , Y , 14 , 12 , 8 , -1 , SCALE , AUX1 , 1000 , AUX2 , 0 , AUX3 , 0 )
```

INIT = 1 (for initialization)

INIT = 0 (for computation)

SCALE = 1.0/96.0

X is an array with 7 rows and 8 columns with (1.0, 0.0) in all locations.

#### Output:

$$Y = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \end{bmatrix}$$

### Example 2

This example shows another transform computation with different data using the same initialized array AUX1 in Example 1.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

## SCRFT2 and DCRFT2

### Call Statement and Input:

```

          INIT X INC2X Y  INC2Y N1  N2 ISIGN SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
          |   |   |   |   |   |   |   |   |   |   |   |   |   |
CALL SCRFT2( 0 , X , 7 , Y , 14 , 12 , 8 , -1 , SCALE , AUX1 , 1000 , AUX2 , 0 , AUX3 , 0 )

```

SCALE = 1.0/96.0

X is an array with 7 rows and 8 columns having (96.0, 0.0) in location X(0,0) and (0.0, 0.0) in all others.

### Output:

```

Y =
  [ 1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
    .   .   .   .   .   .   .   .
    .   .   .   .   .   .   .   . ]

```

### Example 3

This example shows the same array being used for input and output. The arrays are declared as follows:

```

REAL*8      Y(0:17,0:7)
COMPLEX*16  X(0:8,0:7)
REAL*8      AUX1(1000), AUX2(1), AUX3(1)

```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage.

```
EQUIVALENCE (X,Y)
```

This requires  $inc2y = 2(inc2x)$ . First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```

          INIT X INC2X Y  INC2Y N1  N2 ISIGN SCALE  AUX1  NAUX1  AUX2  NAUX2  AUX3  NAUX3
          |   |   |   |   |   |   |   |   |   |   |   |   |   |
CALL DCRFT2(INIT, X , 9 , Y , 18 , 16 , 8 , 1 , SCALE , AUX1 , 1000 , AUX2 , 0 , AUX3 , 0 )

```

INIT = 1 (for initialization)

INIT = 0 (for computation)

SCALE = 1.0

X is an array with 9 rows and 8 columns having (1.0, 1.0) in location X(4,2) and (0.0, 0.0) in all others.

Output:

$$Y = \begin{bmatrix} 2.0 & 2.0 & -2.0 & -2.0 & 2.0 & 2.0 & -2.0 & -2.0 \\ 2.0 & -2.0 & -2.0 & 2.0 & 2.0 & -2.0 & -2.0 & 2.0 \\ -2.0 & -2.0 & 2.0 & 2.0 & -2.0 & -2.0 & 2.0 & 2.0 \\ -2.0 & 2.0 & 2.0 & -2.0 & -2.0 & 2.0 & 2.0 & -2.0 \\ 2.0 & 2.0 & -2.0 & -2.0 & 2.0 & 2.0 & -2.0 & -2.0 \\ 2.0 & -2.0 & -2.0 & 2.0 & 2.0 & -2.0 & -2.0 & 2.0 \\ -2.0 & -2.0 & 2.0 & 2.0 & -2.0 & -2.0 & 2.0 & 2.0 \\ -2.0 & 2.0 & 2.0 & -2.0 & -2.0 & 2.0 & 2.0 & -2.0 \\ 2.0 & 2.0 & -2.0 & -2.0 & 2.0 & 2.0 & -2.0 & -2.0 \\ 2.0 & -2.0 & -2.0 & 2.0 & 2.0 & -2.0 & -2.0 & 2.0 \\ 2.0 & -2.0 & -2.0 & 2.0 & 2.0 & -2.0 & -2.0 & 2.0 \\ -2.0 & -2.0 & 2.0 & 2.0 & -2.0 & -2.0 & 2.0 & 2.0 \\ -2.0 & 2.0 & 2.0 & -2.0 & -2.0 & 2.0 & 2.0 & -2.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

## SCFT3 and DCFT3 — Complex Fourier Transform in Three Dimensions

### Purpose

These subroutines compute the three-dimensional discrete Fourier transform of complex data.

Table 149. Data Types

X, Y	scale	Subroutine
Short-precision complex	Short-precision real	SCFT3
Long-precision complex	Long-precision real	DCFT3

**Note:** For each use, only one invocation of this subroutine is necessary. The initialization phase, preparing the working storage, is a relatively small part of the total computation, so it is performed on each invocation.

### Syntax

<b>Fortran</b>	CALL SCFT3   DCFT3 ( <i>x</i> , <i>inc2x</i> , <i>inc3x</i> , <i>y</i> , <i>inc2y</i> , <i>inc3y</i> , <i>n1</i> , <i>n2</i> , <i>n3</i> , <i>isign</i> , <i>scale</i> , <i>aux</i> , <i>naux</i> )
<b>C and C++</b>	scft3   dcft3 ( <i>x</i> , <i>inc2x</i> , <i>inc3x</i> , <i>y</i> , <i>inc2y</i> , <i>inc3y</i> , <i>n1</i> , <i>n2</i> , <i>n3</i> , <i>isign</i> , <i>scale</i> , <i>aux</i> , <i>naux</i> );

### On Entry

*x* is the array X, containing the three-dimensional data to be transformed, where each element  $x_{j1,j2,j3}$ , using zero-based indexing, is stored in  $X(j1+j2(inc2x)+j3(inc3x))$  for  $j1 = 0, 1, \dots, n1-1$ ,  $j2 = 0, 1, \dots, n2-1$ , and  $j3 = 0, 1, \dots, n3-1$ . The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2x (\geq n1)$ , and  $inc3x (\geq (n2)(inc2x))$ , respectively.

Specified as: an array, containing numbers of the data type indicated in Table 149. This array must be aligned on a doubleword boundary. If the array is dimensioned  $X(LDA1, LDA2, LDA3)$ , then  $LDA1 = inc2x$ ,  $(LDA1)(LDA2) = inc3x$ , and  $LDA3 \geq n3$ . For information on how to set up this array, see "Setting Up Your Data" on page 782. For more details, see "Notes" on page 852.

*inc2x* is the stride between the elements in array X for the second dimension.

Specified as: a fullword integer;  $inc2x \geq n1$ .

*inc3x* is the stride between the elements in array X for the third dimension.

Specified as: a fullword integer;  $inc3x \geq (n2)(inc2x)$ .

*y* See "On Return" on page 852.

*inc2y* is the stride between the elements in array Y for the second dimension.

Specified as: a fullword integer;  $inc2y \geq n1$ .

*inc3y* is the stride between the elements in array Y for the third dimension.

Specified as: a fullword integer;  $inc3y \geq (n2)(inc2y)$ .

- n1* is the length of the first dimension of the three-dimensional data in the array to be transformed.
- Specified as: a fullword integer;  $n1 \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- n2* is the length of the second dimension of the three-dimensional data in the array to be transformed.
- Specified as: a fullword integer;  $n2 \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- n3* is the length of the third dimension of the three-dimensional data in the array to be transformed.
- Specified as: a fullword integer;  $n3 \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- isign* controls the direction of the transform, determining the sign *Isign* of the exponents of  $W_{n1}$ ,  $W_{n2}$ , and  $W_{n3}$ , where:
- If *isign* = positive value, *Isign* = + (transforming time to frequency).
- If *isign* = negative value, *Isign* = - (transforming frequency to time).
- Specified as: a fullword integer;  $isign > 0$  or  $isign < 0$ .
- scale* is the scaling constant *scale*. See “Function” on page 853 for its usage.
- Specified as: a number of the data type indicated in Table 149 on page 850, where  $scale > 0.0$  or  $scale < 0.0$ .
- aux* has the following meaning:
- If  $n_{aux} = 0$  and error 2015 is unrecoverable, *aux* is ignored.
- Otherwise, it is a storage work area used by this subroutine.
- Specified as: an area of storage, containing  $n_{aux}$  long-precision real numbers. On output, the contents are overwritten.
- n<sub>aux</sub>* is the number of doublewords in the working storage specified in *aux*.
- Specified as: a fullword integer, where:
- If  $n_{aux} = 0$  and error 2015 is unrecoverable, SCFT3 and DCFT3 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.

### On Return

$y$  is the array  $Y$ , containing the elements resulting from the three-dimensional discrete Fourier transform of the data in  $X$ . Each element  $y_{k1,k2,k3}$ , using zero-based indexing, is stored in  $Y(k1+k2(inc2y)+k3(inc3y))$  for  $k1 = 0, 1, \dots, n1-1$ ,  $k2 = 0, 1, \dots, n2-1$ , and  $k3 = 0, 1, \dots, n3-1$ . The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2y (\geq n1)$ , and  $inc3y (\geq (n2)(inc2y))$ , respectively.

Returned as: an array, containing numbers of the data type indicated in Table 149 on page 850. This array must be aligned on a doubleword boundary. If the array is dimensioned  $Y(LDA1, LDA2, LDA3)$ , then  $LDA1 = inc2y$ ,  $(LDA1)(LDA2) = inc3y$ , and  $LDA3 \geq n3$ . For information on how to set up this array, see “Setting Up Your Data” on page 782. For more details, see “Notes.”

### Notes

1. If you specify the same array for  $X$  and  $Y$ , then  $inc2x$  must be greater than or equal to  $inc2y$ , and  $inc3x$  must be greater than or equal to  $inc3y$ . In this case, output overwrites input. When using the ESSL SMP library in a multithreaded environment, if  $inc2x > inc2y$  or  $inc3x > inc3y$ , these subroutines run on a single thread and issue an attention message.  
If you specify different arrays  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
2. You should use “STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines” on page 1017 to determine the optimal values for the strides  $inc2y$  and  $inc3y$  for your output array. The strides for your input array do not affect performance. Example 7 in the STRIDE subroutine description explains how it is used for these subroutines. For additional information on how to set up your data, see “Setting Up Your Data” on page 782.

### Formulas

#### Processor-Independent Formulas for SCFT3 for NAUX

Use the following formulas for calculating  $naux$ :

1. If  $\max(n2, n3) < 252$  and:

If  $n1 \leq 8192$ , use  $naux = 60000$ .

If  $n1 > 8192$ , use  $naux = 60000 + 2.28n1$ .

2. If  $n2 \geq 252$ ,  $n3 < 252$ , and:

If  $n1 \leq 8192$ , use  $naux = 60000 + \lambda$ .

If  $n1 > 8192$ , use  $naux = 60000 + 2.28n1 + \lambda$ ,

where  $\lambda = (n2 + 256)(s + 2.28)$

and  $s = \min(64, n1)$ .

3. If  $n_2 < 252$ ,  $n_3 \geq 252$ , and:

If  $n_1 \leq 8192$ , use  $naux = 60000 + \psi$ .  
 If  $n_1 > 8192$ , use  $naux = 60000 + 2.28n_1 + \psi$ ,

where  $\psi = (n_3 + 256)(s + 2.28)$   
 and  $s = \min(64, (n_1)(n_2))$ .

4. If  $n_2 \geq 252$  and  $n_3 \geq 252$ , use the larger of the values calculated for cases 2 and 3 above.

### Processor-Independent Formulas for DCFT3 for NAUX

Use the following formulas for calculating  $naux$ :

1. If  $\max(n_2, n_3) < 252$  and:

If  $n_1 \leq 2048$ , use  $naux = 60000$ .  
 If  $n_1 > 2048$ , use  $naux = 60000 + 4.56n_1$ .

2. If  $n_2 \geq 252$ ,  $n_3 < 252$ , and:

If  $n_1 \leq 2048$ , use  $naux = 60000 + \lambda$ .  
 If  $n_1 > 2048$ , use  $naux = 60000 + 4.56n_1 + \lambda$ ,

where  $\lambda = ((2)n_2 + 256)(s + 4.56)$   
 and  $s = \min(64, n_1)$ .

3. If  $n_2 < 252$ ,  $n_3 \geq 252$ , and:

If  $n_1 \leq 2048$ , use  $naux = 60000 + \psi$ .  
 If  $n_1 > 2048$ , use  $naux = 60000 + 4.56n_1 + \psi$ ,

where  $\psi = ((2)n_3 + 256)(s + 4.56)$   
 and  $s = \min(64, (n_1)(n_2))$ .

4. If  $n_2 \geq 252$  and  $n_3 \geq 252$ , use the larger of the values calculated for cases 2 and 3 above.

### Function

The three-dimensional discrete Fourier transform of complex data in array  $X$ , with results going into array  $Y$ , is expressed as follows:

$$y_{k_1, k_2, k_3} = scale \sum_{j_1=0}^{n_1-1} \sum_{j_2=0}^{n_2-1} \sum_{j_3=0}^{n_3-1} x_{j_1, j_2, j_3} W_{n_1}^{(l_{sign}j_1k_1)} W_{n_2}^{(l_{sign}j_2k_2)} W_{n_3}^{(l_{sign}j_3k_3)}$$

for:

$k_1 = 0, 1, \dots, n_1-1$   
 $k_2 = 0, 1, \dots, n_2-1$   
 $k_3 = 0, 1, \dots, n_3-1$

where:

$$W_{n1} = e^{-2\pi(\sqrt{-1})/n1}$$

$$W_{n2} = e^{-2\pi(\sqrt{-1})/n2}$$

$$W_{n3} = e^{-2\pi(\sqrt{-1})/n3}$$

and where:

$x_{j1,j2,j3}$  are elements of array  $X$ .

$y_{k1,k2,k3}$  are elements of array  $Y$ .

$isign$  is + or - (determined by argument  $isign$ ).

$scale$  is a scalar value.

For  $scale = 1.0$  and  $isign$  being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with  $scale = 1.0/((n1)(n2)(n3))$  and  $isign$  being negative. See references [1], [4], [5], [21], and [22].

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n1 > 37748736$
2.  $n2 > 37748736$
3.  $n3 > 37748736$
4.  $inc2x < n1$
5.  $inc3x < (n2)(inc2x)$
6.  $inc2y < n1$
7.  $inc3y < (n2)(inc2y)$
8.  $scale = 0.0$
9.  $isign = 0$
10. The length of one of the transforms in  $n1$ ,  $n2$ , or  $n3$  is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
11. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example

This example shows how to compute a three-dimensional transform. In this example,  $INC2X \geq INC2Y$  and  $INC3X \geq INC3Y$ , so that the same array can be used for both input and output. The STRIDE subroutine is called to select good values for the  $INC2Y$  and  $INC3Y$  strides. (As explained below, STRIDE is not called for  $INC2X$  and  $INC3X$ .) Using the transform lengths ( $N1 = 32$ ,  $N2 = 64$ , and  $N3 = 40$ ) along with the output data type (short-precision complex: 'C'), STRIDE is called once for each stride needed. First, it is called for  $INC2Y$ :

```
CALL STRIDE (N2,N1,INC2Y,'C',0)
```

The output value returned for  $INC2Y$  is 32. Then STRIDE is called again for  $INC3Y$ :



```
CALL STRIDE (N3,N2*INC2Y,INC3Y,'C',0)
```

The output value returned for INC3Y is 2056. Because INC3Y is not a multiple of INC2Y, Y is not declared as a three-dimensional array. It is declared as a two-dimensional array, Y(INC3Y,N3).

To equivalence the X and Y arrays requires  $INC2X \geq INC2Y$  and  $INC3X \geq INC3Y$ . Therefore, INC2X is set equal to INC2Y( = 32). Also, to declare the X array as a three-dimensional array, INC3X must be a multiple of INC2X. Therefore, its value is set as  $INC3X = (65)(INC2X) = 2080$ .

The arrays are declared as follows:

```
COMPLEX*8  X(32,65,40),Y(2056,40)
REAL*8     AUX(1)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage:

```
EQUIVALENCE (X,Y)
```

**Note:** Because NAUX = 0, this subroutine dynamically allocates the AX working storage.

**Call Statement and Input:**

```

      X  INC2X INC3X  Y  INC2Y INC3Y  N1  N2  N3  ISIGN  SCALE  AUX  NAUX
CALL SCFT3( X , 32 , 2080 , Y , 32 , 2056 , 32 , 64 , 40 , 1 , SCALE , AUX , 0 )

```

SCALE = 1.0

X has (1.0,2.0) in location X(1,1,1) and (0.0,0.0) in all other locations.

**Output:** Y has (1.0,2.0) in locations Y(ij,k), where  $ij = 1, 2048$  and  $j = 1, 40$ . It remains unchanged elsewhere.

## SRCFT3 and DRCFT3 — Real-to-Complex Fourier Transform in Three Dimensions

### Purpose

These subroutines compute the three-dimensional discrete Fourier transform of real data in a three-dimensional array.

Table 150. Data Types

$X$ , <i>scale</i>	$Y$	Subroutine
Short-precision real	Short-precision complex	SRCFT3
Long-precision real	Long-precision complex	DRCFT3

**Note:** For each use, only one invocation of this subroutine is necessary. The initialization phase, preparing the working storage, is a relatively small part of the total computation, so it is performed on each invocation.

### Syntax

<b>Fortran</b>	CALL SRCFT3   DRCFT3 ( <i>x</i> , <i>inc2x</i> , <i>inc3x</i> , <i>y</i> , <i>inc2y</i> , <i>inc3y</i> , <i>n1</i> , <i>n2</i> , <i>n3</i> , <i>isign</i> , <i>scale</i> , <i>aux</i> , <i>naux</i> )
<b>C and C++</b>	srcft3   drcft3 ( <i>x</i> , <i>inc2x</i> , <i>inc3x</i> , <i>y</i> , <i>inc2y</i> , <i>inc3y</i> , <i>n1</i> , <i>n2</i> , <i>n3</i> , <i>isign</i> , <i>scale</i> , <i>aux</i> , <i>naux</i> );

### On Entry

*x* is the array  $X$ , containing the three-dimensional data to be transformed, where each element  $x_{j1,j2,j3}$ , using zero-based indexing, is stored in  $X(j1+j2(inc2x)+j3(inc3x))$  for  $j1 = 0, 1, \dots, n1-1$ ,  $j2 = 0, 1, \dots, n2-1$ , and  $j3 = 0, 1, \dots, n3-1$ . The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2x (\geq n1)$ , and  $inc3x (\geq (n2)(inc2x))$ , respectively.

Specified as: an array, containing numbers of the data type indicated in Table 150. If the array is dimensioned  $X(LDA1, LDA2, LDA3)$ , then  $LDA1 = inc2x$ ,  $(LDA1)(LDA2) = inc3x$ , and  $LDA3 \geq n3$ . For information on how to set up this array, see “Setting Up Your Data” on page 782. For more details, see “Notes” on page 858.

*inc2x* is the stride between the elements in array  $X$  for the second dimension.

Specified as: a fullword integer;  $inc2x \geq n1$ .

*inc3x* is the stride between the elements in array  $X$  for the third dimension.

Specified as: a fullword integer;  $inc3x \geq (n2)(inc2x)$ .

*y* See “On Return” on page 858.

*inc2y* is the stride between the elements in array  $Y$  for the second dimension.

Specified as: a fullword integer;  $inc2y \geq n1/2+1$ .

*inc3y* is the stride between the elements in array  $Y$  for the third dimension.

- Specified as: a fullword integer;  $inc3y \geq (n2)(inc2y)$ .
- n1* is the length of the first dimension of the three-dimensional data in the array to be transformed.
- Specified as: a fullword integer;  $n1 \leq 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 42.
- n2* is the length of the second dimension of the three-dimensional data in the array to be transformed.
- Specified as: a fullword integer;  $n2 \leq 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 42.
- n3* is the length of the third dimension of the three-dimensional data in the array to be transformed.
- Specified as: a fullword integer;  $n3 \leq 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 42.
- isign* controls the direction of the transform, determining the sign *Isign* of the exponents of  $W_{n1}$ ,  $W_{n2}$ , and  $W_{n3}$ , where:
- If *isign* = positive value, *Isign* = + (transforming time to frequency).
- If *isign* = negative value, *Isign* = - (transforming frequency to time).
- Specified as: a fullword integer;  $isign > 0$  or  $isign < 0$ .
- scale* is the scaling constant *scale*. See "Function" on page 859 for its usage.
- Specified as: a number of the data type indicated in Table 150 on page 856, where  $scale > 0.0$  or  $scale < 0.0$ .
- aux* has the following meaning:
- If  $n_{aux} = 0$  and error 2015 is unrecoverable, *aux* is ignored.
- Otherwise, it is a storage work area used by this subroutine.
- Specified as: an area of storage, containing  $n_{aux}$  long-precision real numbers. On output, the contents are overwritten.
- n<sub>aux</sub>* is the number of doublewords in the working storage specified in *aux*.
- Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, SRCFT3 and DRCFT3 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.

### On Return

$y$  is the array  $Y$ , containing the elements resulting from the three-dimensional discrete Fourier transform of the data in  $X$ . Each element  $y_{k1,k2,k3}$ , using zero-based indexing, is stored in  $Y(k1+k2(inc2y)+k3(inc3y))$  for  $k1 = 0, 1, \dots, n1/2$ ,  $k2 = 0, 1, \dots, n2-1$ , and  $k3 = 0, 1, \dots, n3-1$ . Due to complex conjugate symmetry, the output consists of only the first  $n1/2+1$  values along the first dimension of the array, for  $k1 = 0, 1, \dots, n1/2$ . The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2y (\geq n1/2+1)$ , and  $inc3y (\geq (n2)(inc2y))$ , respectively.

Returned as: an array, containing numbers of the data type indicated in Table 150 on page 856. This array must be aligned on a doubleword boundary. If the array is dimensioned  $Y(LDA1, LDA2, LDA3)$ , then  $LDA1 = inc2y$ ,  $(LDA1)(LDA2) = inc3y$ , and  $LDA3 \geq n3$ . For information on how to set up this array, see “Setting Up Your Data” on page 782. For more details, see “Notes.”

### Notes

1. If you specify the same array for  $X$  and  $Y$ , then  $inc2x$  must be greater than or equal to  $(2)(inc2y)$ , and  $inc3x$  must be greater than or equal to  $(2)(inc3y)$ . In this case, output overwrites input. When using the ESSL SMP library in a multithreaded environment, if  $inc2x > (2)(inc2y)$  or  $inc3x > (2)(inc3y)$ , these subroutines run on a single thread and issue an attention message.

If you specify different arrays  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.

2. To achieve the best performance, you should align array  $X$  on a doubleword boundary, and  $inc2x$  and  $inc3x$  should be even numbers. The strides for your input array do not affect performance as long as they are even numbers. In addition, you should use “STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines” on page 1017 to determine the optimal values for the strides  $inc2y$  and  $inc3y$  for your output array. Example 8 in the STRIDE subroutine description explains how it is used for these subroutines. For additional information on how to set up your data, see “Setting Up Your Data” on page 782.

### Formulas

#### Processor-Independent Formulas for SRCFT3 for NAUX

Use the following formulas for calculating  $naux$ :

1. If  $\max(n2, n3) < 252$  and:

- If  $n1 \leq 16384$ , use  $naux = 65000$ .  
 If  $n1 > 16384$ , use  $naux = 60000 + 1.39n1$ .
2. If  $n2 \geq 252$ ,  $n3 < 252$ , and:
- If  $n1 \leq 16384$ , use  $naux = 65000 + \lambda$ .  
 If  $n1 > 16384$ , use  $naux = 60000 + 1.39n1 + \lambda$ ,
- where  $\lambda = (n2 + 256)(s + 2.28)$  and  $s = \min(64, 1 + n1/2)$ .
3. If  $n2 < 252$ ,  $n3 \geq 252$ , and:
- If  $n1 \leq 16384$ , use  $naux = 65000 + \psi$ .  
 If  $n1 > 16384$ , use  $naux = 60000 + 1.39n1 + \psi$ ,
- where  $\psi = (n3 + 256)(s + 2.28)$  and  $s = \min(64, (n2)(1 + n1/2))$ .
4. If  $n2 \geq 252$  and  $n3 \geq 252$ , use the larger of the values calculated for cases 2 and 3 above.

If  $inc2x$  or  $inc3x$  is an odd number, or if array  $X$  is not aligned on a doubleword boundary, you should add the following amount to all the formulas given above:

$$n2(1 + n1/2)$$

### Processor-Independent Formulas for DRCFT3 for NAUX

Use the following formulas for calculating  $naux$ :

1. If  $\max(n2, n3) < 252$  and:
- If  $n1 \leq 4096$ , use  $naux = 62000$ .  
 If  $n1 > 4096$ , use  $naux = 60000 + 2.78n1$ .
2. If  $n2 \geq 252$ ,  $n3 < 252$ , and:
- If  $n1 \leq 4096$ , use  $naux = 62000 + \lambda$ .  
 If  $n1 > 4096$ , use  $naux = 60000 + 2.78n1 + \lambda$ ,
- where  $\lambda = ((2)n2 + 256)(s + 4.56)$   
 and  $s = \min(64, n1/2)$ .
3. If  $n2 < 252$ ,  $n3 \geq 252$ , and:
- If  $n1 \leq 4096$ , use  $naux = 62000 + \psi$ .  
 If  $n1 > 4096$ , use  $naux = 60000 + 2.78n1 + \psi$ ,
- where  $\psi = ((2)n3 + 256)(s + 4.56)$   
 and  $s = \min(64, n2(1 + n1/2))$ .
4. If  $n2 \geq 252$  and  $n3 \geq 252$ , use the larger of the values calculated for cases 2 and 3 above.

## Function

The three-dimensional complex conjugate even discrete Fourier transform of real data in array  $X$ , with results going into array  $Y$ , is expressed as follows:

$$Y_{k1,k2,k3} = scale \sum_{j1=0}^{n1-1} \sum_{j2=0}^{n2-1} \sum_{j3=0}^{n3-1} x_{j1,j2,j3} W_{n1}^{(l\text{sign})j1k1} W_{n2}^{(l\text{sign})j2k2} W_{n3}^{(l\text{sign})j3k3}$$

## SRCFT3 and DRCFT3

for:

$$k1 = 0, 1, \dots, n1-1$$

$$k2 = 0, 1, \dots, n2-1$$

$$k3 = 0, 1, \dots, n3-1$$

where:

$$W_{n1} = e^{-2\pi(\sqrt{-1})/n1}$$

$$W_{n2} = e^{-2\pi(\sqrt{-1})/n2}$$

$$W_{n3} = e^{-2\pi(\sqrt{-1})/n3}$$

and where:

$x_{j1,j2,j3}$  are elements of array X.

$y_{k1,k2,k3}$  are elements of array Y.

*isign* is + or - (determined by argument *isign*).

*scale* is a scalar value.

The output in array Y is complex. For *scale* = 1.0 and *isign* being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with *scale* = 1.0/((*n1*)(*n2*)(*n3*)) and *isign* being negative. See references [1], [4], [5], [21], and [22].

## Error conditions

### Resource Errors

Error 2015 is unrecoverable, *naux* = 0, and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1. *n1* > 37748736
2. *n2* > 37748736
3. *n3* > 37748736
4. *inc2x* < *n1*
5. *inc3x* < (*n2*)(*inc2x*)
6. *inc2y* < *n1*/2+1
7. *inc3y* < (*n2*)(*inc2y*)
8. *scale* = 0.0
9. *isign* = 0
10. The length of one of the transforms in *n1*, *n2*, or *n3* is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
11. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example

This example shows how to compute a three-dimensional transform. In this example, *INC2X* ≥ (2)(*INC2Y*) and *INC3X* ≥ (2)(*INC3Y*), so that the same array can be

used for both input and output. The STRIDE subroutine is called to select good values for the INC2Y and INC3Y strides. Using the transform lengths ( $N1 = 32$ ,  $N2 = 64$ , and  $N3 = 40$ ) along with the output data type (short-precision complex: 'C'), STRIDE is called once for each stride needed. First, it is called for INC2Y:

```
CALL STRIDE (N2,N1/2+1,INC2Y,'C',0)
```

The output value returned for INC2Y is 17. (This value is equal to  $N1/2+1$ .) Then STRIDE is called again for INC3Y:

```
CALL STRIDE (N3,N2*INC2Y,INC3Y,'C',0)
```

The output value returned for INC3Y is 1088. Because INC3Y is a multiple of INC2Y—that is,  $INC3Y = (N2)(INC2Y)$ —Y is declared as a three-dimensional array, Y(17,64,40). (In general, for larger arrays, these types of values for INC2Y and INC3Y are not returned by STRIDE, and you are probably not able to declare Y as a three-dimensional array.)

To equivalence the X and Y arrays requires  $INC2X \geq (2)(INC2Y)$  and  $INC3X \geq (2)(INC3Y)$ . Therefore, the values  $INC2X = (2)(INC2Y) = 34$  and  $INC3X = (2)(INC3Y) = 2176$  are set, and X is declared as a three-dimensional array, X(34,64,40).

The arrays are declared as follows:

```
REAL*4    X(34,64,40)
COMPLEX*8 Y(17,64,40)
REAL*8    AUX(1)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage:

```
EQUIVALENCE (X,Y)
```

**Note:** Because  $NAUX = 0$ , this subroutine dynamically allocates the AX working storage.

**Call Statement and Input:**

```

      X  INC2X  INC3X  Y  INC2Y  INC3Y  N1  N2  N3  ISIGN  SCALE  AUX  NAUX
      |   |   |   |   |   |   |   |   |   |   |   |
CALL SRCFT3( X , 34 , 2176 , Y , 17 , 1088 , 32 , 64 , 40 , 1 , SCALE , AUX , 0 )

```

SCALE = 1.0

X has 1.0 in location X(1,1,1) and 0.0 in all other locations.

**Output:** Y has (1.0,0.0) in all locations.

## SCRFT3 and DCRFT3 — Complex-to-Real Fourier Transform in Three Dimensions

### Purpose

These subroutines compute the three-dimensional discrete Fourier transform of complex conjugate even data in a three-dimensional array.

Table 151. Data Types

X	Y, scale	Subroutine
Short-precision complex	Short-precision real	SCRFT2
Long-precision complex	Long-precision real	DCRFT2

**Note:** For each use, only one invocation of this subroutine is necessary. The initialization phase, preparing the working storage, is a relatively small part of the total computation, so it is performed on each invocation.

### Syntax

<b>Fortran</b>	CALL SCRFT3   DCRFT3 ( <i>x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux</i> )
<b>C and C++</b>	scrft3   dcrft3 ( <i>x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux</i> );

### On Entry

*x* is the array  $X$ , containing the three-dimensional data to be transformed, where each element  $x_{j1,j2,j3}$ , using zero-based indexing, is stored in  $X(j1+j2(inc2x)+j3(inc3x))$  for  $j1 = 0, 1, \dots, n1/2$ ,  $j2 = 0, 1, \dots, n2-1$ , and  $j3 = 0, 1, \dots, n3-1$ . Due to complex conjugate symmetry, the input consists of only the first  $n1/2+1$  values along the first dimension of the array, for  $j1 = 0, 1, \dots, n1/2$ . The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2x (\geq n1/2+1)$ , and  $inc3x (\geq (n2)(inc2x))$ , respectively.

Specified as: an array, containing numbers of the data type indicated in Table 151. This array must be aligned on a doubleword boundary. If the array is dimensioned  $X(LDA1,LDA2,LDA3)$ , then  $LDA1 = inc2x$ ,  $(LDA1)(LDA2) = inc3x$ , and  $LDA3 \geq n3$ . For information on how to set up this array, see “Setting Up Your Data” on page 782. For more details, see “Notes” on page 864.

*inc2x* is the stride between the elements in array  $X$  for the second dimension.

Specified as: a fullword integer;  $inc2x \geq n1/2+1$ .

*inc3x* is the stride between the elements in array  $X$  for the third dimension.

Specified as: a fullword integer;  $inc3x \geq (n2)(inc2x)$ .

*y* See “On Return” on page 864.

*inc2y* is the stride between the elements in array  $Y$  for the second dimension.

Specified as: a fullword integer;  $inc2y \geq n1+2$ .



- inc3y* is the stride between the elements in array *Y* for the third dimension.  
Specified as: a fullword integer;  $inc3y \geq (n2)(inc2y)$ .
- n1* is the length of the first dimension of the three-dimensional data in the array to be transformed.  
Specified as: a fullword integer;  $n1 \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- n2* is the length of the second dimension of the three-dimensional data in the array to be transformed.  
Specified as: a fullword integer;  $n2 \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- n3* is the length of the third dimension of the three-dimensional data in the array to be transformed.  
Specified as: a fullword integer;  $n3 \leq 37748736$  and must be one of the values listed in “Acceptable Lengths for the Transforms” on page 779. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see “Providing a Correct Transform Length to ESSL” on page 42.
- isign* controls the direction of the transform, determining the sign *Isign* of the exponents of  $W_{n1}$ ,  $W_{n2}$ , and  $W_{n3}$ , where:  
If *isign* = positive value, *Isign* = + (transforming time to frequency).  
If *isign* = negative value, *Isign* = - (transforming frequency to time).  
Specified as: a fullword integer;  $isign > 0$  or  $isign < 0$ .
- scale* is the scaling constant *scale*. See “Function” on page 865 for its usage.  
Specified as: a number of the data type indicated in Table 151 on page 862, where  $scale > 0.0$  or  $scale < 0.0$ .
- aux* has the following meaning:  
If  $naux = 0$  and error 2015 is unrecoverable, *aux* is ignored.  
Otherwise, it is a storage work area used by this subroutine.  
Specified as: an area of storage, containing *naux* long-precision real numbers. On output, the contents are overwritten.
- naux* is the number of doublewords in the working storage specified in *aux*.  
Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, SCRFT3 and DCRFT3 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.

### On Return

$y$  is the array Y, containing the elements resulting from the three-dimensional discrete Fourier transform of the data in X. Each element  $y_{k1,k2,k3}$ , using zero-based indexing, is stored in  $Y(k1+k2(inc2y)+k3(inc3y))$  for  $k1 = 0, 1, \dots, n1-1$ ,  $k2 = 0, 1, \dots, n2-1$ , and  $k3 = 0, 1, \dots, n3-1$ . The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2y (\geq n1+2)$ , and  $inc3y (\geq (n2)(inc2y))$ , respectively.

Returned as: an array, containing numbers of the data type indicated in Table 151 on page 862. If the array is dimensioned  $Y(LDA1, LDA2, LDA3)$ , then  $LDA1 = inc2y$ ,  $(LDA1)(LDA2) = inc3y$ , and  $LDA3 \geq n3$ . For information on how to set up this array, see “Setting Up Your Data” on page 782. For more details, see “Notes.”

### Notes

1. If you specify the same array for X and Y, then  $inc2y$  must equal  $(2)(inc2x)$  and  $inc3y$  must equal  $(2)(inc3x)$ . In this case, output overwrites input. If you specify different arrays X and Y, they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
2. To achieve the best performance, you should align array Y on a doubleword boundary, and  $inc2y$  and  $inc3y$  should be even numbers. In addition, you should use “STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines” on page 1017 to determine the optimal values for the strides  $inc2y$  and  $inc3y$  for your output array. To obtain the best performance, you should use  $inc2x = inc2y/2$  and  $inc3x = inc3y/2$ . Example 9 in the STRIDE subroutine description explains how it is used for these subroutines. For additional information on how to set up your data, see “Setting Up Your Data” on page 782.

### Formulas

#### Processor-Independent Formulas for SCRFT3 for Calculating NAUX

Use the following formulas for calculating  $naux$ :

1. If  $\max(n2, n3) < 252$  and:

If  $n1 \leq 16384$ , use  $naux = 65000$ .

If  $n1 > 16384$ , use  $naux = 60000 + 1.39n1$ .

2. If  $n2 \geq 252$ ,  $n3 < 252$ , and:

If  $n1 \leq 16384$ , use  $naux = 65000 + \lambda$ .

If  $n1 > 16384$ , use  $naux = 60000 + 1.39n1 + \lambda$ ,

where  $\lambda = (n2+256)(s+2.28)$   
and  $s = \min(64, 1+n1/2)$ .

3. If  $n2 < 252, n3 \geq 252$ , and:

If  $n1 \leq 16384$ , use  $naux = 65000+\psi$ .  
If  $n1 > 16384$ , use  $naux = 60000+1.39n1+\psi$ ,

where  $\psi = (n3+256)(s+2.28)$   
and  $s = \min(64, (n2)(1+n1/2))$ .

4. If  $n2 \geq 252$  and  $n3 \geq 252$ , use the larger of the values calculated for cases 2 and 3 above.

If  $inc2y$  or  $inc3y$  is an odd number, or if array  $Y$  is not aligned on a doubleword boundary, you should add the following amount to all the formulas given above:

$$(1+n1/2)(\max(n2, n3))$$

### Processor-Independent Formulas for DCRFT3 for NAUX

Use the following formulas for calculating  $naux$ :

1. If  $\max(n2, n3) < 252$  and:

If  $n1 \leq 4096$ , use  $naux = 62000$ .  
If  $n1 > 4096$ , use  $naux = 60000+2.78n1$ .

2. If  $n2 \geq 252, n3 < 252$ , and:

If  $n1 \leq 4096$ , use  $naux = 62000+\lambda$ .  
If  $n1 > 4096$ , use  $naux = 60000+2.78n1+\lambda$ ,

where  $\lambda = ((2)n2+256)(s+4.56)$   
and  $s = \min(64, n1/2)$ .

3. If  $n2 < 252, n3 \geq 252$ , and:

If  $n1 \leq 4096$ , use  $naux = 62000+\psi$ .  
If  $n1 > 4096$ , use  $naux = 60000+2.78n1+\psi$ ,

where  $\psi = ((2)n3+256)(s+4.56)$   
and  $s = \min(64, n2(1+n1/2))$ .

4. If  $n2 \geq 252$  and  $n3 \geq 252$ , use the larger of the values calculated for cases 2 and 3 above.

## Function

The three-dimensional discrete Fourier transform of complex conjugate even data in array  $X$ , with results going into array  $Y$ , is expressed as follows:

$$Y_{k1,k2,k3} = scale \sum_{j1=0}^{n1-1} \sum_{j2=0}^{n2-1} \sum_{j3=0}^{n3-1} X_{j1,j2,j3} W_{n1}^{(lsign)j1k1} W_{n2}^{(lsign)j2k2} W_{n3}^{(lsign)j3k3}$$

for:

## SCRFT3 and DCRFT3

$$k1 = 0, 1, \dots, n1-1$$

$$k2 = 0, 1, \dots, n2-1$$

$$k3 = 0, 1, \dots, n3-1$$

where:

$$W_{n1} = e^{-2\pi(\sqrt{-1})/n1}$$

$$W_{n2} = e^{-2\pi(\sqrt{-1})/n2}$$

$$W_{n3} = e^{-2\pi(\sqrt{-1})/n3}$$

and where:

$x_{j1,j2,j3}$  are elements of array X.

$y_{k1,k2,k3}$  are elements of array Y.

*isign* is + or - (determined by argument *isign*).

*scale* is a scalar value.

Because of the complex conjugate symmetry, the output in array Y is real. For *scale* = 1.0 and *isign* being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with *scale* = 1.0/((*n1*)(*n2*)(*n3*)) and *isign* being negative. See references [1], [4], [5], [21], and [22].

## Error conditions

### Resource Errors

Error 2015 is unrecoverable, *naux* = 0, and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n1 > 37748736$
2.  $n2 > 37748736$
3.  $n3 > 37748736$
4.  $inc2x < n1/2+1$
5.  $inc3x < (n2)(inc2x)$
6.  $inc2y < n1+2$
7.  $inc3y < (n2)(inc2y)$
8.  $scale = 0.0$
9.  $isign = 0$
10. The length of one of the transforms in *n1*, *n2*, or *n3* is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
11. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example

This example shows how to compute a three-dimensional transform. In this example,  $INC2Y = (2)(INC2X)$  and  $INC3Y = (2)(INC3X)$ , so that the same array can be used for both input and output. The STRIDE subroutine is called to select good

values for the INC2Y and INC3Y strides. (As explained below, STRIDE is not called for INC2X and INC3X.) Using the transform lengths ( $N1 = 32$ ,  $N2 = 64$ , and  $N3 = 40$ ) along with the output data type (short-precision real: 'S'), STRIDE is called once for each stride needed. First, it is called for INC2Y:

```
CALL STRIDE (N2,N1+2,INC2Y,'S',0)
```

The output value returned for INC2Y is 34. (This value is equal to  $N1+2$ .) Then STRIDE is called again for INC3Y:

```
CALL STRIDE (N3,N2*INC2Y,INC3Y,'S',0)
```

The output value returned for INC3Y is 2176. Because INC3Y is a multiple of INC2Y—that is,  $INC3Y = (N2)(INC2Y)$ —Y is declared as a three-dimensional array,  $Y(34,64,40)$ . (In general, for larger arrays, these types of values for INC2Y and INC3Y are not returned by STRIDE, and you are probably not able to declare Y as a three-dimensional array.)

A good stride value for INC2X is  $INC2Y/2$ , and a good stride value for INC3X is  $INC3Y/2$ . Also, to equivalence the X and Y arrays requires  $INC2Y = (2)(INC2X)$  and  $INC3Y = (2)(INC3X)$ . Therefore, the values  $INC2X = INC2Y/2 = 17$  and  $INC3X = INC3Y/2 = 1088$  are set, and X is declared as a three-dimensional array,  $X(17,64,40)$ .

The arrays are declared as follows:

```
COMPLEX*8 X(17,64,40)
REAL*4    Y(34,64,40)
REAL*8    AUX(1)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage:

```
EQUIVALENCE (X,Y)
```

**Note:** Because  $NAUX = 0$ , this subroutine dynamically allocates the AX working storage.

**Call Statement and Input:**

```

      X  INC2X INC3X  Y  INC2Y INC3Y  N1  N2  N3  ISIGN SCALE  AUX  NAUX
      |   |   |   |   |   |   |   |   |   |   |   |
CALL SCRFT3( X , 17 , 1088 , Y , 34 , 2176 , 32 , 64 , 40 , 1 , SCALE , AUX , 0 )

```

SCALE = 1.0

X has (1.0,0.0) in location X(1,1,1) and (0.0,0.0) in all other locations.

**Output:** Y has 1.0 in all locations.

---

## Convolution and Correlation Subroutines

This section contains the convolution and correlation subroutine descriptions.

## SCON and SCOR — Convolution or Correlation of One Sequence with One or More Sequences

### Purpose

These subroutines compute the convolutions and correlations of a sequence with one or more sequences using a direct method. The input and output sequences contain short-precision real numbers.

**Note:** These subroutines are considered obsolete. They are provided in ESSL only for compatibility with earlier releases. You should use `SCOND`, `SCORD`, `SDCON`, `SDCOR`, `SCONF`, and `SCORF` instead, because they provide **better performance**. For further details, see “Convolution and Correlation Considerations” on page 783.

### Syntax

<b>Fortran</b>	CALL SCON   SCOR ( <i>init</i> , <i>h</i> , <i>inc1h</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>nh</i> , <i>nx</i> , <i>m</i> , <i>iy0</i> , <i>ny</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
<b>C and C++</b>	<code>scon   scor (<i>init</i>, <i>h</i>, <i>inc1h</i>, <i>x</i>, <i>inc1x</i>, <i>inc2x</i>, <i>y</i>, <i>inc1y</i>, <i>inc2y</i>, <i>nh</i>, <i>nx</i>, <i>m</i>, <i>iy0</i>, <i>ny</i>, <i>aux1</i>, <i>naux1</i>, <i>aux2</i>, <i>naux2</i>);</code>

### On Entry

<i>init</i>	is a flag, where:  If <i>init</i> $\neq$ 0, no computation is performed, error checking is performed, and the subroutine exits back to the calling program.  If <i>init</i> = 0, the convolutions or correlations of the sequence in <i>h</i> with the sequences in <i>x</i> are computed.  Specified as: a fullword integer. It can have any value.
<i>h</i>	is the array H, consisting of the sequence of length $N_h$ to be convolved or correlated with the sequences in array X.  Specified as: an array of (at least) length $1+(N_h-1) inc1h $ , containing short-precision real numbers.
<i>inc1h</i>	is the stride between the elements within the sequence in array H.  Specified as: a fullword integer; <i>inc1h</i> > 0.
<i>x</i>	is the array X, consisting of <i>m</i> input sequences of length $N_x$ , each to be convolved or correlated with the sequence in array H.  Specified as: an array of (at least) length $1+(m-1)inc2x+(N_x-1)inc1x$ , containing short-precision real numbers.
<i>inc1x</i>	is the stride between the elements within each sequence in array X.  Specified as: a fullword integer; <i>inc1x</i> > 0.
<i>inc2x</i>	is the stride between the first elements of the sequences in array X.  Specified as: a fullword integer; <i>inc2x</i> > 0.
<i>y</i>	See “On Return” on page 870.
<i>inc1y</i>	is the stride between the elements within each sequence in output array Y.

## SCON and SCOR

	Specified as: a fullword integer; $inc1y > 0$ .
<i>inc2y</i>	is the stride between the first elements of each sequence in output array Y. Specified as: a fullword integer; $inc2y > 0$ .
<i>nh</i>	is the number of elements, $N_h$ , in the sequence in array H. Specified as: a fullword integer; $N_h > 0$ .
<i>nx</i>	is the number of elements, $N_x$ , in each sequence in array X. Specified as: a fullword integer; $N_x > 0$ .
<i>m</i>	is the number of sequences in array X to be convolved or correlated. Specified as: a fullword integer; $m > 0$ .
<i>iy0</i>	is the convolution or correlation index of the element to be stored in the first position of each sequence in array Y. Specified as: a fullword integer. It can have any value.
<i>ny</i>	is the number of elements, $N_y$ , in each sequence in array Y. Specified as: a fullword integer; $N_y > 0$ for SCON and $N_y \geq -N_h + 1$ for SCOR.
<i>aux1</i>	is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.
<i>naux1</i>	is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.
<i>aux2</i>	is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.
<i>naux2</i>	is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.

### On Return

<i>y</i>	is array Y, consisting of $m$ output sequences of length $N_y$ that are the result of the convolutions or correlations of the sequence in array H with the sequences in array X. Returned as: an array of (at least) length $1 + (m-1)inc2y + (N_y-1)inc1y$ , containing short-precision real numbers.
----------	--

### Notes

1. Output should not overwrite input; that is, input arrays X and H must have no common elements with output array Y. Otherwise, results are unpredictable. See "Concepts" on page 59.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for  $init \neq 0$  and  $init = 0$ .
3. Auxiliary storage is not needed, but the arguments *aux1*, *naux1*, *aux2*, and *naux2* must still be specified. You can assign any values to these arguments.



## Function

The convolutions and correlations of a sequence in array H with one or more sequences in array X are expressed as follows:

Convolutions for SCON:

$$y_{ki} = \sum_{j=\max(0, k-N_x+1)}^{\min(N_h-1, k)} h_j x_{k-j, i}$$

Correlations for SCOR:

$$y_{ki} = \sum_{j=\max(0, -k)}^{\min(N_h-1, N_x-1-k)} h_j x_{k+j, i}$$

for:

$$k = iy_0, iy_0+1, \dots, iy_0+N_y-1$$

$$i = 1, 2, \dots, m$$

where:

$y_{ki}$  are elements of the  $m$  sequences of length  $N_y$  in array Y.

$x_{ki}$  are elements of the  $m$  sequences of length  $N_x$  in array X.

$h_j$  are elements of the sequence of length  $N_h$  in array H.

$iy_0$  is the convolution or correlation index of the element to be stored in the first position of each sequence in array Y.

min and max select the minimum and maximum values, respectively.

It is assumed that elements outside the range of definition are zero. See references [19] and [88].

Only one invocation of this subroutine is needed:

1. You do not need to invoke the subroutine with  $init \neq 0$ . If you do, however, the subroutine performs error checking, exits back to the calling program, and no computation is performed.
2. With  $init = 0$ , the subroutine performs the calculation of the convolutions or correlations.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $nh, nx, ny$ , or  $m \leq 0$
2.  $inc1h, inc1x, inc2x, inc1y$ , or  $inc2y \leq 0$

## Examples

### Example 1

This example shows how to compute a convolution of a sequence in H, which is a ramp function, and three sequences in X, a triangular function and its cyclic translates. It computes the full range of nonzero values of the convolution plus two extra points, which are set to 0. The arrays are declared as follows:

```
REAL*4  H(0:4999), X(0:49999), Y(0:49999)
REAL*8  AUX1, AUX2
```

#### Call Statement and Input:

```

      INIT  H  INC1H  X  INC1X  INC2X  Y  INC1Y  INC2Y  NH  NX  M  IY0  NY  AUX1  NAUX1  AUX2  NAUX2
      |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SCON(INIT, H , 1 , X , 1 , 10 , Y , 1 , 15 , 4 , 10 , 3 , 0 , 15 , AUX1 , 0 , AUX2 , 0)

```

```
INIT      = 0(for computation)
H         = (1.0, 2.0, 3.0, 4.0)
```

X contains the following three sequences:

```

1.0  2.0  3.0
2.0  1.0  2.0
3.0  2.0  1.0
4.0  3.0  2.0
5.0  4.0  3.0
6.0  5.0  4.0
5.0  6.0  5.0
4.0  5.0  6.0
3.0  4.0  5.0
2.0  3.0  4.0

```

**Output:** Y contains the following three sequences:

```

1.0  2.0  3.0
4.0  5.0  8.0
10.0 10.0 14.0
20.0 18.0 22.0
30.0 20.0 18.0
40.0 30.0 20.0
48.0 40.0 30.0
52.0 48.0 40.0
50.0 52.0 48.0
40.0 50.0 52.0
29.0 38.0 47.0
18.0 25.0 32.0
8.0  12.0 16.0
0.0  0.0  0.0
0.0  0.0  0.0

```

### Example 2

This example shows how the output from Example 1 differs when the values for NY and *inc2y* are 10 rather than 15. The output is the same except that it consists of only the first 10 values produced in Example 1.

**Output:** Y contains the following three sequences:

```

1.0  2.0  3.0
4.0  5.0  8.0
10.0 10.0 14.0
20.0 18.0 22.0
30.0 20.0 18.0
40.0 30.0 20.0

```

```
48.0 40.0 30.0
52.0 48.0 40.0
50.0 52.0 48.0
40.0 50.0 52.0
```

### Example 3

This example shows how the output from Example 2 differs if the value for IY0 is 3 rather than 0. The output is the same except it starts at element 3 of the convolution sequences rather than element 0.

**Output:** Y contains the following three sequences:

```
20.0 18.0 22.0
30.0 20.0 18.0
40.0 30.0 20.0
48.0 40.0 30.0
52.0 48.0 40.0
50.0 52.0 48.0
40.0 50.0 52.0
29.0 38.0 47.0
18.0 25.0 32.0
8.0 12.0 16.0
```

### Example 4

This example shows how to compute a correlation of a sequence in H, which is a ramp function, and three sequences in X, a triangular function and its cyclic translates. It computes the full range of nonzero values of the correlation plus two extra points, which are set to 0. The arrays are declared as follows:

```
REAL*4 H(0:4999), X(0:49999), Y(0:49999)
REAL*8 AUX1, AUX2
```

**Call Statement and Input:**

```
INIT H INC1H X INC1X INC2X Y INC1Y INC2Y NH NX M IY0 NY AUX1 NAUX1 AUX2 NAUX2
CALL SCOR(INIT, H, 1, X, 1, 10, Y, 1, 15, 4, 10, 3, -3, 15, AUX1, 0, AUX2, 0)
```

```
INIT = 0(for computation)
H = (1.0, 2.0, 3.0, 4.0)
```

X contains the following three sequences:

```
1.0 2.0 3.0
2.0 1.0 2.0
3.0 2.0 1.0
4.0 3.0 2.0
5.0 4.0 3.0
6.0 5.0 4.0
5.0 6.0 5.0
4.0 5.0 6.0
3.0 4.0 5.0
2.0 3.0 4.0
```

**Output:** Y contains the following three sequences:

```
4.0 8.0 12.0
11.0 10.0 17.0
20.0 15.0 16.0
30.0 22.0 18.0
40.0 30.0 22.0
50.0 40.0 30.0
52.0 50.0 40.0
48.0 52.0 50.0
40.0 48.0 52.0
```

## SCON and SCOR

```
30.0 40.0 48.0
16.0 22.0 28.0
 7.0 10.0 13.0
 2.0  3.0  4.0
 0.0  0.0  0.0
 0.0  0.0  0.0
```

### Example 5

This example shows how the output from Example 4 differs when the values for NY and INC2Y are 10 rather than 15. The output is the same except that it consists of only the first 10 values produced in Example 4.

**Output:** Y contains the following three sequences:

```
 4.0  8.0 12.0
11.0 10.0 17.0
20.0 15.0 16.0
30.0 22.0 18.0
40.0 30.0 22.0
50.0 40.0 30.0
52.0 50.0 40.0
48.0 52.0 50.0
40.0 48.0 52.0
30.0 40.0 48.0
```

### Example 6

This example shows how the output from Example 5 differs if the value for IY0 is 0 rather than -3. The output is the same except it starts at element 0 of the correlation sequences rather than element -3.

**Output:** Y contains the following three sequences:

```
30.0 22.0 18.0
40.0 30.0 22.0
50.0 40.0 30.0
52.0 50.0 40.0
48.0 52.0 50.0
40.0 48.0 52.0
30.0 40.0 48.0
16.0 22.0 28.0
 7.0 10.0 13.0
 2.0  3.0  4.0
```

## SCOND and SCORD — Convolution or Correlation of One Sequence with Another Sequence Using a Direct Method

### Purpose

These subroutines compute the convolution and correlation of a sequence with another sequence using a direct method. The input and output sequences contain short-precision real numbers.

#### Notes:

1. These subroutines compute the convolution and correlation using direct methods. In most cases, these subroutines provide **better performance** than using SCON or SCOR, if you determine that SCON or SCOR would have used a direct method for its computation. For information on how to make this determination, see reference [4].
2. For long-precision data, you should use DDCON or DDCOR with the decimation rate, *id*, equal to 1.

### Syntax

Fortran	CALL SCOND   SCORD ( <i>h</i> , <i>inch</i> , <i>x</i> , <i>incx</i> , <i>y</i> , <i>incy</i> , <i>nh</i> , <i>nx</i> , <i>iy0</i> , <i>ny</i> )
C and C++	scond   scord ( <i>h</i> , <i>inch</i> , <i>x</i> , <i>incx</i> , <i>y</i> , <i>incy</i> , <i>nh</i> , <i>nx</i> , <i>iy0</i> , <i>ny</i> );

### On Entry

<i>h</i>	is the array H, consisting of the sequence of length $N_h$ to be convolved or correlated with the sequence in array X.  Specified as: an array of (at least) length $1+(N_h-1) inch $ , containing short-precision real numbers.
<i>inch</i>	is the stride between the elements within the sequence in array H.  Specified as: a fullword integer; $inch > 0$ or $inch < 0$ .
<i>x</i>	is the array X, consisting of the input sequence of length $N_x$ to be convolved or correlated with the sequence in array H.  Specified as: an array of (at least) length $1+(N_x-1) incx $ , containing short-precision real numbers.
<i>incx</i>	is the stride between the elements within the sequence in array X.  Specified as: a fullword integer; $incx > 0$ or $incx < 0$ .
<i>y</i>	See "On Return" on page 876.
<i>incy</i>	is the stride between the elements within the sequence in output array Y.  Specified as: a fullword integer; $incy > 0$ or $incy < 0$ .
<i>nh</i>	is the number of elements, $N_h$ , in the sequence in array H.  Specified as: a fullword integer; $N_h > 0$ .
<i>nx</i>	is the number of elements, $N_x$ , in the sequence in array X.  Specified as: a fullword integer; $N_x > 0$ .
<i>iy0</i>	is the convolution or correlation index of the element to be stored in the first position of the sequence in array Y.

## SCOND and SCORD

Specified as: a fullword integer. It can have any value.

*ny* is the number of elements,  $N_y$ , in the sequence in array Y.

Specified as: a fullword integer;  $N_y > 0$ .

### On Return

*y* is the array Y of length  $N_y$ , consisting of the output sequence that is the result of the convolution or correlation of the sequence in array H with the sequence in array X. Returned as: an array of (at least) length  $1+(N_y-1)|incy|$ , containing short-precision real numbers.

### Notes

1. Output should not overwrite input—that is, input arrays X and H must have no common elements with output array Y. Otherwise, results are unpredictable. See “Concepts” on page 59.
2. If *iy0* and *ny* are such that output outside the basic range is needed, where the basic range is  $0 \leq k \leq (nh+nx-2)$  for SCOND and  $(-nh+1) \leq k \leq (nx-1)$  for SCORD, the subroutine stores zeros using scalar code. It is not efficient to store many zeros in this manner. It is more efficient to set *iy0* and *ny* so that the output is produced within the above range of *k* values.

### Function

The convolution and correlation of a sequence in array H with a sequence in array X are expressed as follows:

Convolution for SCOND:

$$y_k = \sum_{j=\max(0, k-N_x+1)}^{\min(N_h-1, k)} h_j x_{k-j}$$

Correlation for SCORD:

$$y_k = \sum_{j=\max(0, -k)}^{\min(N_h-1, N_x-1-k)} h_j x_{k+j}$$

for  $k = iy0, iy0+1, \dots, iy0+N_y-1$

where:

$y_k$  are elements of the sequence of length  $N_y$  in array Y.

$x_k$  are elements of the sequence of length  $N_x$  in array X.  $h_j$  are elements of the sequence of length  $N_h$  in array H.

*iy0* is the convolution or correlation index of the element to be stored in the first position of each sequence in array Y.

min and max select the minimum and maximum values, respectively.

It is assumed that elements outside the range of definition are zero. See reference [4].

## Special Usage

SCORD can also perform the functions of SCON and SACOR; that is, it can compute convolutions and autocorrelations. To compute a convolution, you must specify a negative stride for H (see Example 9). To compute the autocorrelation, you must specify the two input sequences to be the same (see Example 10). In fact, you can also compute the autoconvolution by using both of these techniques together, letting the two input sequences be the same, and specifying a negative stride for the first input sequence.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $nh$ ,  $nx$ , or  $ny \leq 0$
2.  $inch$ ,  $incx$ , or  $incy = 0$

## Examples

### Example 1

This example shows how to compute a convolution of a sequence in H with a sequence in X, where both sequences are ramp functions.

#### Call Statement and Input:

```

          H  INCH X  INCX Y  INCY NH  NX  IY0  NY
          |  |   |  |   |  |   |  |   |  |
CALL SCORD( H , 1 , X , 1 , Y , 1 , 4 , 8 , 0 , 11 )

H          = (1.0, 2.0, 3.0, 4.0)
X          = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)

```

#### Output:

```

Y          = (11.0, 34.0, 70.0, 120.0, 130.0, 140.0, 150.0, 160.0,
             151.0, 122.0, 72.0)

```

### Example 2

This example shows how the output from Example 1 differs when the value for IY0 is -2 rather than 0, and NY is 15 rather than 11. The output has two zeros at the beginning and end of the sequence, for points outside the range of nonzero output.

#### Call Statement and Input:

```

          H  INCH X  INCX Y  INCY NH  NX  IY0  NY
          |  |   |  |   |  |   |  |   |  |
CALL SCORD( H , 1 , X , 1 , Y , 1 , 4 , 8 , -2 , 15 )

H          = (1.0, 2.0, 3.0, 4.0)
X          = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)

```

#### Output:

```

Y          = (0.0, 0.0, 11.0, 34.0, 70.0, 120.0, 130.0, 140.0, 150.0,
             160.0, 151.0, 122.0, 72.0, 0.0, 0.0)

```

**Example 3**

This example shows how the same output as Example 1 can be obtained when H and X are interchanged, because the convolution is symmetric in H and X. (The arguments are switched in the calling sequence.)

**Call Statement and Input:**

```

          H INCH X INCX Y INCY NH NX IY0 NY
          | | | | | | | | | |
CALL SCOND( X , 1 , H , 1 , Y , 1 , 4 , 8 , 0 , 11 )

H      = (1.0, 2.0, 3.0, 4.0)
X      = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)

```

**Output:**

```

Y      = (11.0, 34.0, 70.0, 120.0, 130.0, 140.0, 150.0, 160.0,
          151.0, 122.0, 72.0)

```

**Example 4**

This example shows how the output from Example 1 differs when a negative stride is specified for the sequence in H. By reversing the H sequence, the correlation is computed.

**Call Statement and Input:**

```

          H INCH X INCX Y INCY NH NX IY0 NY
          | | | | | | | | | |
CALL SCOND( H , -1 , X , 1 , Y , 1 , 4 , 8 , 0 , 11 )

H      = (1.0, 2.0, 3.0, 4.0)
X      = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)

```

**Output:**

```

Y      = (44.0, 81.0, 110.0, 130.0, 140.0, 150.0, 160.0, 170.0,
          104.0, 53.0, 18.0)

```

**Example 5**

This example shows how to compute the autoconvolution of a sequence by letting the two input sequences for H and X be the same. (X is specified for both arguments in the calling sequence.)

**Call Statement and Input:**

```

          H INCH X INCX Y INCY NH NX IY0 NY
          | | | | | | | | | |
CALL SCOND( X , 1 , X , 1 , Y , 1 , 4 , 4 , 0 , 7 )

X      = (11.0, 12.0, 13.0, 14.0)

```

**Output:**

```

Y      = (121.0, 264.0, 430.0, 620.0, 505.0, 364.0, 196.0)

```

**Example 6**

This example shows how to compute a correlation of a sequence in H with a sequence in X, where both sequences are ramp functions.

**Call Statement and Input:**

```

          H INCH X INCX Y INCY NH NX IY0 NY
          | | | | | | | | | |
CALL SCOND( H , 1 , X , 1 , Y , 1 , 4 , 8 , -3 , 11 )

```



```
H      = (1.0, 2.0, 3.0, 4.0)
X      = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)
```

**Output:**

```
Y      = (44.0, 81.0, 110.0, 130.0, 140.0, 150.0, 160.0, 170.0,
          104.0, 53.0, 18.0)
```

**Example 7**

This example shows how the output from Example 6 differs when the value for IY0 is -5 rather than -3 and NY is 15 rather than 11. The output has two zeros at the beginning and end of the sequence, for points outside the range of nonzero output.

**Call Statement and Input:**

```
          H INCH X INCX Y INCY NH NX IY0 NY
          | |   | |   | |   | |   | |
CALL SCORD( H , 1 , X , 1 , Y , 1 , 4 , 8 , -5 , 15 )
```

```
H      = (1.0, 2.0, 3.0, 4.0)
X      = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)
```

**Output:**

```
Y      = (0.0, 0.0, 44.0, 81.0, 110.0, 130.0, 140.0, 150.0, 160.0,
          170.0, 104.0, 53.0, 18.0, 0.0, 0.0)
```

**Example 8**

This example shows how the output from Example 6 differs when H and X are interchanged (in the calling sequence). The output sequence is the reverse of that in Example 6. To get the full range of output, IY0 is set to -NX+1.

**Call Statement and Input:**

```
          H INCH X INCX Y INCY NH NX IY0 NY
          | |   | |   | |   | |   | |
CALL SCORD( X , 1 , H , 1 , Y , 1 , 4 , 8 , -7 , 11 )
```

```
H      = (1.0, 2.0, 3.0, 4.0)
X      = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)
```

**Output:**

```
Y      = (18.0, 53.0, 104.0, 170.0, 160.0, 150.0, 140.0, 130.0,
          110.0, 81.0, 44.0)
```

**Example 9**

This example shows how the output from Example 6 differs when a negative stride is specified for the sequence in H. By reversing the H sequence, the convolution is computed.

**Call Statement and Input:**

```
          H INCH X INCX Y INCY NH NX IY0 NY
          | |   | |   | |   | |   | |
CALL SCORD( H , -1 , X , 1 , Y , 1 , 4 , 8 , -3 , 11 )
```

```
H      = (1.0, 2.0, 3.0, 4.0)
X      = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)
```

**Output:**

```
Y      = (11.0, 34.0, 70.0, 120.0, 130.0, 140.0, 150.0, 160.0,
          151.0, 122.0, 72.0)
```

## SCOND and SCORD

### Example 10

This example shows how to compute the autocorrelation of a sequence by letting the two input sequences for H and X be the same. (X is specified for both arguments in the calling sequence.)

#### Call Statement and Input:

```
          H  INCH  X  INCX  Y  INCY  NH  NX  IY0  NY
          |  |    |  |    |  |    |  |  |    |
CALL SCORD( X , 1 , X , 1 , Y , 1 , 4 , 4 , -3 , 7 )

X          = (11.0, 12.0, 13.0, 14.0)
```

#### Output:

```
Y          = (154.0, 311.0, 470.0, 630.0, 470.0, 311.0, 154.0)
```

## SCONF and SCORF — Convolution or Correlation of One Sequence with One or More Sequences Using the Mixed-Radix Fourier Method

### Purpose

These subroutines compute the convolutions and correlations, respectively, of a sequence with one or more sequences using the mixed-radix Fourier method. The input and output sequences contain short-precision real numbers.

**Note:** Two invocations of these subroutines are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

<b>Fortran</b>	CALL SCONF   SCORF ( <i>init</i> , <i>h</i> , <i>inc1h</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>nh</i> , <i>nx</i> , <i>m</i> , <i>iy0</i> , <i>ny</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
<b>C and C++</b>	scnf   scorf ( <i>init</i> , <i>h</i> , <i>inc1h</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>nh</i> , <i>nx</i> , <i>m</i> , <i>iy0</i> , <i>ny</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

*init* is a flag, where:

If  $init \neq 0$ , trigonometric functions, the transform of the sequence in  $h$ , and other parameters, depending on arguments other than  $x$ , are computed and saved in  $aux1$ . The contents of  $x$  and  $y$  are not used or changed.

If  $init = 0$ , the convolutions or correlations of the sequence that was in  $h$  at initialization with the sequences in  $x$  are computed.  $h$  is not used or changed. The only arguments that may change after initialization are  $x$ ,  $y$ , and  $aux2$ . All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .

Specified as: a fullword integer. It can have any value.

*h* is the array H, consisting of the sequence of length  $N_h$  to be convolved or correlated with the sequences in array X.

Specified as: an array of (at least) length  $1+(N_h-1)|inc1h|$ , containing short-precision real numbers.

*inc1h* is the stride between the elements within the sequence in array H.

Specified as: a fullword integer;  $inc1h > 0$ .

*x* is the array X, consisting of  $m$  input sequences of length  $N_x$ , each to be convolved or correlated with the sequence in array H.

Specified as: an array of (at least) length  $1+(N_x-1)inc1x+(m-1)inc2x$ , containing short-precision real numbers.

*inc1x* is the stride between the elements within each sequence in array X.

Specified as: a fullword integer;  $inc1x > 0$ .

*inc2x* is the stride between the first elements of the sequences in array X.

Specified as: a fullword integer;  $inc2x > 0$ .

## SCONF and SCORF

<i>y</i>	See “On Return” on page 883.
<i>inc1y</i>	is the stride between the elements within each sequence in output array <i>Y</i> . Specified as: a fullword integer; <i>inc1y</i> > 0.
<i>inc2y</i>	is the stride between the first elements of each sequence in output array <i>Y</i> . Specified as: a fullword integer; <i>inc2y</i> > 0.
<i>nh</i>	is the number of elements, $N_h$ , in the sequence in array <i>H</i> . Specified as: a fullword integer; $N_h$ > 0.
<i>nx</i>	is the number of elements, $N_x$ , in each sequence in array <i>X</i> . Specified as: a fullword integer; $N_x$ > 0.
<i>m</i>	is the number of sequences in array <i>X</i> to be convolved or correlated. Specified as: a fullword integer; <i>m</i> > 0.
<i>iy0</i>	is the convolution or correlation index of the element to be stored in the first position of each sequence in array <i>Y</i> . Specified as: a fullword integer. It can have any value.
<i>ny</i>	is the number of elements, $N_y$ , in each sequence in array <i>Y</i> . Specified as: a fullword integer; $N_y$ > 0.
<i>aux1</i>	is the working storage for this subroutine, where: If <i>init</i> ≠ 0, the working storage is computed. If <i>init</i> = 0, the working storage is used in the computation of the convolutions. Specified as: an area of storage, containing <i>naux1</i> long-precision real numbers.
<i>naux1</i>	is the number of doublewords in the working storage specified in <i>aux1</i> . Specified as: a fullword integer; <i>naux1</i> > 23 and <i>naux1</i> ≥ (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For values between 23 and the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.
<i>aux2</i>	has the following meaning: If <i>naux2</i> = 0 and error 2015 is unrecoverable, <i>aux2</i> is ignored. Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine. Specified as: an area of storage, containing <i>naux2</i> long-precision real numbers. On output, the contents are overwritten.
<i>naux2</i>	is the number of doublewords in the working storage specified in <i>aux2</i> .

Specified as: a fullword integer, where:

If  $naux2 = 0$  and error 2015 is unrecoverable, SCONF and SCORF dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## On Return

$y$

has the following meaning, where:

If  $init \neq 0$ , this argument is not used, and its contents remain unchanged.

If  $init = 0$ , this is array  $Y$ , consisting of  $m$  output sequences of length  $N_y$  that are the result of the convolutions or correlations of the sequence in array  $H$  with the sequences in array  $X$ .

Returned as: an array of (at least) length  $1+(N_y-1)inc1y+(m-1)inc2y$ , containing short-precision real numbers.

$aux1$

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If  $init = 0$ , its contents are unchanged.

Returned as: the contents are not relevant.

## Notes

1.  $aux1$  should **not** be used by the calling program between calls to this subroutine with  $init \neq 0$  and  $init = 0$ . However, it can be reused after intervening calls to this subroutine with different arguments.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for  $init \neq 0$  and  $init = 0$ .
3. If you specify the same array for  $X$  and  $Y$ , then  $inc1x$  and  $inc1y$  must be equal, and  $inc2x$  and  $inc2y$  must be equal. In this case, output overwrites input.
4. If you specify different arrays for  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.
5. If  $iy0$  and  $ny$  are such that output outside the basic range is needed, the subroutine stores zeros. These ranges are:  $0 \leq k \leq N_x+N_h-2$  for SCONF and  $1-N_h \leq k \leq N_x-1$  for SCORF.

## Formulas

### Formulas for the Length of the Fourier Transform

Before calculating the necessary sizes of  $naux1$  and  $naux2$ , you must determine the length  $n$  of the Fourier transform. The value of  $n$  is based on  $nf$ . You can use one of two techniques to determine  $nf$ :

- Use the simple overestimate of  $nf = nx+nh-1$ . (If  $iy0 = 0$  and  $ny > nh+nx$ , this is the actual value, not an overestimate.)

## SCONF and SCORF

- Use the values of the arguments  $iy0$ ,  $nh$ ,  $nx$ , and  $ny$  inserted into the following formulas to get a value for the variable  $nf$ :

$$\begin{aligned}iy0p &= \max(iy0, 0) \\ix0 &= \max((iy0p+1)-nh, 0) \\ih0 &= \max((iy0p+1)-nx, 0) \\nd &= ix0+ih0 \\n1 &= iy0+ny \\nxx &= \min(n1, nx)-ix0 \\nhh &= \min(n1, nh)-ih0 \\ntt &= nx+n1-1 \\nn1 &= n1-nd \\iyy0 &= iy0p-nd \\nzleft &= \max(0, nhh-iyy0-1) \\nzrt &= \min(nn1, ntt)-nxx \\nf &= \max(12, nx+\max(nzleft, nzrt))\end{aligned}$$

After calculating the value for  $nf$ , using one of these two techniques, refer to the formula or table of allowable values of  $n$  in "Acceptable Lengths for the Transforms" on page 779, selecting the value equal to or greater than  $nf$ .

### Processor-Independent Formulas for NAUX1 and NAUX2

The required values of  $naux1$  and  $naux2$  depend on the value determined for  $n$  in "Formulas for the Length of the Fourier Transform" on page 883.

#### NAUX1 Formulas:

If  $n \leq 16384$ , use  $naux1 = 58000$ .  
If  $n > 16384$ , use  $naux1 = 40000+2.14n$ .

#### NAUX2 Formulas:

If  $n \leq 16384$ , use  $naux2 = 30000$ .  
If  $n > 16384$ , use  $naux2 = 20000+1.07n$ .

## Function

The convolutions and correlations of a sequence in array H with one or more sequences in array X are expressed as follows.

Convolutions for SCONF:

$$y_{ki} = \sum_{j=\max(0, k-N_x+1)}^{\min(N_h-1, k)} h_j x_{k-j, i}$$

Correlations for SCORF:

$$y_{ki} = \sum_{j=\max(0, -k)}^{\min(N_h-1, N_x-1-k)} h_j x_{k+j, i}$$

for:

$$k = iy0, iy0+1, \dots, iy0+N_y-1$$

$$i = 1, 2, \dots, m$$

where:

$y_{ki}$  are elements of the  $m$  sequences of length  $N_y$  in array  $Y$ .

$x_{ki}$  are elements of the  $m$  sequences of length  $N_x$  in array  $X$ .

$h_j$  are elements of the sequence of length  $N_h$  in array  $H$ .

$iy0$  is the convolution or correlation index of the element to be stored in the first position of each sequence in array  $Y$ .

min and max select the minimum and maximum values, respectively.

These subroutines use a Fourier transform method with a mixed-radix capability. This provides maximum performance for your application. The length of the transform,  $n$ , that you must calculate to determine the correct sizes for  $naux1$  and  $naux2$  is the same length used by the Fourier transform subroutines called by this subroutine. It is assumed that elements outside the range of definition are zero. See references [19] and [88].

Two invocations of this subroutine are necessary:

1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the  $aux1$  working storage.
2. With  $init = 0$ , the subroutine checks that the initialization arguments in the  $aux1$  working storage correspond to the present arguments, and if so, performs the calculation of the convolutions.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux2 = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $nh, nx, ny$ , or  $m \leq 0$
2.  $inc1h, inc1x, inc2x, inc1y$ , or  $inc2y \leq 0$
3. The resulting internal Fourier transform length  $n$ , is too large. See "Convolutions and Correlations by Fourier Methods" on page 784.
4. The subroutine has not been initialized with the present arguments.
5.  $naux1 \leq 23$
6.  $naux1$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
7. Error 2015 is recoverable or  $naux2 \neq 0$ , and  $naux2$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to compute a convolution of a sequence in H, where H and X are ramp functions. It calculates all nonzero values of the convolution of the sequences in H and X. The arrays are declared as follows:

```
REAL*4 H(8), X(10,1), Y(17)
```

Because this convolution is symmetric in H and X, you can interchange the H and X sequences, leaving all other arguments the same, and you get the same output shown below. First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

#### Call Statement and Input:

```

      INIT  H  INC1H X  INC1X  INC2X  Y  INC1Y  INC2Y  NH  NX  M  IY0  NY  AUX1  NAUX1  AUX2  NAUX2
      |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SCONF(INIT, H , 1 , X , 1 , 1 , Y, 1 , 1 , 8, 10, 1, 0, 17, AUX1, 128, AUX2, 0)

```

```

INIT      = 1(for initialization)
INIT      = 0(for computation)
H         = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0)
X         = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0, 19.0, 20.0)

```

#### Output:

```

Y         = (11.0, 34.0, 70.0, 120.0, 185.0, 266.0, 364.0, 480.0,
            516.0, 552.0, 567.0, 560.0, 530.0, 476.0, 397.0, 292.0,
            160.0)

```

### Example 2

This example shows how the output from Example 1 differs when the value for NY is 21 rather than 17, and the value for IY0 is -2 rather than 0. This yields two zeros on each end of the convolution.

#### Output:

```

Y         = (0.0, 0.0, 11.0, 34.0, 70.0, 120.0, 185.0, 266.0, 364.0,
            480.0, 516.0, 552.0, 567.0, 560.0, 530.0, 476.0, 397.0,
            292.0, 160.0, 0.0, 0.0)

```

### Example 3

This example shows how to compute the autoconvolution by letting the two input sequences be the same for Example 2. First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

#### Call Statement and Input:

```

      INIT  H  INC1H X  INC1X  INC2X  Y  INC1Y  INC2Y  NH  NX  M  IY0  NY  AUX1  NAUX1  AUX2  NAUX2
      |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SCONF(INIT, H , 1 , H , 1 , 1 , Y, 1 , 1 , 8, 10, 1, -2, 21, AUX1, 128, AUX2, 0)

```



INIT = 1(for initialization)  
 INIT = 0(for computation)

**Output:**

Y = (1.0, 4.0, 10.0, 20.0, 35.0, 56.0, 84.0, 120.0, 147.0,  
 164.0, 170.0, 164.0, 145.0, 112.0, 64.0)

**Example 4**

This example shows how to compute all nonzero values of the convolution of the sequence in H with the two sequences in X. First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Note:** Because NAUX2 = 0, this subroutine dynamically allocates the AUX2 working storage.

**Call Statement and Input:**

```

      INIT  H  INC1H X  INC1X  INC2X Y  INC1Y  INC2Y NH  NX  M  IY0 NY  AUX1  NAUX1  AUX2  NAUX2
      |    |  |    |  |    |  |    |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |
CALL SCONF(INIT, H , 1 , X, 1 , 10 , Y, 1 , 17 , 8, 10, 2, 0, 17, AUX1, 148, AUX2, 0)
  
```

INIT = 1(for initialization)  
 INIT = 0(for computation)  
 H = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0)

X contains the following two sequences:

```

11.0 12.0
12.0 13.0
13.0 14.0
14.0 15.0
15.0 16.0
16.0 17.0
17.0 18.0
18.0 19.0
19.0 20.0
20.0 11.0
  
```

**Output:** Y contains the following two sequences:

```

11.0 12.0
34.0 37.0
70.0 76.0
120.0 130.0
185.0 200.0
266.0 287.0
364.0 392.0
480.0 516.0
516.0 552.0
552.0 578.0
567.0 582.0
560.0 563.0
530.0 520.0
476.0 452.0
397.0 358.0
292.0 237.0
160.0 88.0
  
```

**Example 5**

This example shows how to compute a correlation of a sequence in H, where H and X are ramp functions. It calculates all nonzero values of the correlation of the sequences in H and X. The arrays are declared as follows:

## SCONF and SCORF

```
REAL*4 H(8), X(10,1)
```

First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```
INIT H INC1H X INC1X INC2X Y INC1Y INC2Y NH NX M IY0 NY AUX1 NAUX1 AUX2 NAUX2
| | | | | | | | | | | | | | | | | | | | | |
CALL SCORF(INIT, H, 1, X, 1, 1, Y, 1, 1, 8, 10, 1, -7, 17, AUX1, 128, AUX2, 0)
```

INIT = 1(for initialization)  
INIT = 0(for computation)  
H =(same as input H in Example 1)  
X =(same as input X in Example 1)

### Output:

Y = (88.0, 173.0, 254.0, 330.0, 400.0, 463.0, 518.0, 564.0,  
600.0, 636.0, 504.0, 385.0, 280.0, 190.0, 116.0,  
59.0, 20.0)

### Example 6

This example shows how the output from Example 5 differs when the value for NY is 21 rather than 17, and the value for IY0 is -9 rather than 0. This yields two zeros on each end of the correlation.

### Output:

Y = (0.0, 0.0, 88.0, 173.0, 254.0, 330.0, 400.0, 463.0, 518.0,  
564.0, 600.0, 636.0, 504.0, 385.0, 280.0, 190.0, 116.0,  
59.0, 20.0, 0.0, 0.0)

### Example 7

This example shows the effect of interchanging H and X. It uses the same input as Example 5, with H and X switched in the calling sequence, and with IY0 with a value of -9. Unlike convolution, as noted in Example 1, the correlation is not symmetric in H and X. First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```
INIT H INC1H X INC1X INC2X Y INC1Y INC2Y NH NX M IY0 NY AUX1 NAUX1 AUX2 NAUX2
| | | | | | | | | | | | | | | | | | | | | |
CALL SCONF(INIT, X, 1, H, 1, 1, Y, 1, 1, 8, 10, 1, -9, 17, AUX1, 128, AUX2, 0)
```

INIT = 1(for initialization)  
INIT = 0(for computation)

### Output:

Y = (20.0, 59.0, 116.0, 190.0, 280.0, 385.0, 504.0, 636.0,  
600.0, 564.0, 518.0, 463.0, 400.0, 330.0, 254.0, 173.0,  
88.0)

**Example 8**

This example shows how to compute the autocorrelation by letting the two input sequences be the same. First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation. Because there is only one H input sequence, only one autocorrelation can be computed. Furthermore, this usage does not take advantage of the fact that the output is symmetric. Therefore, you should use SACORF to compute autocorrelations, because it does not have either of these problems.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

**Call Statement and Input:**

```

      INIT  H  INC1H X  INC1X  INC2X Y  INC1Y  INC2Y  NH  NX  M  IY0  NY  AUX1  NAUX1  AUX2  NAUX2
      |    |  |    |  |    |  |    |  |    |  |  |  |  |    |  |    |  |    |
CALL SCONF(INIT, H , 1 , H, 1 , 1 , Y, 1 , 1 , 8, 8, 1, -7, 15, AUX1, 148, AUX2, 0)

```

INIT = 1(for initialization)  
 INIT = 0(for computation)

**Output:**

Y = (8.0, 23.0, 44.0, 70.0, 100.0, 133.0, 168.0, 204.0, 168.0,  
 133.0, 100.0 , 70.0, 44.0, 23.0, 8.0)

**Example 9**

This example shows how to compute all nonzero values of the correlation of the sequence in H with the two sequences in X. First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

**Call Statement and Input:**

```

      INIT  H  INC1H X  INC1X  INC2X Y  INC1Y  INC2Y  NH  NX  M  IY0  NY  AUX1  NAUX1  AUX2  NAUX2
      |    |  |    |  |    |  |    |  |    |  |  |  |  |    |  |    |  |    |
CALL SCONF(INIT, H , 1 , X, 1 , 10 , Y, 1 , 17 , 8, 10, 2, -7, 17, AUX1, 148, AUX2, 0)

```

INIT = 1(for initialization)  
 INIT = 0(for computation)  
 H = (same as input H in Example 4)  
 X = (same as input X in Example 4)

**Output:** Y contains the following two sequences:

```

88.0  96.0
173.0 188.0
254.0 275.0
330.0 356.0
400.0 430.0
463.0 496.0
518.0 553.0
564.0 600.0
600.0 636.0
636.0 592.0
504.0 462.0
385.0 346.0
280.0 245.0

```

## SCONF and SCORF

190.0	160.0
116.0	92.0
59.0	42.0
20.0	11.0

## SDCON, DDCON, SDCOR, and DDCOR — Convolution or Correlation with Decimated Output Using a Direct Method

### Purpose

These subroutines compute the convolution and correlation of a sequence with another sequence, with decimated output, using a direct method.

Table 152. Data Types

<i>h, x, y</i>	Subroutine
Short-precision real	SDCON
Long-precision real	DDCON
Short-precision real	SDCOR
Long-precision real	DDCOR

**Note:** These subroutines are the short- and long-precision equivalents of SCOND and SCORD when the decimation interval  $id$  is equal to 1. Because there is no long-precision version of SCOND and SCORD, you can use DDCON and DDCOR, respectively, with decimation interval  $id = 1$  to perform the same function.

### Syntax

Fortran	CALL SDCON   DDCON   SDCOR   DDCOR ( <i>h, inch, x, incx, y, incy, nh, nx, iy0, ny, id</i> )
C and C++	sdcon   ddcon   sdcor   ddcor ( <i>h, inch, x, incx, y, incy, nh, nx, iy0, ny, id</i> );

### On Entry

- h* is the array H, consisting of the sequence of length  $N_h$  to be convolved or correlated with the sequence in array X.  
Specified as: an array of (at least) length  $1+(N_h-1)|inch|$ , containing numbers of the data type indicated in Table 152.
- inch* is the stride between the elements within the sequence in array H.  
Specified as: a fullword integer;  $inch > 0$  or  $inch < 0$ .
- x* is the array X, consisting of the input sequence of length  $N_x$  to be convolved or correlated with the sequence in array H.  
Specified as: an array of (at least) length  $1+(N_x-1)|incx|$ , containing numbers of the data type indicated in Table 152.
- incx* is the stride between the elements within the sequence in array X.  
Specified as: a fullword integer;  $incx > 0$  or  $incx < 0$ .
- y* See “On Return” on page 892.
- incy* is the stride between the elements within the sequence in output array Y.  
Specified as: a fullword integer;  $incy > 0$  or  $incy < 0$ .
- nh* is the number of elements,  $N_h$ , in the sequence in array H.  
Specified as: a fullword integer;  $N_h > 0$ .

## SDCON, DDCON, SDCOR, and DDCOR

$nx$	is the number of elements, $N_x$ , in the sequence in array $X$ . Specified as: a fullword integer; $N_x > 0$ .
$iy0$	is the convolution or correlation index of the element to be stored in the first position of the sequence in array $Y$ . Specified as: a fullword integer. It can have any value.
$ny$	is the number of elements, $N_y$ , in the sequence in array $Y$ . Specified as: a fullword integer; $N_y > 0$ .
$id$	is the decimation interval $id$ for the output sequence in array $Y$ ; that is, every $id$ -th value of the convolution or correlation is produced. Specified as: a fullword integer; $id > 0$ .

### On Return

$y$	is the array $Y$ of length $N_y$ , consisting of the output sequence that is the result of the convolution or correlation of the sequence in array $H$ with the sequence in array $X$ , given for every $id$ -th value in the convolution or correlation.  Returned as: an array of (at least) length $1+(N_y-1)  incy $ , containing numbers of the data type indicated in Table 152 on page 891.
-----	--

### Notes

1. If you specify the same array for  $X$  and  $Y$ , the following conditions must be true:  $incx = incy$ ,  $incx > 0$ ,  $incy > 0$ ,  $id = 1$ , and  $iy0 \geq N_h - 1$  for `_DCON` and  $iy0 \geq 0$  for `_DCOR`. In this case, output overwrites input. In all other cases, output should not overwrite input; that is, input arrays  $X$  and  $H$  must have no common elements with output array  $Y$ . Otherwise, results are unpredictable. See "Concepts" on page 59.
2. If  $iy0$  and  $ny$  are such that output outside the basic range is needed, where the basic range is  $0 \leq k \leq (nh+nx-2)$  for `SDCON` and `DDCON` and is  $(-nh+1) \leq k \leq (nx-1)$  for `SDCOR` and `DDCOR`, the subroutine stores zeros using scalar code. It is not efficient to store many zeros in this manner. If you anticipate that this will happen, you may want to adjust  $iy0$  and  $ny$ , so the subroutine computes only for  $k$  in the above range, or use the ESSL subroutine `SSCAL` or `DSCAL` to store the zeros, so you achieve better performance.

### Function

The convolution and correlation of a sequence in array  $H$  with a sequence in array  $X$ , with decimated output, are expressed as follows:

Convolution for `SDCON` and `DDCON`:

$$y_k = \sum_{j=\max(0, k-N_x+1)}^{\min(N_h-1, k)} h_j x_{k-j}$$

Correlation for `SDCOR` and `DDCOR`:

$$y_k = \sum_{j=\max(0,-k)}^{\min(N_h-1, N_x-1-k)} h_j x_{k+j}$$

for  $k = iy0, iy0+id, iy0+(2)id, \dots, iy0+(N_y-1)id$

where:

$y_k$  are elements of the sequence of length  $N_y$  in array  $Y$ .

$x_k$  are elements of the sequence of length  $N_x$  in array  $X$ .

$h_j$  are elements of the sequence of length  $N_h$  in array  $H$ .

$iy0$  is the convolution or correlation index of the element to be stored in the first position of the sequence in array  $Y$ .

min and max select the minimum and maximum values, respectively.

It is assumed that elements outside the range of definition are zero. See reference [4].

## Special Usage

SDCON and DDCON can also perform a correlation, autoconvolution, or autocorrelation. To compute a correlation, you must specify a negative stride for  $H$ . To compute the autoconvolution, you must specify the two input sequences to be the same. You can also compute the autocorrelation by using both of these techniques together, letting the two input sequences be the same, and specifying a negative stride for the first input sequence. For examples of this, see the examples for SCOND on page 877. Because SCOND and SDCON are functionally the same, their results are the same as long as the decimation interval  $id = 1$  for SDCON.

SDCOR and DDCOR can also perform a convolution, autocorrelation, or autoconvolution. To compute a convolution, you must specify a negative stride for  $H$ . To compute the autocorrelation, you must specify the two input sequences to be the same. You can also compute the autoconvolution by using both of these techniques together, letting the two input sequences be the same and specifying a negative stride for the first input sequence. For examples of these, see the examples for SCORD on page 878. Because SCORD and SDCOR are functionally the same, their results are the same as long as the decimation interval  $id = 1$  for SDCOR.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $nh, nx,$  or  $ny \leq 0$
2.  $inch, incx,$  or  $incy = 0$
3.  $id \leq 0$

## Examples

### Example 1

This example shows how to compute a convolution of a sequence in H with a sequence in X, where both sequences are ramp functions. It shows how a decimated output can be obtained, using the same input as “Example 1” on page 877 for SCOND and using a decimation interval ID = 2.

**Note:** For further examples of use, see the examples for SCOND on page 877. Because SCOND and SDCON are functionally the same, their results are the same as long as the decimation interval ID = 1 for SDCON.

#### Call Statement and Input:

```

          H  INCH  X  INCX  Y  INCY  NH  NX  IY0  NY  ID
CALL SDCON( |  |  |  |  |  |  |  |  |  |  |
            H , 1 , X , 1 , Y , 1 , 4 , 8 , 0 , 6 , 2 )

H          = (1.0, 2.0, 3.0, 4.0)
X          = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)

```

#### Output:

```
Y          = (11.0, 70.0, 130.0, 150.0, 151.0, 72.0)
```

### Example 2

This example shows how to compute a correlation of a sequence in H with a sequence in X, where both sequences are ramp functions. It shows how a decimated output can be obtained, using the same input as “Example 6” on page 878 for SCORD and using a decimation interval ID = 2.

**Note:** For further examples of use, see the examples for SCORD on page 878. Because SCORD and SDCOR are functionally the same, their results are the same as long as the decimation interval ID = 1 for SDCOR.

#### Call Statement and Input:

```

          H  INCH  X  INCX  Y  INCY  NH  NX  IY0  NY  ID
CALL SDCOR( |  |  |  |  |  |  |  |  |  |  |
            H , 1 , X , 1 , Y , 1 , 4 , 8 , -3 , 6 , 2 )

H          = (1.0, 2.0, 3.0, 4.0)
X          = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)

```

#### Output:

```
Y          = (44.0, 110.0, 140.0, 160.0, 104.0, 18.0)
```

### Example 3

This example shows how to compute the same function as computed in “Example 1” on page 877 for SCOND. The input sequences and arguments are the same as that example, except a decimation interval ID = 1 is specified here for SDCON.

#### Call Statement and Input:

```

          H  INCH  X  INCX  Y  INCY  NH  NX  IY0  NY  ID
CALL SDCON( |  |  |  |  |  |  |  |  |  |  |
            H , 1 , X , 1 , Y , 1 , 4 , 8 , 0 , 11 , 1 )

H          = (1.0, 2.0, 3.0, 4.0)
X          = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)

```

#### Output:



## SDCON, DDCON, SDCOR, and DDCOR

Y = (11.0, 34.0, 70.0, 120.0, 130.0, 140.0, 150.0, 160.0,  
151.0, 122.0, 72.0)

---

## SACOR — Autocorrelation of One or More Sequences

### Purpose

This subroutine computes the autocorrelations of one or more sequences using a direct method. The input and output sequences contain short-precision real numbers.

**Note:** This subroutine is considered obsolete. It is provided in ESSL only for compatibility with earlier releases. You should use SCORD, SDCOR, SCORF and SACORF instead, because they provide **better performance**. For further details, see reference [4].

### Syntax

Fortran	CALL SACOR ( <i>init</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>nx</i> , <i>m</i> , <i>ny</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
C and C++	sacor ( <i>init</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>nx</i> , <i>m</i> , <i>ny</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

<i>init</i>	is a flag, where:  If <i>init</i> ≠ 0, no computation is performed, error checking is performed, and the subroutine exits back to the calling program.  If <i>init</i> = 0, the autocorrelations of the sequence in <i>x</i> are computed.  Specified as: a fullword integer. It can have any value.
<i>x</i>	is the array <i>X</i> , consisting of <i>m</i> input sequences of length $N_x$ , to be autocorrelated. Specified as: an array of (at least) length $1+(N_x-1)inc1x+(m-1)inc2x$ , containing short-precision real numbers.
<i>inc1x</i>	is the stride between the elements within each sequence in array <i>X</i> .  Specified as: a fullword integer; <i>inc1x</i> > 0.
<i>inc2x</i>	is the stride between the first elements of the sequences in array <i>X</i> .  Specified as: a fullword integer; <i>inc2x</i> > 0.
<i>y</i>	See "On Return" on page 897.
<i>inc1y</i>	is the stride between the elements within each sequence in output array <i>Y</i> .  Specified as: a fullword integer; <i>inc1y</i> > 0.
<i>inc2y</i>	is the stride between the first elements of each sequence in output array <i>Y</i> .  Specified as: a fullword integer; <i>inc2y</i> > 0.
<i>nx</i>	is the number of elements, $N_x$ , in each sequence in array <i>X</i> .  Specified as: a fullword integer; $N_x$ > 0.
<i>m</i>	is the number of sequences in array <i>X</i> to be correlated.  Specified as: a fullword integer; <i>m</i> > 0.
<i>ny</i>	is the number of elements, $N_y$ , in each sequence in array <i>Y</i> .  Specified as: a fullword integer; $N_y$ > 0.

<i>aux1</i>	is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.
<i>naux1</i>	is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.
<i>aux2</i>	is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.
<i>naux2</i>	is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.

### On Return

<i>y</i>	is array $Y$ , consisting of $m$ output sequences of length $N_y$ that are the autocorrelation functions of the sequences in array $X$ . Returned as: an array of (at least) length $1 + (N_y-1)inc1y + (m-1)inc2y$ , containing short-precision real numbers.
----------	--

### Notes

1. Output should not overwrite input; that is, input arrays  $X$  and  $H$  must have no common elements with output array  $Y$ . Otherwise, results are unpredictable. See "Concepts" on page 59.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for  $init \neq 0$  and  $init = 0$ .
3. Auxiliary storage is not needed, but the arguments *aux1*, *naux1*, *aux2*, and *naux2* must still be specified. You can assign any values to these arguments.

### Function

The autocorrelations of the sequences in array  $X$  are expressed as follows:

$$y_{ki} = \sum_{j=0}^{N_x-1-k} x_{ji} x_{j+k,i}$$

for:

$$\begin{aligned} k &= 0, 1, \dots, N_y-1 \\ i &= 1, 2, \dots, m \end{aligned}$$

where:

$y_{ki}$  are elements of the  $m$  sequences of length  $N_y$  in array  $Y$ .  
 $x_{ji}$  and  $x_{j+k,i}$  are elements of the  $m$  sequences of length  $N_x$  in array  $X$ .

See references [19] and [88].

Only one invocation of this subroutine is needed:

1. You do not need to invoke the subroutine with  $init \neq 0$ . If you do, however, the subroutine performs error checking, exits back to the calling program, and no computation is performed.

- With *init* = 0, the subroutine performs the calculation of the convolutions or correlations.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

- $nx$ ,  $ny$ , or  $m \leq 0$
- $inc1x$ ,  $inc2x$ ,  $inc1y$ , or  $inc2y \leq 0$  (or incompatible)

## Examples

### Example 1

This example shows how to compute an autocorrelation for three short sequences in array *X*, where the input sequence length *NX* is equal to the output sequence length *NY*. This gives all nonzero autocorrelation values.

The arrays are declared as follows:

```
REAL*4  X(0:49999), Y(0:49999)
REAL*8  AUX1, AUX2
```

### Call Statement and Input:

```

      INIT  X  INC1X  INC2X  Y  INC1Y  INC2Y  NX  M  NY  AUX1  NAUX1  AUX2  NAUX2
      |    |    |    |    |    |    |    |    |    |    |    |    |
CALL SACOR(INIT, X , 1 , 7 , Y , 1 , 7 , 7 , 3 , 7 , AUX1 , 0 , AUX2 , 0)
```

INIT = 0(for computation)

*X* contains the following three sequences:

```
1.0  2.0  3.0
2.0  1.0  2.0
3.0  2.0  1.0
4.0  3.0  2.0
4.0  4.0  3.0
3.0  4.0  4.0
2.0  3.0  4.0
```

**Output:** *Y* contains the following three sequences:

```
59.0  59.0  59.0
54.0  50.0  44.0
43.0  39.0  30.0
29.0  27.0  24.0
16.0  18.0  21.0
 7.0  11.0  20.0
 2.0   6.0  12.0
```

### Example 2

This example shows how the output from Example 1 differs when the values for *NY* and *INC2Y* are 9 rather than 7. This shows that when *NY* is greater than *NX*, the output array is longer, and that part is filled with zeros.

**Output:** *Y* contains the following three sequences:

```
59.0  59.0  59.0
54.0  50.0  44.0
43.0  39.0  30.0
29.0  27.0  24.0
```

```
16.0 18.0 21.0
 7.0 11.0 20.0
 2.0  6.0 12.0
 0.0  0.0  0.0
 0.0  0.0  0.0
```

### Example 3

This example shows how the output from Example 1 differs when the value for  $NY$  is 5 rather than 7. Also, the values for  $INC1X$  and  $INC1Y$  are 3, and the values for  $INC2X$  and  $INC2Y$  are 1 rather than 7. This shows that when  $NY$  is less than  $NX$ , the output array is shortened.

**Output:**  $Y$  contains the following three sequences:

```
59.0 59.0 59.0
54.0 50.0 44.0
43.0 39.0 30.0
29.0 27.0 24.0
16.0 18.0 21.0
```

## SACORF — Autocorrelation of One or More Sequences Using the Mixed-Radix Fourier Method

### Purpose

This subroutine computes the autocorrelations of one or more sequences using the mixed-radix Fourier method. The input and output sequences contain short-precision real numbers.

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

Fortran	CALL SACORF ( <i>init</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>nx</i> , <i>m</i> , <i>ny</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> )
C and C++	sacorf ( <i>init</i> , <i>x</i> , <i>inc1x</i> , <i>inc2x</i> , <i>y</i> , <i>inc1y</i> , <i>inc2y</i> , <i>nx</i> , <i>m</i> , <i>ny</i> , <i>aux1</i> , <i>naux1</i> , <i>aux2</i> , <i>naux2</i> );

### On Entry

<i>init</i>	is a flag, where:  If <i>init</i> $\neq$ 0, trigonometric functions and other parameters, depending on arguments other than <i>x</i> , are computed and saved in <i>aux1</i> . The contents of <i>x</i> and <i>y</i> are not used or changed.  If <i>init</i> = 0, the autocorrelations of the sequence in <i>x</i> are computed. The only arguments that may change after initialization are <i>x</i> , <i>y</i> , and <i>aux2</i> . All scalar arguments must be the same as when the subroutine was called for initialization with <i>init</i> $\neq$ 0.  Specified as: a fullword integer. It can have any value.
<i>x</i>	is the array $\chi$ , consisting of <i>m</i> input sequences of length $N_x$ , to be autocorrelated. Specified as: an array of (at least) length $1+(N_x-1)inc1x+(m-1)inc2x$ , containing short-precision real numbers.
<i>inc1x</i>	is the stride between the elements within each sequence in array $\chi$ .  Specified as: a fullword integer; <i>inc1x</i> > 0.
<i>inc2x</i>	is the stride between the first elements of the sequences in array $\chi$ .  Specified as: a fullword integer; <i>inc2x</i> > 0.
<i>y</i>	See "On Return" on page 901.
<i>inc1y</i>	is the stride between the elements within each sequence in output array $\Upsilon$ .  Specified as: a fullword integer; <i>inc1y</i> > 0.
<i>inc2y</i>	is the stride between the first elements of each sequence in output array $\Upsilon$ .  Specified as: a fullword integer; <i>inc2y</i> > 0.
<i>nx</i>	is the number of elements, $N_x$ , in each sequence in array $\chi$ .  Specified as: a fullword integer; $N_x$ > 0.
<i>m</i>	is the number of sequences in array $\chi$ to be correlated.

- Specified as: a fullword integer;  $m > 0$ .
- ny* is the number of elements,  $N_y$ , in each sequence in array  $Y$ .  
Specified as: a fullword integer;  $N_y > 0$ .
- aux1* is the working storage for this subroutine, where:  
If  $init \neq 0$ , the working storage is computed.  
If  $init = 0$ , the working storage is used in the computation of the autocorrelations.  
Specified as: an area of storage, containing *naux1* long-precision real numbers.
- naux1* is the number of doublewords in the working storage specified in *aux1*.  
Specified as: a fullword integer;  $naux1 > 21$  and  $naux1 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For values between 21 and the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 36.
- aux2* has the following meaning:  
If  $naux2 = 0$  and error 2015 is unrecoverable, *aux2* is ignored.  
Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.  
Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.
- naux2* is the number of doublewords in the working storage specified in *aux2*.  
Specified as: a fullword integer, where:  
If  $naux2 = 0$  and error 2015 is unrecoverable, SACORF dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.  
Otherwise,  $naux2 \geq$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 36.

### On Return

- y* has the following meaning, where:  
If  $init \neq 0$ , this argument is not used, and its contents remain unchanged.  
If  $init = 0$ , this is array  $Y$ , consisting of  $m$  output sequences of length  $N_y$  that are the autocorrelation functions of the sequences in array  $X$ .

Returned as: an array of (at least) length  $1+(N_y-1)inc1y+(m-1)inc2y$ , containing short-precision real numbers.

*aux1*

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If  $init = 0$ , its contents are unchanged.

Returned as: the contents are not relevant.

## Notes

1. *aux1* should **not** be used by the calling program between calls to this subroutine with  $init \neq 0$  and  $init = 0$ . However, it can be reused after intervening calls to this subroutine with different arguments.
2. When using the ESSL SMP library, for optimal performance, the number of threads specified should be the same for  $init \neq 0$  and  $init = 0$ .
3. If you specify the same array for  $X$  and  $Y$ , then  $inc1x$  and  $inc1y$  must be equal and  $inc2x$  and  $inc2y$  must be equal. In this case, output overwrites input.
4. If you specify different arrays for  $X$  and  $Y$ , they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.
5. If  $ny$  is such that output outside the basic range is needed, the subroutine stores zeros. This range is:  $0 \leq k \leq nx-1$ .

## Formulas

### Formula for Calculating the Length of the Fourier Transform

Before calculating the necessary sizes of  $naux1$  and  $naux2$ , you must determine the length  $n$  of the Fourier transform. To do this, you use the values of the arguments  $nx$  and  $ny$ , inserted into the following formula, to get a value for the variable  $nf$ . After calculating  $nf$ , reference the formula or table of allowable values of  $n$  in "Acceptable Lengths for the Transforms" on page 779, selecting the value equal to or greater than  $nf$ . Following is the formula for determining  $nf$ :

$$nf = \min(ny, nx) + nx + 1$$

### Processor-Independent Formulas for NAUX1 and NAUX2

The required values of  $naux1$  and  $naux2$  depend on the value determined for  $n$  in "Formula for Calculating the Length of the Fourier Transform" and the argument  $m$ .

#### NAUX1 Formulas:

If  $n \leq 16384$ , use  $naux1 = 55000$ .

If  $n > 16384$ , use  $naux1 = 40000 + 1.89n$ .

#### NAUX2 Formulas:

If  $n \leq 16384$ , use  $naux2 = 50000$ .

If  $n > 16384$ , use  $naux2 = 40000 + 1.64n$ .

## Function

The autocorrelations of the sequences in array  $X$  are expressed as follows:



$$y_{ki} = \sum_{j=0}^{N_x-1-k} x_{ji} x_{j+k,i}$$

for:

$$k = 0, 1, \dots, N_y-1$$

$$i = 1, 2, \dots, m$$

where:

$y_{ki}$  are elements of the  $m$  sequences of length  $N_y$  in array  $Y$ .  
 $x_{ji}$  and  $x_{j+k,i}$  are elements of the  $m$  sequences of length  $N_x$  in array  $X$ .

This subroutine uses a Fourier transform method with a mixed-radix capability. This provides maximum performance for your application. The length of the transform,  $n$ , that you must calculate to determine the correct sizes for  $naux1$  and  $naux2$  is the same length used by the Fourier transform subroutines called by this subroutine. See references [19] and [88].

Two invocations of this subroutine are necessary:

1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the  $aux1$  working storage.
2. With  $init = 0$ , the subroutine checks that the initialization arguments in the  $aux1$  working storage correspond to the present arguments, and if so, performs the calculation of the autocorrelations.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux2 = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $nx$ ,  $ny$ , or  $m \leq 0$
2.  $inc1x$ ,  $inc2x$ ,  $inc1y$ , or  $inc2y \leq 0$  (or incompatible)
3. The resulting correlation is too long.
4. The subroutine has not been initialized with the present arguments.
5.  $naux1 \leq 21$
6.  $naux1$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
7. Error 2015 is recoverable or  $naux2 \neq 0$ , and  $naux2$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to compute an autocorrelation for three short sequences in array  $X$ , where the input sequence length  $NX$  is equal to the output sequence length  $NY$ . This gives all nonzero autocorrelation values. The arrays are declared as follows:

## SACORF

```
REAL*4 X(0:49999), Y(0:49999)
REAL*8 AUX1(2959), AUX2(1)
```

First, initialize AUX1 using the calling sequence shown below with  $INIT \neq 0$ . Then use the same calling sequence with  $INIT = 0$  to do the calculation.

**Note:** Because  $NAUX2 = 0$ , this subroutine dynamically allocates the AUX2 working storage.

### Call Statement and Input:

```
INIT X INC1X INC2X Y INC1Y INC2Y NX M NY AUX1 NAUX1 AUX2 NAUX2
|   |   |   |   |   |   |   |   |   |   |   |   |
CALL SACORF(INIT, X, 1, 7, Y, 1, 7, 7, 3, 7, AUX1, 2959, AUX2, 0)
```

INIT = 1(for initialization)

INIT = 0(for computation)

X contains the following three sequences:

```
1.0 2.0 3.0
2.0 1.0 2.0
3.0 2.0 1.0
4.0 3.0 2.0
4.0 4.0 3.0
3.0 4.0 4.0
2.0 3.0 4.0
```

**Output:** Y contains the following three sequences:

```
59.0 59.0 59.0
54.0 50.0 44.0
43.0 39.0 30.0
29.0 27.0 24.0
16.0 18.0 21.0
7.0 11.0 20.0
2.0 6.0 12.0
```

### Example 2

This example shows how the output from Example 1 differs when the value for NY and INC2Y are 9 rather than 7. This shows that when NY is greater than NX, the output array is longer and that part is filled with zeros.

**Output:** Y contains the following three sequences:

```
59.0 59.0 59.0
54.0 50.0 44.0
43.0 39.0 30.0
29.0 27.0 24.0
16.0 18.0 21.0
7.0 11.0 20.0
2.0 6.0 12.0
0.0 0.0 0.0
0.0 0.0 0.0
```

### Example 3

This example shows how the output from Example 1 differs when the value for NY is 5 rather than 7. Also, the values for INC1X and INC1Y are 3 rather than 1, and the values for INC2X and INC2Y are 1 rather than 7. This shows that when NY is less than NX, the output array is shortened.

**Output:** Y contains the following three sequences:

59.0	59.0	59.0
54.0	50.0	44.0
43.0	39.0	30.0
29.0	27.0	24.0
16.0	18.0	21.0

---

## **Related-Computation Subroutines**

This section contains the related-computation subroutine descriptions.

## SPOLY and DPOLY — Polynomial Evaluation

### Purpose

These subroutines evaluate a polynomial of degree  $k$ , using coefficient vector  $u$ , input vector  $x$ , and output vector  $y$ :

$$y_i = u_0 + u_1 x_i + u_2 x_i^2 + \dots + u_k x_i^k \quad \text{for } i = 1, 2, \dots, n$$

where  $u_k$ ,  $x_i$ , and  $y_i$  are elements of  $u$ ,  $x$ , and  $y$ , respectively.

Table 153. Data Types

$u$ , $x$ , $y$	Subroutine
Short-precision real	SPOLY
Long-precision real	DPOLY

### Syntax

Fortran	CALL SPOLY   DPOLY ( $u$ , $incu$ , $k$ , $x$ , $incx$ , $y$ , $incy$ , $n$ )
C and C++	spoly   dpoly ( $u$ , $incu$ , $k$ , $x$ , $incx$ , $y$ , $incy$ , $n$ );

### On Entry

- $u$  is the coefficient vector  $u$  of length  $k+1$ . It contains elements  $u_0, u_1, u_0, u_1, u_2, \dots, u_k$ , which are stored in this order. Specified as: a one-dimensional array of (at least) length  $1+k|incu|$ , containing numbers of the data type indicated in Table 153.
- $incu$  is the stride for vector  $u$ .  
Specified as: a fullword integer. It can have any value.
- $k$  is the degree  $k$  of the polynomial.  
Specified as: a fullword integer;  $k \geq 0$ .
- $x$  is the input vector  $x$  of length  $n$ . Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 153.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer. It can have any value.
- $y$  See "On Return."
- $incy$  is the stride for the output vector  $y$ . Specified as: a fullword integer. It can have any value.
- $n$  is the number of elements in input vector  $x$  and the number of resulting elements in output vector  $y$ .  
Specified as: a fullword integer;  $n \geq 0$ .

### On Return

- $y$  is the output vector  $y$  of length  $n$ , containing the results of the

## SPOLY and DPOLY

polynomial evaluation. Returned as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 153 on page 907.

### Notes

Vectors  $u$ ,  $x$ , and  $y$  must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 59.

### Function

The evaluation of the polynomial:

$$y_i = u_0 + u_1x_i + u_2x_i^2 + \dots + u_kx_i^k \quad \text{for } i = 1, 2, \dots, n$$

is expressed as follows:

$$y_i = u_0 + x_i (u_1 + x_i (u_2 + \dots + x_i (u_{k-1} + x_i u_k) \dots)) \quad \text{for } i = 1, 2, \dots, n$$

See reference [84] for Horner's Rule. If  $n$  is 0, no computation is performed. For SPOLY, intermediate results are accumulated in long precision.

SPOLY provides the same function as the IBM 3838 function POLY, with restrictions removed. DPOLY provides a long-precision computation that is not included in the IBM 3838 functions. See the *IBM 3838 Array Processor Functional Characteristics* manual.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

1.  $k < 0$
2.  $n < 0$

### Examples

#### Example 1

This example shows a polynomial evaluation with the degree,  $K$ , equal to 0.

#### Call Statement and Input:

```
          U  INCU  K  X  INCX  Y  INCY  N
          |  |    |  |  |    |  |    |
CALL SPOLY( U , INCU , 0 , X , INCX , Y , 1 , 3 )
```

```
U          = (4.0)
INCX      =(not relevant)
X         =(not relevant)
INCX      =(not relevant)
```

#### Output:

```
Y          = (4.0, 4.0, 4.0)
```

**Example 2**

This example shows a polynomial evaluation, using a negative stride INCU for vector  $u$ . For  $u$ , processing begins at element U(4) which is 1.0.

**Call Statement and Input:**

```

          U  INCU  K  X  INCX  Y  INCY  N
          |  |    |  |  |    |  |    |
CALL SPOLY( U , -1 , 3 , X , 1  , Y , 1  , 3 )

```

```

U      = (4.0, 3.0, 2.0, 1.0)
X      = (2.0, 1.0, -3.0)

```

**Output:**

```

Y      = (49.0, 10.0, -86.0)

```

**Example 3**

This example shows a polynomial evaluation, using a stride INCX of 0 for input vector  $x$ .

**Call Statement and Input:**

```

          U  INCU  K  X  INCX  Y  INCY  N
          |  |    |  |  |    |  |    |
CALL SPOLY( U , 1  , 3 , X , 0  , Y , 1  , 3 )

```

```

U      = (4.0, 3.0, 2.0, 1.0)
X      = (2.0, . , . )

```

**Output:**

```

Y      = (26.0, 26.0, 26.0)

```

**Example 4**

This example shows a polynomial evaluation, using a stride INCX greater than 1 for input vector  $x$ , and a negative stride INCY for output vector  $y$ . For  $y$ , results are stored beginning at element Y(5).

**Call Statement and Input:**

```

          U  INCU  K  X  INCX  Y  INCY  N
          |  |    |  |  |    |  |    |
CALL SPOLY( U , 1  , 3 , X , 2  , Y , -2 , 3 )

```

```

U      = (4.0, 3.0, 2.0, 1.0)
X      = (2.0, . , -3.0, . , 1.0)

```

**Output:**

```

Y      = (10.0, . , -14.0, . , 26.0)

```

---

## SIZC and DIZC — I-th Zero Crossing

### Purpose

These subroutines find the position of the  $i$ -th zero crossing in vector  $x$ . This is the  $i$ -th transition between positive and negative or negative and positive, where 0 is considered a positive value. It returns the position of the element in vector  $x$  where the  $i$ -th zero crossing is detected. The direction of the scan is either from the first element to the last or from the last element to the first, depending on the value you specify for the scan direction argument.

Table 154. Data Types

$x$	Subroutine
Short-precision real	SIZC
Long-precision real	DIZC

### Syntax

Fortran	CALL SIZC   DIZC ( $x$ , $idrx$ , $n$ , $i$ , $ky$ )
C and C++	size   dizc ( $x$ , $idrx$ , $n$ , $i$ , $ky$ );

### On Entry

- $x$  is the target vector  $x$  of length  $n$ .  
Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 154.
- $idrx$  indicates the scan direction. If it is positive or 0,  $x$  is scanned from the first element to the last ( $1, n$ ). If it is negative,  $x$  is scanned from the last element to the first ( $n, 1$ ).  
Specified as: a fullword integer. It can have any value.
- $n$  is the number of elements in vector  $x$ . Specified as: a fullword integer;  $n > 1$ .
- $i$  is the number of the zero crossing to be identified.  
Specified as: a fullword integer;  $i > 0$ .
- $ky$  See "On Return."

### On Return

- $ky$  is the integer vector  $ky$  of length 2, containing elements  $ky_1$  and  $ky_2$ , where:
- If the  $i$ -th zero crossing is found:
- $ky_1 = j$ , where  $j$  is the position of the element  $x_j$  at the point that the  $i$ -th zero crossing is found. The position is always relative to the beginning of the vector regardless of the scan direction.
  - $ky_2 = i$
- If the  $i$ -th zero crossing is not found:
- $ky_1 = 0$
  - $ky_2 =$  the total number of zero crossings encountered in the scan.



Returned as: an array of (at least) length 2, containing fullword integers.

## Notes

The *aux* and *naux* arguments, required in some earlier releases of ESSL, are no longer required by these subroutines. If your program still includes them, you do not have to change your program; it continues to run normally. It ignores these arguments. However, if you did any program checking for error code 2015, you may want to remove it, because this error no longer occurs. (You must not code these arguments in your C program.)

## Function

The *i*-th zero crossing in vector *x* is found by scanning vector *x* for *i* occurrences of TRUE for the following logical expressions. A zero crossing is defined here as a crossing either from a positive value to a negative value or from a negative value to a positive value, where 0 is considered a positive value. If the *i*-th zero crossing is found, the value of *j* at that point is returned in *ky*<sub>1</sub> as the position of the *i*-th zero crossing, and *i* is returned in *ky*<sub>2</sub>.

If *idrx* ≥ 0:

TRUE = ( $x_{j-1} < 0$  and  $x_j \geq 0$ ) or ( $x_{j-1} \geq 0$  and  $x_j < 0$ ) for  $j = 2, n$

If *idrx* < 0:

TRUE = ( $x_{j+1} < 0$  and  $x_j \geq 0$ ) or ( $x_{j+1} \geq 0$  and  $x_j < 0$ ) for  $j = n-1, 1$

If the position of the *i*-th zero crossing is not found, 0 is returned in *y*<sub>1</sub> and the number of zero crossings encountered in the scan is returned in *y*<sub>2</sub>.

SIZC provides the same functions as the IBM 3838 functions NZCP and NZCN, with restrictions removed. It combines these functions into one ESSL subroutine. DIZC provides a long-precision computation that is not included in the IBM 3838 functions. See the *IBM 3838 Array Processor Functional Characteristics* manual.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $n \leq 1$
2.  $i \leq 0$

## Examples

### Example 1

This example shows a scan of a vector *x* from the first element to the last. It is looking for the fifth zero crossing, which is encountered at position 9.

**Call Statement and Input:**

## SIZC and DIZC

```
          X  IDRX  N    I    KY
          |  |    |    |    |
CALL SIZC( X , 1 , 12 , 5 , KY )
```

```
X          = (2.0, -1.0, -3.0, 3.0, 0.0, 8.0, -2.0, 0.0, -5.0, -3.0,
              2.0, -9.0)
```

### Output:

```
KY          = (9, 5)
```

### Example 2

This example shows a scan of a vector  $x$  from the last element to the first. It is looking for the seventh zero crossing, which is encountered at position 3. Because IDRX is negative,  $X$  is scanned from the last element,  $X(12)$ , to the first element,  $X(1)$ .

### Call Statement and Input:

```
          X  IDRX  N    I    KY
          |  |    |    |    |
CALL SIZC( X , -1 , 12 , 7 , KY )
```

```
X          = (2.0, -1.0, 3.0, -3.0, 0.0, -8.0, -2.0, 0.0, -5.0, -3.0,
              2.0, -9.0)
```

### Output:

```
KY          = (3, 7)
```

### Example 3

This example shows a scan of a vector  $x$  when the  $i$ -th zero crossing is not found. It encounters seven zero crossings and returns this value in  $KY(2)$ .

### Call Statement and Input:

```
          X  IDRX  N    I    KY
          |  |    |    |    |
CALL SIZC( X , 1 , 12 , 10 , KY )
```

```
X          = (2.0, -1.0, -3.0, 3.0, 0.0, 8.0, -2.0, 0.0, -5.0, -3.0,
              2.0, -9.0)
```

### Output:

```
KY          = (0, 7)
```

## STREC and DTREC — Time-Varying Recursive Filter

### Purpose

These subroutines implement the first-order time-varying recursive equation, using initial value  $s$ , target vectors  $u$  and  $x$ , and output vector  $y$ .

Table 155. Data Types

$s, u, x, y$	Subroutine
Short-precision real	STREC
Long-precision real	DTREC

### Syntax

Fortran	CALL STREC   DTREC ( $s, u, incu, x, incx, y, incy, n, iopt$ )
C and C++	strec   dtrec ( $s, u, incu, x, incx, y, incy, n, iopt$ );

### On Entry

- $s$  is the scalar  $s$  used in the initial computation for  $y_1$ .  
Specified as: a number of the data type indicated in Table 155.
- $u$  is the target vector  $u$  of length  $n$ .  
Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incu|$ , containing numbers of the data type indicated in Table 155.
- $incu$  is the stride for target vector  $u$ .  
Specified as: a fullword integer. It can have any value.
- $x$  is the target vector  $x$  of length  $n$ .  
Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 155.
- $incx$  is the stride for target vector  $x$ . Specified as: a fullword integer. It can have any value.
- $y$  See "On Return."
- $incy$  is the stride for output vector  $y$ . Specified as: a fullword integer;  $incy > 0$  or  $incy < 0$ .
- $n$  is the number of elements in vectors  $u$  and  $x$  and the number of resulting elements in output vector  $y$ .  
Specified as: a fullword integer;  $n \geq 0$ .
- $iopt$  this argument has no effect on the performance of the computation, but still must be specified as: a fullword integer;  $iopt = 0$  or  $1$ .

### On Return

- $y$  is the vector  $y$  of length  $n$ , containing the results of the implementation of the first-order time-varying recursive equation.

## STREC and DTREC

Returned as: a one-dimensional array of (at least) length  $1+(n-1)|incy|$ , containing numbers of the data type indicated in Table 155 on page 913.

### Notes

Vectors  $u$ ,  $x$ , and  $y$  must have no common elements; otherwise, results are unpredictable. See “Concepts” on page 59.

### Function

The first-order time-varying recursive equation is expressed as follows:

$$\begin{aligned}y_1 &= s+u_1x_1 \\y_2 &= u_2y_1+u_1x_2 \\&\cdot \\&\cdot \\y_i &= u_iy_{i-1}+u_1x_i \text{ for } i = 3, 4, \dots, n\end{aligned}$$

STREC provides the same function as the IBM 3838 function REC, with restrictions removed. DTREC provides a long-precision computation that is not included in the IBM 3838 functions. See the *IBM 3838 Array Processor Functional Characteristics* manual.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

1.  $incy = 0$
2.  $n < 0$
3.  $iopt \neq 0$  or 1

### Examples

#### Example 1

This example shows all strides INCU, INCX, and INCY equal to 1 for vectors  $u$ ,  $x$ , and  $y$ , respectively.

#### Call Statement and Input:

```
          S   U   INCU  X   INCX  Y   INCY  N   IOPT
          |   |   |     |   |     |   |     |
CALL STREC( 1.0 , U , 1 , X , 1 , Y , 1 , 8 , 0 )
```

```
U       = (1.0, 2.0, 3.0, 3.0, 2.0, 1.0, 1.0, 2.0)
X       = (3.0, 2.0, 1.0, 1.0, 2.0, 3.0, 3.0, 2.0)
```

#### Output:

```
Y       = (4.0, 10.0, 31.0, 94.0, 190.0, 193.0, 196.0, 394.0)
```

#### Example 2

This example shows a stride, INCU, that is greater than 1 for vector  $u$ . The strides INCX and INCY for vectors  $x$  and  $y$ , respectively, are 1.

#### Call Statement and Input:

```

          S   U  INCU X  INCX Y  INCY N  IOPT
          |   |   |   |   |   |   |   |
CALL STREC( 1.0 , U , 2 , X , 1 , Y , 1 , 4 , 0 )

```

```

U      = (1.0, . , 3.0, . , 2.0, . , 1.0, . )
X      = (3.0, 2.0, 1.0, 1.0, 2.0, 3.0, 3.0, 2.0)

```

**Output:**

```

Y      = (4.0, 14.0, 29.0, 30.0)

```

**Example 3**

This example shows a stride, *INCX*, of 1 for vector *u*, a stride, *INCX*, that is greater than 1 for vector *x*, and a negative stride, *INCY*, for vector *y*. For *y*, results are stored beginning at element *Y*(4).

**Call Statement and Input:**

```

          S   U  INCU X  INCX Y  INCY N  IOPT
          |   |   |   |   |   |   |   |
CALL STREC( 1.0 , U , 1 , X , 2 , Y , -1 , 4 , 1 )

```

```

U      = (1.0, 2.0, 3.0, 3.0, 2.0, 1.0, 1.0, 2.0)
X      = (3.0, . , 1.0, . , 2.0, . , 3.0)

```

**Output:**

```

Y      = (90.0, 29.0, 9.0, 4.0)

```

---

## SQINT and DQINT — Quadratic Interpolation

### Purpose

These subroutines perform a quadratic interpolation at specified points in the vector  $x$ , using initial linear displacement in the samples  $s$ , sample interval  $g$ , output scaling parameter  $\Omega$ , and sample reflection times in vector  $t$ . The result is returned in vector  $y$ .

Table 156. Data Types

$x, s, g, \Omega, t, y$	Subroutine
Short-precision real	SQINT
Long-precision real	DQINT

### Syntax

Fortran	CALL SQINT   DQINT ( $s, g, \omega, x, incx, n, t, inct, y, incy, m$ )
C and C++	sqint   dqint ( $s, g, \omega, x, incx, n, t, inct, y, incy, m$ );

### On Entry

- $s$  is the scalar  $s$ , containing the initial linear displacement in samples.  
Specified as: a number of the data type indicated in Table 156.
- $g$  is the scalar  $g$ , containing the sample interval.  
Specified as: a number of the data type indicated in Table 156;  
 $g > 0.0$ .
- $\omega$  is the output scaling parameter  $\Omega$ .  
Specified as: a number of the data type indicated in Table 156.
- $x$  is the vector  $x$  of length  $n$ , containing the trace data.  
Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 156.
- $incx$  is the stride for vector  $x$ .  
Specified as: a fullword integer;  $incx > 0$  or  $incx < 0$ .
- $n$  is the number of elements in vector  $x$ .  
Specified as: a fullword integer;  $n \geq 3$ .
- $t$  is the vector  $t$  of length  $m$ , containing the sample reflection times to be processed.  
Specified as: a one-dimensional array of (at least) length  $1+(m-1)|inct|$ , containing numbers of the data type indicated in Table 156.
- $inct$  is the stride for vector  $t$ .  
Specified as: a fullword integer;  $inct > 0$  or  $inct < 0$ .
- $y$  See "On Return" on page 917.
- $incy$  is the stride for output vector  $y$ .

Specified as: a fullword integer;  $incy > 0$  or  $incy < 0$ .

$m$  is the number of elements in vector  $t$  and the number of elements in output vector  $y$ .

Specified as: a fullword integer;  $m \geq 0$ .

### On Return

$y$  is the vector  $y$  of length  $m$ , containing the results of the quadratic interpolation. Returned as: a one-dimensional array of (at least) length  $1+(m-1)|incy|$ , containing numbers of the data type indicated in Table 156 on page 916.

## Function

The quadratic interpolation, which is expressed as follows:

$$y_i = \Omega \left( trace_{k_i} (f_i^2 - f_i) + 2 trace_{k_i+1} (1 - f_i^2) + trace_{k_i+2} (f_i^2 + f_i) \right)$$

for  $i = 1, 2, \dots, m$

uses the following values:

$x$  is the vector containing the specified points.  
 $s$  is the initial linear displacement in the samples.  
 $g$  is a sample interval.  
 $\Omega$  is the output scaling parameter.  
 $t$  is the vector containing the sample reflection times.

and where  $trace$ ,  $k$ ,  $f$ , and  $w$  are four working vectors, and  $so$  is a working scalar defined as:

$$\begin{aligned} trace_1 &= 3x_1 - 3x_2 + x_3 \\ trace_{i+1} &= x_i \quad \text{for } i = 1, 2, \dots, n \\ so &= s + 2.0 \\ w_i &= so + t_i / g \quad \text{for } i = 1, 2, \dots, m \\ f_i &= \text{fraction part of } w_i \\ k_{i+1} &= \text{integer part of } w_i \end{aligned}$$

**Note:** Allowing  $k_{i+1}$  to have a value of 2 results in performance degradation. If possible, avoid specifying a point at which this occurs.

If  $n$  or  $m$  is 0, no computation is performed.

SQINT provides the same function as the IBM 3838 function INT, with restrictions removed. DQINT provides a long-precision computation that is not included in the IBM 3838 functions. See the *IBM 3838 Array Processor Functional Characteristics* manual.

## Error conditions

### Computational Errors

The condition  $(k_{i+1} > n)$  or  $(k_{i+1} \leq 2)$  has occurred, where  $n$  is the number of elements in vector  $x$ . See "Function" for how to calculate  $k_i$ .

## SQINT and DQINT

- The lower range  $l$  and the upper range  $j$  of the vector are identified in the computational error message.
- The return code is set to 1.
- The ranges  $l$  and  $j$  of the vector can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2100 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see “What Can You Do about ESSL Computational Errors?” on page 51.

### Input-Argument Errors

1.  $n < 3$
2.  $m < 0$
3.  $g \leq 0$
4.  $incx = 0$
5.  $inct = 0$
6.  $incy = 0$

## Examples

### Example 1

This example shows a quadratic interpolation, using vectors with strides of 1.

#### Call Statement and Input:

```
          S      G      OMEGA  X  INCX  N  T  INCT  Y  INCY  M
          |      |      |      |  |    |  |  |    |  |    |
CALL SQINT( 2.0 , 1.0 , 1.0 , X , 1  , 8 , T , 1  , Y , 1  , 4 )
```

```
X      = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0)
T      = (1.5, 2.5, 3.5, 4.5)
```

#### Output:

```
Y      = (9.0, 11.0, 13.0, 15.0)
```

### Example 2

This example shows a quadratic interpolation, using vectors with a positive stride of 1 and negative strides of -1.

#### Call Statement and Input:

```
          S      G      OMEGA  X  INCX  N  T  INCT  Y  INCY  M
          |      |      |      |  |    |  |  |    |  |    |
CALL SQINT( 2.0 , 1.0 , 1.0 , X , -1 , 8 , T , -1 , Y , 1  , 4 )
```

```
X      = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0)
T      = (1.5, 2.5, 3.5, 4.5)
```

#### Output:

```
Y      = (3.0, 5.0, 7.0, 9.0)
```

### Example 3

This example shows a quadratic interpolation, using vectors with a positive stride greater than 1 and negative strides less than -1.

#### Call Statement and Input:

```
          S      G      OMEGA  X  INCX  N  T  INCT  Y  INCY  M
          |      |      |      |  |    |  |  |    |  |    |
CALL SQINT( 2.0 , 1.0 , 1.0 , X , -2 , 8 , T , -1 , Y , 2  , 4 )
```



```

X      = (1.0, . , 3.0, . , 5.0, . , 7.0, . , 9.0, . , 11.0, . ,
          13.0, . , 15.0)
T      = (1.36, 2.36, 3.36, 4.36)

```

**Output:**

```
Y      = (4.56, . , 8.56, . , 12.56, . , 16.56)
```

**Example 4**

This example shows a quadratic interpolation, using vectors with positive strides and larger values for S and G than shown in the previous examples.

**Call Statement and Input:**

```

          S      G  OMEGA X  INCX  N  T  INCT  Y  INCY  M
          |      |      |  |  |    |  |  |    |  |  |
CALL SQINT( 3.0 , 10.0 , 1.0 , X , 1 , 8 , T , 2 , Y , 3 , 4 )

```

```

X      = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0)
T      = (1.5, . , 2.5, . , 3.5, . , 4.5)

```

**Output:**

```
Y      = (8.3, . , . , 8.5, . , . , 8.7, . , . , 8.9)
```

## SWLEV, DWLEV, CWLEV, and ZWLEV — Wiener-Levinson Filter Coefficients

### Purpose

These subroutines compute the coefficients of an  $n$ -point Wiener-Levinson filter, using vector  $x$ , the trace for which the filter is to be designed, and vector  $u$ , the right-hand side of the system, chosen to remove reverberations or sharpen the wavelet. The result is returned in vector  $y$ .

Table 157. Data Types

$x, u, y$	$aux$	Subroutine
Short-precision real	Long-precision real	SWLEV
Long-precision real	Long-precision real	DWLEV
Short-precision complex	Long-precision complex	CWLEV
Long-precision complex	Long-precision complex	ZWLEV

### Syntax

<b>Fortran</b>	CALL SWLEV   DWLEV   CWLEV   ZWLEV   ( $x, incx, u, incu, y, incy, n, aux, naux$ )
<b>C and C++</b>	swlev   dwlev   cwlev   zwlev ( $x, incx, u, incu, y, incy, n, aux, naux$ );

### On Entry

- $x$  is the vector  $x$  of length  $n$ , containing the trace data for which the filter is to be designed.
- For SWLEV and DWLEV,  $x$  represents the first row (or the first column) of a positive definite or negative definite symmetric Toeplitz matrix, which is the autocorrelation matrix for which the filter is designed.
- For CWLEV and ZWLEV,  $x$  represents the first row of a positive definite or negative definite complex Hermitian Toeplitz matrix, which is the autocorrelation matrix for which the filter is designed.
- Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 157.
- $incx$  is the stride for vector  $x$ .
- Specified as: a fullword integer;  $incx > 0$ .
- $u$  is the vector  $u$  of length  $n$ , containing the right-hand side of the system to be solved.
- Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incu|$ , containing numbers of the data type indicated in Table 157.
- $incu$  is the stride for vector  $u$ .
- Specified as: a fullword integer. It can have any value.
- $y$  See "On Return" on page 921.
- $incy$  is the stride for vector  $y$ .

	Specified as: a fullword integer; $incy > 0$ or $incy < 0$ .
$n$	is the number of elements in vectors $x$ , $u$ , and $y$ . Specified as: a fullword integer; $n \geq 0$ .
$aux$	has the following meaning: If $naux = 0$ and error 2015 is unrecoverable, $aux$ is ignored. Otherwise, it is the storage work area used by these subroutines. Specified as: an area of storage of length $naux$ , containing numbers of the data type indicated in Table 157 on page 920.
$naux$	is the size of the work area specified by $aux$ —that is, the number of elements in $aux$ . Specified as: a fullword integer, where: If $naux = 0$ and error 2015 is unrecoverable, SWLEV, DWLEV, CWLEV, and ZWLEV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program. Otherwise, $naux \geq 3n$ . You cannot use dynamic allocation if you need the information returned in AUX(1).

### On Return

$y$	is the vector $y$ of length $n$ , containing the solution vector—that is, the coefficients of the $n$ -point Wiener-Levinson filter. Returned as: a one-dimensional array of (at least) length $1+(n-1) incy $ , containing numbers of the data type indicated in Table 157 on page 920.
$aux$	is the storage work area used by these subroutines, where if $naux \neq 0$ : If AUX(1) = 0.0, the input Toeplitz matrix is positive definite or negative definite. If AUX(1) > 0.0, the input Toeplitz matrix is indefinite (that is, it is not positive definite and it is not negative definite). The value returned in AUX(1) is the order of the first submatrix of $A$ that is indefinite. The subroutine continues processing. See reference [64] for information about under what circumstances your solution vector $y$ would be valid. All other values in $aux$ are overwritten and are not significant. Returned as: an area of storage of length $naux$ , containing numbers of the data type indicated in Table 157 on page 920, where AUX(1) $\geq$ 0.0.

### Notes

1. For a description of a positive definite or negative definite symmetric Toeplitz matrix, see “Positive Definite or Negative Definite Symmetric Toeplitz Matrix” on page 75.
2. For a description of a positive definite or negative definite complex Hermitian Toeplitz matrix, see “Positive Definite or Negative Definite Complex Hermitian Toeplitz Matrix” on page 76.

## SWLEV, DWLEV, CWLEV, and ZWLEV

3. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

### Function

The computation of the coefficients of an *n*-point Wiener-Levinson filter in vector *y* is expressed as solving the following system:

$$Ay = u$$

where:

- For SWLEV and DWLEV, matrix *A* is a real symmetric Toeplitz matrix whose first row (or first column) is represented by vector *x*.  
For CWLEV and ZWLEV, matrix *A* is a complex Hermitian Toeplitz matrix whose first row is represented by vector *x*.
- *u* is the vector specifying the right side of the system, chosen to remove reverberations or to sharpen the wavelet.
- *y* is the solution vector.

See reference [64], [29], and the *IBM 3838 Array Processor Functional Characteristics*.

If *n* is 0, no computation is performed. For SWLEV and CWLEV, intermediate results are accumulated in long precision.

SWLEV provides the same function as the IBM 3838 function WLEV, with restrictions removed. See the *IBM 3838 Array Processor Functional Characteristics* manual.

### Error conditions

#### Resource Errors

Error 2015 is unrecoverable, *naux* = 0, and unable to allocate work area.

#### Computational Errors

None

#### Input-Argument Errors

1. *n* < 0
2. *incx* ≤ 0
3. *incy* = 0
4. Error 2015 is recoverable or *naux* ≠ 0, and *naux* is too small—that is, less than the minimum required value specified in the syntax for this argument. Return code 1 is returned if error 2015 is recoverable.

### Examples

#### Example 1

This example shows how to compute filter coefficients in vector *y* by solving the system  $Ay = u$ . Matrix *A* is:

$$\begin{bmatrix} 50.0 & -8.0 & 7.0 & -5.0 \\ -8.0 & 50.0 & -8.0 & 7.0 \\ 7.0 & -8.0 & 50.0 & -8.0 \\ -5.0 & 7.0 & -8.0 & 50.0 \end{bmatrix}$$

This input Toeplitz matrix is positive definite, as indicated by the zero value in AUX(1) on output.

**Call Statement and Input:**

```

          X  INCX  U  INCU  Y  INCY  N  AUX  NAUX
          |  |    |  |    |  |    |  |    |
CALL SWLEV( X , 1 , U , 1 , Y , 1 , 4 , AUX , 12 )
    
```

```

X      = (50.0, -8.0, 7.0, -5.0)
U      = (40.0, -10.0, 30.0, 20.0)
AUX    =(not relevant)
    
```

**Output:**

```

Y      = (0.7667, -0.0663, 0.5745, 0.5778)
AUX    = (0.0, . . . . .)
    
```

**Example 2**

This example shows how to compute filter coefficients in vector *y* by solving the system *Ay* = *u*. Matrix *A* is:

$$\begin{bmatrix}
 10.0 & -8.0 & 7.0 & -5.0 \\
 -8.0 & 10.0 & -8.0 & 7.0 \\
 7.0 & -8.0 & 10.0 & -8.0 \\
 -5.0 & 7.0 & -8.0 & 10.0
 \end{bmatrix}$$

This input Toeplitz matrix is not positive definite, as indicated by the zero value in AUX(1) on output.

**Call Statement and Input:**

```

          X  INCX  U  INCU  Y  INCY  N  AUX  NAUX
          |  |    |  |    |  |    |  |    |
CALL SWLEV( X , 1 , U , 1 , Y , 1 , 4 , AUX , 12 )
    
```

```

X      = (10.0, -8.0, 7.0, -5.0)
U      = (40.0, -10.0, 30.0, 20.0)
AUX    =(not relevant)
    
```

**Output:**

```

Y      = (5.1111, 5.5555, 12.2222, 10.4444)
AUX    = (0.0, . . . . .)
    
```

**Example 3**

This example shows a vector *x* with a stride greater than 1, a vector *u* with a negative stride, and a vector *y* with a stride of 1. It uses the same input Toeplitz matrix as in Example 2, which is not positive definite.

**Call Statement and Input:**

```

          X  INCX  U  INCU  Y  INCY  N  AUX  NAUX
          |  |    |  |    |  |    |  |    |
CALL SWLEV( X , 2 , U , -2 , Y , 1 , 4 , AUX , 12 )
    
```

```

X      = (10.0, . . , -8.0, . . , 7.0, . . , -5.0)
U      = (20.0, . . , 30.0, . . , -10.0, . . , 40.0)
AUX    =(not relevant)
    
```

**Output:**

## SWLEV, DWLEV, CWLEV, and ZWLEV

```

Y      = (5.1111, 5.5555, 12.2222, 10.4444)
AUX    = (0.0, . , . , . , . , . , . , . , . , . , . , . , . , . , . , . )

```

### Example 4

This example shows how to compute filter coefficients in vector  $y$  by solving the system  $Ay = u$ . Matrix  $A$  is:

$$\begin{bmatrix} (10.0, 0.0) & (2.0, -3.0) & (-3.0, 1.0) & (1.0, 1.0) \\ (2.0, 3.0) & (10.0, 0.0) & (2.0, -3.0) & (-3.0, 1.0) \\ (-3.0, -1.0) & (2.0, 3.0) & (10.0, 0.0) & (2.0, -3.0) \\ (1.0, -1.0) & (-3.0, -1.0) & (2.0, 3.0) & (10.0, 0.0) \end{bmatrix}$$

This input complex Hermitian Toeplitz matrix is positive definite, as indicated by the zero value in AUX(1) on output.

#### Call Statement and Input:

```

          X  INCX  U  INCU  Y  INCY  N  AUX  NAUX
          |  |    |  |    |  |    |  |    |
CALL ZWLEV( X , 1 , U , 1 , Y , 1 , 4 , AUX , 12 )

```

```

X      = ((10.0, 0.0), (2.0, -3.0), (-3.0, 1.0), (1.0, 1.0))
U      = ((8.0, 3.0), (21.0, -5.0), (67.0, -13.0), (72.0, 11.0))
AUX    =(not relevant)

```

#### Output:

```

Y      = ((1.0, 0.0), (3.0, 0.0), (5.0, 0.0), (7.0, 0.0))
AUX    = ((0.0, 0.0), . , . , . , . , . , . , . , . , . , . , . , . , . , . , . )

```

### Example 5

This example shows a vector  $x$  with a stride greater than 1, a vector  $u$  with a negative stride, and a vector  $y$  with a stride of 1. It uses the same input complex Hermitian Toeplitz matrix as in Example 4.

This input complex Hermitian Toeplitz matrix is positive definite, as indicated by the zero value in AUX(1) on output.

#### Call Statement and Input:

```

          X  INCX  U  INCU  Y  INCY  N  AUX  NAUX
          |  |    |  |    |  |    |  |    |
CALL ZWLEV( X , 2 , U , -2 , Y , 1 , 4 , AUX , 12 )

```

```

X      = ((10.0, 0.0), . , (2.0, -3.0), . , (-3.0, 1.0), .
,
          (1.0, 1.0))
U      = ((72.0, 11.0), . , (67.0, -13.0), . , (21.0, -5.0), . ,
          (8.0, 3.0), . )
AUX    =(not relevant)

```

#### Output:

```

Y      = ((1.0, 0.0), (3.0, 0.0), (5.0, 0.0), (7.0, 0.0))
AUX    = ((0.0, 0.0), . , . , . , . , . , . , . , . , . , . , . , . , . , . , . )

```

---

## Chapter 13. Sorting and Searching

The sorting and searching subroutines are described in this chapter.

---

### Overview of the Sorting and Searching Subroutines

The sorting and searching subroutines operate on three types of data: integer, short-precision real, and long-precision-real ( Table 158). The sorting subroutines perform sorts with or without index designations. The searching subroutines perform either a binary or sequential search.

Table 158. List of Sorting and Searching Subroutines

Descriptive Name	Integer Subroutine	Short- Precision Subroutine	Long- Precision Subroutine	Page
Sort the Elements of a Sequence	ISORT	SSORT	DSORT	927
Sort the Elements of a Sequence and Note the Original Element Positions	ISORTX	SSORTX	DSORTX	929
Sort the Elements of a Sequence Using a Stable Sort and Note the Original Element Positions	ISORTS	SSORTS	DSORTS	932
Binary Search for Elements of a Sequence X in a Sorted Sequence Y	IBSRCH	SBSRCH	DBSRCH	936
Sequential Search for Elements of a Sequence X in the Sequence Y	ISSRCH	SSSRCH	DSSRCH	940

---

### Use Considerations

It is important to understand the concept of stride for sequences when using these subroutines. For example, in the sort subroutines, a negative stride causes a sequence to be sorted into descending order in an array. In the search subroutines, a negative stride reverses the direction of the search. See “How Stride Is Used for Vectors” on page 62.

---

### Performance and Accuracy Considerations

1. The binary search subroutines provide better performance than the sequential search subroutines because of the nature of the searching algorithms. However, the binary search subroutines require that, before the subroutine is called, the sequence to be searched is sorted into ascending order. Therefore, if your data is already sorted, a binary search subroutine is faster. On the other hand, if your data is in random order and the number of elements being searched for is small, a sequential search subroutine is faster than doing a sort and binary search.
2. When doing multiple invocations of the binary search subroutines, you get better overall performance from the searching algorithms by doing fewer invocations and specifying larger search element arrays for argument *x*.
3. If you do not need the results provided in array RC by these subroutine, you get better performance if you do not request it. That is, specify 0 for the *iopt* argument.

---

## Sorting and Searching Subroutines

This section contains the sorting and searching subroutine descriptions.



## ISORT, SSORT, and DSORT — Sort the Elements of a Sequence

### Purpose

These subroutines sort the elements of sequence  $x$ .

Table 159. Data Types

$x$	Subroutine
Integer	ISORT
Short-precision real	SSORT
Long-precision real	DSORT

### Syntax

<b>Fortran</b>	CALL ISORT   SSORT   DSORT ( $x, incx, n$ )
<b>C and C++</b>	isort   ssort   dsort ( $x, incx, n$ );

### On Entry

$x$  is the sequence  $x$  of length  $n$ , to be sorted.

Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 159.

$incx$  is the stride for both the input sequence  $x$  and the output sequence  $x$ . If it is positive, elements are sorted into ascending order in the array, and if it is negative, elements are sorted into descending order in the array.

Specified as: a fullword integer. It can have any value.

$n$  is the number of elements in sequence  $x$ . Specified as: a fullword integer;  $n \geq 0$ .

### On Return

$x$  is the sequence  $x$  of length  $n$ , with its elements sorted into designated order in the array. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 159.

### Function

The elements of input sequence  $x$  are sorted into ascending order, in place and using a partition sort. The elements of output sequence  $x$  can be expressed as follows:

$$x_1 \leq x_2 \leq x_3 \leq \dots \leq x_n$$

By specifying a negative stride for sequence  $x$ , the elements of sequence  $x$  are assumed to be reversed in the array,  $(x_n, x_{n-1}, \dots, x_1)$ , thus producing a sort into descending order within the array. If  $n$  is 0 or 1 or if  $incx$  is 0, no sort is performed. See reference [78].

## Error conditions

### Resource Errors

Unable to allocate internal work area.

### Computational Errors

None

### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows a sequence  $x$  with a positive stride.

#### Call Statement and Input:

```
          X  INCX  N  
          |  |    |  
CALL ISORT( X , 2 , 5 )
```

X = (2, . , -1, . , 5, . , 4, . , -2)

#### Output:

X = (-2, . , -1, . , 2, . , 4, . , 5)

### Example 2

This example shows a sequence  $x$  with a negative stride.

#### Call Statement and Input:

```
          X  INCX  N  
          |  |    |  
CALL ISORT( X , -1 , 5 )
```

X = (2, -1, 5, 4, -2)

#### Output:

X = (5, 4, 2, -1, -2)

## ISORTX, SSORTX, and DSORTX — Sort the Elements of a Sequence and Note the Original Element Positions

### Purpose

These subroutines sort the elements of sequence  $x$ . The original positions of the elements in sequence  $x$  are returned in the indices array,  $INDX$ . Where equal elements occur in the input sequence, they do not necessarily remain in the same relative order in the output sequence.

**Note:** If you need a stable sort, you should use ISORTS, SSORTS, or DSORTS rather than these subroutines.

Table 160. Data Types

$x$	Subroutine
Integer	ISORTX
Short-precision real	SSORTX
Long-precision real	DSORTX

### Syntax

<b>Fortran</b>	CALL ISORTX   SSORTX   DSORTX ( $x, incx, n, indx$ )
<b>C and C++</b>	isortx   ssortx   dsortx ( $x, incx, n, indx$ );

### On Entry

$x$  is the sequence  $x$  of length  $n$ , to be sorted.

Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$  elements, containing numbers of the data type indicated in Table 160.

$incx$  is the stride for both the input sequence  $x$  and the output sequence  $x$ . If it is positive, elements are sorted into ascending order in the array, and if it is negative, elements are sorted into descending order in the array.

Specified as: a fullword integer. It can have any value.

$n$  is the number of elements in sequence  $x$ . Specified as: a fullword integer;  $n \geq 0$ .

$indx$  See "On Return."

### On Return

$x$  is the sequence  $x$  of length  $n$ , with its elements sorted into designated order in the array. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 160.

$indx$  is the array, referred to as  $INDX$ , containing the  $n$  indices that indicate, for the elements in the sorted output sequence, the original positions of those elements in input sequence  $x$ .

**Note:** It is important to remember that when you specify a negative stride, ESSL assumes that the order of the input

## ISORTX, SSORTX, and DSORTX

and output sequence elements in the  $X$  array is reversed; however, the elements in  $INDX$  are not reversed. See "Function."

Returned as: a one-dimensional array of length  $n$ , containing fullword integers;  $1 \leq (INDX \text{ elements}) \leq n$ .

### Function

The elements of input sequence  $x$  are sorted into ascending order, in place and using a partition sort. The elements of output sequence  $x$  can be expressed as follows:

$$x_1 \leq x_2 \leq x_3 \leq \dots \leq x_n$$

Where equal elements occur in the input sequence, they do not necessarily remain in the same relative order in the output sequence.

By specifying a negative stride for  $x$ , the elements of input sequence  $x$  are assumed to be reversed in the array,  $(x_n, x_{n-1}, \dots, x_1)$ , thus producing a sort into descending order within the array.

In addition, the  $INDX$  array contains the  $n$  indices that indicate, for the elements in the sorted output sequence, the original positions of those elements in input sequence  $x$ . (These are not the positions in the array, but rather the positions in the sequence.) For each element  $x_j$  in the input sequence, becoming element  $xx_k$  in the output sequence, the elements in  $INDX$  are defined as follows:

$$INDX(k) = j \quad \text{for } j = 1, n \text{ and } k = 1, n$$

where  $xx_k = x_j$

To understand  $INDX$  when you specify a negative stride, you should remember that both the input and output sequences,  $x$ , are assumed to be in reverse order in array  $X$ , but  $INDX$  is not affected by stride. The sequence elements of  $x$  are assumed to be stored in your input array as follows:

$$X = (x_n, x_{n-1}, \dots, x_1)$$

The sequence elements of  $x$  are stored in your output array by ESSL as follows:

$$X = (xx_n, xx_{n-1}, \dots, xx_1)$$

where the elements  $xx_k$  are the elements  $x_j$ , sorted into descending order in  $X$ . As an example of how  $INDX$  is calculated, if  $xx_1 = x_{n-1}$ , then  $INDX(1) = n-1$ .

If  $n$  is 0, no computation is performed. See reference [78].

### Error conditions

#### Resource Errors

Unable to allocate internal work area.

#### Computational Errors

None

#### Input-Argument Errors

$n < 0$

## Examples

### Example 1

This example shows how to sort a sequence  $x$  into ascending order by specifying a positive stride.

#### Call Statement and Input:

```

          X  INCX  N  INDX
          |  |    |  |
CALL ISORTX( X , 2 , 5 , INDX )

X      = (2, . , -1, . , 5, . , 1, . , -2)

```

#### Output:

```

X      = (-2, . , -1, . , 1, . , 2, . , 5)
INDX   = (5, 2, 4, 1, 3)

```

### Example 2

This example shows how to sort a sequence  $x$  into descending order by specifying a negative stride. Therefore, both the input and output sequences are assumed to be reversed in the array  $X$ . The input sequence is assumed to be stored as follows:

$$X = (x_5, x_4, x_3, x_2, x_1) = (2, -1, 5, 1, -2)$$

The output sequence is stored by ESSL as follows:

$$X = (xx_5, xx_4, xx_3, xx_2, xx_1) = (5, 2, 1, -1, -2)$$

As a result,  $INDX$  is defined as follows:

$$INDX = (indx_1, indx_2, indx_3, indx_4, indx_5) = (1, 4, 2, 5, 3)$$

For example, because output sequence element  $xx_4 = 2$  is input sequence element  $x_5$ , then  $INDX(4) = 5$ .

#### Call Statement and Input:

```

          X  INCX  N  INDX
          |  |    |  |
CALL ISORTX( X , -1 , 5 , INDX )

X      = (2, -1, 5, 1, -2)

```

#### Output:

```

X      = (5, 2, 1, -1, -2)
INDX   = (1, 4, 2, 5, 3)

```

## ISORTS, SSORTS, and DSORTS — Sort the Elements of a Sequence Using a Stable Sort and Note the Original Element Positions

### Purpose

These subroutines sort the elements of sequence  $x$  using a stable sort; that is, where equal elements occur in the input sequence, they remain in the same relative order in the output sequence. The original positions of the elements in sequence  $x$  are returned in the indices array  $INDX$ .

**Note:** If you need a stable sort, then you should use these subroutines rather than ISORTX, SSORTX, or DSORTX.

Table 161. Data Types

$x, work$	Subroutine
Integer	ISORTS
Short-precision real	SSORTS
Long-precision real	DSORTS

### Syntax

<b>Fortran</b>	CALL ISORTS   SSORTS   DSORTS ( $x, incx, n, indx, work, lwork$ )
<b>C and C++</b>	isorts   ssorts   dsorts ( $x, incx, n, indx, work, lwork$ );

### On Entry

- $x$  is the sequence  $x$  of length  $n$ , to be sorted.  
Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$  elements, containing numbers of the data type indicated in Table 161.
- $incx$  is the stride for both the input sequence  $x$  and the output sequence  $x$ . If it is positive, elements are sorted into ascending order in the array, and if it is negative, elements are sorted into descending order in the array.  
Specified as: a fullword integer. It can have any value.
- $n$  is the number of elements in sequence  $x$ . Specified as: a fullword integer;  $n \geq 0$ .
- $indx$  See “On Return” on page 933.
- $work$  is the storage work area used by this subroutine. Its size is specified by  $lwork$ .  
Specified as: an area of storage, containing numbers of the data type indicated in Table 161.
- $lwork$  is the size of the work area specified by  $work$ — that is, the number of elements in  $work$ .  
Specified as: a fullword integer;  $lwork \geq n/2$ .

**Note:** This is the value to achieve optimal performance. The sort is performed regardless of the value you specify for *lwork*, but you may receive an attention message.

### On Return

*x* is the sequence *x* of length *n*, with its elements sorted into designated order in the array. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 161 on page 932.

*indx* is the array, referred to as INDX, containing the *n* indices that indicate, for the elements in the sorted output sequence, the original positions of those elements in input sequence *x*.

**Note:** It is important to remember that when you specify a negative stride, ESSL assumes that the order of the input and output sequence elements in the *X* array is reversed; however, the elements in INDX are not reversed. See "Function."

Returned as: a one-dimensional array of length *n*, containing fullword integers;  $1 \leq (\text{INDX elements}) \leq n$ .

### Function

The elements of input sequence *x* are sorted into ascending order using a partition sort. The sorting is stable; that is, where equal elements occur in the input sequence, they remain in the same relative order in the output sequence. The elements of output sequence *x* can be expressed as follows:

$$x_1 \leq x_2 \leq x_3 \leq \dots \leq x_n$$

By specifying a negative stride for *x*, the elements of input sequence *x* are assumed to be reversed in the array,  $(x_n, x_{n-1}, \dots, x_1)$ , thus producing a sort into descending order within the array.

In addition, the INDX array contains the *n* indices that indicate, for the elements in the sorted output sequence, the original positions of those elements in input sequence *x*. (These are not the positions in the array, but rather the positions in the sequence.) For each element  $x_j$  in the input sequence, becoming element  $xx_k$  in the output sequence, the elements in INDX are defined as follows:

$$\text{INDX}(k) = j \quad \text{for } j = 1, n \text{ and } k = 1, n$$

where  $xx_k = x_j$

To understand INDX when you specify a negative stride, you should remember that both the input and output sequences, *x*, are assumed to be in reverse order in array *X*, but INDX is not affected by stride. The sequence elements of *x* are assumed to be stored in your input array as follows:

$$X = (x_n, x_{n-1}, \dots, x_1)$$

The sequence elements of *x* are stored in your output array by ESSL as follows:

$$X = (xx_n, xx_{n-1}, \dots, xx_1)$$

## ISORTS, SSORTS, and DSORTS

where the elements  $xx_k$  are the elements  $x_j$ , sorted into descending order in  $X$ . As an example of how  $INDX$  is calculated, if  $xx_1 = x_{n-1}$ , then  $INDX(1) = n-1$ .

If  $n$  is 0, no computation is performed. See references [30] and [78].

### Error conditions

#### Resource Errors

Unable to allocate internal work area.

#### Computational Errors

None

#### Input-Argument Errors

$n < 0$

### Examples

#### Example 1

This example shows how to sort a sequence  $x$  into ascending order by specifying a positive stride. Because this is a stable sort, the  $-1$  elements remain in the same relative order in the output sequence, indicated by  $INDX(2) = 2$  and  $INDX(3) = 4$ .

#### Call Statement and Input:

```

          X  INCX  N  INDX  WORK  LWORK
          |  |    |  |    |    |    |
CALL ISORTS( X , 2 , 5 , INDX , WORK , 5 )
X          = ( 2, . , -1, . , 5, . , -1, . , -2)
```

#### Output:

```
X          = (-2, . , -1, . , -1, . , 2, . , 5)
INDX       = ( 5, 2, 4, 1, 3)
```

#### Example 2

This example shows how to sort a sequence  $x$  into descending order by specifying a negative stride. Therefore, both the input and output sequences are assumed to be reversed in the array  $X$ . The input sequence is assumed to be stored as follows:

```
X = (x5, x4, x3, x2, x1) = (2, -1, 5, -1, -2)
```

The output sequence is stored by ESSL as follows:

```
X = (xx5, xx4, xx3, xx2, xx1) = (5, 2, -1, -1, -2)
```

As a result,  $INDX$  is defined as follows:

```
INDX = (indx1, indx2, indx3, indx4, indx5) = (1, 2, 4, 5, 3)
```

For example, because output sequence element  $xx_4 = 2$  is input sequence element  $x_5$ , then  $INDX(4) = 5$ . Also, because this is a stable sort, the  $-1$  elements remain in the same relative order in the output sequence, indicated by  $INDX(2) = 2$  and  $INDX(3) = 4$ .

#### Call Statement and Input:



```
          X  INCX  N  INDX  WORK  LWORK
          |  |    |  |    |  |    |
CALL ISORTS( X , -1 , 5 , INDX , WORK , 5 )
```

```
X          = (2, -1, 5, -1, -2)
```

**Output:**

```
X          = (5, 2, -1, -1, -2)
INDX       = (1, 2, 4, 5, 3)
```

## IBSRCH, SBSRCH, and DBSRCH — Binary Search for Elements of a Sequence X in a Sorted Sequence Y

### Purpose

These subroutines perform a binary search for the locations of the elements of sequence  $x$  in another sequence  $y$ , where  $y$  has been sorted into ascending order. The first occurrence of each element is found. When an exact match is not found, the position of the next larger element in  $y$  is indicated. The locations are returned in the indices array `INDX`, and, optionally, return codes indicating whether the exact elements were found are returned in array `RC`.

Table 162. Data Types

$x, y$	Subroutine
Integer	IBSRCH
Short-precision real	SBSRCH
Long-precision real	DBSRCH

### Syntax

<b>Fortran</b>	CALL IBSRCH   SBSRCH   DBSRCH ( $x, incx, n, y, incy, m, indx, rc, iopt$ )
<b>C and C++</b>	ibsrch   sbsrch   dbsrch ( $x, incx, n, y, incy, m, indx, rc, iopt$ );

### On Entry

$x$  is the sequence  $x$  of length  $n$ , containing the elements for which sequence  $y$  is searched.

Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 162. It must have at least  $1+(n-1)|incx|$  elements.

$incx$  is the stride for sequence  $x$ .

Specified as: a fullword integer. It can have any value.

$n$  is the number of elements in sequence  $x$  and arrays `INDX` and `RC`.

Specified as: a fullword integer;  $n \geq 0$ .

$y$  is the sequence  $y$  of length  $m$ , to be searched, where  $y$  must be sorted into ascending order.

**Note:** Be careful in specifying the stride for sequence  $y$ . A negative stride reverses the direction of the search, because the order of the sequence elements is reversed in the array.

Specified as: a one-dimensional array of (at least) length  $1+(m-1)|incy|$ , containing numbers of the data type indicated in Table 162.

$incy$  is the stride for sequence  $y$ .

Specified as: a fullword integer. It can have any value.

$m$  is the number of elements in sequence  $y$ . Specified as: a fullword integer;  $m \geq 0$ .

<i>indx</i>	See “On Return.”
<i>rc</i>	See “On Return.”
<i>iopt</i>	has the following meaning, where: If <i>iopt</i> = 0, the <i>rc</i> argument is not used in the computation. If <i>iopt</i> = 1, the <i>rc</i> argument is used in the computation. Specified as: a fullword integer; <i>iopt</i> = 0 or 1.

### On Return

<i>indx</i>	is the array, referred to as INDX, containing the <i>n</i> indices that indicate the positions of the elements of sequence <i>x</i> in sequence <i>y</i> . The first occurrence of the element found in sequence <i>y</i> is indicated in array INDX. When an exact match between an element of sequence <i>x</i> and an element of sequence <i>y</i> is not found, the position of the next larger element in sequence <i>y</i> is indicated. When the element in sequence <i>x</i> is larger than all the elements in sequence <i>y</i> , then <i>m</i> +1 is indicated in array INDX.  Returned as: a one-dimensional array of length <i>n</i> , containing fullword integers; $1 \leq (\text{INDX elements}) \leq m+1$ .
<i>rc</i>	has the following meaning, where:  If <i>iopt</i> = 0, then <i>rc</i> is not used, and its contents remain unchanged.  If <i>iopt</i> = 1, it is the array, referred to as RC, containing the <i>n</i> return codes that indicate whether the elements in sequence <i>x</i> were found in sequence <i>y</i> . For <i>i</i> = 1, <i>n</i> , elements $\text{RC}(i) = 0$ if $x_i$ matches an element in sequence <i>y</i> , and $\text{RC}(i) = 1$ if an exact match is not found in sequence <i>y</i> .  Returned as: a one-dimensional array of length <i>n</i> , containing fullword integers; $\text{RC}(i) = 0$ or 1.

### Notes

1. The elements of *y* must be sorted into ascending order; otherwise, results are unpredictable. For details on how to do this, see “ISORT, SSORT, and DSORT — Sort the Elements of a Sequence” on page 927.
2. If you do not need the results provided in array RC by these subroutines, you get better performance if you do not request it. That is, specify 0 for the *iopt* argument.

### Function

These subroutines perform a binary search for the first occurrence (or last occurrence, using negative stride) of the locations of the elements of sequence *x* in another sequence *y*, where *y* must be sorted into ascending order before calling this subroutine. The first occurrence of each element is found. Two arrays are returned, containing the results of the binary searches:

- INDX, the indices array, contains the positions of the elements of sequence *x* in sequence *y*. When an exact match between values of elements in sequences *x* and *y* is not found, the location of the next larger element in sequence *y* is indicated in array INDX.
- RC, the return codes array, indicates for each element in sequence *x* whether the exact element was found in sequence *y*. If you do not need these results, you get better performance if you set *iopt* = 0.

## IBSRCH, SBSRCH, and DBSRCH

The results returned for the INDX and RC arrays are expressed as follows:

For  $i = 1, n$

for all  $y_j \geq x_i, j = 1, m, \text{INDX}(i) = \min(j)$   
if all  $y_j < x_i, j = 1, m, \text{INDX}(i) = m+1$

And for  $i = 1, n$

if  $x_i = y_{\text{INDX}(i)}, \text{RC}(i) = 0$

if  $x_i \neq y_{\text{INDX}(i)}, \text{RC}(i) = 1$

where:

$x$  is a sequence of length  $n$ , containing the search elements.

$y$  is a sequence of length  $m$  to be searched. It must be sorted into ascending order.

INDX is the array of length  $n$  of indices.

RC is the array of length  $n$  of return codes.

See reference [78]. If  $n$  is 0, no search is performed. If  $m$  is 0, then:

$\text{INDX}(i) = 1$  and  $\text{RC}(i) = 1$  for  $i = 1, n$

It is important to note that a negative stride for sequence  $y$  reverses the direction of the search, because the order of the sequence elements is reversed in the array. For more details on sorting sequences, see "Function" on page 927.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $n < 0$
2.  $m < 0$
3.  $iopt \neq 0$  or 1

## Examples

### Example 1

This example shows a search where sequences  $x$  and  $y$  have positive strides, and where the optional return codes are returned as part of the output.

#### Call Statement and Input:

```
          X  INCX  N  Y  INCY  M  INDX  RC  IOPT
          |  |    |  |  |    |  |    |  |
CALL IBSRCH( X , 2 , 5 , Y , 1 , 10 , INDX , RC , 1 )
```

```
X      = (-3, . , 125, . , 30, . , 20, . , 70)
Y      = (10, 20, 30, 30, 40, 50, 60, 80, 90, 100)
```

#### Output:

```
INDX   = (1, 11, 3, 2, 8)
RC     = (1, 1, 0, 0, 1)
```

**Example 2**

This example shows the same calling sequence as in Example 1, except that it includes the IOPT argument, specified as 1. This is equivalent to using the calling sequence in Example 1 and gives the same results.

**Call Statement and Input:**

```

           X  INCX  N  Y  INCY  M  INDX  RC  IOPT
           |  |    |  |  |    |  |    |  |
CALL IBSRCH( X , 2 , 5 , Y , 1 , 10 , INDX , RC , 1 )

```

**Example 3**

This example shows a search where sequence  $x$  has a negative stride, and sequence  $y$  has a positive stride. The optional return codes are not requested, because IOPT is specified as 0.

**Call Statement and Input:**

```

           X  INCX  N  Y  INCY  M  INDX  RC  IOPT
           |  |    |  |  |    |  |    |  |
CALL IBSRCH( X , -2 , 5 , Y , 1 , 10 , INDX , RC , 0 )

```

```

X      = (-3, . , 125, . , 30, . , 20, . , 70)
Y      = (10, 20, 30, 30, 40, 50, 60, 80, 90, 100)

```

**Output:**

```

INDX   = (8, 2, 3, 11, 1)
RC     =(not relevant)

```

**Example 4**

This example shows a search where sequence  $x$  has a positive stride, and sequence  $y$  has a negative stride. As shown below, elements of  $y$  are in descending order in array Y. The optional return codes are not requested, because IOPT is specified as 0.

**Call Statement and Input:**

```

           X  INCX  N  Y  INCY  M  INDX  RC  IOPT
           |  |    |  |  |    |  |    |  |
CALL IBSRCH( X , 2 , 5 , Y , -1 , 10 , INDX , RC , 0 )

```

```

X      = (-3, . , 125, . , 30, . , 20, . , 70)
Y      = (100, 90, 80, 60, 50, 40, 30, 30, 20, 10)
RC     =(not relevant)

```

**Output:**

```

INDX   = (1, 11, 3, 2, 8)

```

## ISSRCH, SSSRCH, and DSSRCH — Sequential Search for Elements of a Sequence X in the Sequence Y

### Purpose

These subroutines perform a sequential search for the locations of the elements of sequence  $x$  in another sequence  $y$ . Depending on the sign of the *idir* argument, the search direction indicator, the location of either the first or last occurrence of each element is indicated in the resulting indices array *INDX*. When an exact match between elements is not found, the position is indicated as 0.

Table 163. Data Types

$x, y$	Subroutine
Integer	ISSRCH
Short-precision real	SSSRCH
Long-precision real	DSSRCH

### Syntax

<b>Fortran</b>	CALL ISSRCH   SSSRCH   DSSRCH ( $x, incx, n, y, incy, m, idir, indx$ )
<b>C and C++</b>	issrch   sssrch   dssrch ( $x, incx, n, y, incy, m, idir, indx$ );

### On Entry

$x$  is the sequence  $x$  of length  $n$ , containing the elements for which sequence  $y$  is searched.

Specified as: a one-dimensional array of (at least) length  $1+(n-1)|incx|$ , containing numbers of the data type indicated in Table 163.

$incx$  is the stride for sequence  $x$ .

Specified as: a fullword integer. It can have any value.

$n$  is the number of elements in sequence  $x$  and array *INDX*.

Specified as: a fullword integer;  $n \geq 0$ .

$y$  is the sequence  $y$  of length  $m$  to be searched.

**Note:** Be careful in specifying the stride for sequence  $y$ . A negative stride reverses the direction of the search, because the order of the sequence elements is reversed in the array.

Specified as: a one-dimensional array of (at least) length  $1+(m-1)|incy|$ , containing numbers of the data type indicated in Table 163.

$incy$  is the stride for sequence  $y$ .

Specified as: a fullword integer. It can have any value.

$m$  is the number of elements in sequence  $y$ . Specified as: a fullword integer;  $m \geq 0$ .

*idir* indicates the search direction, where:

If  $idir \geq 0$ , sequence  $y$  is searched from the first element to the last ( $1, n$ ), thus finding the first occurrence of the element in the sequence.

If  $idir < 0$ , sequence  $y$  is searched from the last element to the first ( $n, 1$ ), thus finding the last occurrence of the element in the sequence.

Specified as: a fullword integer. It can have any value.

*indx* See On Return.

### On Return

*indx* is the array, referred to as INDX, containing the  $n$  indices that indicate the positions of the elements of sequence  $x$  in sequence  $y$ , where:

If  $idir \geq 0$ , the first occurrence of the element found in sequence  $y$  is indicated in array INDX.

If  $idir < 0$ , the last occurrence of the element found in sequence  $y$  is indicated in array INDX.

In all cases, if no match is found, 0 is indicated in array INDX.

Returned as: a one-dimensional array of length  $n$ , containing fullword integers;  $0 \leq (\text{INDX elements}) \leq m$ .

## Function

These subroutines perform a sequential search for the first occurrence (or last occurrence, using a negative *idir*) of the locations of the elements of sequence  $x$  in another sequence  $y$ . The results of the sequential searches are returned in the indices array INDX, indicating the positions of the elements of sequence  $x$  in sequence  $y$ . The positions indicated in array INDX are calculated relative to the first sequence element position—that is, the position of  $y_1$ . When an exact match between values of elements in sequences  $x$  and  $y$  is not found, 0 is indicated in array INDX for that position.

The results returned in array INDX are expressed as follows:

For  $i = 1, n$

for all  $y_j = x_i, j = 1, m$   
 $\text{INDX}(i) = \min(j)$ , if  $idir \geq 0$   
 $\text{INDX}(i) = \max(j)$ , if  $idir < 0$

if all  $y_j \neq x_i, j = 1, m$   
 $\text{INDX}(i) = 0$

where:

$x$  is a sequence of length  $n$ , containing the search elements.

$y$  is a sequence of length  $m$  to be searched.

INDX is the array of length  $n$  of indices.

See reference [78]. If  $n$  is 0, no search is performed.

It is important to note that a negative stride for sequence  $y$  reverses the direction of the search, because the order of the sequence elements is reversed in the array.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $n < 0$
2.  $m < 0$

## Examples

### Example 1

This example shows a search where sequences  $x$  and  $y$  have positive strides, and the search direction indicator,  $idir$ , is positive.

#### Call Statement and Input:

```

          X  INCX  N  Y  INCY  M  IDIR  INDX
          |  |    |  |  |    |  |    |
CALL ISSRCH( X , 1 , 3 , Y , 2 , 8 , 1 , INDX )

```

```

X      = (0, 12, 3)
Y      = (0, . , 8, . , 12, . , 0, . , 1, . , 4, . , 0, . , 2)

```

#### Output:

```
INDX   = (1, 3, 0)
```

### Example 2

This example shows a search where sequences  $x$  and  $y$  have positive strides, and the search direction indicator,  $idir$ , is negative.

#### Call Statement and Input:

```

          X  INCX  N  Y  INCY  M  IDIR  INDX
          |  |    |  |  |    |  |    |
CALL ISSRCH( X , 2 , 3 , Y , 2 , 8 , -1 , INDX )

```

```

X      = (0, . , 12, . , 3)
Y      = (0, . , 8, . , 12, . , 0, . , 1, . , 4, . , 0, . , 2)

```

#### Output:

```
INDX   = (7, 3, 0)
```

### Example 3

This example shows a search where sequences  $x$  and  $y$  have negative strides, and the search direction indicator,  $idir$ , is positive.

#### Call Statement and Input:

```

          X  INCX  N  Y  INCY  M  IDIR  INDX
          |  |    |  |  |    |  |    |
CALL ISSRCH( X , -1 , 3 , Y , -2 , 8 , 1 , INDX )

```

```

X      = (0, 12, 3)
Y      = (0, . , 8, . , 12, . , 0, . , 1, . , 4, . , 0, . , 2)

```

#### Output:

```
INDX   = (0, 6, 2)
```



**Example 4**

This example shows a search where sequences  $x$  and  $y$  have negative strides, and the search direction indicator,  $idir$ , is negative.

**Call Statement and Input:**

	X	INCX	N	Y	INCY	M	IDIR	INDX								
CALL ISSRCH(	X	,	-2	,	3	,	Y	,	-1	,	8	,	-1	,	INDX	)

X = (0, . , 12, . , 3)  
 Y = (0, 8, 12, 0, 1, 4, 0, 2)

**Output:**

INDX = (0, 6, 8)



---

## Chapter 14. Interpolation

The interpolation subroutines are described in this chapter.

---

### Overview of the Interpolation Subroutines

The interpolation subroutines provide the capabilities of doing polynomial interpolation, local polynomial interpolation, and one- and two-dimensional cubic spline interpolation (Table 164).

Table 164. List of Interpolation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Polynomial Interpolation	SPINT	DPINT	947
Local Polynomial Interpolation	STPINT	DTPINT	952
Cubic Spline Interpolation	SCSINT	DCSINT	955
Two-Dimensional Cubic Spline Interpolation	SCSIN2	DCSIN2	961

---

### Use Considerations

Polynomial interpolation (SPINT and DPINT) is a global scheme. As the number of data points increases, the degree of the interpolating polynomial is raised; therefore, the graph of the interpolating polynomial tends to be oscillatory.

Local polynomial interpolation (STPINT and DTPINT) is a local scheme. The data generated is affected only by locally grouped data points. The degree of the local interpolating polynomial is usually lower than a global interpolating polynomial.

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### Performance and Accuracy Considerations

1. Doing extrapolation with SPINT and DPINT is not encouraged unless you know the consequences of doing polynomial extrapolation.
2. If performance is the overriding consideration, you should investigate using the general signal processing subroutines, DQINT and SQINT.
3. There are some ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 48.

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## Interpolation Subroutines

This section contains the interpolation subroutine descriptions.

## SPINT and DPINT — Polynomial Interpolation

### Purpose

These subroutines compute the Newton divided difference coefficients and perform a polynomial interpolation through a set of data points at specified abscissas.

Table 165. Data Types

$x, y, c, t, s$	Subroutine
Short-precision real	SPINT
Long-precision real	DPINT

### Syntax

Fortran	CALL SPINT   DPINT ( $x, y, n, c, ninit, t, s, m$ )
C and C++	spint   dpint ( $x, y, n, c, ninit, t, s, m$ );

### On Entry

- $x$  is the vector  $x$  of length  $n$ , containing the abscissas of the data points used in the interpolations. The elements of  $x$  must be distinct.
- Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 165.
- $y$  is the vector  $y$  of length  $n$ , containing the ordinates of the data points used in the interpolations.
- Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 165.
- $n$  is the number of elements in vectors  $x$ ,  $y$ , and  $c$ —that is, the number of data points. Specified as: a fullword integer;  $n \geq 0$ .
- $c$  is the vector  $c$  of length  $n$ , where:
- If  $ninit \leq 0$ , all elements of  $c$  are undefined on entry.
- If  $ninit > 0$ ,  $c$  contains the Newton divided difference coefficients,  $c_j$  for  $j = 1, ninit$ , for the interpolating polynomial through the data points  $(x_j, y_j)$  for  $j = 1, ninit$ . If  $ninit < n$ , the values of  $c_j$  for  $j = ninit+1, n$  are undefined.
- Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 165.
- $ninit$  indicates the following:
- If  $ninit \leq 0$ , this is the first call to this subroutine with the data in  $x$  and  $y$ ; therefore, none of the Newton divided difference coefficients in  $c$  have been initialized.
- If  $ninit > 0$ , a previous call to this subroutine was made with the data points  $(x_j, y_j)$  for  $j = 1, ninit$ , where:
- If  $ninit = n$ , all the Newton divided difference coefficients in  $c$  were computed for the data points. No additional coefficients are computed on this entry.

## SPINT and DPINT

- If  $ninit < n$ , the first  $ninit$  Newton divided difference coefficients in  $c$  were computed for the data points  $(x_j, y_j)$  for  $j = 1, ninit$ . The coefficients are updated for the additional data points  $(x_j, y_j)$  for  $j = ninit+1, n$  on this entry.

Specified as: a fullword integer;  $ninit \leq n$ .

$t$  is the vector  $t$  of length  $m$ , containing the abscissas at which interpolation is to be done.

Specified as: a one-dimensional array of (at least) length  $m$ , containing numbers of the data type indicated in Table 165 on page 947.

$s$  See "On Return."

$m$  is the number of elements in vectors  $t$  and  $s$ —that is, the number of interpolations to be performed.

Specified as: a fullword integer;  $m \geq 0$ .

### On Return

$c$  is the vector  $c$  of length  $n$ , containing the coefficients of the Newton divided difference form of the interpolating polynomial through the data points  $(x_j, y_j)$  for  $j = 1, n$ . Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 165 on page 947.

$ninit$  is the number of coefficients,  $n$ , in output vector  $c$ . (If you call this subroutine again with the same data, this value should be specified for  $ninit$ .) Returned as: a fullword integer;  $ninit = n$ .

$s$  is the vector  $s$  of length  $m$ , containing the resulting interpolated values; that is, each  $s_i$  is the value of the interpolating polynomial evaluated at  $t_i$ . Returned as: a one-dimensional array of (at least) length  $m$ , containing numbers of the data type indicated in Table 165 on page 947.

## Notes

1. In your C program, argument  $ninit$  must be passed by reference.
2. Vectors  $x$ ,  $y$ , and  $t$  must have no common elements with vectors  $c$  and  $s$ , and vector  $c$  must have no common element with vector  $s$ ; otherwise, results are unpredictable.
3. The elements of vector  $x$  must be distinct; that is,  $x_i \neq x_j$  if  $i \neq j$  for  $i, j = 1, n$ .

## Function

Polynomial interpolation is performed at specified abscissas,  $t_i$  for  $i = 1, m$ , in vector  $t$ , using the method of Newton divided differences through the data points:

$(x_j, y_j)$  for  $j = 1, n$

where:

$x_j$  are elements of vector  $x$ .  
 $y_j$  are elements of vector  $y$ .

The interpolated value at each  $t_i$  is returned in  $s_i$  for  $i = 1, m$ . See references [17] and [56]. The interpolating values returned in  $s$  are computed using the Newton divided difference coefficients, as defined in the following section.

The divided difference coefficients,  $c_j$  for  $j = 1, n$ , are returned in vector  $c$ . These coefficients can then be reused on subsequent calls to this subroutine, using the same data points  $(x_j, y_j)$ , but with new values of  $t_i$ . If the number of data points is increased from one call this subroutine to the next, the new coefficients are computed, and the existing coefficients are updated (not recomputed). This feature can be used to test for the convergence of the interpolations through a sequence of an increasingly larger set of points.

The values specified for  $ninit$  and  $m$  indicate which combination of functions are performed by this subroutine: computing the coefficients, performing the interpolation, or both. If  $m = 0$ , only the divided difference coefficients are computed. No interpolation is performed. If  $n = 0$ , no computation or interpolation is performed.

For SPINT, the Newton divided differences and interpolating values are accumulated in long precision.

### Newton Divided Differences and Interpolating Values

The Newton divided differences of the following data points:

$$(x_j, y_j) \quad \text{for } j = 1, n$$

$$\text{where } x_j \neq x_l \text{ if } j \neq l \quad \text{for } j, l = 1, n$$

are denoted by  $\delta_k y_j$  for  $k = 0, 1, 2, \dots, n-1$  and  $j = 1, 2, \dots, n-k$ , and are defined as follows:

For  $k = 0$  and 1:

$$\delta_0 y_j = y_j \quad \text{for } j = 1, 2, \dots, n$$

$$\delta_1 y_j = (y_{j+1} - y_j) / (x_{j+1} - x_j) \quad \text{for } j = 1, 2, \dots, n-1$$

For  $k = 2, 3, \dots, n-1$ :

$$\delta_k y_j = (\delta_{k-1} y_{j+1} - \delta_{k-1} y_j) / (x_{j+k} - x_j) \quad \text{for } j = 1, 2, \dots, n-k$$

The value  $s$  of the Newton divided difference form of the interpolating polynomial evaluated at an abscissa  $t$  is given by:

$$s = y_n + (t-x_n) \delta_1 y_{n-1}$$

$$+ (t-x_{n-1}) (t-x_n) \delta_2 y_{n-2}$$

$$+ \dots + (t-x_2) (t-x_3) \dots (t-x_n) \delta_{n-1} y_1$$

Therefore, on output, the coefficients in vector  $c$  are as follows:

$$c_n = y_n$$

$$c_{n-1} = \delta_1 y_{n-1}$$

$$c_{n-2} = \delta_2 y_{n-2}$$

$$\cdot$$

$$\cdot$$

$$\cdot$$

$$c_1 = \delta_{n-1} y_1$$

Also, the interpolating values in  $s$ , in terms of  $c$ , are as follows for  $i = 1, m$ :

## SPINT and DPINT

$$\begin{aligned} s_i &= c_n + (t_i - x_n) c_{n-1} \\ &+ (t_i - x_{n-1}) (t_i - x_n) c_{n-2} \\ &+ \dots \\ &+ (t_i - x_2) (t_i - x_3) \dots (t_i - x_n) c_1 \end{aligned}$$

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

1.  $n < 0$
2.  $ninit > n$
3.  $m < 0$

### Examples

#### Example 1

This example shows a quadratic polynomial interpolation on the initial call with the specified data points; that is, NINIT = 0, and C contains all undefined values. On output, NINIT and C are updated with new values.

#### Call Statement and Input:

	X	Y	N	C	NINIT	T	S	M
CALL SPINT(	X	Y	3	C	0	T	S	2
X	=	(-0.50, 0.00, 1.00)						
Y	=	(0.25, 0.00, 1.00)						
C	=	(. , . , .)						
T	=	(-0.2, 0.2)						

#### Output:

C	=	(1.00, 1.00, 1.00)
NINIT	=	3
S	=	(0.04, 0.04)

#### Example 2

This example shows a quadratic polynomial interpolation on a subsequent call with the same data points specified in Example 1, but using a different set of abscissas in T. In this case, NINIT = N = 3, and C contains the values defined on output in Example 1. On output here, the values in NINIT and C are unchanged.

#### Call Statement and Input:

	X	Y	N	C	NINIT	T	S	M
CALL SPINT(	X	Y	3	C	3	T	S	2
X	=	(-0.50, 0.00, 1.00)						
Y	=	(0.25, 0.00, 1.00)						
C	=	(1.00, 1.00, 1.00)						
T	=	(-0.10, 0.10)						

#### Output:

C	=	(1.00, 1.00, 1.00)
NINIT	=	3
S	=	(0.01, 0.01)



**Example 3**

This example is the same as Example 2 except that it specifies additional data points on the subsequent call to the subroutine. In this case,  $0 < \text{NINIT} < N$ . On output here, the values in NINIT and C are updated. The interpolating polynomial is a degree of 4.

**Call Statement and Input:**

	X	Y	N	C	NINIT	T	S	M
CALL SPINT(								
	X	Y	5	C	3	T	S	2
X	=	(-0.50, 0.00, 1.00, -1.00, 0.50)						
Y	=	(0.25, 0.00, 1.00, 1.10, 0.26)						
C	=	(1.00, 1.00, 1.00, . , . )						
T	=	(-0.10, 0.10)						

**Output:**

C	=	(0.04, -0.06, 1.02, -0.56, 0.26)						
NINIT	=	5						
S	=	(0.0072, 0.0130)						

---

## STPINT and DTPINT — Local Polynomial Interpolation

### Purpose

These subroutines perform a polynomial interpolation at specified abscissas, using data points selected from a table of data.

Table 166. Data Types

$x, y, t, s, aux$	Subroutine
Short-precision real	STPINT
Long-precision real	DTPINT

### Syntax

Fortran	CALL STPINT   DTPINT ( $x, y, n, nint, t, s, m, aux, naux$ )
C and C++	stpint   dtpint ( $x, y, n, nint, t, s, m, aux, naux$ );

### On Entry

- $x$  is the vector  $x$  of length  $n$ , containing the abscissas of the data points used in the interpolations. The elements of  $x$  must be distinct and sorted into ascending order.
- Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 166.
- $y$  is the vector  $y$  of length  $n$ , containing the ordinates of the data points used in the interpolations.
- Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 166.
- $n$  is the number of elements in vectors  $x$  and  $y$ —that is, the number of data points. Specified as: a fullword integer;  $n \geq 0$ .
- $nint$  is the number of data points to be used in the interpolation at any given point.
- Specified as: a fullword integer;  $0 \leq nint \leq n$ .
- $t$  is the vector  $t$  of length  $m$ , containing the abscissas at which interpolation is to be done. For optimal performance,  $t$  should be sorted into ascending order.
- Specified as: a one-dimensional array of (at least) length  $m$ , containing numbers of the data type indicated in Table 166.
- $s$  See “On Return” on page 953.
- $m$  is the number of elements in vectors  $t$  and  $s$ —that is, the number of interpolations to be performed.
- Specified as: a fullword integer;  $m \geq 0$ .
- $aux$  has the following meaning:
- If  $naux = 0$  and error 2015 is unrecoverable,  $aux$  is ignored.
- Otherwise, it is the storage work area used by this subroutine. Its size is specified by  $naux$ .

Specified as: an area of storage, containing numbers of the data type indicated in Table 166 on page 952. On output, the contents are overwritten.

*naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.

Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, STPINT and DTPINT dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \geq nint+m$ .

### On Return

*s* is the vector *s* of length *m*, containing the resulting interpolated values; that is, each  $s_i$  is the value of the interpolating polynomial evaluated at  $t_i$ . Returned as: a one-dimensional array of (at least) length *m*, containing numbers of the data type indicated in Table 166 on page 952.

### Notes

1. Vectors *x*, *y*, and *t* must have no common elements with vector *s* or work area *aux*; otherwise, results are unpredictable. See “Concepts” on page 59.
2. The elements of vector *x* must be distinct and must be sorted into ascending order; that is,  $x_1 < x_2 < \dots < x_n$ . Otherwise, results are unpredictable. For details on how to do this, see “ISORT, SSORT, and DSORT — Sort the Elements of a Sequence” on page 927.
3. The elements of vector *t* should be sorted into ascending order; that is,  $t_1 \leq t_2 \leq t_3 \leq \dots \leq t_m$ . Otherwise, performance is affected.
4. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

### Function

Polynomial interpolation is performed at specified abscissas,  $t_i$  for  $i = 1, m$ , in vector *t*, using *nint* points selected from the following data:

$(x_j, y_j)$  for  $j = 1, n$

where:

$x_1 < x_2 < x_3 < \dots < x_n$

$x_j$  are elements of vector *x*.

$y_j$  are elements of vector *y*.

The points  $(x_j, y_j)$ , used in the interpolation at a given abscissa  $t_i$ , are chosen as follows, where  $k = nint/2$ :

For  $t_i \leq x_{k+1}$ , the first *nint* points are used.

For  $t_i > x_{n-nint+k}$ , the last *nint* points are used.

Otherwise, points *h* through  $h+nint-1$  are used, where:

$x_{h+k-1} < t_i \leq x_{h+k}$

## STPINT and DTPINT

The interpolated value at each  $t_i$  is returned in  $s_i$  for  $i = 1, m$ . See references [17] and [56]. If  $n$ ,  $nint$ , or  $m$  is 0, no computation is performed. For a definition of the polynomial interpolation function performed through a set of data points, see "Function" on page 948.

For STPINT, the Newton divided differences and interpolating values are accumulated in long precision.

### Error conditions

#### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

#### Computational Errors

None

#### Input-Argument Errors

1.  $n < 0$
2.  $nint < 0$  or  $nint > n$
3.  $m < 0$
4. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value specified in the syntax for this argument. Return code 1 is returned if error 2015 is recoverable.

### Examples

#### Example 1

This example shows interpolation using two data points—that is, linear interpolation—at each  $t_i$  value.

##### Call Statement and Input:

```
CALL STPINT( X , Y , 10 , 2 , T , S , 5 , AUX , 7 )
```

```
X      = (0.0, 0.4, 1.0, 1.5, 2.1, 2.6, 3.0, 3.4, 3.9, 4.3)
Y      = (1.0, 2.0, 3.0, 4.0, 5.0, 5.0, 4.0, 3.0, 2.0, 1.0)
T      = (-1.0, 0.1, 1.1, 1.2, 3.9)
```

##### Output:

```
S      = (-1.5000, 1.2500, 3.2000, 3.4000, 2.0000)
```

#### Example 2

This example shows interpolation using three data points—that is, quadratic interpolation—at each  $t_i$  value.

##### Call Statement and Input:

```
CALL STPINT( X , Y , 10 , 3 , T , S , 5 , AUX , 8 )
```

```
X      = (0.0, 0.4, 1.0, 1.5, 2.1, 2.6, 3.0, 3.4, 3.9, 4.3)
Y      = (1.0, 2.0, 3.0, 4.0, 5.0, 5.0, 4.0, 3.0, 2.0, 1.0)
T      = (-1.0, 0.1, 1.1, 1.2, 3.9)
```

##### Output:

```
S      = (-2.6667, 1.2750, 3.2121, 3.4182, 2.0000)
```

## SCSINT and DCSINT — Cubic Spline Interpolation

### Purpose

These subroutines compute the coefficients of the cubic spline through a set of data points and evaluate the spline at specified abscissas.

Table 167. Data Types

$x, y, C, t, s$	Subroutine
Short-precision real	SCSINT
Long-precision real	DCSINT

### Syntax

Fortran	CALL SCSINT   DCSINT ( $x, y, c, n, init, t, s, m$ )
C and C++	scsint   dcsint ( $x, y, c, n, init, t, s, m$ );

### On Entry

- $x$  is the vector  $x$  of length  $n$ , containing the abscissas of the data points that define the spline. The elements of  $x$  must be distinct and sorted into ascending order. Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 167.
- $y$  is the vector  $y$  of length  $n$ , containing the ordinates of the data points that define the spline.  
Specified as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 167.
- $c$  is the matrix  $C$  with elements  $c_{jk}$  for  $j = 1, n$  and  $k = 1, 4$  that contain the following:  
If  $init \leq 0$ , all elements of  $c$  are undefined on entry.  
If  $init = 1$ ,  $c_{11}$  contains the spline derivative at  $x_1$ .  
If  $init = 2$ ,  $c_{21}$  contains the spline derivative at  $x_n$ .  
If  $init = 3$ ,  $c_{11}$  contains the spline derivative at  $x_1$ , and  $c_{21}$  contains the spline derivative at  $x_n$ .  
If  $init > 3$ ,  $c$  contains the coefficients of the spline computed for the data points  $(x_j, y_j)$  for  $j = 1, n$  on a previous call to this subroutine.  
Specified as: an  $n$  by (at least) 4 array, containing numbers of the data type indicated in Table 167.
- $n$  is the number of elements in vectors  $x$  and  $y$  and the number of rows in matrix  $C$ —that is, the number of data points.  
Specified as: a fullword integer;  $n \geq 0$ .
- $init$  indicates the following, where in those cases for uninitialized coefficients, this is the first call to this subroutine with the data in  $x$  and  $y$ :

## SCSINT and DCSINT

If  $init \leq 0$ , the coefficients are uninitialized. The second derivatives of the spline at  $x_1$  and  $x_n$  are set to zero. (These are free end conditions, also called natural boundary conditions.)

If  $init = 1$ , the coefficients are uninitialized. The value in  $c_{11}$  is used as the spline derivative at  $x_1$ .

If  $init = 2$ , the coefficients are uninitialized. The value in  $c_{21}$  is used as the spline derivative at  $x_n$ .

If  $init = 3$ , the coefficients are uninitialized. The value in  $c_{11}$  is used as the spline derivative at  $x_1$  and the value in  $c_{21}$  is used as the spline derivative at  $x_n$ .

If  $init > 3$ , the coefficients in  $c$  were computed for data points  $(x_j, y_j)$  for  $j = 1, n$  on a previous call to this subroutine.

Specified as: a fullword integer. It can have any value.

$t$  is the vector  $t$  of length  $m$ , containing the abscissas at which the spline is evaluated.

Specified as: a one-dimensional array of (at least) length  $m$ , containing numbers of the data type indicated in Table 167 on page 955.

$s$  See "On Return."

$m$  is the number of elements in vectors  $t$  and  $s$ —that is, the number of points at which the spline interpolation is evaluated.

Specified as: a fullword integer;  $m \geq 0$ .

### On Return

$c$  is the matrix  $C$ , containing the coefficients of the spline through the data points  $(x_j, y_j)$  for  $j = 1, n$ . Returned as: an  $n$  by (at least) 4 array, containing numbers of the data type indicated in Table 167 on page 955.

$init$  is an indicator that is set to indicate that the coefficients have been initialized. (If you call this subroutine again with the same data, this value should be specified for  $init$ .) Returned as: a fullword integer;  $init = 4$ .

$s$  is the vector  $s$  of length  $m$ , containing the resulting values of the spline; that is, each  $s_i$  is the value of the spline evaluated at  $t_i$ . Returned as: a one-dimensional array of (at least) length  $m$ , containing numbers of the data type indicated in Table 167 on page 955.

### Notes

1. In your C program, argument  $init$  must be passed by reference.
2. Vectors  $x$ ,  $y$ , and  $t$  must have no common elements with matrix  $C$  and vector  $s$ , and matrix  $C$  must have no common elements with vector  $s$ ; otherwise, results are unpredictable.
3. The elements of vector  $x$  must be distinct and must be sorted into ascending order; that is,  $x_1 < x_2 < \dots < x_n$ . Otherwise, results are unpredictable. For details on how to do this, see "ISORT, SSORT, and DSORT — Sort the Elements of a Sequence" on page 927.

## Function

Interpolation is performed at specified abscissas,  $t_i$  for  $i = 1, m$ , in vector  $t$ , using the cubic spline passing through the data points:

$$(x_j, y_j) \quad \text{for } j = 1, n$$

where:

$$x_1 < x_2 < x_3 < \dots < x_n$$

$x_j$  are elements of vector  $x$ .  
 $y_j$  are elements of vector  $y$ .

The value of the cubic spline at each  $t_i$  is returned in  $s_i$  for  $i = 1, m$ . See references [17] and [56]. The coefficients of the spline,  $c_{jk}$  for  $j = 1, n$  and  $k = 1, 4$ , are returned in matrix  $C$ . These coefficients can then be reused on subsequent calls to this subroutine, using the same data points  $(x_j, y_j)$ , but with new values of  $t_i$ . The cubic spline values returned in  $s$  are computed using the coefficients as follows:

$$s_i = c_{j1} + c_{j2} (x_j - t_i) + c_{j3} (x_j - t_i)^2 + c_{j4} (x_j - t_i)^3 \quad \text{for } i = 1, m$$

where:

$$j = 1 \quad \text{for } t_i \leq x_1$$

$$j = k \quad \text{for } x_1 < t_i \leq x_n, \text{ such that } x_{k-1} < t_i \leq x_k$$

$$j = n \quad \text{for } x_n < t_i$$

The values specified for  $m$  and  $init$  indicate which combination of functions are performed by this subroutine:

- If  $m = 0$  and  $init > 3$ , no computation is performed.
- If  $m = 0$  and  $init \leq 3$ , only the coefficients are computed, and no interpolation is performed.
- If  $m \neq 0$  and  $init > 3$ , the coefficients are not computed, and the interpolation is performed.
- If  $m \neq 0$  and  $init \leq 3$ , the coefficients are computed, and the interpolation is performed.

In addition, if  $n = 0$ , no computation is performed.

The values specified for  $n$  and  $init$  determine the type of spline function:

- If  $n = 1$ , the constructed spline is a constant function.
- If  $n = 2$  and  $init = 0$ , the constructed spline is a line through the points.
- If  $n = 2$  and  $init = 1$ , the constructed spline is a cubic function through the points whose derivative at  $x_1$  is  $c_{11}$ .
- If  $n = 2$  and  $init = 2$ , the constructed spline is a cubic function through the points whose derivative at  $x_n$  is  $c_{21}$ .
- If  $n = 2$  and  $init = 3$ , the constructed spline is a cubic function through the points whose derivative at  $x_1$  is  $c_{11}$  and at  $x_n$  is  $c_{21}$ .

## Error conditions

### Computational Errors

None

**Input-Argument Errors**

1.  $n < 0$
2.  $m < 0$

**Examples****Example 1**

This example computes the spline coefficients through a set of data points with no derivative value specified. It also evaluates the spline at the abscissas specified in T. On output, INIT and C are updated with new values.

**Call Statement and Input:**

```

          X   Y   C   N   INIT   T   S   M
          |   |   |   |   |     |   |   |
CALL SCSINT( X , Y , C , 6 , 0 , T , S , 4 )

```

```

X       = (1.000, 2.000, 3.000, 4.000, 5.000, 6.000)
Y       = (0.000, 1.000, 2.000, 1.100, 0.000, -1.000)
C       =(not relevant)
T       = (-1.000, 2.500, 4.000, 7.000)

```

**Output:**

```

C       = [
           0.000  -0.868   0.000  -0.132
           1.000  -1.264   0.396  -0.132
           2.000  -0.076  -1.585   0.660
           1.100   1.267   0.243  -0.609
           0.000   1.010   0.014   0.076
           -1.000   0.995   0.000   0.005
         ]

```

```

INIT    = 4
S       = (-2.792, 1.649, 1.100, -2.000)

```

**Example 2**

This example computes the spline coefficients through a set of data points with a derivative value specified at the right endpoint. It also evaluates the spline at the abscissas specified in T. On output, INIT and C are updated with new values.

**Call Statement and Input:**

```

          X   Y   C   N   INIT   T   S   M
          |   |   |   |   |     |   |   |
CALL SCSINT( X , Y , C , 6 , 2 , T , S , 4 )

```

```

X       = (1.000, 2.000, 3.000, 4.000, 5.000, 6.000)
Y       = (0.000, 1.000, 2.000, 1.100, 0.000, -1.000)

```

```

C       = [
           .   .   .   .
          0.1 .   .   .
           .   .   .   .
           .   .   .   .
           .   .   .   .

```

```

T       = (-1.000, 2.500, 4.000, 7.000)

```

**Output:**



$$C = \begin{bmatrix} 0.000 & -0.865 & 0.000 & -0.135 \\ 1.000 & -1.270 & 0.405 & -0.135 \\ 2.000 & -0.054 & -1.621 & 0.675 \\ 1.100 & 1.188 & 0.379 & -0.667 \\ 0.000 & 1.303 & -0.494 & 0.291 \\ -1.000 & 0.100 & 1.897 & -0.797 \end{bmatrix}$$

$$\begin{aligned} \text{INIT} &= 4 \\ S &= (-2.810, 1.652, 1.100, 1.794) \end{aligned}$$

### Example 3

This example computes the spline coefficients through a set of data points with a derivative value specified at both endpoints. It does not evaluate the spline at any points. On output, INIT and C are updated with new values. Because arrays are not needed for arguments  $t$  and  $s$ , the value 0 is specified in their place.

#### Call Statement and Input:

```

          X   Y   C   N   INIT  T   S   M
          |   |   |   |   |    |   |   |
CALL SCSINT( X , Y , C , 6 , 3 , 0 , 0 , 0 )

```

$$\begin{aligned} X &= (1.000, 2.000, 3.000, 4.000, 5.000, 6.000) \\ Y &= (0.000, 1.000, 2.000, 1.100, 0.000, -1.000) \end{aligned}$$

$$C = \begin{bmatrix} -1.0 & . & . & . \\ 0.1 & . & . & . \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \end{bmatrix}$$

#### Output:

$$C = \begin{bmatrix} 0.000 & 1.000 & 3.230 & 1.230 \\ 1.000 & -1.770 & -0.460 & 1.230 \\ 2.000 & 0.079 & -1.389 & 0.310 \\ 1.100 & 1.152 & 0.316 & -0.568 \\ 0.000 & 1.312 & -0.476 & 0.264 \\ -1.000 & -0.100 & 1.888 & -0.788 \end{bmatrix}$$

$$\text{INIT} = 4$$

### Example 4

This example evaluates the spline at a set of points, using the coefficients obtained in Example 3.

#### Call Statement and Input:

```

          X   Y   C   N   INIT  T   S   M
          |   |   |   |   |    |   |   |
CALL SCSINT( X , Y , C , 6 , 4 , T , S , 4 )

```

$$\begin{aligned} X &= (1.000, 2.000, 3.000, 4.000, 5.000, 6.000) \\ Y &= (0.000, 1.000, 2.000, 1.100, 0.000, -1.000) \\ C &= (\text{same as output } C \text{ in Example 3}) \\ T &= (-1.000, 2.500, 4.000, 7.000) \end{aligned}$$

#### Output:

## SCSINT and DCSINT

C        =(same as output C in Example 3 )  
S        = (24.762, 1.731, 1.100, 1.776)  
INIT     = 4

## SCSIN2 and DCSIN2 — Two-Dimensional Cubic Spline Interpolation

### Purpose

These subroutines compute the interpolation values at a specified set of points, using data defined on a rectangular mesh in the x-y plane.

Table 168. Data Types

$x, y, Z, t, u, aux, S$	Subroutine
Short-precision real	SCSIN2
Long-precision real	DCSIN2

### Syntax

Fortran	CALL SCSIN2   DCSIN2 ( $x, y, z, n1, n2, ldz, t, u, m1, m2, s, lds, aux, naux$ )
C and C++	scsin2   dcsin2 ( $x, y, z, n1, n2, ldz, t, u, m1, m2, s, lds, aux, naux$ );

### On Entry

- $x$  is the vector  $x$  of length  $n1$ , containing the x-coordinates of the data points that define the spline. The elements of  $x$  must be distinct and sorted into ascending order.
- Specified as: a one-dimensional array of (at least) length  $n1$ , containing numbers of the data type indicated in Table 168.
- $y$  is the vector  $y$  of length  $n2$ , containing the y-coordinates of the data points that define the spline. The elements of  $y$  must be distinct and sorted into ascending order.
- Specified as: a one-dimensional array of (at least) length  $n2$ , containing numbers of the data type indicated in Table 168.
- $z$  is the matrix  $Z$ , containing the data at  $(x_i, y_j)$  for  $i = 1, n1$  and  $j = 1, n2$  that defines the spline.
- Specified as: an  $ldz$  by (at least)  $n2$  array, containing numbers of the data type indicated in Table 168.
- $n1$  is the number of elements in vector  $x$  and the number of rows in matrix  $Z$ —that is, the number of x-coordinates at which the spline is defined.
- Specified as: a fullword integer;  $n1 \geq 0$ .
- $n2$  is the number of elements in vector  $y$  and the number of columns in matrix  $Z$ —that is, the number of y-coordinates at which the spline is defined.
- Specified as: a fullword integer;  $n2 \geq 0$ .
- $ldz$  is the leading dimension of the array specified for  $z$ .
- Specified as: a fullword integer;  $ldz > 0$  and  $ldz \geq n1$ .
- $t$  is the vector  $t$  of length  $m1$ , containing the x-coordinates at which the spline is evaluated.
- Specified as: a one-dimensional array of (at least) length  $m1$ , containing numbers of the data type indicated in Table 168.

## SCSIN2 and DCSIN2

<i>u</i>	is the vector <i>u</i> of length <i>m2</i> , containing the y-coordinates at which the spline is evaluated.  Specified as: a one-dimensional array of (at least) length <i>m2</i> , containing numbers of the data type indicated in Table 168 on page 961.
<i>m1</i>	is the number of elements in vector <i>t</i> —that is, the number of x-coordinates at which the spline interpolation is evaluated. Specified as: a fullword integer; $m1 \geq 0$ .
<i>m2</i>	is the number of elements in vector <i>u</i> —that is, the number of y-coordinates at which the spline interpolation is evaluated. Specified as: a fullword integer; $m2 \geq 0$ .
<i>s</i>	See “On Return.”
<i>lds</i>	is the leading dimension of the array specified for <i>s</i> .  Specified as: a fullword integer; $lds > 0$ and $lds \geq m1$ .
<i>aux</i>	has the following meaning:  If $naux = 0$ and error 2015 is unrecoverable, <i>aux</i> is ignored.  Otherwise, it is the storage work area used by this subroutine. Its size is specified by <i>naux</i> .  Specified as: an area of storage, containing numbers of the data type indicated in Table 166 on page 952. On output, the contents are overwritten.
<i>naux</i>	is the size of the work area specified by <i>aux</i> —that is, the number of elements in <i>aux</i> .  Specified as: a fullword integer, where:  If $naux = 0$ and error 2015 is unrecoverable, SCSIN2 and DCSIN2 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.  Otherwise, $naux \geq (10)(\max(n1, n2)) + (n2+1)(m1) + 2(m2)$ .

### On Return

<i>s</i>	is the matrix <i>S</i> with elements $s_{kh}$ that contain the interpolation values at $(t_k, u_h)$ for $k = 1, m1$ and $h = 1, m2$ . Returned as: an <i>lds</i> by (at least) <i>m2</i> array, containing numbers of the data type indicated in Table 168 on page 961.
----------	---

### Notes

1. The cyclic reduction method used to solve the equations in this subroutine can generate underflows on well-scaled problems. This does not affect accuracy, but it may decrease performance. For this reason, you may want to disable underflow before calling this subroutine.
2. Vectors *x*, *y*, *t*, and *u*, matrix *Z*, and the *aux* work area must have no common elements with matrix *S*; otherwise, results are unpredictable.
3. The elements within vectors *x* and *y* must be distinct. In addition, the elements in the vectors must be sorted into ascending order; that is,  $x_1 < x_2 < \dots < x_{n1}$  and  $y_1 < y_2 < \dots < y_{n2}$ . Otherwise, results are unpredictable. For details on how to do this, see “ISORT, SSORT, and DSORT — Sort the Elements of a Sequence” on page 927.

4. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## Function

Interpolation is performed at a specified set of points:

$$(t_k, u_h) \quad \text{for } k = 1, m1 \text{ and } h = 1, m2$$

by fitting bicubic spline functions with natural boundary conditions, using the following set of data, defined on a rectangular grid,  $(x_i, y_j)$  for  $i = 1, n1$  and  $j = 1, n2$ :

$$z_{ij} \quad \text{for } i = 1, n1 \text{ and } j = 1, n2$$

where  $t_k, u_h, x_i, y_j$ , and  $z_{ij}$  are elements of vectors  $\mathbf{t}$ ,  $\mathbf{u}$ ,  $\mathbf{x}$ , and  $\mathbf{y}$  and matrix  $\mathbf{Z}$ , respectively. In vectors  $\mathbf{x}$  and  $\mathbf{y}$ , elements are assumed to be sorted into ascending order.

The interpolation involves two steps:

1. For each  $j$  from 1 to  $n2$ , the single variable cubic spline:

$$s_{y_j}(x)$$

with natural boundary conditions, is constructed using the data points:

$$(x_i, z_{ij}) \quad \text{for } i = 1, n1$$

The following interpolation values are then computed:

$$s_{y_j}(t_k) \quad \text{for } k = 1, m1$$

2. For each  $k$  from 1 to  $m1$ , the single variable cubic spline:

$$s_{t_k}(y),$$

with natural boundary conditions, is constructed using the data points:

$$(y_j, s_{y_j}(t_k)) \quad \text{for } j = 1, n2$$

The following interpolation values are then computed:

$$s_{kh} = s_{t_k}(u_h) \quad \text{for } l = 1, m2$$

See references [56] and [62]. Because natural boundary conditions (zero second derivatives at the end of the ranges) are used for the splines, unless the underlying function has these properties, interpolated values near the boundaries may be less satisfactory than elsewhere. If  $n1, n2, m1$ , or  $m2$  is 0, no computation is performed.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n1 < 0$  or  $n1 > ldz$
2.  $n2 < 0$
3.  $m1 < 0$  or  $m1 > lds$
4.  $m2 < 0$
5.  $ldz < 0$
6.  $lds < 0$
7. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value specified in the syntax for this argument. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example

This example computes the interpolated values at a specified set of points, given by T and U, from a set of data points defined on a rectangular mesh in the x-y plane, using X, Y, and Z.

#### Call Statement and Input:

```

          X   Y   Z   N1  N2  LDZ  T   U   M1  M2  S   LDS  AUX  NAUX
          |   |   |   |   |   |   |   |   |   |   |   |   |
CALL SCSIN2( X , Y , Z , 6 , 5 , 6 , T , U , 4 , 3 , S , 4 , AUX , 90 )

```

```

X       = (0.0, 0.2, 0.3, 0.4, 0.5, 0.7)
Y       = (0.0, 0.2, 0.3, 0.4, 0.6)

```

```

Z       = [ 0.000  0.008  0.027  0.064  0.216
           0.008  0.016  0.035  0.072  0.224
           0.027  0.035  0.054  0.091  0.243
           0.064  0.072  0.091  0.128  0.280
           0.125  0.133  0.152  0.189  0.341
           0.343  0.351  0.370  0.407  0.559 ]

```

```

T       = (0.10, 0.15, 0.25, 0.35)
U       = (0.05, 0.25, 0.45)

```

#### Output:

```

S       = [ 0.001  0.017  0.095
           0.003  0.019  0.097
           0.016  0.031  0.110
           0.043  0.059  0.137 ]

```

---

## Chapter 15. Numerical Quadrature

The numerical quadrature subroutines are described in this chapter.

---

### Overview of the Numerical Quadrature Subroutines

The numerical quadrature subroutines provide Gaussian quadrature methods for integrating a tabulated function and a user-supplied function over a finite, semi-infinite, or infinite region of integration (Table 169).

Table 169. List of Numerical Quadrature Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Numerical Quadrature Performed on a Set of Points	SPTNQ	DPTNQ	969
Numerical Quadrature Performed on a Function Using Gauss-Legendre Quadrature	SGLNQ <sup>+</sup>	DGLNQ <sup>+</sup>	972
Numerical Quadrature Performed on a Function Over a Rectangle Using Two-Dimensional Gauss-Legendre Quadrature	SGLNQ2 <sup>+</sup>	DGLNQ2 <sup>+</sup>	975
Numerical Quadrature Performed on a Function Using Gauss-Laguerre Quadrature	SGLGQ <sup>+</sup>	DGLGQ <sup>+</sup>	981
Numerical Quadrature Performed on a Function Using Gauss-Rational Quadrature	SGRAQ <sup>+</sup>	DGRAQ <sup>+</sup>	984
Numerical Quadrature Performed on a Function Using Gauss-Hermite Quadrature	SGHMQ <sup>+</sup>	DGHMQ <sup>+</sup>	988

<sup>+</sup> This subprogram is invoked as a function in a Fortran program.

---

### Use Considerations

This section contains some key points about using the numerical quadrature subroutines.

#### Choosing the Method

The theoretical aspects of choosing the method to use for integration can be found in the references [28], [63], and [96].

---

### Performance and Accuracy Considerations

1. There are  $n$  function evaluations for a method of order  $n$ . Because function evaluations are expensive in terms of computing time, you should weigh the considerations for computing time and accuracy in choosing a value for  $n$ .
2. To achieve optimal performance in the `_GLNQ2` subroutines, specify the first variable integrated to be the variable having more points. This allows both the subroutine and the function evaluation to achieve optimal performance. Details on how to do this are given in "Notes" on page 976.
3. There are some ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 48.

---

## Programming Considerations for the SUBF Subroutine

This section describes how to design and code the *subf* subroutine for use by the numerical quadrature subroutines.

### Designing SUBF

For the Gaussian quadrature subroutines, you must supply a separate subroutine that is callable by ESSL. You specify the name of the subroutine in the *subf* argument. This subroutine name is selected by you. You should design the *subf* subroutine so it receives, as input, a tabulated set of points at which the integrand is evaluated, and it returns, as output, the values of the integrand evaluated at these points.

Depending on the numerical quadrature subroutine that you use, the *subf* subroutine is defined in one of the two following ways:

- For `_GLNQ`, `_GLGQ`, `_GRAQ`, and `_GHMQ`, you define the *subf* subroutine with three arguments: *t*, *y*, and *n*, where:

*t* is an input array, referred to as T, of tabulated Gaussian quadrature abscissas, containing *n* real numbers,  $t_i$ , where  $t_i$  is automatically provided by the ESSL subroutine and is determined by *n* and the Gaussian quadrature method chosen.

*y* is an output array, referred to as Y, containing *n* real numbers, where for the integrand, the following is true:  $y_i = f(t_i)$  for  $i = 1, n$ .

*n* is a positive integer indicating the number of elements in T and Y.

- For `_GLNQ2`, you define the *subf* subroutine with six arguments: *s*, *n1*, *t*, *n2*, *z*, and *ldz*, where:

*s* is an input array, referred to as S, of tabulated Gaussian quadrature abscissas, containing *n1* real numbers,  $s_i$ , where  $s_i$  is automatically provided by the ESSL subroutine and is determined by *n1* and the Gaussian quadrature method.

*n1* is a positive integer indicating the number of elements in S and the number of rows to be used in array Z.

*t* is an input array, referred to as T, of tabulated Gaussian quadrature abscissas, containing *n2* real numbers,  $t_i$ , where  $t_i$  is automatically provided by the ESSL subroutine and is determined by *n2* and the Gaussian quadrature method.

*n2* is a positive integer indicating the number of elements in T and the number of columns to be used in array Z.

*z* is an *ldz* by (at least) *n2* output array, referred to as Z, of real numbers, where for the integrand, the following is true:  $z_{ij} = f(s_i, t_j)$  for  $i = 1, n1$  and  $j = 1, n2$ .

*ldz* is a positive integer indicating the size of the leading dimension of the array Z.

### Coding and Setting Up SUBF in Your Program

Examples of coding a *subf* subroutine in Fortran are provided for each subroutine in this chapter. Examples of coding a *subf* subroutine in C, and C++ are provided in "Example 1" on page 978.



Depending on the programming language you use for your program that calls the numerical quadrature subroutines, you have a choice of one or more languages that you can use for writing *subf*. These rules and other language-related coding rules for setting up *subf* in your program are described in the following sections:

- “Setting Up a User-Supplied Subroutine for ESSL in Fortran” on page 111
- “Setting Up a User-Supplied Subroutine for ESSL in C” on page 131
- “Setting Up a User-Supplied Subroutine for ESSL in C++” on page 147

---

## Numerical Quadrature Subroutines

This section contains the numerical quadrature subroutine descriptions.

## SPTNQ and DPTNQ — Numerical Quadrature Performed on a Set of Points

### Purpose

These subroutines approximate the integral of a real valued function specified in tabular form,  $(x_i, y_i)$  for  $i = 1, n$ . For more than four points, an error estimate is returned along with the resulting value.

Table 170. Data Types

$x, y, xyint, eest$	Subroutine
Short-precision real	SPTNQ
Long-precision real	DPTNQ

### Syntax

Fortran	CALL SPTNQ   DPTNQ ( $x, y, n, xyint, eest$ )
C and C++	sptnq   dptnq ( $x, y, n, xyint, eest$ );

### On Entry

$x$	is the vector $x$ of length $n$ , containing the abscissas of the data points to be integrated. The elements of $x$ must be distinct and sorted into ascending or descending order.  Specified as: a one-dimensional array of (at least) length $n$ , containing numbers of the data type indicated in Table 170.
$y$	is the vector $y$ of length $n$ , containing the ordinates of the data points to be integrated.  Specified as: a one-dimensional array of (at least) length $n$ , containing numbers of the data type indicated in Table 170.
$n$	is the number of elements in vectors $x$ and $y$ —that is, the number of data points. The value of $n$ determines the algorithm used by this subroutine. For details, see “Function” on page 970.  Specified as: a fullword integer; $n \geq 2$ .
$xyint$	See “On Return.”
$eest$	See “On Return.”

### On Return

$xyint$	is the approximation $xyint$ of the integral. Returned as: a number of the data type indicated in Table 170.
$eest$	has the following meaning, where:  If $n < 5$ , it is undefined and is set to 0.  If $n \geq 5$ , it is an estimate, $eest$ , of the error in the integral, where $xyint+eest$ tends to give a better approximation to the integral than $xyint$ . For details, see references [28] and [63].  Returned as: a number of the data type indicated in Table 170.

## Notes

1. In your C program, arguments *xyint* and *eest* must be passed by reference.
2. The elements of vector *x* must be distinct—that is,  $x_i \neq x_j$  for  $i \neq j$ ,—and they must be sorted into ascending or descending order; otherwise, results are unpredictable. For how to do this, see “ISORT, SSORT, and DSORT — Sort the Elements of a Sequence” on page 927.

## Function

The integral is approximated for a real valued function specified in tabular form,  $(x_i, y_i)$  for  $i = 1, n$ , where  $x_i$  are distinct and sorted into ascending or descending order, and  $n \geq 2$ . If  $y_i = f(x_i)$  for  $i = 1, n$ , then on output, *xyint* is an approximation to the integral of the following form:

$$\int_{x_1}^{x_n} f(x) dx$$

The algorithm used by this subroutine is based on the number of data points used in the computation, where:

- If  $n = 2$ , the trapezoid rule is used to do the integration.
- If  $n = 3$ , the parabola through the three points is integrated.
- If  $n \geq 4$ , the method of Gill and Miller is used to do the integration.

For  $n \geq 5$ , an estimate of the error *eest* is returned. For the method of Gill and Miller, it is shown that adding the estimate of the error *eest* to the result *xyint* often gives a better approximation to the integral than the result *xyint* by itself. For  $n < 5$ , an estimate of the error is not returned. In this case, a value of 0 is returned for *eest*. See references [63] and [28].

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n < 2$

## Examples

### Example 1

This example shows the result of an integration, where the abscissas in *X* are sorted into ascending order.

#### Call Statement and Input:

```

          X   Y   N   XYINT   EEST
          |   |   |   |       |
CALL SPTNQ( X , Y , 10 , XYINT , EEST )

```

```

X       = (0.0, 0.4, 1.0, 1.5, 2.1, 2.6, 3.0, 3.4, 3.9, 4.3)
Y       = (1.0, 2.0, 3.0, 4.0, 5.0, 4.5, 4.0, 3.0, 3.5, 3.3)

```

#### Output:

```

XYINT   = 15.137
EEST    = -0.003

```

**Example 2**

This example shows the result of an integration, where the abscissas in  $X$  are sorted into descending order.

**Call Statement and Input:**

```

           X   Y   N   XYINT   EEST
           |   |   |   |       |
CALL SPTNQ( X , Y , 10 , XYINT , EEST )

```

```

X       = (4.3, 3.9, 3.4, 3.0, 2.6, 2.1, 1.5, 1.0, 0.4, 0.0)
Y       = (3.3, 3.5, 3.0, 4.0, 4.5, 5.0, 4.0, 3.0, 2.0, 1.0)

```

**Output:**

```

XYINT   = -15.137
EEST     =  0.003

```

## SGLNQ and DGLNQ — Numerical Quadrature Performed on a Function Using Gauss-Legendre Quadrature

### Purpose

These functions approximate the integral of a real valued function over a finite interval, using the Gauss-Legendre Quadrature method of specified order.

Table 171. Data Types

<i>a, b</i> , Result	Subroutine
Short-precision real	SGLNQ
Long-precision real	DGLNQ

### Syntax

Fortran	SGLNQ   DGLNQ ( <i>subf</i> , <i>a</i> , <i>b</i> , <i>n</i> )
C and C++	sglnq   dglng ( <i>subf</i> , <i>a</i> , <i>b</i> , <i>n</i> );

### On Entry

- subf* is the user-supplied subroutine that evaluates the integrand function. The subroutine should be defined with three arguments: *t*, *y*, and *n*. For details, see “Programming Considerations for the SUBF Subroutine” on page 966.
- Specified as: *subf* must be declared as an external subroutine in your application program. It can be whatever name you choose.
- a* is the lower limit of integration, *a*.
- Specified as: a number of the data type indicated in Table 171.
- b* is the upper limit of integration, *b*.
- Specified as: a number of the data type indicated in Table 171.
- n* is the order of the quadrature method to be used.
- Specified as: a fullword integer; *n* = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 64, 96, 128, or 256.

### On Return

- Function value* is the approximation of the integral. Returned as: a number of the data type indicated in Table 171.

### Notes

1. Declare the DGLNQ function in your program as returning a long-precision real number. Declare the SGLNQ, if necessary, as returning a short-precision real number.
2. The subroutine specified for *subf* must be declared as external in your program. Also, data types used by *subf* must agree with the data types specified by this ESSL subroutine. The variable *x*, described under “Function” on page 973, and the argument *n* correspond to the *subf* arguments *t* and *n*, respectively. For details on how to set up the subroutine, see “Programming Considerations for the SUBF Subroutine” on page 966.

## Function

The integral is approximated for a real valued function over a finite interval, using the Gauss-Legendre Quadrature method of specified order. The region of integration is from  $a$  to  $b$ . The method of order  $n$  is theoretically exact for integrals of the following form, where  $f$  is a polynomial of degree less than  $2n$ :

$$\int_a^b f(x) dx$$

The method of order  $n$  is a good approximation when your integrand is closely approximated by a function of the form  $f(x)$ , where  $f$  is a polynomial of degree less than  $2n$ . See references [28] and [96]. The result is returned as the function value.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

$n$  is not an allowable value, as listed in the syntax for this argument.

## Examples

### Example

This example shows how to compute the integral of the function  $f$  given by:

$$f(x) = x^2 + e^x$$

over the interval (0.0, 2.0), using the Gauss-Legendre method with 10 points:

$$\int_{0.0}^{2.0} (x^2 + e^x) dx$$

The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in Fortran as follows:

```

SUBROUTINE FUN1 (T,Y,N)
  INTEGER*4 N
  REAL*4 T(*),Y(*)
  DO 1 I=1,N
1    Y(I)=T(I)**2+EXP(T(I))
  RETURN
  END

```

### Program Statements and Input:

```

EXTERNAL FUN1
.
.
.
          SUBF   A   B   N
          |     |   |   |
XINT = SGLNQ( FUN1 , 0.0 , 2.0 , 10 )
.
.
.

```

## SGLNQ and DGLNQ

FUN1 = (see above)

### **Output:**

XINT = 9.056



## SGLNQ2 and DGLNQ2 — Numerical Quadrature Performed on a Function Over a Rectangle Using Two-Dimensional Gauss-Legendre Quadrature

### Purpose

These functions approximate the integral of a real valued function of two variables over a rectangular region, using the Gauss-Legendre Quadrature method of specified order in each variable.

Table 172. Data Types

<i>a, b, c, d, Z, Result</i>	Subroutine
Short-precision real	SGLNQ2
Long-precision real	DGLNQ2

### Syntax

Fortran	SGLNQ2   DGLNQ2 ( <i>subf, a, b, n1, c, d, n2, z, ldz</i> )
C and C++	sglnq2   dglng2 ( <i>subf, a, b, n1, c, d, n2, z, ldz</i> );

### On Entry

*subf* is the user-supplied subroutine that evaluates the integrand function. The subroutine should be defined with six arguments: *s*, *n1*, *t*, *n2*, *z*, and *ldz*. For details, see “Programming Considerations for the SUBF Subroutine” on page 966.

Specified as: *subf* must be declared as an external subroutine in your application program. It can be whatever name you choose.

*a* is the lower limit of integration, *a*, for the first variable integrated.  
Specified as: a number of the data type indicated in Table 172.

*b* is the upper limit of integration, *b*, for the first variable integrated.  
Specified as: a number of the data type indicated in Table 172.

*n1* is the order of the quadrature method to be used for the first variable integrated.  
Specified as: a fullword integer; *n1* = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 64, 96, 128, or 256.

*c* is the lower limit of integration, *c*, for the second variable integrated.  
Specified as: a number of the data type indicated in Table 172.

*d* is the upper limit of integration, *d*, for the second variable integrated.  
Specified as: a number of the data type indicated in Table 172.

*n2* is the order of the quadrature method to be used for the second variable integrated.  
Specified as: a fullword integer; *n2* = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 64, 96, 128, or 256.

## SGLNQ2 and DGLNQ2

- z* is the matrix *Z*, containing the *n1* rows and *n2* columns of data used to evaluate the integrand function. (The output values from the *subf* subroutine are placed in *Z*.) Specified as: an *ldz* by (at least) *n2* array, containing numbers of the data type indicated in Table 172 on page 975.
- ldz* is the size of the leading dimension of the array specified for *z*. Specified as: a fullword integer;  $ldz > 0$  and  $ldz \geq n1$ .

### On Return

#### *Function value*

is the approximation of the integral. Returned as: a number of the data type indicated in Table 172 on page 975.

### Notes

1. Declare the DGLNQ2 function in your program as returning a long-precision real number. Declare the SGLNQ2 function, if necessary, as returning a short-precision real number.
2. The subroutine specified for *subf* must be declared as external in your program. Also, data types used by *subf* must agree with the data types specified by this ESSL subroutine. For details on how to set up the subroutine, see “Programming Considerations for the SUBF Subroutine” on page 966.

### Function

The integral:

$$\int_c^d \int_a^b f(s,t) ds dt$$

is approximated for a real valued function of two variables *s* and *t*, over a rectangular region, using the Gauss-Legendre Quadrature method of specified order in each variable. The region of integration is:

$$\begin{array}{ll} (a, b) & \text{for } s \\ (c, d) & \text{for } t \end{array}$$

The method gives a good approximation when your integrand is closely approximated by a function of the form  $f(s, t)$ , where  $f$  is a polynomial of degree less than  $2(n1)$  for  $s$  and  $2(n2)$  for  $t$ . See the function description for “SGLNQ and DGLNQ — Numerical Quadrature Performed on a Function Using Gauss-Legendre Quadrature” on page 972 and references [28] and [96]. The result is returned as the function value.

### Special Usage

To achieve optimal performance in this subroutine and in the functional evaluation, specify the first variable integrated in this subroutine as the variable having more points. The first variable integrated is the variable in the inner integral. For example, in the following integration,  $x$  is the first variable integrated:

$$\int_{u1}^{u2} \int_{r1}^{r2} f(x,y) dx dy$$

This is the suggested order of integration if the  $x$  variable has more points than the  $y$  variable. On the other hand, if the  $y$  variable has more points, you make  $y$  the first variable integrated.

Because the order of integration does not matter to the resulting approximation, you may be able to reverse the order that  $x$  and  $y$  are integrated and get better performance. This can be expressed as:

$$\int_{u1}^{u2} \int_{r1}^{r2} f(x,y) dx dy = \int_{r1}^{r2} \int_{u1}^{u2} f(x,y) dy dx$$

Results are mathematically equivalent. However, because the algorithm is computed in a different way, results may not be bitwise identical.

Table 173 shows how to assign your variables to the `_GLNQ2` and `subf` arguments for the  $x$ - $y$  integration shown on the left and for the  $y$ - $x$  integration shown on the right. For examples of how to do each of these, see “Example 1” on page 978 and “Example 2” on page 979.

Table 173. How to Assign Your Variables for  $x$ - $y$  Integration Versus  $y$ - $x$  Integration

<code>_GLNQ2</code> and <code>SUBF</code> Arguments	Variables for $x$ - $y$ Integration	Variables for $y$ - $x$ Integration
For <code>_GLNQ2</code> :		
<code>a</code>	<code>r1</code>	<code>u1</code>
<code>b</code>	<code>r2</code>	<code>u2</code>
<code>n1</code>	(order for $x$ )	(order for $y$ )
<code>c</code>	<code>u1</code>	<code>r1</code>
<code>d</code>	<code>u2</code>	<code>r2</code>
<code>n2</code>	(order for $y$ )	(order for $x$ )
For <code>subf</code> :		
<code>s</code>	<code>x</code>	<code>y</code>
<code>t</code>	<code>y</code>	<code>x</code>
<code>n1</code>	(order for $x$ )	(order for $y$ )
<code>n2</code>	(order for $y$ )	(order for $x$ )

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $ldz \leq 0$
2.  $n1 > ldz$
3.  $n1$  or  $n2$  is not an allowable value, as listed in the syntax for this argument.

## Examples

### Example 1

This example shows how to compute the integral of the function  $f$  given by:

$$f(x, y) = e^x \sin y$$

over the intervals (0.0, 2.0) for the first variable  $x$  and (-2.0, -1.0) for the second variable  $y$ , using the Gauss-Legendre method with 10 points in the  $x$  variable and 5 points in the  $y$  variable:

$$\int_{-2.0}^{-1.0} \int_{0.0}^{2.0} (e^x \sin y) dx dy$$

Because the variable  $x$  has more points, it is the first variable integrated. This allows the SGLNQ2 subroutine and the FUN1 evaluation to achieve optimal performance. Therefore, the  $x$  and  $y$  variables correspond to S and T in the FUN1 subroutine. Also, the  $x$  and  $y$  variables correspond to the A, B, N1 and C, D, N2 sets of arguments, respectively, for SGLNQ2.

**Using Fortran for SUBF:** The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in Fortran as follows:

```

SUBROUTINE FUN1 (S,N1,T,N2,Z,LDZ)
  INTEGER*4 N1,N2,LDZ
  REAL*4 S(*),T(*),Z(LDZ,*)
  DO 1 J=1,N2
  DO 2 I=1,N1
2    Z(I,J)=EXP(S(I))*SIN(T(J))
1    CONTINUE
  RETURN
  END

```

**Note:** The computation for this user-supplied subroutine FUN1 can also be performed by using the following statements in place of the above DO loops, using T1 and T2 as temporary storage areas:

```

.
.
.
DO 1 I=1,N1
1  T1(I)=EXP(S(I))
DO 2 J=1,N2
2  T2(J)=SIN(T(J))
DO 3 J=1,N2
DO 4 I=1,N1
4  Z(I,J)=T1(I)*T2(J)
3  CONTINUE
.
.
.

```

When coding your application, this is the preferred technique. It reduces the number of evaluations performed and, therefore, provides better performance.

**Using C for SUBF:** The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in C as follows:

```

void fun1(s, n1, t, n2, z, ldz)
float *s, *t, *z;
int *n1, *n2, *ldz;

```

```

{
  int i, j;
  for(j = 0; j < *n2; ++j, z += *ldz)
  {
    for(i = 0; i < *n1; ++i)
      z[i] = exp(s[i]) * sin(t[j]);
  }
}

```

**Using C++ for SUBF:** The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in C++ as follows:

```

void fun1(float *s, int *n1, float *t, int *n2, float *z, int *ldz)
{
  int i, j;
  for(j = 0; j < *n2; ++j, z += *ldz)
  {
    for(i = 0; i < *n1; ++i)
      z[i] = exp(s[i]) * sin(t[j]);
  }
}

```

### Program Statements and Input:

```

EXTERNAL FUN1
.
.
.
          SUBF   A   B   N1   C   D   N2   Z   LDZ
XYINT = SGLNQ2( FUN1 , 0.0 , 2.0 , 10 , -2.0 , -1.0 , 5 , Z , 10 )
.
.
.

```

FUN1 = (see sections above)  
Z = (not relevant)

### Output:

XYINT = -6.1108

### Example 2

This example shows how to reverse the order of integration of the variables  $x$  and  $y$ . It computes the integral of the function  $f$  given by:

$$f(x, y) = \cos x \sin y$$

over the intervals (0.0, 1.0) for the variable  $x$  and (0.0, 20.0) for the variable  $y$ , using the Gauss-Legendre method with 5 points in the  $x$  variable and 48 points in the  $y$  variable. Because the order of integration does not matter to the approximation:

$$\int_{0.0}^{20.0} \int_{0.0}^{1.0} (\cos x \sin y) dx dy = \int_{0.0}^{1.0} \int_{0.0}^{20.0} (\cos x \sin y) dy dx$$

the variable  $y$ , having more points, is the first variable integrated (performing the integration shown on the right.) This allows the SGLNQ2 subroutine and the FUN1 evaluation to achieve optimal performance. Therefore, the  $x$  and  $y$  variables correspond to T and S in the FUN2 subroutine. Also, the  $x$  and  $y$  variables correspond to the C, D, N2 and A, B, N1 sets of arguments, respectively, for SGLNQ2.

## SGLNQ2 and DGLNQ2

The user-supplied subroutine FUN2, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN2 (S,N1,T,N2,Z,LDZ)
  INTEGER*4 N1,N2,LDZ
  REAL*4 S(*),T(*),Z(LDZ,*)
  DO 1 J=1,N2
  DO 2 I=1,N1
2    Z(I,J)=COS(T(J))*SIN(S(I))
1    CONTINUE
  RETURN
  END
```

**Note:** The same coding principles for achieving good performance that are noted in “Example 1” on page 978 also apply to this user-supplied subroutine FUN2.

### Program Statements and Input:

```
EXTERNAL FUN2.
.
.
.
          SUBF   A   B   N1   C   D   N2   Z   LDZ
YXINT = SGLNQ2( FUN2 , 0.0 , 20.0 , 48 , 0.0 , 1.0 , 5 , Z , 48 )
.
.
.
```

FUN2 = (see above)  
Z = (not relevant)

### Output:

YXINT = 0.4981

## SGLGQ and DGLGQ — Numerical Quadrature Performed on a Function Using Gauss-Laguerre Quadrature

### Purpose

These functions approximate the integral of a real valued function over a semi-infinite interval, using the Gauss-Laguerre Quadrature method of specified order.

Table 174. Data Types

<i>a</i> , <i>b</i> , <b>Result</b>	<b>Subroutine</b>
Short-precision real	SGLGQ
Long-precision real	DGLGQ

### Syntax

<b>Fortran</b>	SGLGQ   DGLGQ ( <i>subf</i> , <i>a</i> , <i>b</i> , <i>n</i> )
<b>C and C++</b>	sglgq   dglgq ( <i>subf</i> , <i>a</i> , <i>b</i> , <i>n</i> );

### On Entry

*subf* is the user-supplied subroutine that evaluates the integrand function. The subroutine should be defined with three arguments: *t*, *y*, and *n*. For details, see “Programming Considerations for the SUBF Subroutine” on page 966.

Specified as: *subf* must be declared as an external subroutine in your application program. It can be whatever name you choose.

*a* has the following meaning, where:

If  $b > 0$ , it is the lower limit of integration.

If  $b < 0$ , it is the upper limit of integration.

Specified as: a number of the data type indicated in Table 174.

*b* is the scaling constant *b* for the exponential.

Specified as: a number of the data type indicated in Table 174;  $b > 0$  or  $b < 0$ .

*n* is the order of the quadrature method to be used.

Specified as: a fullword integer;  $n = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, \text{ or } 64$ .

### On Return

*Function value*

is the approximation of the integral. Returned as: a number of the data type indicated in Table 174.

### Notes

1. Declare the DGLGQ function in your program as returning a long-precision real number. Declare the SGLGQ function, if necessary, as returning a short-precision real number.

- The subroutine specified for *subf* must be declared as external in your program. Also, data types used by *subf* must agree with the data types specified by this ESSL subroutine. The variable  $x$ , described under "Function," and the argument  $n$  correspond to the *subf* arguments  $t$  and  $n$ , respectively. For details on how to set up the subroutine, see "Programming Considerations for the SUBF Subroutine" on page 966.

## Function

The integral is approximated for a real valued function over a semi-infinite interval, using the Gauss-Laguerre Quadrature method of specified order. The region of integration is:

$$\begin{aligned} (a, \infty) & \quad \text{if } b > 0 \\ (-\infty, a) & \quad \text{if } b < 0 \end{aligned}$$

The method of order  $n$  is theoretically exact for integrals of the following form, where  $f$  is a polynomial of degree less than  $2n$ :

$$\int_a^{\infty} f(x)e^{-bx} dx \quad \text{if } b > 0$$

$$\int_{-\infty}^a f(x)e^{-bx} dx \quad \text{if } b < 0$$

The method of order  $n$  is a good approximation when your integrand is closely approximated by a function of the form  $f(x)e^{-bx}$ , where  $f$  is a polynomial of degree less than  $2n$ . See references [28] and [96]. The result is returned as the function value.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

- $b = 0$
- $n$  is not an allowable value, as listed in the syntax for this argument.

## Examples

### Example 1

This example shows how to compute the integral of the function  $f$  given by:

$$f(x) = \sin(3.0x)e^{-1.5x}$$

over the interval  $(-2.0, \infty)$ , using the Gauss-Laguerre method with 20 points:

$$\int_{-2.0}^{\infty} (\sin(3.0x)e^{-1.5x}) dx$$

The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in Fortran as follows:



```

SUBROUTINE FUN1 (T,Y,N)
INTEGER*4 N
REAL*4 T(*),Y(*)
DO 1 I=1,N
1  Y(I)=SIN(3.0*T(I))*EXP(-1.5*T(I))
RETURN
END

```

**Program Statements and Input:**

```

EXTERNAL FUN1
.
.
.
      SUBF      A      B      N
      |        |        |        |
XINT = SGLGQ( FUN1 , -2.0 , 1.5 , 20 )
.
.
.

```

FUN1 = (see above)

**Output:**

XINT = 5.891

**Example 2**

This example shows how to compute the integral of the function  $f$  given by:

$$f(x) = \sin(3.0x)e^{1.5x}$$

over the interval  $(-\infty, -2.0)$ , using the Gauss-Laguerre method with 20 points:

$$\int_{-\infty}^{-2.0} \sin(3.0x)e^{1.5x} dx$$

The user-supplied subroutine FUN2, which evaluates the integrand function, is coded in Fortran as follows:

```

SUBROUTINE FUN2 (T,Y,N)
INTEGER*4 N
REAL*4 T(*),Y(*),TEMP
DO 1 I=1,N
1  Y(I)=SIN(3.0*T(I))*EXP(1.5*T(I))
RETURN
END

```

**Program Statements and Input:**

```

EXTERNAL FUN2
.
.
.
      SUBF      A      B      N
      |        |        |        |
XINT = SGLGQ( FUN2 , -2.0 , -1.5 , 20 )
.
.
.
FUN2 = (see above)

```

**Output:**

XINT = -0.011

## SGRAQ and DGRAQ — Numerical Quadrature Performed on a Function Using Gauss-Rational Quadrature

### Purpose

These functions approximate the integral of a real valued function over a semi-infinite interval, using the Gaussian-Rational quadrature method of specified order.

Table 175. Data Types

<i>a, b</i> , <b>Result</b>	<b>Subroutine</b>
Short-precision real	SGRAQ
Long-precision real	DGRAQ

### Syntax

<b>Fortran</b>	SGRAQ   DGRAQ ( <i>subf</i> , <i>a</i> , <i>b</i> , <i>n</i> )
<b>C and C++</b>	sgraq   dgraq ( <i>subf</i> , <i>a</i> , <i>b</i> , <i>n</i> );

### On Entry

*subf* is the user-supplied subroutine that evaluates the integrand function. The subroutine should be defined with three arguments: *t*, *y*, and *n*. For details, see “Programming Considerations for the SUBF Subroutine” on page 966.

Specified as: *subf* must be declared as an external subroutine in your application program. It can be whatever name you choose.

*a* has the following meaning, where:

If  $a+b > 0$ , it is the lower limit of integration.

If  $a+b < 0$ , it is the upper limit of integration.

Specified as: a number of the data type indicated in Table 175.

*b* is the centering constant *b* for the integrand.

Specified as: a number of the data type indicated in Table 175.

*n* is the order of the quadrature method to be used.

Specified as: a fullword integer;  $n = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 64, 96, 128, \text{ or } 256$ .

### On Return

*Function value*

is the approximation of the integral. Returned as: a number of the data type indicated in Table 175.

### Notes

1. Declare the DGRAQ function in your program as returning a long-precision real number. Declare the SGRAQ function, if necessary, as returning a short-precision real number.

2. The subroutine specified for *subf* must be declared as external in your program. Also, data types used by *subf* must agree with the data types specified by this ESSL subroutine. The variable  $x$ , described under “Function,” and the argument  $n$  correspond to the *subf* arguments  $t$  and  $n$ , respectively. For details on how to set up the subroutine, see “Programming Considerations for the SUBF Subroutine” on page 966.

## Function

The integral is approximated for a real valued function over a semi-infinite interval, using the Gauss-Rational quadrature method of specified order. The region of integration is:

$$\begin{aligned} (a, \infty) & \quad \text{if } a+b > 0 \\ (-\infty, a) & \quad \text{if } a+b < 0 \end{aligned}$$

The method of order  $n$  is theoretically exact for integrals of the following form, where  $f$  is a polynomial of degree less than  $2n$ :

$$\int_a^{\infty} f\left(\frac{1}{x+b}\right) \frac{1}{(x+b)^2} dx \quad \text{if } a+b > 0$$

$$\int_{-\infty}^a f\left(\frac{1}{x+b}\right) \frac{1}{(x+b)^2} dx \quad \text{if } a+b < 0$$

The method of order  $n$  is a good approximation when your integrand is closely approximated by a function of the following form, where  $f$  is a polynomial of degree less than  $2n$ :

$$f\left(\frac{1}{x+b}\right) \frac{1}{(x+b)^2}$$

See references [28] and [96]. The result is returned as the function value to a Fortran, C, or C++ program.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $a+b = 0$
2.  $n$  is not an allowable value, as listed in the syntax for this argument.

## Examples

### Example 1

This example shows how to compute the integral of the function  $f$  given by:

$$f(x) = (e^{1.0/x}) / x^2$$

## SGRAQ and DGRAQ

over the interval  $(-\infty, -2.0)$ , using the Gauss-Rational method with 10 points:

$$\int_{-\infty}^{-2.0} \left( \frac{e^{1.0/x}}{x^2} \right) dx$$

The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN1 (T,Y,N)
  INTEGER*4 N
  REAL*4 T(*),Y(*),TEMP
  DO 1 I=1,N
    TEMP=1.0/T(I)
1    Y(I)=EXP(TEMP)*TEMP**2
  RETURN
  END
```

### Program Statements and Input:

```
EXTERNAL FUN1
.
.
.
      SUBF      A      B      N
XINT = SGRAQ(  FUN1 , -2.0 , 0.0 , 10 )
.
.
.
```

FUN1 = (see above)

### Output:

XINT = 0.393

## Example 2

This example shows how to compute the integral of the function  $f$  given by:

$$f(x) = (x-3.0)^{-2} + 10(x-3.0)^{-11}$$

over the interval  $(4.0, \infty)$ , using the Gauss-Rational method with 6 points:

$$\int_{4.0}^{\infty} \left( (x-3.0)^{-2} + 10(x-3.0)^{-11} \right) dx$$

The user-supplied subroutine FUN2, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN2 (T,Y,N)
  INTEGER*4 N
  REAL*4 T(*),Y(*),TEMP
  DO 1 I=1,N
    TEMP=1.0/(T(I)-3.0)
1    Y(I)=TEMP**2+10.0*TEMP**11
  RETURN
  END
```

### Program Statements and Input:

```

EXTERNAL FUN2
      .
      .
      .
      SUBF   A   B   N
      |     |   |   |
XINT = SGRAQ( FUN2 , 4.0 , -3.0 , 6 )
      .
      .
      .
FUN2      = (see above)

```

**Output:**

```

XINT      = 2.00

```

## SGHMQ and DGHMQ — Numerical Quadrature Performed on a Function Using Gauss-Hermite Quadrature

### Purpose

These functions approximate the integral of a real valued function over the entire real line, using the Gauss-Hermite Quadrature method of specified order.

Table 176. Data Types

<i>a, b</i> , Result	Subroutine
Short-precision real	SGHMQ
Long-precision real	DGHMQ

### Syntax

Fortran	SGHMQ   DGHMQ ( <i>subf, a, b, n</i> )
C and C++	sghmq   dghmq ( <i>subf, a, b, n</i> );

### On Entry

- subf* is the user-supplied subroutine that evaluates the integrand function. The subroutine should be defined with three arguments: *t*, *y*, and *n*. For details, see “Programming Considerations for the SUBF Subroutine” on page 966.
- Specified as: *subf* must be declared as an external subroutine in your application program. It can be whatever name you choose.
- a* is the centering constant *a* for the exponential.
- Specified as: a number of the data type indicated in Table 176.
- b* is the scaling constant *b* for the exponential.
- Specified as: a number of the data type indicated in Table 176;  $b > 0$ .
- n* is the order of the quadrature method to be used.
- Specified as: a fullword integer;  $n = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 64, \text{ or } 96$ .

### On Return

*Function value*

is the approximation of the integral. Returned as: a number of the data type indicated in Table 176.

### Notes

1. Declare the DGHMQ function in your program as returning a long-precision real number. Declare the SGHMQ function, if necessary, as returning a short-precision real number.
2. The subroutine specified for *subf* must be declared as external in your program. Also, data types used by *subf* must agree with the data types specified by this ESSL subroutine. The variable *x*, described under “Function” on page 989, and

the argument  $n$  correspond to the *subf* arguments  $t$  and  $n$ , respectively. For details on how to set up the subroutine, see “Programming Considerations for the SUBF Subroutine” on page 966.

## Function

The integral is approximated for a real valued function over the entire real line, using the Gauss-Hermite Quadrature method of specified order. The region of integration is from  $-\infty$  to  $\infty$ . The method of order  $n$  is theoretically exact for integrals of the following form, where  $f$  is a polynomial of degree less than  $2n$ :

$$\int_{-\infty}^{\infty} f(x)e^{-b(x-a)^2} dx$$

The method of order  $n$  is a good approximation when your integrand is closely approximated by a function of the following form, where  $f$  is a polynomial of degree less than  $2n$ :

$$f(x)e^{-b(x-a)^2}$$

See references [28] and [96]. The result is returned as the function value to a Fortran, C, or C++ program.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $b \leq 0$
2.  $n$  is not an allowable value, as listed in the syntax for this argument.

## Examples

### Example

This example shows how to compute the integral of the function  $f$  given by:

$$f(x) = x^2 e^{-2(x+5.0)^2}$$

over the interval  $(-\infty, \infty)$ , using the Gauss-Hermite method with 4 points:

$$\int_{-\infty}^{\infty} \left( x^2 e^{-2(x+5.0)^2} \right) dx$$

The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN1 (T,Y,N)
  INTEGER*4 N
  REAL*4 T(*),Y(*)
```

## SGHMQ and DGHMQ

```
DO 1 I=1,N
1  Y(I)=T(I)**2*EXP(-2.0*(T(I)+5.0)**2)
RETURN
END
```

### Program Statements and Input:

```
EXTERNAL FUN1
.
.
.
      SUBF      A      B      N
      |         |         |         |
XINT = SGHMQ( FUN1 , -5.0 , 2.0 , 4 )
.
.
.
```

FUN1 = (see above)

### Output:

XINT = 31.646



---

## Chapter 16. Random Number Generation

The random number generation subroutines are described in this chapter.

---

### Overview of the Random Number Generation Subroutines

Random number generation subroutines generate uniformly distributed random numbers or normally distributed random numbers (Table 177).

Table 177. List of Random Number Generation Subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Generate a Vector of Uniformly Distributed Random Numbers	SURAND	DURAND	993
Generate a Vector of Normally Distributed Random Numbers	SNRAND	DNRAND	996
Generate a Vector of Long Period Uniformly Distributed Random Numbers	SURXOR	DURXOR	1000

---

### Use Considerations

If you need a very long period random number generator, you should use SURXOR and DURXOR, rather than SURAND and DURAND, respectively. The very long period of the generator used by SURXOR and DURXOR,  $2^{1279}-1$ , makes it useful in modern statistical simulations in which the shorter period of other generators can be exhausted during a single run. As a result, if you need a large number of random numbers, you can use these subroutines, because with this generator, you are not be requesting more than a small percentage of the entire period of the generator.

---

## **Random Number Generation Subroutines**

This section contains the random number generation subroutine descriptions.

## SURAND and DURAND — Generate a Vector of Uniformly Distributed Random Numbers

### Purpose

These subroutines generate vector  $x$  of uniform (0,1) pseudo-random numbers, using the multiplicative congruential method with a user-specified seed.

Table 178. Data Types

$x$	$seed$	Subroutine
Short-precision real	Long-precision real	SURAND
Long-precision real	Long-precision real	DURAND

**Note:** If you need a very long period random number generator, use SURXOR and DURXOR instead of these subroutines.

### Syntax

<b>Fortran</b>	CALL SURAND   DURAND ( $seed, n, x$ )
<b>C and C++</b>	surand   durand ( $seed, n, x$ );

### On Entry

$seed$

is the initial value used to generate the random numbers.

Specified as: a number of the data type indicated in Table 178. It should be a whole number; that is, the fraction part should be 0. (If you specify a mixed number, it is truncated.) Its value must be  $1.0 \leq seed < (2147483647.0 = 2^{31}-1)$ .

**Note:**  $seed$  is always a long-precision real number, even in SURAND.

$n$

is the number of random numbers to be generated.

Specified as: a fullword integer;  $n \geq 0$ .

$x$

See "On Return."

### On Return

$seed$

is the new seed that is to be used to generate additional random numbers in subsequent invocations of SURAND or DURAND.

Returned as: a number of the data type indicated in Table 178. It is a whole number whose value is  $1.0 \leq seed < (2147483647.0 = 2^{31}-1)$ .

$x$

is a vector of length  $n$ , containing the uniform pseudo-random numbers with values between 0 and 1. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 178.

### Notes

In your C program, argument  $seed$  must be passed by reference.

## Function

The uniform (0,1) pseudo-random numbers are generated as follows, using the multiplicative congruential method:

$$s_i = (a(s_{i-1})) \bmod(m) = (a^i s_0) \bmod(m)$$

$$x_i = s_i/m \quad \text{for } i = 1, 2, \dots, n$$

where:

$s_i$  is a random sequence.

$x_i$  is a random number.

$s_0$  is the initial seed provided by the caller.

$a = 7^5 = 16807.0$

$m = 2^{31}-1 = 2147483647.0$

$n$  is the number of random numbers to be generated.

See references [79] and [83]. If  $n$  is 0, no computation is performed, and the initial seed is unchanged.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $n < 0$
2.  $seed < 1.0$  or  $seed \geq 2147483647.0$

## Examples

### Example 1

This example shows a call to SURAND to generate 10 random numbers.

#### Call Statement and Input:

```

          SEED   N   X
          |     |   |
CALL SURAND( SEED , 10 , X )

```

SEED = 80629.0

**Note:** It is important to note that SEED is a long-precision number, even though X contains short-precision numbers.

#### Output:

SEED = 759150100.0

X = (0.6310323,  
0.7603202,  
0.7015232,  
0.5014868,  
0.4895853,  
0.4602344,  
0.1603608,  
0.1832564,  
0.9899062,  
0.3535068)

**Example 2**

This example shows a call to DURAND to generate 10 random numbers.

**Call Statement and Input:**

```
          SEED  N  X  
          |    |  |  
CALL DURAND( SEED , 10 , X )
```

```
SEED      = 80629.0
```

**Output:**

```
SEED      = 759150100.0
```

```
X         = (0.6310323270182275,  
            0.7603201953509451,  
            0.7015232633340746,  
            0.5014868557925740,  
            0.4895853057920864,  
            0.4602344475967038,  
            0.1603607578018497,  
            0.1832563756887132,  
            0.9899062002030695,  
            0.3535068129904134)
```

## SNRAND and DNRAND — Generate a Vector of Normally Distributed Random Numbers

### Purpose

These subroutines generate vector  $x$  of normally distributed pseudo-random numbers, with a mean of 0 and a standard deviation of 1, using Polar methods with a user-specified seed.

Table 179. Data Types

$x, aux$	$seed$	Subroutine
Short-precision real	Long-precision real	SNRAND
Long-precision real	Long-precision real	DNRAND

### Syntax

Fortran	CALL SNRAND   DNRAND ( $seed, n, x, aux, naux$ )
C and C++	snrand   dnrnd ( $seed, n, x, aux, naux$ );

### On Entry

- $seed$  is the initial value used to generate the random numbers.  
Specified as: a number of the data type indicated in Table 179. It must be a whole number; that is, the fraction part must be 0. Its value must be  $1.0 \leq seed < (2147483647.0 = 2^{31}-1)$ .
- Note:**  $seed$  is always a long-precision real number, even in SNRAND.
- $n$  is the number of random numbers to be generated.  
Specified as: a fullword integer;  $n$  must be an even number and  $n \geq 0$ .
- $x$  See "On Return" on page 997.
- $aux$  has the following meaning:  
If  $naux = 0$  and error 2015 is unrecoverable,  $aux$  is ignored.  
Otherwise, it is the storage work area used by this subroutine. Its size must be greater than or equal to  $n/2$ .  
Specified as: an area of storage, containing numbers of the data type indicated in Table 179. They can have any value.
- $naux$  is the size of the work area specified by  $aux$ .  
Specified as: a fullword integer, where:  
If  $naux = 0$  and error 2015 is unrecoverable, SNRAND and DNRAND dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.  
Otherwise,  $naux \geq n/2$ .

**On Return**

- seed* is the new seed that is to be used to generate additional random numbers in subsequent invocations of SNRAND or DNRAND. Returned as: a number of the data type indicated in Table 179 on page 996. It is a whole number whose value is  $1.0 \leq \text{seed} < (2147483647.0 = 2^{31}-1)$ .
- x* is a vector of length  $n$ , containing the normally distributed pseudo-random numbers. Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 179 on page 996.

**Notes**

1. In your C program, argument *seed* must be passed by reference.
2. Vector *x* must have no common elements with the storage area specified for *aux*; otherwise, results are unpredictable.
3. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 36.

**Function**

The normally distributed pseudo-random numbers, with a mean of 0 and a standard deviation of 1, are generated as follows, using Polar methods with a user-specified seed. The Polar method, which this technique is based on, was developed by G. E. P. Box, M. E. Muller, and G. Marsaglia and is described in reference [79].

1. Using *seed*, a vector of uniform (0,1) pseudo-random numbers,  $u_i$  for  $i = 1, n$ , is generated by calling SURAND or DURAND, respectively. These  $u_i$  values are then used in the subsequent steps.
2. All  $(y_j, z_j)$  for  $j = 1, n/2$  are set as follows, where each  $(y, z)$  is a point in the square  $-1$  to  $1$ :

$$\begin{aligned} y_j &= 2u_{2j-1}-1 \\ z_j &= 2u_{2j}-1 \end{aligned}$$

3. All  $p_j$  for  $j = 1, n/2$  are set as follows, where each  $p$  measures the square of the radius of  $(y, z)$ :

$$p_j = y_j^2 + z_j^2$$

If  $p_j \geq 1$ , then  $p_j$  is discarded, and steps 1 through 3 are repeated until  $p_j < 1$ .

4. All  $x_i$  for  $i = 1, n$  are set as follows to produce the normally distributed random numbers:

$$\begin{aligned} x_{2j-1} &= y_j ((-2 \ln p_j) / p_j)^{0.5} \\ x_{2j} &= z_j ((-2 \ln p_j) / p_j)^{0.5} \\ &\text{for } j = 1, n/2 \end{aligned}$$

If  $n$  is 0, no computation is performed, and the initial seed is unchanged.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n < 0$  or  $n$  is an odd number
2.  $seed < 1.0$  or  $seed \geq 2147483647.0$
3. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows a call to SNRAND to generate 10 random numbers.

#### Call Statement and Input:

```

          SEED  N    X    AUX  NAUX
          |    |    |    |    |
CALL SNRAND( SEED , 10 , X , AUX , 5 )

```

```
SEED      = 80629.0
```

**Note:** It is important to note that SEED is a long-precision number, even though X contains short-precision numbers.

#### Output:

```
SEED      = 48669425.0
```

```
X         = (0.660649538,
            1.312503695,
            1.906438112,
            0.014065863,
            -0.800935328,
            -3.058144093,
            -0.397426069,
            -0.370634943,
            -0.064151444,
            -0.275887042)
```

### Example 2

This example shows a call to DNRAND to generate 10 random numbers.

#### Call Statement and Input:

```

          SEED  N    X    AUX  NAUX
          |    |    |    |    |
CALL DNRAND( SEED , 10 , X , AUX , 5 )

```

```
SEED      = 80629.0
```

#### Output:

```
SEED      = 48669425.0
```

```
X         = (0.6606495655963802,
            1.3125037758861060,
            1.9064381379483730,
            0.0140658628770495,
```



```
-0.8009353314494653,  
-3.0581441239248530,  
-0.3974260845722100,  
-0.3706349643478605,  
-0.0641514443372939,  
-0.2758870630332470)
```

## SURXOR and DURXOR — Generate a Vector of Long Period Uniformly Distributed Random Numbers

### Purpose

These subroutines generate a vector  $x$  of uniform  $[0,1)$  pseudo-random numbers, using the Tausworthe exclusive-or algorithm.

Table 180. Data Types

$x, vseed$	$iseed$	Subroutine
Short-precision real	Integer	SURXOR
Long-precision real	Integer	DURXOR

### Syntax

<b>Fortran</b>	CALL SURXOR   DURXOR ( $iseed, n, x, vseed$ )
<b>C and C++</b>	surxor   durxor ( $iseed, n, x, vseed$ );

### On Entry

$iseed$

has the following meaning, where:

If  $iseed \neq 0$ ,  $iseed$  is the initial value used to generate the random numbers. You specify  $iseed \neq 0$  when you call this subroutine for the first time or when you changed  $vseed$  between calls to this subroutine.

If  $iseed = 0$ ,  $vseed$  is used to generate the random numbers, where  $vseed$  was initialized by an earlier call to this subroutine. ESSL assumes you have not changed  $vseed$  between calls to this subroutine, when you specify  $iseed = 0$ .

Specified as: a fullword integer, as indicated in Table 180.

$n$

is the number of random numbers to be generated.

Specified as: a fullword integer;  $n \geq 0$ .

$x$

See "On Return."

$vseed$

is the work area used by this subroutine and has the following meaning, where:

If  $iseed \neq 0$ ,  $vseed$  is not used for input. The work area can contain anything.

If  $iseed = 0$ ,  $vseed$  contains the seed vector generated by a preceding call to this subroutine.  $vseed$  is used in this computation to generate the new random numbers. It should not be changed between calls to this subroutine.

Specified as: a one-dimensional array of (at least) length 10000, containing numbers of the data type indicated in Table 180.

### On Return

$iseed$

is set to 0 for subsequent calls to SURXOR or DURXOR. Returned as: a fullword integer, as indicated in Table 180.

$x$

is a vector of length  $n$ , containing the uniform pseudo-random

numbers with the following values:  $0 \leq x < 1$ . Returned as: a one-dimensional array of (at least) length  $n$ , containing numbers of the data type indicated in Table 180 on page 1000.

*vseed* is the work area used by these subroutines, containing the new seed that is to be used in subsequent calls to this subroutine. Returned as: a one-dimensional array of (at least) length 10000, containing numbers of the data type indicated in Table 180 on page 1000.

## Notes

1. You can generate the same vector  $x$  of random numbers by starting over and specifying your original nonzero *iseed* value.
2. Multiple calls to these subroutines with mixed sizes generate the same sequence of numbers as a single call the total length, assuming you specify the same initial *iseed* in both cases. For example, you can generate the same vector  $x$  of random numbers by calling this subroutine twice and specifying  $n = 10$  or by calling this subroutine once and specifying  $n = 20$ . You need to specify the same *iseed* in the initial call in both cases, and *iseed* = 0 in the second call with  $n = 10$ .
3. Vector  $x$  must have no common elements with the storage area specified for *vseed*; otherwise, results are unpredictable.
4. In your C program, argument *iseed* must be passed by reference.

## Function

The pseudo-random numbers uniformly distributed in the interval [0,1) are generated using the Tausworthe exclusive-or algorithm. This is based on a linear-feedback shift-register sequence. The very long period of the generator,  $2^{1279}-1$ , makes it useful in modern statistical simulations where the shorter period of other generators could be exhausted during a single run. If you need a large number of random numbers, you can use these subroutines, because with this generator you do not request more than a small percentage of the entire period of the generator.

This generator is based on two feedback positions to generate a new binary digit:

$$z_k = z_{(k-p)} \oplus z_{(k-q)}$$

where:

$p > q$   
 $k = 1, 2, \dots$   
 $z$  is a bit vector.  
 and where:

$\oplus$  is the bitwise exclusive-or operation.

For details, see references [55], [77], and [98]. The values of  $p$  and  $q$  are selected according to the criteria stated in reference [104].

## SURXOR and DURXOR

The algorithm initializes a seed vector of length  $p$ , starting with *iseed*. The seed vector is stored in *vseed* for use in subsequent calls to this subroutine with *iseed* = 0.

If  $n$  is 0, no computation is performed, and the initial seed is unchanged.

### Special Usage

For some specialized applications, if you need multiple sources of random numbers, you can specify different *vseed* areas, which are initialized with different seeds on multiple calls to this subroutine. You then get multiple sequences of the random number sequence provided by the generator that are sufficiently far apart for most purposes.

### Error conditions

#### Computational Errors

None.

#### Input-Argument Errors

1.  $n < 0$
2. *iseed* = 0 and *vseed* does not contain valid data.

### Examples

#### Example 1

This example shows a call to SURXOR to generate 10 random numbers.

##### Call Statement and Input:

```
          ISEED   N   X   VSEED
          |       |   |   |
CALL SURXOR( ISEED , 10 , X , VSEED )
```

```
ISEED   = 137
```

##### Output:

```
ISEED   = 0
X       = (0.6440868,
          0.5105118,
          0.4878680,
          0.3209075,
          0.6624528,
          0.2499877,
          0.0056630,
          0.7329214,
          0.7486335,
          0.8050517)
```

#### Example 2

This example shows a call to SURXOR to generate 10 random numbers. This example specifies *iseed* = 0 and uses the *vseed* output generated from Example 1.

##### Call Statement and Input:

```
          ISEED   N   X   VSEED
          |       |   |   |
CALL SURXOR( ISEED , 10 , X , VSEED )
```

```
ISEED   = 0
```

**Output:**

```

ISEED   =  0

X       = (0.9930249,
           0.0441873,
           0.6891295,
           0.3101060,
           0.6324178,
           0.3299408,
           0.3553145,
           0.0100013,
           0.0214620,
           0.8059390)

```

**Example 3**

This example shows a call to DURXOR to generate 20 random numbers. This sequence of numbers generated are like those generated in Examples 1 and 2.

**Call Statement and Input:**

```

           ISEED   N   X   VSEED
           |       |   |   |
CALL DURXOR( ISEED , 20 , X , VSEED )

```

```

ISEED   =  137

```

**Output:**

```

ISEED   =  0

X       = (0.64408693438956721,
           0.51051182536460882,
           0.48786801310787142,
           0.32090755617007050,
           0.66245283144861666,
           0.24998782843358081,
           0.00566308101257373,
           0.73292147005172925,
           0.74863359794102236,
           0.80505169697755319,
           0.99302499462139138,
           0.04418740640269125,
           0.68912952155409579,
           0.31010611495627916,
           0.63241786342211936,
           0.32994081459690583,
           0.35531452631408911,
           0.01000134413132581,
           0.02146199494672940,
           0.80593898487597615)

```

## SURXOR and DURXOR

---

## Chapter 17. Utilities

The utility subroutines are described in this chapter.

---

### Overview of the Utility Subroutines

The utility subroutines perform general service functions that support ESSL, rather than mathematical computations (Table 181).

Table 181. List of Utility Subroutines

Descriptive Name	Subroutine	Page
ESSL Error Information-Handler Subroutine	EINFO	1008
ESSL ERRSAV Subroutine	ERRSAV	1011
ESSL ERRSET Subroutine	ERRSET	1012
ESSL ERRSTR Subroutine	ERRSTR	1014
Set the Vector Section Size (VSS) for the ESSL/370 Scalar Library	IVSSET <sup>‡</sup>	
Set the Extended Vector Operations Indicator for the ESSL/370 Scalar Library	IEVOPS <sup>‡</sup>	
Determine the Level of ESSL Installed	IESSL	1015
Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines	STRIDE	1017
Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode	DSRSM	1026
For a General Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode	DGKTRN	1030
For a Symmetric Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode	DSKTRN	1035
<sup>‡</sup> This subroutine is provided for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutines is no longer provided.		

---

### Use Considerations

This section describes what you use the utility subroutines for.

#### Determining the Level of ESSL Installed

IESSL gets the level of ESSL and returns it to your program. The level consists of the following: version number, release number, modification number, and number of the most recently installed ESSL PTF. You can use this function to verify that you are running on or using the capabilities of the desired level.

#### Finding the Optimal Stride(s) for Your Fourier Transforms

STRIDE is used to determine optimal stride values for your Fourier transforms when using any of the Fourier transform subroutines, except `_RCFT` and `_CRFT`. You must invoke STRIDE for each optimal stride you want computed. Sometimes you need a separate stride for your input and output data. For the three-dimensional Fourier transforms, you need an optimal stride for both the second and third dimensions of the array. The examples provided for STRIDE explain how it is used for each of the subroutines listed above.

## Utility Subroutines

After obtaining the optimal strides from `STRIDE`, you should arrange your data using these stride values. After the data is set up, call the Fourier transform subroutine. For additional information on how to set up your data, see “Setting Up Your Data” on page 782.

### Converting Sparse Matrix Storage

`DSRSM` is used to migrate your existing program from sparse matrices stored by rows to sparse matrices stored in compressed-matrix storage mode. This converts the matrices into a storage format that is compatible with the input requirements for some ESSL sparse matrix subroutines, such as `DSMMX`.

`DGKTRN` and `DSKTRN` are used to convert your sparse matrix from one skyline storage mode to another, if necessary, before calling the subroutines `DGKFS/DGKFSP` or `DSKFS/DSKFSP`, respectively.



---

## Utility Subroutines

This section contains the utility subroutine descriptions.

## EINFO — ESSL Error Information-Handler Subroutine

### Purpose

This subroutine returns information to your program about the data involved in a computational error that occurred in an ESSL subroutine. This is the same information that is provided in the ESSL messages; however, it allows you to check the information in your program at run time and continue processing. You pass the computational error code of interest to this subroutine in *icode*, and it passes back one or more pieces of information in the output arguments *inf1* and, optionally, *inf2*, as defined in Table 182. **You should use this subroutine only for those computational errors listed in the table. It does not apply to computational errors that do not return information.**

For multithreaded application programs, if you want the error handling capabilities that this subroutine provides to be implemented on each thread created by your program, this subroutine must be called from each thread. If your application creates multiple threads, the action performed by a call to this subroutine applies to the thread that this subroutine was invoked from. For an example, see “Example of Handling Errors in a Multithreaded Application Program” on page 127.

Table 182. Computational Error Information Returned by EINFO

Error Code	Receiver	Type of Information
2100	<i>inf1</i>	Lower range of a vector
	<i>inf2</i>	Upper range of a vector
2101	<i>inf1</i>	Index of the eigenvalue that failed to converge
	<i>inf2</i>	Number of iterations after which it failed to converge
2102	<i>inf1</i>	Index of the last eigenvector that failed to converge
	<i>inf2</i>	Number of iterations after which it failed to converge
2103	<i>inf1</i>	Index of the pivot with zero value
2104	<i>inf1</i>	Index of the last pivot with nonpositive value
2105	<i>inf1</i>	Index of the pivot element near zero causing factorization to fail
2107	<i>inf1</i>	Index of the singular value that failed to converge
	<i>inf2</i>	Number of iterations after which it failed to converge
2109	<i>inf1</i>	Iteration count when it was determined that the matrix was not definite
2114	<i>inf1</i>	Index of the last eigenvalue that failed to converge
	<i>inf2</i>	Number of iterations after which it failed to converge
2115	<i>inf1</i>	Order of the leading minor that was discovered to have a nonpositive determinant
2117	<i>inf1</i>	Column number for which pivot value was near zero
2118	<i>inf1</i>	Row number for which pivot value was near zero
2120	<i>inf1</i>	Row number of empty row where factorization failed
2121	<i>inf1</i>	Column number of empty column where factorization failed

Table 182. Computational Error Information Returned by EINFO (continued)

Error Code	Receiver	Type of Information
2126	<i>inf1</i>	Row number for which pivot value was unacceptable
2145	<i>inf1</i>	First diagonal element with zero value
2150	<i>inf1</i>	First diagonal element with zero value

## Syntax

<b>Fortran</b>	CALL EINFO ( <i>icode</i> [, <i>inf1</i> [, <i>inf2</i> ]])
<b>C and C++</b>	einfo ( <i>icode</i> , <i>inf1</i> , <i>inf2</i> );

### On Entry

*icode* has the following meaning, where:

If *icode* = 0, this indicates that the ESSL error option table is to be initialized. (You specify this value once in the beginning of your program before calls to ERRSET.)

If *icode* has any of the allowable error code values listed in Table 182 on page 1008, this is the computational error code of interest. (You specify one of these values whenever you want information returned about a computational error.)

Specified as: a fullword integer; *icode* = 0 or an error code value indicated in Table 182 on page 1008.

*inf1* See "On Return."

*inf2* See "On Return."

### On Return

*inf1* has the following meaning, where:

If *icode* = 0, this argument is not used in the computation. In this case, *inf1* is an optional argument, except in C and C++ programs.

If *icode* ≠ 0, then *inf1* is the first information receiver, containing numerical information related to the computational error.

Returned as: a fullword integer.

*inf2* has the following meaning, where:

If *icode* = 0, this argument is not used in the computation.

If *icode* ≠ 0, then *inf2* is the second information receiver, containing numerical information related to the computational error. It should be specified when the error code provides a second piece of information, and you want the information.

In both of these cases, *inf2* is an optional argument, except in C and C++ programs. For more details, see "Notes" on page 1010.

Returned as: a fullword integer.

### Notes

1. If *icode* is not 0 and is not one of the error codes specified in Table 182 on page 1008, this subroutine returns to the caller, and no information is provided in *inf1* and *inf2*.
2. If there are two pieces of information for the error and you specify one output argument, the second piece of information is not returned to the caller.
3. If there is one piece of information for the error and you specify two output arguments, the second output argument is not set by this subroutine.
4. In C and C++ programs you must code the *inf1* and *inf2* arguments, because they are not optional arguments.
5. In Fortran programs, *inf1* and *inf2* are optional arguments. This is an exception to the rule, because other ESSL subroutines do not allow optional arguments.
6. Examples of how to use EINFO are provided in Chapter 4, “Coding Your Program,” on page 111.

---

## ERRSAV — ESSL ERRSAV Subroutine

### Purpose

The ERRSAV subroutine copies an ESSL error option table entry into an 8-byte storage area that is accessible to your program.

For multithreaded application programs, if you want the error handling capabilities that this subroutine provides to be implemented on each thread created by your program, this subroutine must be called from each thread. If your application creates multiple threads, the action performed by a call to this subroutine applies to the thread that this subroutine was invoked from. For an example, see “Example of Handling Errors in a Multithreaded Application Program” on page 127.

### Syntax

Fortran	CALL ERRSAV ( <i>ierno</i> , <i>tabent</i> )
C and C++	errsav ( <i>ierno</i> , <i>tabent</i> );

### On Entry

*ierno* is the error number in the option table. The entry for *ierno* in the ESSL error option table is stored in the 8-byte storage area *tabent*.

Specified as: a fullword integer; *ierno* must be one of the error numbers in the option table. For a list of these numbers, see Table 34 on page 54.

### On Return

*tabent* is the storage area where the option table entry is stored.

Specified as: an area of storage of length 8-bytes.

### Notes

Examples of how to use ERRSAV are provided in Chapter 4, “Coding Your Program,” on page 111.

---

## ERRSET — ESSL ERRSET Subroutine

### Purpose

The ERRSET subroutine allows you to control execution when error conditions occur. It modifies the information in the ESSL error option table for the error number indicated. For a range of error messages, you can specify the following:

- How many times a particular error is allowed to occur before the program is terminated
- How many times a particular error message is printed before printing is suppressed
- Whether the ESSL error exit routine is to be invoked

For multithreaded application programs, if you want the error handling capabilities that this subroutine provides to be implemented on each thread created by your program, this subroutine must be called from each thread. If your application creates multiple threads, the action performed by a call to this subroutine applies to the thread that this subroutine was invoked from. For an example, see “Example of Handling Errors in a Multithreaded Application Program” on page 127.

### Syntax

Fortran	CALL ERRSET ( <i>ierno</i> , <i>inoal</i> , <i>inomes</i> , <i>itrace</i> , <i>iusadr</i> , <i>irange</i> )
C and C++	errset ( <i>ierno</i> , <i>inoal</i> , <i>inomes</i> , <i>itrace</i> , <i>iusadr</i> , <i>irange</i> );

### On Entry

- ierno* is the error number in the option table. The entry for *ierno* in the ESSL error option table is updated as indicated by the other arguments. Specified as: a fullword integer; *ierno* must be one of the error numbers in the option table. For a list of these numbers, see Table 34 on page 54.
- inoal* indicates the number of errors allowed before each execution is terminated, where:
- If  $inoal \leq 0$ , the specification is ignored, and the number-of-errors option is not changed.
- If  $inoal = 1$ , execution is terminated after one error.
- If  $2 \leq inoal \leq 255$ , then *inoal* specifies the number of errors allowed before each execution is terminated.
- If  $inoal > 255$ , an unlimited number of errors is allowed.
- Specified as: a fullword integer, where:
- If  $iusadr = ENOTRM$ , then  $2 \leq inoal \leq 255$ .
- inomes* indicates the number of messages to be printed, where:
- If  $inomes < 0$ , all messages are suppressed.
- If  $inomes = 0$ , the number-of-messages option is not changed.
- If  $0 < inomes \leq 255$ , then *inomes* specifies the number of messages to be printed.

If *inomes* > 255, an unlimited number of error messages is allowed.  
Specified as: a fullword integer.

*itrace* this argument is ignored, but must be specified.  
Specified as: a fullword integer where, *itrace* = 0, 1, or 2 (for migration purposes).

*iusadr* indicates whether or not the ESSL error exit routine is to be invoked, where:  
If *iusadr* is zero, the option table is not altered.  
If *iusadr* is one, the option table is set to show no exit routine. Therefore, standard corrective action is to be used when continuing execution.  
If *iusadr* = ENOTRM, the option table entry is set to the ESSL error exit routine ENOTRM. Therefore, the ENOTRM subroutine is to be invoked after the occurrence of the indicated errors. (ENOTRM must appear in an EXTERNAL statement in your program.)  
Specified as: a 32-bit integer in a 32-bit environment or the name of a subroutine; *iusadr* = 0, 1, or ENOTRM.  
Specified as: a 64-bit integer in a 64-bit environment or the name of a subroutine; *iusadr* = 0\_8, 1\_8, or ENOTRM.

*irange* indicates the range of errors to be updated in the ESSL error option table, where:  
If *irange* < *ierno*, the parameter is ignored.  
If *irange* ≥ *ierno*, the options specified for the other parameters are to be applied to the entire range of error conditions encompassed by *ierno* and *irange*.  
Specified as: a fullword integer.

## Notes

1. Examples of how to use ERRSET are provided in Chapter 4, "Coding Your Program," on page 111.
2. If you specify ENOTRM for *iusadr*, then *inoal* must be in the following range:  
 $2 \leq \textit{inoal} \leq 255$ .

---

## ERRSTR — ESSL ERRSTR Subroutine

### Purpose

The ERRSTR subroutine stores an entry in the ESSL error option table.

For multithreaded application programs, if you want the error handling capabilities that this subroutine provides to be implemented on each thread created by your program, this subroutine must be called from each thread. If your application creates multiple threads, the action performed by a call to this subroutine applies to the thread that this subroutine was invoked from. For an example, see “Example of Handling Errors in a Multithreaded Application Program” on page 127.

### Syntax

Fortran	CALL ERRSTR ( <i>ierno</i> , <i>tabent</i> )
C and C++	errstr ( <i>ierno</i> , <i>tabent</i> );

### On Entry

*ierno* is the error number in the option table. The information in the 8-byte storage area *tabent* is stored into the entry for *ierno* in the ESSL error option table.

Specified as: a fullword integer; *ierno* must be one of the error numbers in the option table. For a list of these numbers, see Table 34 on page 54.

*tabent* is the storage area containing the table entry data.  
Specified as: an area of storage of length 8-bytes.

### Notes

Examples of how to use ERRSTR are provided in Chapter 4, “Coding Your Program,” on page 111.



## IESSL — Determine the Level of ESSL Installed

### Purpose

This function returns the level of ESSL installed on your system, where the level consists of a version number, release number, and modification number, plus the fix number of the most recent PTF installed.

### Syntax

Fortran	IESSL ()
C and C++	iessl ();

### On Return

*Function value*

is the level of ESSL installed on your system. It is provided as a fullword integer in the form *vvrrmmff*, where each two digits represents a part of the level:

- *vv* is the version number.
- *rr* is the release number.
- *mm* is the modification number.
- *ff* is the fix number of the most recent PTF installed.

Returned as: a fullword integer; *vvrrmmff* > 0.

### Notes

1. To use IESSL effectively, you must install your ESSL PTFs in their proper sequential order. As part of the result, IESSL returns the value *ff* of the **most recent** PTF installed, rather than the **highest number** PTF installed. Therefore, if you do not install your PTFs sequentially, the *ff* value returned by IESSL does not reflect the actual level of ESSL.
2. Declare the IESSL function in your program as returning a fullword integer value.

### Function

The IESSL function enables you to determine the current level of ESSL installed on your system. It is useful to you in those instances where your program is using a subroutine or feature that exists only in certain levels of ESSL. It is also useful when your program is dependent upon certain PTFs being applied to ESSL.

### Examples

#### Example

This example shows several ways to use the IESSL function. Most typically, you use IESSL for checking the version and release level of ESSL. Suppose you are dependent on a new capability in ESSL, such as a new subroutine or feature, provided for the first time in ESSL Version 3. You can add the following check in your program before using the new capability:

```
IF IESSL() ≥ 3010000
```

By specifying 0000 for *mmff*, the modification and fix level, you are independent of the order in which your modifications and PTFs are installed.

## IESSL

Less typically, you use IESSL for checking the PTF level of ESSL. Suppose you are dependent on PTF 2 being installed on your ESSL Version 3 system. You want to know whether to call a different user-callable subroutine to set up your array data. You can add the following check in your program before making the call:

```
IF IESSL() ≥ 3010002
```

If your system support group installed the ESSL PTFs in their proper sequential order, this test works properly; otherwise, it is unpredictable.

## STRIDE — Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines

### Purpose

This subroutine determines an optimal stride value for you to use for your input or output data when you are computing large row Fourier transforms in any of the Fourier transform subroutines, except `_RCFT` and `_CRFT`. The strides determined by this subroutine allow your arrays to fit comfortably in various levels of storage hierarchy on your particular processor, thus allowing you to improve your run-time performance.

**Note:** This subroutine returns a single stride value. Where you need multiple strides, you must invoke this subroutine multiple times; for example, in the multidimensional Fourier transforms and, also, when input and output data types differ. For more details, see “Function” on page 1018.

### Syntax

Fortran	CALL STRIDE ( <i>n</i> , <i>incd</i> , <i>incr</i> , <i>dt</i> , <i>iopt</i> )
C and C++	stride ( <i>n</i> , <i>incd</i> , <i>incr</i> , <i>dt</i> , <i>iopt</i> );

### On Entry

- n* is the length *n* of the Fourier transform for which the optimal stride is being determined. The transform corresponding to *n* is usually a row transform; that is, the data elements are stored using a stride value.
- Specified as: a fullword integer;  $n > 0$ .
- incd* is the minimum allowable stride for the Fourier transform for which the optimal stride is being determined. For each situation in each subroutine, there is a specific way to compute this minimum value. This is explained in the examples starting on page 1019.
- Specified as: a fullword integer;  $incd > 0$  or  $incd < 0$ .
- incr* See “On Return.”
- dt* is the data type of the numbers for the Fourier transform for which the optimal stride is being determined, where:
- If *dt* = 'S', the numbers are short-precision real.
- If *dt* = 'D', the numbers are long-precision real.
- If *dt* = 'C', the numbers are short-precision complex.
- If *dt* = 'Z', the numbers are long-precision complex.
- Specified as: a single character; *dt* = 'S', 'D', 'C', or 'Z'.
- iopt* is provided only for migration purposes from ESSL Version 1 and is no longer used; however, you must still specify it as a dummy argument.
- Specified as: a fullword integer; *iopt* = 0, 1, or 2.

### On Return

- incr* is the stride that allows you to improve your run-time performance

in your Fourier transform computation on your particular processor. In general, this value differs for each processor you are running on.

Returned as: a fullword integer;  $incr > 0$  or  $incr < 0$  and  $|incr| \geq |incd|$ , where  $incr$  has the same sign (+ or -) as  $incd$ .

## Notes

1. In your C program, argument *incr* must be passed by reference.
2. All subroutines accept lowercase letters for the *dt* argument.
3. For each situation in each of the Fourier transform subroutines, there is a specific way to compute the value you should specify for the *incd* argument. Details on how to compute each of these values is given in the examples starting on page 1019. See the example corresponding to the Fourier transform subroutine you are using.
4. Where different data types are specified for the input and output data in your Fourier transform subroutine, you should be careful to indicate the correct data type in the *dt* argument in this subroutine.
5. For additional information on how to set up your data, see "Setting Up Your Data" on page 782.

## Function

This subroutine determines an optimal stride, *incr*, for you to use for your input or output data when computing large row Fourier transforms. The stride value returned by this subroutine is based on the size and structure of your transform data, using:

- The size of each data item (*dt*)
- The minimum allowable stride for this transform (*incd*)
- The length of the transform (*n*)

This information is used in determining the optimal stride for the processor you are currently running on. The stride determined by this subroutine allows your arrays to fit comfortably in various levels of storage hierarchy for that processor, thus giving you the ability to improve your run-time performance.

You get only one stride value returned by this subroutine on each invocation. Therefore, in many instances, you may need to invoke this subroutine multiple times to obtain several stride values to use in your Fourier transform computation:

- For multidimensional Fourier transforms using several strides, this subroutine must be called once for each optimal stride you want to obtain. Successive invocations should go from the lower (earlier) dimensions to the higher (later) dimensions, because the results from the lower dimensions are used to calculate the *incd* values for the higher dimensions.
- Where input and output data have different data types and you want to obtain optimal strides for each, this subroutine must be called once for each data type.

Where multiple invocations are necessary, they are explained in the examples starting on page 1019. The examples also explain how to calculate the *incd* values for each invocation. There are nine examples to cover the Fourier transform subroutines that can use the STRIDE subroutine.

After calling this subroutine and obtaining the optimal stride value, you then set up your input or output array accordingly. This may involve movement of data for input arrays or increasing the sizes of input or output arrays. To accomplish this,

you may want to set up a separate subroutine with the stride values passed into it as arguments. You can then dimension your arrays in that subroutine, depending on the values calculated by STRIDE. For additional information on how to set up your data, see “Setting Up Your Data” on page 782.

## Error conditions

### Computational Errors

None

### Input-Argument Errors

1.  $n \leq 0$
2.  $incd = 0$
3.  $iopt \neq 0, 1, \text{ or } 2$
4.  $dt \neq S, D, C, \text{ or } Z$

## Examples

### Example 1—SCFT

This example shows the use of the STRIDE subroutine in computing one-dimensional row transforms using the SCFT subroutine.

If  $inc2x = 1$ , the input sequences are stored in the transposed form as rows of a two-dimensional array  $X(INC1X, N)$ . In this case, the STRIDE subroutine helps in determining a good value of  $inc1x$  for this array. The required minimum value of  $inc1x$  is  $m$ , the number of Fourier transforms being computed. To find a good value of  $inc1x$ , use STRIDE as follows:

```

          N  INCD  INCR   DT   IOPT
          |  |    |    |    |
CALL STRIDE( N , M , INC1X , 'C' , 0 )

```

Here, the arguments refer to the SCFT subroutine. In the following table, values of  $inc1x$  are given (as obtained from the STRIDE subroutine) for some combinations of  $n$  and  $m$  and for POWER3 with 64KB level 1 cache:

N	M	INC1X
128	64	64
240	32	32
240	64	65
256	256	264
512	60	60
1024	64	65

The above example also applies when the output sequences are stored in the transposed form ( $inc2y = 1$ ). In that case, in the above example,  $inc1x$  is replaced by  $inc1y$ .

In computing column transforms ( $inc1x = inc1y = 1$ ), the values of  $inc2x$  and  $inc2y$  are not very important. For these, any value over the required minimum of  $n$  can be used.

### Example 2—DCOSF

This example shows the use of the STRIDE subroutine in computing one-dimensional row transforms using the DCOSF subroutine.

If  $inc2x = 1$ , the input sequences are stored in the transposed form as rows of a two-dimensional array  $X(INC1X, N/2+1)$ . In this case, the STRIDE subroutine helps

## STRIDE

in determining a good value of *inc1x* for this array. The required minimum value of *inc1x* is *m*, the number of Fourier transforms being computed. To find a good value of *inc1x*, use STRIDE as follows:

```
          N   INCD  INCR   DT  IOPT
          |   |    |    |   |    |
CALL STRIDE( N/2+1 , M , INC1X , 'D' , 0 )
```

Here, the arguments refer to the DCOSF subroutine. In the following table, values of *inc1x* are given (as obtained from the STRIDE subroutine) for some combinations of *n* and *m* and for POWER3 with 64KB level 1 cache:

N	M	INC1X
128	64	64
240	32	32
240	64	64
256	256	264
512	60	60
1024	64	65

The above example also applies when the output sequences are stored in the transposed form (*inc2y* = 1). In that case, in the above example, *inc1x* is replaced by *inc1y*.

In computing column transforms (*inc1x* = *inc1y* = 1), the values of *inc2x* and *inc2y* are not very important. For these, any value over the required minimum of *n/2+1* can be used.

### Example 3—DSINF

This example shows the use of the STRIDE subroutine in computing one-dimensional row transforms using the DSINF subroutine.

If *inc2x* = 1, the input sequences are stored in the transposed form as rows of a two-dimensional array X(INC1X,N/2). In this case, the STRIDE subroutine helps in determining a good value of *inc1x* for this array. The required minimum value of *inc1x* is *m*, the number of Fourier transforms being computed. To find a good value of *inc1x*, use STRIDE as follows:

```
          N   INCD  INCR   DT  IOPT
          |   |    |    |   |    |
CALL STRIDE( N/2 , M , INC1X , 'D' , 0 )
```

Here, the arguments refer to the DSINF subroutine. In the following table, values of *inc1x* are given (as obtained from the STRIDE subroutine) for some combinations of *n* and *m* and for POWER3 with 64KB level 1 cache:

N	M	INC1X
128	64	64
240	32	32
240	64	64
256	256	264
512	60	60
1024	64	65

The above example also applies when the output sequences are stored in the transposed form (*inc2y* = 1). In that case, in the above example, *inc1x* is replaced by *inc1y*.

In computing column transforms ( $inc1x = inc1y = 1$ ), the values of  $inc2x$  and  $inc2y$  are not very important. For these, any value over the required minimum of  $n/2$  can be used.

### Example 4—SCFT2

This example shows the use of the STRIDE subroutine in computing two-dimensional transforms using the SCFT2 subroutine.

If  $inc1y = 1$ , the two-dimensional output array is stored in the normal form. In this case, the output array can be declared as  $Y(INC2Y, N2)$ , where the required minimum value of  $inc2y$  is  $n1$ . The STRIDE subroutine helps in picking a good value of  $inc2y$ . To find a good value of  $inc2y$ , use STRIDE as follows:

```

          N  INCD  INCR  DT  IOPT
          |  |    |    |   |    |
CALL STRIDE( N2 , N1 , INC2Y , 'C' , 0 )

```

Here, the arguments refer to the SCFT2 subroutine. In the following table, values of  $inc2y$  are given (as obtained from the STRIDE subroutine) for some two-dimensional arrays with  $n1 = n2$  and for POWER3 with 64KB level 1 cache:

N1	N2	INC2Y
64	64	64
128	128	136
240	240	240
512	512	520
840	840	848

If the input array is stored in the normal form ( $inc1x = 1$ ), the value of  $inc2x$  is not important. However, if you want to use the same array for input and output, you should use  $inc2x = inc2y$ .

If  $inc2y = 1$ , the two-dimensional output array is stored in the transposed form. In this case, the output array can be declared as  $Y(INC1Y, N1)$ , where the required minimum value of  $inc1y$  is  $n2$ . The STRIDE subroutine helps in picking a good value of  $inc1y$ . To find a good value of  $inc1y$ , use STRIDE as follows:

```

          N  INCD  INCR  DT  IOPT
          |  |    |    |   |    |
CALL STRIDE( N1 , N2 , INC1Y , 'C' , 0 )

```

Here, the arguments refer to the SCFT2 subroutine. In the following table, values of  $inc1y$  are given (as obtained from the STRIDE subroutine) for some combinations of  $n1$  and  $n2$  and for POWER3 with 64K level 1 cache:

N1	N2	INC1Y
60	64	64
120	128	136
256	240	240
512	512	520
840	840	848

If the input array is stored in the transposed form ( $inc2x = 1$ ), the value of  $inc1x$  is also important. The above example can be used to find a good value of  $inc1x$ , by replacing  $inc1y$  with  $inc1x$ . If both arrays are stored in the transposed form, a good value for  $inc1y$  is also a good value for  $inc1x$ . In that situation, the two arrays can also be made equivalent.

**Example 5—SRCFT2**

This example shows the use of the STRIDE subroutine in computing two-dimensional transforms using the SRCFT2 subroutine.

For this subroutine, the output array is declared as  $Y(INC2Y, N2)$ , where the required minimum value of  $inc2y$  is  $n1/2+1$ . The STRIDE subroutine helps in picking a good value of  $inc2y$ . To find a good value of  $inc2y$ , use STRIDE as follows:

```

          N      INCD      INCR      DT      IOPT
          |      |      |      |      |
CALL STRIDE( N2 , N1/2 + 1 , INC2Y , 'C' , 0 )

```

Here, the arguments refer to the SRCFT2 subroutine. In the following table, values of  $inc2y$  are given (as obtained from the STRIDE subroutine) for some two-dimensional arrays with  $n1 = n2$  and for POWER3 with 64KB level 1 cache:

N1	N2	INC2Y
240	240	121
420	420	211
512	512	257
840	840	421
1024	1024	513
2048	2048	1032

For this subroutine, the leading dimension of the input array ( $inc2x$ ) is not important. If you want to use the same array for input and output, you should use  $inc2x \geq 2(inc2y)$ .

**Example 6—SCRFT2**

This example shows the use of the STRIDE subroutine in computing two-dimensional transforms using the SCRFT2 subroutine.

For this subroutine, the output array is declared as  $Y(INC2Y, N2)$ , where the required minimum value of  $inc2y$  is  $n1+2$ . The STRIDE subroutine helps in picking a good value of  $inc2y$ . To find a good value of  $inc2y$ , use STRIDE as follows:

```

          N      INCD      INCR      DT      IOPT
          |      |      |      |      |
CALL STRIDE( N2 , N1 + 2 , INC2Y , 'S' , 0 )

```

Here, the arguments refer to the SCRFT2 subroutine. In the following table, values of  $inc2y$  are given (as obtained from the STRIDE subroutine) for some two-dimensional arrays with  $n1 = n2$  and for POWER3 with 64KB level 1 cache:

N1	N2	INC2Y
240	240	242
420	420	422
512	512	514
840	840	842
1024	1024	1026
2048	2048	2064

For this subroutine, the leading dimension of the input array ( $inc2x$ ) is also important. In general,  $inc2x = inc2y/2$  is a good choice. This is also the requirement if you want to use the same array for input and output.

**Example 7—SCFT3**

This example shows the use of the STRIDE subroutine in computing three-dimensional transforms using the SCFT3 subroutine.



For this subroutine, the strides for the input array are not important. They are important for the output array. The STRIDE subroutine helps in picking good values of  $inc2y$  and  $inc3y$ . This requires two calls to the STRIDE subroutine as shown below. First, you should find a good value for  $inc2y$ . The minimum acceptable value for  $inc2y$  is  $n1$ .

```

      N   INCD  INCR   DT   IOPT
      |   |    |    |    |
CALL STRIDE( N2 , N1 , INC2Y , 'C' , 0 )

```

Here, the arguments refer to the SCFT3 subroutine. Next, you should find a good value for  $inc3y$ . The minimum acceptable value for  $inc3y$  is  $(n2)(inc2y)$ .

```

      N   INCD  INCR   DT   IOPT
      |   |    |    |    |
CALL STRIDE( N3 , N2*INC2Y, INC3Y , 'C' , 0 )

```

If  $inc3y$  turns out to be a multiple of  $inc2y$ , then  $Y$  can be declared a three-dimensional array as  $Y(inc2y, inc3y/inc2y, n3)$ . For large problems, this may not happen. In that case, you can declare the  $Y$  array as a two-dimensional array  $Y(0:inc3y-1, 0:n3-1)$  or a one-dimensional array  $Y(0:inc3y*n3-1)$ . Using zero-based indexing, the element  $y(k1, k2, k3)$  is stored in the following location in these arrays:

- For the two-dimensional array, location  $(k1+k2*inc2y, k3)$
- For the one-dimensional array, location  $(k1+k2*inc2y+k3*inc3y)$

In the following table, values of  $inc2y$  and  $inc3y$  are given (as obtained from the STRIDE subroutine) for some three-dimensional arrays with  $n1 = n2 = n3$  and for POWER3 with 64KB level 1 cache:

N1,N2,N3	INC2Y	INC3Y
30	30	900
32	32	1032
64	64	4112
120	120	14408
128	136	17416
240	240	57608
256	264	67592
420	420	176400

As mentioned before, the strides of the input array are not important. The array can be declared as a three-dimensional array. If you want to use the same array for input and output, the requirements are  $inc2x \geq inc2y$  and  $inc3x \geq inc3y$ . A simple thing to do is to use  $inc2x = inc2y$  and make  $inc3x$  a multiple of  $inc2x$  not smaller than  $inc3y$ . Then  $X$  can be declared as a three-dimensional array  $X(inc2x, inc3x/inc2x, n3)$ .

### Example 8—SRCFT3

This example shows the use of the STRIDE subroutine in computing three-dimensional transforms using the SRCFT3 subroutine.

For this subroutine, the strides for the input array are not important. They are important for the output array. The STRIDE subroutine helps in picking good values of  $inc2y$  and  $inc3y$ . This requires two calls to the STRIDE subroutine as shown below. First, you should find a good value for  $inc2y$ . The minimum acceptable value for  $inc2y$  is  $n1/2+1$ .

```

      N   INCD  INCR   DT   IOPT
      |   |    |    |    |
CALL STRIDE( N2 , N1/2 + 1 , INC2Y , 'C' , 0 )

```

## STRIDE

Here, the arguments refer to the SRCFT3 subroutine. Next, you should find a good value for *inc3y*. The minimum acceptable value for *inc3y* is  $(n2)(inc2y)$ .

```
      N      INCD      INCR      DT      IOPT
      |      |      |      |      |
CALL STRIDE( N3 , N2*INC2Y , INC3Y , 'C' , 0 )
```

If *inc3y* turns out to be a multiple of *inc2y*, then Y can be declared a three-dimensional array as  $Y(INC2Y, INC3Y/INC2Y, N3)$ . For large problems, this may not happen. In that case, you can declare the Y array as a two-dimensional array  $Y(0:INC3Y-1, 0:N3-1)$  or a one-dimensional array  $Y(0:INC3Y*N3-1)$ . Using zero-based indexing, the element  $y(k1, k2, k3)$  is stored in the following location in these arrays:

- For the two-dimensional array, location  $(k1+k2*inc2y, k3)$
- For the one-dimensional array, location  $(k1+k2*inc2y+k3*inc3y)$

In the following table, values of *inc2y* and *inc3y* are given (as obtained from the STRIDE subroutine) for some three-dimensional arrays with  $n1 = n2 = n3$  and for POWER3 with 64KB level 1 cache:

N1,N2,N3	INC2Y	INC3Y
30	16	488
32	17	552
64	33	2128
120	61	7320
128	65	8328
240	121	29064
256	129	33032
420	211	88620

As mentioned before, the strides of the input array are not important. The array can be declared as a three-dimensional array. If you want to use the same array for input and output, the requirements are  $inc2x \geq 2(inc2y)$  and  $inc3x \geq 2(inc3y)$ . A simple thing to do is to use  $inc2x = 2(inc2y)$  and make *inc3x* a multiple of *inc2x* not smaller than  $2(inc3y)$ . Then X can be declared as a three-dimensional array  $X(INC2X, INC3X/INC2X, N3)$ .

### Example 9—SCRFT3

This example shows the use of the STRIDE subroutine in computing three-dimensional transforms using the SCRFT3 subroutine.

The STRIDE subroutine helps in picking good values of *inc2y* and *inc3y*. This requires two calls to the STRIDE subroutine as shown below. First, you should find a good value for *inc2y*. The minimum acceptable value for *inc2y* is  $n1+2$ .

```
      N      INCD      INCR      DT      IOPT
      |      |      |      |      |
CALL STRIDE( N2 , N1 + 2 , INC2Y , 'S' , 0 )
```

Here, the arguments refer to the SCRFT3 subroutine. Next, you should find a good value for *inc3y*. The minimum acceptable value for *inc3y* is  $(n2)(inc2y)$ .

```
      N      INCD      INCR      DT      IOPT
      |      |      |      |      |
CALL STRIDE( N3 , N2*INC2Y , INC3Y , 'S' , 0 )
```

If *inc3y* turns out to be a multiple of *inc2y*, then Y can be declared a three-dimensional array as  $Y(INC2Y, INC3Y/INC2Y, N3)$ . For large problems, this may not happen. In that case, you can declare the Y array as a two-dimensional array

$Y(0:INC3Y-1,0:N3-1)$  or a one-dimensional array  $Y(0:INC3Y*N3-1)$ . Using zero-based indexing, the element  $y(k1,k2,k3)$  is stored in the following location in these arrays:

- For the two-dimensional array, location  $(k1+k2*inc2y,k3)$
- For the one-dimensional array, location  $(k1+k2*inc2y+k3*inc3y)$

In the following table, values of  $inc2y$  and  $inc3y$  are given (as obtained from the STRIDE subroutine) for some three-dimensional arrays with  $n1 = n2 = n3$  and for POWER3 with 64KB level 1 cache:

N1,N2,N3	INC2Y	INC3Y
30	32	976
32	34	1104
64	66	4256
128	122	14640
128	130	16656
240	242	58128
256	258	66064
420	422	177240

For this subroutine, the strides ( $inc2x$  and  $inc3x$ ) of the input array are also important. In general,  $inc2x = inc2y/2$  and  $inc3x = inc3y/2$  are good choices. These are also the requirement if you want to use the same array for input and output.

## DSRSM — Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode

### Purpose

This subroutine converts either  $m$  by  $n$  general sparse matrix  $A$  or symmetric sparse matrix  $A$  of order  $n$  from storage-by-rows to compressed-matrix storage mode, where matrix  $A$  contains long-precision real numbers.

### Syntax

Fortran	CALL DSRSM ( <i>iopt</i> , <i>ar</i> , <i>ja</i> , <i>ia</i> , <i>m</i> , <i>nz</i> , <i>ac</i> , <i>ka</i> , <i>lda</i> )
C and C++	dsrsm ( <i>iopt</i> , <i>ar</i> , <i>ja</i> , <i>ia</i> , <i>m</i> , <i>nz</i> , <i>ac</i> , <i>ka</i> , <i>lda</i> );

### On Entry

<i>iopt</i>	<p>indicates the storage variation used for sparse matrix <math>A</math> storage-by-rows:</p> <p>If <math>iopt = 0</math>, matrix <math>A</math> is a general sparse matrix, where all the nonzero elements in matrix <math>A</math> are used to set up the storage arrays.</p> <p>If <math>iopt = 1</math>, matrix <math>A</math> is a symmetric sparse matrix, where only the upper triangle and diagonal elements are used to set up the storage arrays.</p> <p>Specified as: a fullword integer; <math>iopt = 0</math> or <math>1</math>.</p>
<i>ar</i>	<p>is the sparse matrix <math>A</math>, stored by rows in an array, referred to as AR. The <math>iopt</math> argument indicates the storage variation used for storing matrix <math>A</math>. Specified as: a one-dimensional array, containing long-precision real numbers. The number of elements, <math>ne</math>, in this array can be determined by subtracting 1 from the value in <math>IA(m+1)</math>.</p>
<i>ja</i>	<p>is the array, referred to as JA, containing the column numbers of each nonzero element in sparse matrix <math>A</math>.</p> <p>Specified as: a one-dimensional array, containing fullword integers; <math>1 \leq (JA \text{ elements}) \leq n</math>. The number of elements, <math>ne</math>, in this array can be determined by subtracting 1 from the value in <math>IA(m+1)</math>.</p>
<i>ia</i>	<p>is the row pointer array, referred to as IA, containing the starting positions of each row of matrix <math>A</math> in array AR and one position past the end of array AR. Specified as: a one-dimensional array of (at least) length <math>m+1</math>, containing fullword integers; <math>IA(i+1) \geq IA(i)</math> for <math>i = 1, m+1</math>.</p>
<i>m</i>	<p>is the number of rows in sparse matrix <math>A</math>. Specified as: a fullword integer; <math>m \geq 0</math>.</p>
<i>nz</i>	<p>is the number of columns in output arrays AC and KA that are available for use.</p> <p>Specified as: a fullword integer; <math>nz &gt; 0</math>.</p>
<i>ac</i>	See "On Return" on page 1027.
<i>ka</i>	See "On Return" on page 1027.

*lda* is the size of the leading dimension of the arrays specified for *ac* and *ka*.  
Specified as: a fullword integer;  $0 < lda \leq m$ .

### On Return

*nz* is the maximum number of nonzero elements, *nz*, in each row of matrix *A*, which is stored in compressed-matrix storage mode. Returned as: a fullword integer; (input argument) *nz*  $\leq$  (output argument) *nz*.

*ac* is the *m* by *n* general sparse matrix *A* or symmetric matrix *A* of order *n* stored in compressed-matrix storage mode in an array, referred to as AC. Returned as: an *lda* by at least (input argument) *nz* array, containing long-precision real numbers, where only the first (output argument) *nz* columns are used to store the matrix.

*ka* is the array, referred to as KA, containing the column numbers of the matrix *A* elements that are stored in the corresponding positions in array AC. Returned as: an *lda* by at least (input argument) *nz* array, containing fullword integers, where only the first (output argument) *nz* columns are used to store the column numbers.

### Notes

1. In your C program, argument *nz* must be passed by reference.
2. The value specified for input argument *nz* should be greater than or equal to the number of nonzero elements you estimate to be in each row of sparse matrix *A*. The value returned in output argument *nz* corresponds to the *nz* value defined for compressed-matrix storage mode. This value is less than or equal to the value specified for input argument *nz*.
3. For a description of the storage modes for sparse matrices, see “Compressed-Matrix Storage Mode” on page 95 and “Storage-by-Rows” on page 100.

### Function

A sparse matrix *A* is converted from storage-by-rows (using arrays AR, JA, and IA) to compressed-matrix storage mode (using arrays AC and KA). The argument *iopt* indicates whether the input matrix *A* is stored by rows using the storage variation for general sparse matrices or for symmetric sparse matrices. See reference [76].

This subroutine is meant for existing programs that need to convert their sparse matrices to a storage mode compatible with some of the ESSL sparse matrix subroutines, such as DSMMX.

### Error conditions

#### Computational Errors

None

#### Input-Argument Errors

1. *iopt*  $\neq$  0 or 1
2. *m*  $<$  0
3. *lda*  $<$  1
4. *lda*  $<$  *m*
5. *nz*  $\leq$  0

6.  $IA(m+1) < 1$
7.  $IA(i+1)-IA(i) < 0$ , for any  $i = 1, m$
8.  $nz$  is too small to store matrix  $A$  in array  $AC$ , where:
  - If  $iopt = 0$ ,  $AC$  and  $KA$  are not modified.
  - If  $iopt = 1$ ,  $AC$  and  $KA$  are modified.

## Examples

### Example 1

This example shows a general sparse matrix  $A$ , which is stored by rows and converted to compressed-matrix storage mode, where sparse matrix  $A$  is:

$$\begin{bmatrix} 11.0 & 0.0 & 0.0 & 14.0 \\ 0.0 & 22.0 & 0.0 & 24.0 \\ 0.0 & 0.0 & 33.0 & 34.0 \\ 0.0 & 0.0 & 0.0 & 44.0 \end{bmatrix}$$

Because there is a maximum of only two nonzero elements in each row of  $A$ , and argument  $nz$  is specified as 5, columns 3 through 5 of arrays  $AC$  and  $KA$  are not used.

#### Call Statement and Input:

```

          IOPT  AR   JA   IA   M   NZ   AC   KA   LDA
CALL DSRSM( 0 , AR , JA , IA , 4 , 5 , AC , KA , 4 )
    
```

```

AR      = (11.0, 14.0, 22.0, 24.0, 33.0, 34.0, 44.0)
JA      = (1, 4, 2, 4, 3, 4, 4)
IA      = (1, 3, 5, 7, 8)
    
```

#### Output:

```
NZ      = 2
```

$$AC = \begin{bmatrix} 11.0 & 14.0 & . & . & . \\ 22.0 & 24.0 & . & . & . \\ 33.0 & 34.0 & . & . & . \\ 44.0 & 0.0 & . & . & . \end{bmatrix}$$

$$KA = \begin{bmatrix} 1 & 4 & . & . & . \\ 2 & 4 & . & . & . \\ 3 & 4 & . & . & . \\ 4 & 4 & . & . & . \end{bmatrix}$$

### Example 2

This example shows a symmetric sparse matrix  $A$ , which is stored by rows and converted to compressed-matrix storage mode, where sparse matrix  $A$  is:

$$\begin{bmatrix} 11.0 & 0.0 & 0.0 & 14.0 \\ 0.0 & 22.0 & 0.0 & 24.0 \\ 0.0 & 0.0 & 33.0 & 34.0 \\ 14.0 & 24.0 & 34.0 & 44.0 \end{bmatrix}$$

Because there is a maximum of only four nonzero elements in each row of  $A$ , and argument  $nz$  is specified as 6, columns 5 and 6 of arrays  $AC$  and  $KA$  are not used.

**Call Statement and Input:**

	IOPT	AR	JA	IA	M	NZ	AC	KA	LDA									
CALL DSRSM(	1	,	AR	,	JA	,	IA	,	4	,	6	,	AC	,	KA	,	4	)

AR = (11.0, 14.0, 22.0, 24.0, 33.0, 34.0, 44.0)  
 JA = (1, 4, 2, 4, 3, 4, 4)  
 IA = (1, 3, 5, 7, 8)

**Output:**

NZ = 4

$$AC = \begin{bmatrix} 11.0 & 14.0 & 0.0 & 0.0 & . & . \\ 22.0 & 24.0 & 0.0 & 0.0 & . & . \\ 33.0 & 34.0 & 0.0 & 0.0 & . & . \\ 44.0 & 24.0 & 34.0 & 14.0 & . & . \end{bmatrix}$$

$$KA = \begin{bmatrix} 1 & 4 & 4 & 4 & . & . \\ 2 & 4 & 4 & 4 & . & . \\ 3 & 4 & 4 & 4 & . & . \\ 4 & 2 & 3 & 1 & . & . \end{bmatrix}$$

## DGKTRN — For a General Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode

### Purpose

This subroutine converts general sparse matrix  $A$  of order  $n$  from one skyline storage mode to another—that is, between the following:

- Diagonal-out skyline storage mode
- Profile-in skyline storage mode

### Syntax

Fortran	CALL DGKTRN ( $n$ , $au$ , $nu$ , $idu$ , $al$ , $nl$ , $idl$ , $itrans$ , $aux$ , $naux$ )
C and C++	dgktrn ( $n$ , $au$ , $nu$ , $idu$ , $al$ , $nl$ , $idl$ , $itrans$ , $aux$ , $naux$ );

### On Entry

- $n$  is the order of general sparse matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- $au$  is the array, referred to as AU, containing the upper triangular part of general sparse matrix  $A$ , stored as follows, where:  
 If ITRAN(1) = 0,  $A$  is stored in diagonal-out skyline storage mode.  
 If ITRAN(1) = 1,  $A$  is stored in profile-in skyline storage mode.  
 Specified as: a one-dimensional array of (at least) length  $nu$ , containing long-precision real numbers.
- $nu$  is the length of array AU.  
 Specified as: a fullword integer;  $nu \geq 0$  and  $nu \geq (IDU(n+1)-1)$ .
- $idu$  is the array, referred to as IDU, containing the relative positions of the diagonal elements of matrix  $A$  in input array AU.  
 Specified as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.
- $al$  is the array, referred to as AL, containing the lower triangular part of general sparse matrix  $A$ , stored as follows, where:  
 If ITRAN(1) = 0,  $A$  is stored in diagonal-out skyline storage mode.  
 If ITRAN(1) = 1,  $A$  is stored in profile-in skyline storage mode.  
**Note:** Entries in AL for diagonal elements of  $A$  are assumed not to have meaningful values.  
 Specified as: a one-dimensional array of (at least) length  $nl$ , containing long-precision real numbers.
- $nl$  is the length of array AL.  
 Specified as: a fullword integer;  $nl \geq 0$  and  $nl \geq (IDL(n+1)-1)$ .
- $idl$  is the array, referred to as IDL, containing the relative positions of the diagonal elements of matrix  $A$  in input array AL.  
 Specified as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.



*itrans* is an array of parameters,  $ITRAN(i)$ , where:

- $ITRAN(1)$  indicates the input storage mode used for matrix  $A$ . This determines the arrangement of data in arrays AU, IDU, AL, and IDL on input, where:
  - If  $ITRAN(1) = 0$ , diagonal-out skyline storage mode is used.
  - If  $ITRAN(1) = 1$ , profile-in skyline storage mode is used.
- $ITRAN(2)$  indicates the output storage mode used for matrix  $A$ . This determines the arrangement of data in arrays AU, IDU, AL, and IDL on output, where:
  - If  $ITRAN(2) = 0$ , diagonal-out skyline storage mode is used.
  - If  $ITRAN(2) = 1$ , profile-in skyline storage mode is used.
- $ITRAN(3)$  indicates the direction of sweep that ESSL uses through the matrix  $A$ , allowing you to optimize performance (see “Notes” on page 1032), where:
  - If  $ITRAN(3) = 1$ , matrix  $A$  is transformed in the positive direction, starting in row or column 1 and ending in row or column  $n$ .
  - If  $ITRAN(3) = -1$ , matrix  $A$  is transformed in the negative direction, starting in row or column  $n$  and ending in row or column 1.

Specified as: a one-dimensional array of (at least) length 3, containing fullword integers, where:

$ITRAN(1) = 0$  or  $1$   
 $ITRAN(2) = 0$  or  $1$   
 $ITRAN(3) = -1$  or  $1$

*aux* has the following meaning:

If  $naux = 0$  and error 2015 is unrecoverable, *aux* is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing *naux* long-precision real numbers.

*naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.

Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, DGKTRN dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \geq 2n$ .

### On Return

*au* is the array, referred to as AU, containing the upper triangular part of general sparse matrix  $A$ , stored as follows, where:

If  $ITRAN(2) = 0$ ,  $A$  is stored in diagonal-out skyline storage mode.

If  $ITRAN(2) = 1$ ,  $A$  is stored in profile-in skyline storage mode.

Returned as: a one-dimensional array of (at least) length  $nu$ , containing long-precision real numbers.

*idu* is the array, referred to as IDU, containing the relative positions of the diagonal elements of matrix *A* in output array AU. Returned as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.

*al* is the array, referred to as AL, containing the lower triangular part of general sparse matrix *A*, stored as follows, where:

If ITRAN(2) = 0, *A* is stored in diagonal-out skyline storage mode.

If ITRAN(2) = 1, *A* is stored in profile-in skyline storage mode.

**Note:** You should assume that entries in AL for diagonal elements of *A* do not have meaningful values.

Returned as: a one-dimensional array of (at least) length  $nl$ , containing long-precision real numbers.

*idl* is the array, referred to as IDL, containing the relative positions of the diagonal elements of matrix *A* in output array AL. Returned as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.

## Notes

1. Your various arrays must have no common elements; otherwise, results are unpredictable.
2. The ITRAN(3) argument allows you to specify the direction of travel through matrix *A* that ESSL takes during the transformation. By properly specifying ITRAN(3), you can optimize the performance of the transformation, which is especially beneficial when transforming large matrices.

The direction specified by ITRAN(3) should be opposite the most recent direction of access through the matrix performed by the DGKFS or DGKFSP subroutine, as indicated in the following table:

Most Recent Computation Performed by DGKFS/DGKFSP	Direction Used by DGKFS/DGKFSP	Direction to Specify in ITRAN(3)
Factor and Solve	Negative	Positive (ITRAN(3) = 1)
Factor Only	Positive	Negative (ITRAN(3) = -1)
Solve Only	Negative	Positive (ITRAN(3) = 1)

3. For a description of how sparse matrices are stored in skyline storage mode, see “Profile-In Skyline Storage Mode” on page 104 and “Diagonal-Out Skyline Storage Mode” on page 102.
4. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## Function

A general sparse matrix *A*, stored in diagonal-out or profile-in skyline storage mode is converted to either of these same two storage modes. (Generally, you convert from one to the other, but the capability exists to specify the same storage mode for input and output.) The argument ITRAN(3) indicates the direction in

which you want the transformation performed on matrix  $A$ , allowing you to optimize your performance in this subroutine. This is especially beneficial for large matrices.

This subroutine is meant to be used in conjunction with DGKFS and DGKFSP, which process matrices stored in these skyline storage modes.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable,  $naux = 0$ , and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

1.  $n < 0$
2.  $nu < 0$
3.  $IDU(n+1) > nu+1$
4.  $IDU(i+1) \leq IDU(i)$  for  $i = 1, n$
5.  $IDU(i+1) > IDU(i)+i$  and  $ITRAN(1) = 0$  for  $i = 1, n$
6.  $IDU(i) > IDU(i-1)+i$  and  $ITRAN(1) = 1$  for  $i = 2, n$
7.  $nl < 0$
8.  $IDL(n+1) > nl+1$
9.  $IDL(i+1) \leq IDL(i)$  for  $i = 1, n$
10.  $IDL(i+1) > IDL(i)+i$  and  $ITRAN(1) = 0$  for  $i = 1, n$
11.  $IDL(i) > IDL(i-1)+i$  and  $ITRAN(1) = 1$  for  $i = 2, n$
12.  $ITRAN(1) \neq 0$  or  $1$
13.  $ITRAN(2) \neq 0$  or  $1$
14.  $ITRAN(3) \neq -1$  or  $1$
15. Error 2015 is recoverable or  $naux \neq 0$ , and  $naux$  is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to convert a 9 by 9 general sparse matrix  $A$  from diagonal-out skyline storage mode to profile-in skyline storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 11.0 & 12.0 & 13.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 21.0 & 22.0 & 23.0 & 24.0 & 25.0 & 0.0 & 0.0 & 0.0 & 29.0 \\ 31.0 & 32.0 & 33.0 & 34.0 & 35.0 & 0.0 & 37.0 & 0.0 & 39.0 \\ 41.0 & 42.0 & 43.0 & 44.0 & 45.0 & 46.0 & 47.0 & 0.0 & 49.0 \\ 0.0 & 0.0 & 0.0 & 54.0 & 55.0 & 56.0 & 57.0 & 58.0 & 59.0 \\ 0.0 & 62.0 & 63.0 & 64.0 & 65.0 & 66.0 & 67.0 & 68.0 & 69.0 \\ 0.0 & 0.0 & 0.0 & 74.0 & 75.0 & 76.0 & 77.0 & 78.0 & 79.0 \\ 0.0 & 0.0 & 0.0 & 84.0 & 85.0 & 86.0 & 87.0 & 88.0 & 89.0 \\ 91.0 & 92.0 & 93.0 & 94.0 & 95.0 & 96.0 & 97.0 & 98.0 & 99.0 \end{bmatrix}$$

Assuming that DGKFS last performed a solve on matrix  $A$ , the direction of the transformation is positive; that is,  $ITRAN(3)$  is 1. This provides the best performance here.

**Note:** On input and output, the diagonal elements in  $AL$  do not have meaningful values.

**Call Statement and Input:**

```

          N  AU  NU  IDU  AL  NL  IDL  ITRAN  AUX  NAUX
          |  |  |  |  |  |  |  |  |  |
CALL DGKTRN( 9 , AU , 33 , IDU , AL , 35 , IDL , ITRAN , AUX , 18

```

```

AU      = (11.0, 22.0, 12.0, 33.0, 23.0, 13.0, 44.0, 34.0, 24.0,
          55.0, 45.0, 35.0, 25.0, 66.0, 56.0, 46.0, 77.0, 67.0,
          57.0, 47.0, 37.0, 88.0, 78.0, 68.0, 58.0, 99.0, 89.0,
          79.0, 69.0, 59.0, 49.0, 39.0, 29.0)
IDU     = (1, 2, 4, 7, 10, 14, 17, 22, 26, 34)
AL      = ( . , . , 21.0, . , 32.0, 31.0, . , 43.0, 42.0, 41.0, . ,
          54.0, . , 65.0, 64.0, 63.0, 62.0, . , 76.0, 75.0, 74.0,
          . , 87.0, 86.0, 85.0, 84.0, . , 98.0, 97.0, 96.0, 95.0,
          94.0, 93.0, 92.0, 91.0)
IDL     = (1, 2, 4, 7, 11, 13, 18, 22, 27, 36)
ITRAN   = (0, 1, 1)

```

**Output:**

```

AU      = (11.0, 12.0, 22.0, 13.0, 23.0, 33.0, 24.0, 34.0, 44.0,
          25.0, 35.0, 45.0, 55.0, 46.0, 56.0, 66.0, 37.0, 47.0,
          57.0, 67.0, 77.0, 58.0, 68.0, 78.0, 88.0, 29.0, 39.0,
          49.0, 59.0, 69.0, 79.0, 89.0, 99.0)
IDU     = (1, 3, 6, 9, 13, 16, 21, 25, 33, 34)
AL      = ( . , 21.0, . , 31.0, 32.0, . , 41.0, 42.0, 43.0, . , 54.0,
          . , 62.0, 63.0, 64.0, 65.0, . , 74.0, 75.0, 76.0, . ,
          84.0, 85.0, 86.0, 87.0, . , 91.0, 92.0, 93.0, 94.0, 95.0,
          96.0, 97.0, 98.0, . )
IDL     = (1, 3, 6, 10, 12, 17, 21, 26, 35, 36)

```

**Example 2**

This example shows how to convert the same 9 by 9 general sparse matrix *A* in Example 1 from profile-in skyline storage mode to diagonal-out skyline storage mode.

Assuming that DGKFS last performed a factorization on matrix *A*, the direction of the transformation is negative; that is, ITRAN(3) is -1. This provides the best performance here.

**Note:** On input and output, the diagonal elements in AL do not have meaningful values.

**Call Statement and Input:**

```

          N  AU  NU  IDU  AL  NL  IDL  ITRAN  AUX  NAUX
          |  |  |  |  |  |  |  |  |  |
CALL DGKTRN( 9 , AU , 33 , IDU , AL , 35 , IDL , ITRAN , AUX , 18

```

```

AU      =(same as output AU in Example 1)
IDU     =(same as output IDU in Example 1)
AL      =(same as output AL in Example 1)
IDL     =(same as output IDL in Example 1)
ITRAN   = (1, 0, -1)

```

**Output:**

```

AU      =(same as input AU in Example 1)
IDU     =(same as input IDU in Example 1)
AL      =(same as input AL in Example 1)
IDL     =(same as input IDL in Example 1)

```

## DSKTRN — For a Symmetric Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode

### Purpose

This subroutine converts symmetric sparse matrix  $A$  of order  $n$  from one skyline storage mode to another—that is, between the following:

- Diagonal-out skyline storage mode
- Profile-in skyline storage mode

### Syntax

Fortran	CALL DSKTRN ( $n, a, na, idiag, itran, aux, naux$ )
C and C++	dsktrn ( $n, a, na, idiag, itran, aux, naux$ );

### On Entry

- $n$  is the order of symmetric sparse matrix  $A$ . Specified as: a fullword integer;  $n \geq 0$ .
- $a$  is the array, referred to as  $A$ , containing the upper triangular part of symmetric sparse matrix  $A$ , stored as follows, where:
- If ITRAN(1) = 0,  $A$  is stored in diagonal-out skyline storage mode.  
 If ITRAN(1) = 1,  $A$  is stored in profile-in skyline storage mode.
- Specified as: a one-dimensional array of (at least) length  $na$ , containing long-precision real numbers.
- $na$  is the length of array  $A$ .
- Specified as: a fullword integer;  $na \geq 0$  and  $na \geq (\text{IDIAG}(n+1)-1)$ .
- $idiag$  is the array, referred to as IDIAG, containing the relative positions of the diagonal elements of matrix  $A$  in input array  $A$ .
- Specified as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.
- $itrans$  is an array of parameters, ITRAN( $i$ ), where:
- ITRAN(1) indicates the input storage mode used for matrix  $A$ . This determines the arrangement of data in arrays  $A$  and IDIAG on input, where:
    - If ITRAN(1) = 0, diagonal-out skyline storage mode is used.
    - If ITRAN(1) = 1, profile-in skyline storage mode is used.
  - ITRAN(2) indicates the output storage mode used for matrix  $A$ . This determines the arrangement of data in arrays  $A$  and IDAIG on output, where:
    - If ITRAN(2) = 0, diagonal-out skyline storage mode is used.
    - If ITRAN(2) = 1, profile-in skyline storage mode is used.
  - ITRAN(3) indicates the direction of sweep that ESSL uses through the matrix  $A$ , allowing you to optimize performance (see “Notes” on page 1036), where:
    - If ITRAN(3) = 1, matrix  $A$  is transformed in the positive direction, starting in row or column 1 and ending in row or column  $n$ .

If  $\text{ITRAN}(3) = -1$ , matrix  $A$  is transformed in the negative direction, starting in row or column  $n$  and ending in row or column 1.

Specified as: a one-dimensional array of (at least) length 3, containing fullword integers, where:

$\text{ITRAN}(1) = 0$  or  $1$

$\text{ITRAN}(2) = 0$  or  $1$

$\text{ITRAN}(3) = -1$  or  $1$

*aux* has the following meaning:

If  $naux = 0$  and error 2015 is unrecoverable, *aux* is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing *naux* long-precision real numbers.

*naux* is the size of the work area specified by *aux*—that is, the number of elements in *aux*.

Specified as: a fullword integer, where:

If  $naux = 0$  and error 2015 is unrecoverable, DSKTRN dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \geq n$ .

## On Return

*a* is the array, referred to as  $A$ , containing the upper triangular part of symmetric sparse matrix  $A$ , stored as follows, where:

If  $\text{ITRAN}(2) = 0$ ,  $A$  is stored in diagonal-out skyline storage mode.

If  $\text{ITRAN}(2) = 1$ ,  $A$  is stored in profile-in skyline storage mode.

Returned as: a one-dimensional array of (at least) length  $na$ , containing long-precision real numbers.

*idiag* is the array, referred to as IDIAG, containing the relative positions of the diagonal elements of matrix  $A$  in output array  $A$ . Returned as: a one-dimensional array of (at least) length  $n+1$ , containing fullword integers.

## Notes

1. Your various arrays must have no common elements; otherwise, results are unpredictable.
2. The  $\text{ITRAN}(3)$  argument allows you to specify the direction of travel through matrix  $A$  that ESSL takes during the transformation. By properly specifying  $\text{ITRAN}(3)$ , you can optimize the performance of the transformation, which is especially beneficial when transforming large matrices.

The direction specified by  $\text{ITRAN}(3)$  should be opposite the most recent direction of access through the matrix performed by the DSKFS or DSKFSP subroutine, as indicated in the following table:

Most Recent Computation Performed by DSKFS/DSKFSP	Direction Used by DSKFS/DSKFSP	Direction to Specify in ITRAN(3)
Factor and Solve	Negative	Positive (ITRAN(3) = 1)
Factor Only	Positive	Negative (ITRAN(3) = -1)
Solve Only	Negative	Positive (ITRAN(3) = 1)

- For a description of how sparse matrices are stored in skyline storage mode, see “Profile-In Skyline Storage Mode” on page 104 and “Diagonal-Out Skyline Storage Mode” on page 102.
- You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see “Using Auxiliary Storage in ESSL” on page 36.

## Function

A symmetric sparse matrix  $A$ , stored in diagonal-out or profile-in skyline storage mode is converted to either of these same two storage modes. (Generally, you convert from one to the other, but the capability exists to specify the same storage mode for input and output.) The argument ITRAN(3) indicates the direction in which you want the transformation performed on matrix  $A$ , allowing you to optimize your performance in this subroutine. This is especially beneficial for large matrices.

This subroutine is meant to be used in conjunction with DSKFS and DSKFSP, which process matrices stored in these skyline storage modes.

## Error conditions

### Resource Errors

Error 2015 is unrecoverable, *naux* = 0, and unable to allocate work area.

### Computational Errors

None

### Input-Argument Errors

- $n < 0$
- $na < 0$
- $IDIAG(n+1) > na+1$
- $IDIAG(i+1) \leq IDIAG(i)$  for  $i = 1, n$
- $IDIAG(i+1) > IDIAG(i)+i$  and  $ITRAN(1) = 0$  for  $i = 1, n$
- $IDIAG(i) > IDIAG(i-1)+i$  and  $ITRAN(1) = 1$  for  $i = 2, n$
- $ITRAN(1) \neq 0$  or  $1$
- $ITRAN(2) \neq 0$  or  $1$
- $ITRAN(3) \neq -1$  or  $1$
- naux* Error 2015 is recoverable or *naux*  $\neq 0$ , and is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

## Examples

### Example 1

This example shows how to convert a 9 by 9 symmetric sparse matrix  $A$  from diagonal-out skyline storage mode to profile-in skyline storage mode. Matrix  $A$  is:

$$\begin{bmatrix} 11.0 & 12.0 & 13.0 & 14.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 12.0 & 22.0 & 23.0 & 24.0 & 25.0 & 26.0 & 0.0 & 28.0 & 0.0 \\ 13.0 & 23.0 & 33.0 & 34.0 & 35.0 & 36.0 & 0.0 & 38.0 & 0.0 \\ 14.0 & 24.0 & 34.0 & 44.0 & 45.0 & 46.0 & 0.0 & 48.0 & 0.0 \\ 0.0 & 25.0 & 35.0 & 45.0 & 55.0 & 56.0 & 57.0 & 58.0 & 0.0 \\ 0.0 & 26.0 & 36.0 & 46.0 & 56.0 & 66.0 & 67.0 & 68.0 & 69.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 57.0 & 67.0 & 77.0 & 78.0 & 79.0 \\ 0.0 & 28.0 & 38.0 & 48.0 & 58.0 & 68.0 & 78.0 & 88.0 & 89.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 69.0 & 79.0 & 89.0 & 99.0 \end{bmatrix}$$

Assuming that DSKFS last performed a factorization on matrix *A*, the direction of the transformation is negative; that is, ITRAN(3) is -1. This provides the best performance here.

**Call Statement and Input:**

```

          N   A   NA   IDIAG   ITRAN   AUX   NAUX
CALL DSKTRN( 9 , A , 33 , IDIAG , ITRAN , AUX , 9 )

```

```

A          = (11.0, 22.0, 12.0, 33.0, 23.0, 13.0, 44.0, 34.0, 24.0,
             14.0, 55.0, 45.0, 35.0, 25.0, 66.0, 56.0, 46.0, 36.0,
             26.0, 77.0, 67.0, 57.0, 88.0, 78.0, 68.0, 58.0, 48.0,
             38.0, 28.0, 99.0, 89.0, 79.0, 69.0)
IDIAG     = (1, 2, 4, 7, 11, 15, 20, 23, 30, 34)
ITRAN     = (0, 1, -1)

```

**Output:**

```

A          = (11.0, 12.0, 22.0, 13.0, 23.0, 33.0, 14.0, 24.0, 34.0,
             44.0, 25.0, 35.0, 45.0, 55.0, 26.0, 36.0, 46.0, 56.0,
             66.0, 57.0, 67.0, 77.0, 28.0, 38.0, 48.0, 58.0, 68.0,
             78.0, 88.0, 69.0, 79.0, 89.0, 99.0)
IDIAG     = (1, 3, 6, 10, 14, 19, 22, 29, 33, 34)

```

**Example 2**

This example shows how to convert the same 9 by 9 symmetric sparse matrix *A* in Example 1 from profile-in skyline storage mode to diagonal-out skyline storage mode.

Assuming that DSKFS last performed a solve on matrix *A*, the direction of the transformation is positive; that is, ITRAN(3) is 1. This provides the best performance here.

**Call Statement and Input:**

```

          N   A   NA   IDIAG   ITRAN   AUX   NAUX
CALL DSKTRN( 9 , A , 33 , IDIAG , ITRAN , AUX , 9 )

```

```

A          =(same as output A in Example 1)
IDIAG     =(same as output IDIAG in Example 1)
ITRAN     = (1, 0, 1)

```

**Output:**

```

A          =(same as input A in Example 1)
IDIAG     =(same as input IDIAG in Example 1)

```



---

## Part 3. Appendixes



---

## Appendix A. Basic Linear Algebra Subprograms (BLAS)

This appendix lists the ESSL subprograms corresponding to a subprogram in the standard set of BLAS.

---

### Level 1 BLAS

Table 183. Level 1 BLAS Included in ESSL

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram
Position of the First or Last Occurrence of the Vector Element Having the Largest Magnitude	ISAMAX ICAMAX	IDAMAX IZAMAX
Sum of the Magnitudes of the Elements in a Vector	SASUM SCASUM	DASUM DZASUM
Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y	SAXPY CAXPY	DAXPY ZAXPY
Copy a Vector	SCOPY CCOPY	DCOPY ZCOPY
Dot Product of Two Vectors	SDOT CDOTU CDOTC	DDOT ZDOTU ZDOTC
Euclidean Length of a Vector with Scaling of Input to Avoid Destructive Underflow and Overflow	SNRM2 SCNRM2	DNRM2 DZNRM2
Construct a Givens Plane Rotation	SROTG CROTG	DROTG ZROTG
Apply a Plane Rotation	SROT CROT CSROT	DROT ZROT ZDROT
Multiply a Vector X by a Scalar and Store in the Vector X	SSCAL CSCAL CSSCAL	DSCAL ZSCAL ZDSCAL
Interchange the Elements of Two Vectors	SSWAP CSWAP	DSWAP ZSWAP

---

### Level 2 BLAS

Table 184. Level 2 BLAS Included in ESSL

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram
Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose	SGEMV CGEMV	DGEMV ZGEMV
Rank-One Update of a General Matrix	SGER CGERU CGERC	DGER ZGERU ZGERC
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Matrix	SSPMV CHPMV SSYMV CHEMV	DSPMV ZHPMV DSYMV ZHEMV

Table 184. Level 2 BLAS Included in ESSL (continued)

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram
Rank-One Update of a Real Symmetric or Complex Hermitian Matrix	SSPR CHPR SSYR CHER	DSPR ZHPR DSYR ZHER
Rank-Two Update of a Real Symmetric or Complex Hermitian Matrix	SSPR2 CHPR2 SSYR2 CHER2	DSPR2 ZHPR2 DSYR2 ZHER2
Matrix-Vector Product for a General Band Matrix, Its Transpose, or Its Conjugate Transpose	SGBMV CGBMV	DGBMV ZGBMV
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Band Matrix	SSBMV CHBMV	DSBMV ZHBMV
Matrix-Vector Product for a Triangular Matrix, Its Transpose, or Its Conjugate Transpose	STPMV CTPMV STRMV CTRMV	DTPMV ZTPMV DTRMV ZTRMV
Solution of a Triangular System of Equations with a Single Right-Hand Side	STPSV CTPSV STRSV CTRSV	DTPSV ZTPSV DTRSV ZTRSV
Matrix-Vector Product for a Triangular Band Matrix, Its Transpose, or Its Conjugate Transpose	STBMV CTBMV	DTBMV ZTBMV
Triangular Band Equation Solve	STBSV CTBSV	DTBSV ZTBSV

## Level 3 BLAS

Table 185. Level 3 BLAS Included in ESSL

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram
Combined Matrix Multiplication and Addition for General Matrices, Their Transposes, or Conjugate Transposes	SGEMM CGEMM	DGEMM ZGEMM
Matrix-Matrix Product Where One Matrix is Real or Complex Symmetric or Complex Hermitian	SSYMM CSYMM CHEMM	DSYMM ZSYMM ZHEMM
Triangular Matrix-Matrix Product	STRMM CTRMM	DTRMM ZTRMM
Rank-K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYRK CSYRK CHERK	DSYRK ZSYRK ZHERK
Rank-2K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYR2K CSYR2K CHER2K	DSYR2K ZSYR2K ZHER2K
Solution of Triangular Systems of Equations with Multiple Right-Hand Sides	STRSM CTRSM	DTRSM ZTRSM

---

## Appendix B. LAPACK

This appendix contains the following two tables:

- Table 186 on page 1043
- Table 187 on page 1044

---

### LAPACK Subroutines

The following table lists the ESSL subroutines corresponding to subroutines in the standard set of LAPACK.

*Table 186. LAPACK subroutines included in ESSL*

<b>Descriptive Name</b>	<b>Short- Precision Subprogram</b>	<b>Long- Precision Subprogram</b>
General Matrix Factorization and Multiple Right-Hand Side Solve	SGESV CGESV	DGESV ZGESV
General Matrix Factorization	SGETRF CGETRF	DGETRF ZGETRF
General Matrix, Its Transpose, or Its Conjugate Transpose Multiple Right-Hand Side Solve	SGETRS CGETRS	DGETRS ZGETRS
Positive Definite Real Symmetric Matrix Factorization and Multiple Right-Hand Side Solve	SPPSV CPPSV	DPSPV ZPPSV
Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization and Multiple Right-Hand Side Solve	SPOSV CPOSV	DPOSV ZPOSV
Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization	SPOTRF CPOTRF SPPTRF CPPTRF	DPOTRF ZPOTRF DPPTRF ZPPTRF
Positive Definite Real Symmetric or Complex Hermitian Matrix Multiple Right-Hand Side Solve	SPOTRS CPOTRS SPPTRS CPPTRS	DPOTRS ZPOTRS DPPTRS ZPPTRS
General Matrix Inverse	SGETRI CGETRI	DGETRI ZGETRI
Positive Definite Real Symmetric or Complex Hermitian Matrix Inverse	SPOTRI CPOTRI SPPTRI	DPOTRI ZPOTRI DPPTRI
Triangular Matrix Inverse	STRTRI STPTRI CTRTRI CTPTRI	DTRTRI DTPTRI ZTRTRI ZTPTRI
General Matrix QR Factorization		DGEQRF
Linear Least Squares Solution for a General Matrix		DGELS

---

### Non-LAPACK-Conforming Subroutines

The following table lists each ESSL subroutine whose name is the same as an existing LAPACK subroutine, but whose calling-sequence arguments and functionality are different from that LAPACK subroutine.

Table 187. Non-LAPACK subroutines included in ESSL whose names match existing LAPACK subroutines

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine
Eigenvalues and, Optionally, All or Selected Eigenvectors of a General Matrix	SGEEV CGEEV	DGEEV ZGEEV
Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix	SSPEV CHPEV	DSPEV ZHPEV
Extreme Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix	SSPSV CHPSV	DSPSV ZHPSV
Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Eigensystem, $Az=wBz$ , where A and B Are Real General Matrices	SGEGV	DGEGV
Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Symmetric Eigensystem, $Az=wBz$ , where A Is Real Symmetric and B Is Real Symmetric Positive Definite	SSYGV	DSYGV

---

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## Glossary

This glossary defines terms and abbreviations used in this publication. If you do not find the term you are looking for, refer to the index portion of this book. This glossary includes terms and definitions from:

- *American National Standard Dictionary for Information Systems*, ANSI X3.172-1990, copyright 1990 by the American National Standards Institute (ANSI). Copies may be purchased from the American National Standards Institute, 11 West 42nd Street, New York, New York 10036. Definitions are identified by the symbol (A) after the definition.
- *Information Technology Vocabulary*, developed by Subcommittee 1, Joint Technical Committee 1, of the International Organization for Standardization and the International Electrotechnical Commission (ISO/IEC JTC1/SC1). Definitions from published sections of these vocabularies are identified by the symbol (I) after the definition. Definitions taken from draft international standards, committee drafts, and working papers being developed by ISO/IEC JTC1/SC1 are identified by the symbol (T) after the definition, indicating that final agreement has not yet been reached among the participating National Bodies of SC1.

### A

**address.** A character or group of characters that identifies a register, a device, a particular part of storage, or some other data source or destination.

**AIX.** A UNIX operating system developed by IBM that is designed and optimized to run on POWER microprocessor-based hardware such as servers, workstations and blades.

**APAR.** See *authorized program analysis report*.

**application.** A program or set of programs that perform a task; some examples are payroll, inventory, management, and word processing applications.

**argument.** A parameter passed between a calling program and a called program.

**array.** An ordered set of data items identified by a single name.

**array descriptor.** The information required to establish the mapping between an array's global data structure and its corresponding process and memory location.

**array element.** A data item in an array, identified by the array name followed by a subscript indicating its position in the array.

**array name.** The name of an ordered set of data items that make up an array.

**assignment statement.** A statement that gives a value to a variable or array element. It always contains the assignment symbol (=).

**authorized program analysis report (APAR).** A request for correction of a defect in a current release of an IBM-supplied program.

### B

**bandwidth.** The capacity of a communications line, normally expressed in bits per second (bps).

**Basic Linear Algebra Communication Subprograms (BLACS).** A standard set of public domain subroutines that perform message passing (that is, communication) between processes.

**Basic Linear Algebra Subprograms (BLAS).** A standard set of public domain mathematical subroutines that perform linear algebra operations.

**BLACS.** See *Basic Linear Algebra Communication Subprograms*.

**BLAS.** See *Basic Linear Algebra Subprograms*.

### C

**cache.** A special-purpose buffer storage, smaller and faster than main storage, used to hold a copy of instructions and data obtained from main storage and likely to be needed next by the processor.

**Centralized Management Interface (CMI).** A series of menus and dialog boxes based on the System Management Interface Toolkit (SMIT). CMI is used to define and query the SP system configuration.

**character constant.** A string of one or more alphanumeric characters enclosed in apostrophes. The delimiting apostrophes are not part of the value of the constant.

**character expression.** An expression in the form of a single character constant, variable, array element,

substring, function reference, or another expression enclosed in parentheses. A character expression is always of type character.

**character type.** A data type that consists of alphanumeric characters.

**client.** A system or process that is dependent on another system or process (usually called the *server*) to provide it with access to data, services, programs, or resources.

**cluster.** A collection of complete systems that work together to provide a single, unified, computing capability.

**CMI.** See *Centralized Management Interface*.

**column-major order.** A way of storing array elements such that the leftmost subscript varies most rapidly as memory-adjacent elements are accessed.

**complex conjugate even data.** Complex data with an even real part and an odd imaginary part.

**complex constant.** An ordered pair of real or integer constants separated by a comma and enclosed in parentheses. The first constant of the ordered pair represents the real part of a complex number; the second represents the imaginary part.

**complex type.** A data type that represents values of complex numbers. A value is expressed as an ordered pair of real data items separated by a comma and enclosed in parentheses. The first item represents the real part of the complex number, and the second item represents the imaginary part.

**constant.** An unvarying quantity. The four classes of constants specify numbers (arithmetic), truth values (logical), character data (character), and hexadecimal data.

## D

**daemon.** A program that runs unattended to perform continuous or periodic functions, such as network control.

**dataless workstation.** A workstation that has local disks which may be used for **swap**, **tmp**, and **usr** file systems.

**data distribution.** The method in which global data structures are divided among processes. Three types of data distribution are cyclic, block-cyclic, and block distribution.

**data type.** The structural characteristics, features and properties of data that can be directly specified by a programming language. Examples of data types are integers and real numbers in Fortran; arrays in APL; linked lists in LISP; and character strings in SNOBOL.

**decimation.** The formation of a sequence containing every *n*th element of another sequence.

**default.** A value that is automatically supplied or assumed by the system or program when no value is specified by the user.

**dimension.** The attribute of size given to arrays and tables. Contrast with *rank*. See also *extent*.

**direct access storage device.** Peripheral storage equipment in which data access is achieved without the necessity of sequentially traversing the data file.

**diskless.** The property of a workstation that has no local file systems or local boot images to access some of its resources remotely. Diskless clients boot remotely from a diskless server and use the server for remote paging.

**Diskless Workstation Manager (DWM).** Operating-system software that initializes and maintains resources for diskless clients and diskless servers.

**divide-by-zero exception.** The condition recognized by a processor that results from running a program that attempts to divide by zero.

**DNS.** See *domain name server*.

**domain name server (DNS).** In Internet communications, a server program that supplies name-to-address conversion by mapping domain names to IP addresses.

**double precision.** See *long precision*.

**DWM.** See *Diskless Workstation Manager*.

## E

**Ethernet.** A standard protocol for a baseband local area network (LAN) that allows multiple access and manages contention by using carrier sense multiple access with collision detection (CSMA/CD) as the access method.

**expression.** A notation that represents a value: a primary appearing alone, or combinations of primaries and operators. An expression can be arithmetic, character, logical, or relational.

**extent.** The number of different integer values that can be represented by subscript expressions for a particular dimension in a subscript for an array.

**external function.** A procedure or function called from outside the program in which the routine is defined. Contrast with *statement function*.

## F

**file.** A collection of information treated as a unit.

**file server.** A centrally located computer that acts as a storehouse of data and applications for numerous users of a local area network (LAN).

**foreign host.** Any host on a network except the host at which a particular operator is working.

**function.** In Fortran, a procedure that is invoked by referring to it in an expression and that supplies a value to the expression. The value supplied is the value of the function. See also *external function*, *intrinsic function*, and *statement function*.

**function reference.** A Fortran source program reference to an intrinsic function, to an external function, or to a statement function.

## G

**general matrix.** A matrix with no assumed special properties such as symmetry. See also *matrix*.

**global.** Pertaining to information available to more than one program or subroutine. Contrast with *local*.

## H

**home directory.** The directory associated with an individual user.

**host.** A computer that is connected to a network and provides an access point to that network. The host can be a client, a server, or both a client and server simultaneously.

## I

**integer constant.** A decimal constant containing no decimal point.

**integer expression.** An arithmetic expression with only integer type values.

**integer type.** An arithmetic data type capable of expressing the value of an integer. An integer type can have a positive, negative, or 0 value. It must not include a decimal point.

**interim fix.** A noncumulative fix that is made available to all customers. An interim fix is tested by IBM. It contains at least one APAR.

**Internet.** The worldwide collection of interconnected networks that use the Internet suite of protocols and permit public access.

**IP address.** The unique 32-bit address that specifies the location of each device or workstation in the Internet. For example, 9.67.97.103 is an IP address.

**intrinsic function.** In Fortran, a function that is supplied with the runtime environment that performs mathematical, character, logical, or bit-manipulation operations.

## K

**kernel.** The part of an operating system that performs basic functions such as allocating hardware resources.

## L

**LAN.** See *local area network*.

**latency.** The time interval between the instant at which an instruction control unit initiates a call for data and the instant at which the actual transfer of the data starts.

**leading dimension.** For a two-dimensional array, an increment used to find the starting point for the matrix elements in each successive column of the array.

**local.** Pertaining to information that is defined and used only in one subdivision of a computer program. Contrast with *global*.

**local area network.** A network that connects several devices into a limited area (such as a single building or campus) and that can be connected to a larger network.

**local host.** The computer to which a user's terminal is directly connected.

**logical constant.** A constant with a value of true or false.

**logical expression.** An expression consisting of logical operators, relational operators, or both that can be evaluated to a value of either true or false.

**logical type.** A data type that contains the values of true and false. See also *data type*.

**long precision.** Pertaining to the use of two computer words to represent a number in accordance with the required precision. Contrast with *short precision*.

## M

**main program.** A program that performs primary functions, passing control to routines and subroutines for the performance of more specific functions.

**mainframe.** A computer, usually in a computer center, with extensive capabilities and resources to which other computers can be connected so that they can share facilities.

**mask.** To use a pattern of characters to control the retention or elimination of portions of another pattern of characters. (I)

**matrix.** A rectangular array of elements arranged in rows and columns that can be manipulated based on matrix algebra rules.

**menu.** A displayed list of items from which a user can make a selection.

**Message Passing Interface.** A standard for communication among the nodes running a parallel program on a distributed memory system.

**MPI.** See *Message Passing Interface*.

**MPMD.** See *Multiple Program Multiple Data*.

**Multiple Program Multiple Data (MPMD).** A parallel programming model in which different, but related, programs are run on different sets of data.

## N

**name.** An alphanumeric term that identifies a data set, statement, program, or cataloged procedure. The first character of the name must be alphabetic.

**network.** In data communications, a configuration in which two or more locations are physically connected for the purpose of exchanging data.

**Network File System.** A protocol, developed by Sun Microsystems, Incorporated, that allows any host in a network to gain access to another host or netgroup and their file directories.

**NFS.** See *Network File System*.

**node.** In a network, a point at which one or more functional units connect channels or data circuits.

**node ID.** A unique string of characters that identifies the node on a network

## O

**overflow exception.** A condition caused by the result of an arithmetic operation having a magnitude that exceeds the largest possible number.

## P

**parallel processing.** A multiprocessor architecture in which processes are allocated to tightly coupled

processors in a cooperative processing environment, permitting the concurrent execution of tasks.

**parameter.** A value or reference passed to a function, command, or program that serves as input or to control actions. The value is supplied by a user or by another program or process.

**pipe.** In UNIX-based operating systems, a connective symbol used between two commands on a command line, indicating that the output from the preceding command is to be used as the input for the following command.

**port.** (1) A hardware interface to which I/O devices are attached for the purpose of sending and receiving data. (2) A 16-bit number identifying a particular Transmission Control Protocol (TCP) or User Datagram Protocol (UDP) resource within a given Transmission Control Protocol/Internet Protocol (TCP/IP) node.

**primary.** An irreducible unit of data, such as a single constant, variable, or array element.

**process.** A function being performed or waiting to be performed.

**process grid.** A way to view a parallel machine as a logical, one-dimensional or two-dimensional, rectangular grid of processes.

**program exception.** The condition recognized by a processor that results from running a program that incorrectly specifies or uses instructions, operands, or control information.

**protocol.** A set of semantic and syntactic rules that defines the behavior of functional units in achieving communication.

## R

**rank.** In Fortran, the number of dimensions of an array. The rank is zero for scalar.

**real constant.** A string of decimal digits that expresses a real number. A real constant must contain either a decimal point, a decimal exponent, or both.

**real type.** An arithmetic data type that can approximate the values of real numbers.

**reduced instruction set computer (RISC).** A computer that uses a small, simplified set of frequently used instructions for rapid processing.

**remote host.** See *foreign host*.

**RISC.** See *reduced instruction set computing*.

**row-major order.** A method of storing array elements such that the rightmost subscript varies most rapidly as memory-adjacent elements are accessed.

## S

**ScaLAPACK (Scalable Linear Algebra Package).** A linear algebra package (LAPACK) designed for distributed-memory parallel computers.

**scalar.** A quantity characterized by a single value. Contrast with *vector*.

**scope.** The portion of a computer program within which the definition of a variable remains unchanged.

**server.** In a network, hardware or software that provides facilities to other stations. Examples of a server are a file server, a printer server, or a mail server.

**shape.** The extents, listed in order, of all the dimensions of an array. For example, the shape of a three-dimensional array that has four rows, five columns, and three planes is (4,5,3) or 4 by 5 by 3.

**shell.** A software interface between users and the operating system that interprets commands and user interactions and communicates them to the operating system.

**short precision.** The use of one computer word to represent a number, in accordance with the required precision. Contrast with *long precision*.

**single precision.** See *short precision*.

**Single Program Multiple Data (SPMD).** A parallel programming model in which different processors execute the same program on different sets of data.

**size.** The number of elements in an array. The size of an array is the product of the extents of its dimensions.

**SMIT.** See *System Management Interface Toolkit*.

**SMP.** See *symmetric multiprocessor*.

**SPMD .** See *Single Program Multiple Data*.

**statement.** The basic unit of a program, that specifies an action to be performed, the nature and characteristics of the data to be processed, or information about the program itself. Statements fall into two broad classes: executable and nonexecutable.

**statement function.** A procedure specified by a single statement that is similar in form to an arithmetic, a logical, or a character assignment statement. The statement must appear after the specification statements and before the first executable statement; in the remainder of the program, it can be referenced as a function. A statement function can be referred to only in the program unit in which it is defined. Contrast with *external function*.

**statement label.** In Fortran, a number containing one to five decimal digits that is used to identify a statement. A statement label is usually used to transfer control, define the range of a DO loop, or refer to a FORMAT statement.

**statement number.** See *statement label*.

**stride.** The increment used to step through array storage to select the vector or matrix elements from the array.

**subprogram.** A program unit that is invoked by another program unit in the same program. In Fortran, a subprogram has a FUNCTION, SUBROUTINE, or BLOCK DATA statement as its first statement.

**subscript.** (1) A symbol that is associated with the name of a set to identify a particular subset or element. (A) (2) One or more expressions, each enclosed in brackets, that follow an array name. A subscript refers to an element in an array.

**subscript expression.** An integer expression in a subscript whose value and position in the subscript determine the index number for the corresponding dimension in the referenced array.

**system administrator.** The person at a computer installation who designs, controls, and manages the use of the computer system.

**System Management Interface Tool (SMIT).** An interface tool of the AIX operating system for installing, maintaining, configuring, and diagnosing tasks.

**symmetric multiprocessor (SMP).** A system containing multiple processors that are essentially identical and perform identical functions.

## T

**tape archive (tar).** A UNIX utility used to archive files by combining several files into one.

**tar.** See *tape archive*.

**TCP.** See *Transmission Control Protocol*.

**TCP/IP.** See *Transmission Control Protocol/Internet Protocol*.

**Telnet.** In TCP/IP, a protocol that provides remote-terminal connection service. It allows users of one host to log on to a remote host and interact as directly attached terminal users of that host.

**thread.** An element that is scheduled and to which resources such as execution time, locks, and queues may be assigned. There may be one or more threads in a process, and each thread is executed by the operating system concurrently.

**threadsafe.** A function, macro, or operating system service that can be called from multiple threads in a process at the same time.

**thread-tolerant.** A library that can be called from a single thread of a multithreaded application. However, multiple simultaneous calls to the thread-tolerant library from different threads of a single process causes unpredictable results.

**transaction.** An exchange between the user and the system. Each activity the system performs for the user is considered a transaction.

**transfer.** To send data from one location to another.

**transmission.** The sending of data from one place for reception elsewhere.

**Transmission Control Protocol.** A communications protocol used in the Internet and in any network that follows the Internet Engineering Task Force (IETF) standards for internetwork protocol. TCP provides a reliable host-to-host protocol between hosts in packet-switched communications networks and in interconnected systems of such networks. It uses the Internet Protocol (IP) as the underlying protocol.

**Transmission Control Protocol/Internet Protocol.** An industry-standard nonproprietary set of communications protocols that provide reliable end-to-end connections between applications over interconnected networks of different types.

**type declaration.** The specification of the type and, optionally, the length of a variable or function in a specification statement.

## U

**UDP.** See *User Datagram Protocol*.

**underflow exception.** A condition that occurs when the result of an arithmetic operation has a magnitude less than the smallest possible nonzero number.

**Uniform Resource Locator (URL).** The unique address of a file that is accessible in a network such as the Internet. The URL includes the abbreviated name of the protocol used to access the information resource and the information used by the protocol to locate the information resource.

**URL.** See *Uniform Resource Locator*.

**user.** Any person, organization, process, device, program, protocol, or system that uses the services of a computing system.

**User Datagram Protocol (UDP).** An Internet protocol that provides unreliable, connectionless datagram service. It enables an application program on one

machine or process to send a datagram to an application program on another machine or process.

## V

**variable.** A name used to represent data that can be changed while the program or procedure is running.

**vector.** A one-dimensional ordered collection of numbers.

## W

**working directory.** A collection of files to be manipulated by a File Transfer Protocol (FTP) operation.

**workstation.** A configuration of input/output equipment at which an operator works. A workstation is a terminal or microcomputer that is usually connected to a mainframe or a network at which a user can perform applications.

## X

**X Window System.** A software system, developed by the Massachusetts Institute of Technology, that enables the user of a display to concurrently use multiple application programs through different windows of the display. The application programs may execute on different computers.



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## Bibliography

This bibliography lists the publications and related product libraries that you may need to use with ESSL and describes how to obtain them.

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## References

Text books and articles covering the mathematical aspects of ESSL are listed in this section, as well as several software libraries available from other companies. They are listed alphabetically as follows:

- Publications are listed by the author's name. IBM publications that include an order number, other than an *IBM Technical Report* can be ordered through the Subscription Library Services System (SLSS). The non-IBM publications listed here should be obtained through publishers, bookstores, or professional computing organizations.
- Software libraries are listed by their product name. Each reference includes the names, addresses, and phone numbers of the companies from which they can be obtained.

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## ESSL Publications

ESSL publications are all available on the Internet at the URLs listed in Table 7 on page 11.

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## Related Publications

The related publications or libraries at the Web sites listed below may be useful to you when using ESSL.

Product	Web site URL
AIX	<a href="http://www.ibm.com/servers/aix">http://www.ibm.com/servers/aix</a>
Linux	For general information and documentation on Linux: <a href="http://www.tldp.org/">http://www.tldp.org/</a>  For information about the standard Linux installation procedure using the RPM Package Manager (RPM): <a href="http://www.rpm.org/">http://www.rpm.org/</a>  For information about IBM-related offerings for Linux: <a href="http://www.ibm.com/linux/">http://www.ibm.com/linux/</a>
C and C++	<a href="http://www-3.ibm.com/software/awdtools/vacpp/library/">http://www-3.ibm.com/software/awdtools/vacpp/library/</a>
XL Fortran	<a href="http://www-3.ibm.com/software/awdtools/fortran/xlfortran/library/">http://www-3.ibm.com/software/awdtools/fortran/xlfortran/library/</a>
Blue Gene	For general information and documentation about Blue Gene, go to the IBM Redbooks™ Web site at the following URL and search on "Blue Gene": <a href="http://www.redbooks.ibm.com/redbooks.nsf/redbooks/">http://www.redbooks.ibm.com/redbooks.nsf/redbooks/</a>

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# Index

## Numerics

- 3838 Array Processor
  - general signal processing
  - routines 778

## A

- abbreviations
  - for product names xiv
  - interpreting math and programming xviii
- absolute value
  - maximum 199
  - minimum 202
  - notation xviii
  - sum of all absolute values 211
- accuracy
  - considerations for dense and banded linear algebraic equations 449
  - considerations for eigensystem analysis 735
  - considerations for Fourier transforms, convolutions, and correlations 781
  - considerations for interpolation 945
  - considerations for linear algebra subprograms 196
  - considerations for matrix operations 375
  - considerations for numerical quadrature 965
  - considerations for related computations 785
  - considerations for sorting and searching 925
  - error of computation 48
  - of results 5, 47
  - precisions 47
  - what accuracy means 47
  - where to find information on 47
- acronyms
  - associated with programming values xviii
  - product names xiv
- adding
  - absolute values 211
  - general matrices or their transposes 377
  - vector  $x$  to vector  $y$  and store in vector  $z$  257
- address notation xviii
- advantages of ESSL 3
- AIX
  - publications 1060
- AIX, supported versions 8
- algebra 445
- Announcing ESSL brochure 1060
- applications in the industry 4
- architecture supported by ESSL for AIX on the workstations 8

- architecture supported by ESSL for Linux on the workstations 8
- arguments
  - coding rules 34
  - conventions used in the subroutine descriptions xx
  - diagnosing ESSL input-argument errors 177
  - font for ESSL calling xv
  - list of ESSL input-argument errors 180, 188
  - passing in C programs 130
  - passing in C++ programs 145
- array
  - coding in C programs 133
  - coding in C++ programs 150
  - coding in Fortran programs 112
  - conventions for xvii
  - definition of 33
  - real and complex elements 112
  - setting up data structures inside 59
  - storage techniques overview 33
- array data
  - storage and performance tradeoffs 49
- arrow notation, what it means xviii
- ation notation xviii
- attention error messages, interpreting 179
- autocorrelation of one or more sequences 896, 900
- auxiliary working storage
  - calculating 37
  - dynamic allocation 37
  - list of subroutines using 36
  - provided by the user 37

## B

- background books 1055
- band matrix
  - definition of 80
  - storage layout 81, 83, 86, 87, 90, 91
- band matrix subroutines, names of 445
- band width 80, 85
- banded linear algebraic equation subroutines 445
  - SGBF and DGBF 579
  - SGBS and DGBS 583
  - SGTF and DGTG 593
  - SGTNP, DGTNP, CGTNP, and ZGTNP 598
  - SGTNPF, DGTNPF, CGTNPF, and ZGTNPF 601
  - SGTNPS, DGTNPS, CGTNPS, and ZGTNPS 604
  - SGTS and DGTS 596
  - SPBF, DPBF, SPBCHF, and DPBCHF 586
  - SPBS, DPBS, SPBCHS, and DPBCHS 590
  - SPTF and DPTF 607

- banded linear algebraic equation subroutines (*continued*)
  - SPTS and DPTS 609
  - STBSV, DTBSV, CTBSV, and ZTBSV 611
- base program, processing your under AIX 163
- bibliography 1055
- binary search 936
- BLAS (Basic Linear Algebra Subprograms) 193
  - ESSL subprograms 193, 1041
  - Level 1 1041
  - Level 2 1041
  - Level 3 1042
  - migrating from 173
  - migrating to ESSL 25
- BLAS-general-band storage mode 83
- bold letters, usage of xv
- books 1055

## C

- C (C programming language)
  - coding programs 129
  - ESSL header file 129, 132
  - function reference 129
  - handling errors in your program 136
  - how to code arrays 133
  - modifying procedures for using ESSL for AIX 164
  - modifying procedures for using ESSL for Linux 168
  - passing character arguments 130
  - program calling interface 129
  - setting up complex and logical data 132
- C and C++
  - publications 1060
- C libraries 9
- C++ (C++ programming language)
  - coding programs 145
  - ESSL header file 145, 148
  - function reference 145
  - handling errors in your program 152
  - how to code arrays 150
  - modifying procedures for using ESSL for AIX 165
  - modifying procedures for using ESSL for Linux 168
  - passing character arguments 145
  - program calling interface 145
  - setting up complex and logical data 148
- calculating auxiliary working storage 37
- calculating transform lengths 42
- CALL statement 111
- calling sequence
  - for C programs 129
  - for C++ programs 145
  - for Fortran programs 111

- calling sequence (*continued*)
  - specifying the arguments 34
  - subroutines versus functions 111, 129, 145
  - syntax description xx
- cataloged procedures, ESSL 163
- CAXPY 214
- CAXPYI 286
- CCOPY 217
- CDOTC 220
- CDOTCI 289
- CDOTU 220
- CDOTUI 289
- ceiling notation and meaning xviii
- CGBMV 336
- CGEADD 377
- CGEEV 737
- CGEF 467
- CGEMM 404
- CGEMMS 398
- CGEMUL 389
- CGEMV 294
- CGERC 305
- CGERU 305
- CGES 470
- CGESM 474
- CGESUB 383
- CGESV 454
- CGETMI 439
- CGETMO 442
- CGETRF 458
- CGETRI 539
- CGETRS 462
- CGTHR 280
- CGTHRZ 283
- CGTNP 598
- CGTNPf 601
- CGTNPS 604
- character data
  - conventions xv, 33
- characters, special usage of xviii
- CHBMV 343
- CHEMM 412
- CHEMV 312
- CHER 320
- CHER2 327
- CHER2K 432
- CHERK 426
- choosing the ESSL library 25
- choosing the ESSL subroutine 25
- CHPEV 748
- CHPMV 312
- CHPR 320
- CHPR2 327
- CHPSV 757
- citations 1055
- CNORM2 237
- coding your program
  - arguments in ESSL calling sequences 34
  - CALL sequence for C programs 129
  - CALL sequence for C++ programs 145
  - CALL sequence for Fortran programs 111
  - calls to ESSL in C programs 129
  - calls to ESSL in C++ programs 145
- coding your program (*continued*)
  - calls to ESSL in Fortran programs 111
  - data types used in your program 33
  - handling errors with ERRSET, EINFO, ERRSAV, ERRSTR, and return codes 118, 136, 152
  - restrictions for application programs 32
  - techniques that affect performance 49
- column vector 59
- comparison of accuracy for libraries 5
- compilers, required by ESSL for AIX on the workstations 8
- compilers, required by ESSL for Linux on the workstations 9
- compiling your program
  - C programs 164, 168
  - C++ programs 165, 168
  - Fortran programs 163, 167
  - under AIX 163
- complex and real array elements 112
- complex conjugate notation xviii
- complex data
  - conventions xv, 33
  - setting up for C 132
  - setting up for C++ 148
- complex Hermitian band matrix
  - definition of 88
  - storage layout 88
- complex Hermitian matrix
  - definition of 73
  - storage layout 73
- complex Hermitian Toeplitz matrix
  - definition of 76
- complex matrix 65
- complex vector 59
- compressed-diagonal storage mode for sparse matrices 96
- compressed-matrix storage mode for sparse matrices 95
- compressed-vector, definition and storage mode 64
- computational areas, overview 4
- computational errors
  - diagnosing 178
  - list of messages for 186
  - overview 51
- condition number, reciprocal of
  - general matrix 479, 539
  - positive definite complex Hermitian matrix 547
  - positive definite real symmetric matrix 518, 547
- conjugate notation xviii
- conjugate transpose
  - of matrix operation results for multiply 392, 402, 407
- conjugate transpose of a matrix 66
- conjugate transpose of a vector 60
- continuation, convention for numerical data xv
- conventions xv
  - for messages 179
  - mathematical and programming notations xviii
- conventions (*continued*)
  - subroutine descriptions xix
- convolution and correlation
  - autocorrelation of one or more sequences 896
  - direct method
    - one sequence with another sequence 875
    - with decimated output 891
  - mixed radix Fourier method
    - autocorrelation of one or more sequences 900
    - one sequence with one or more sequences 881
  - one sequence with one or more sequences 869
- convolution and correlation subroutines
  - accuracy considerations 781
  - performance and accuracy considerations 783
  - performance considerations 781
  - SACOR 896
  - SACORF 900
  - SCON and SCOR 869
  - SCOND and SCORD 875
  - SCONF and SCORF 881
  - SDCON, DDCON, SDCOR, and DDCOR 891
  - usage considerations 778
- copy a vector 217
- correlation 869
- cosine notation xviii
- cosine transform 812
- courier font usage xv
- CPOF 495
- CPOSM 507
- CPOSV 489
- CPOTRF 495
- CPOTRI 547
- CPOTRS 507
- CPPSV 483
- CPPTRF 495
- CPPTRS 507
- CROT 247
- CROTG 240
- CSCAL 251
- CSCTR 277
- CSROT 247
- CSSCAL 251
- CSWAP 254
- CSYAX 269
- CSYMM 412
- CSYR2K 432
- CSYRK 426
- CTBMV 354
- CTBSV 611
- CTPMV 348
- CTPSV 557
- CTPTRI 570
- CTRMM 419
- CTRMV 348
- CTRSM 563
- CTRSV 557
- CTRTRI 570
- cubic spline interpolating 955, 961
- customer service, IBM 175
- customer support, IBM 175



CVEA 257  
CVEM 265  
CVES 261  
CWLEV 920  
CYAX 269  
CZAXPY 272

## D

DASUM 211  
data  
    array data 33  
    conventions for scalar data xv, 33  
data structures (vectors and matrices) 59  
DAXPY 214  
DAXPYI 286  
DBSRCH 936  
DBSSV 524  
DBSTRF 530  
DBSTRS 535  
DCFT 787  
DCFT2 828  
DCFT3 850  
DCOPY 217  
DCOSF 812  
DCRFT 804  
DCRFT2 842  
DCRFT3 862  
DCSIN2 961  
DCSINT 955  
DDCON 891  
DDCOR 891  
DDOT 220  
DDOTI 289  
default values in the ESSL error option  
    table 54  
dense and banded subroutines  
    performance and accuracy  
    considerations 449  
dense linear algebraic equation  
    subroutines 445  
        CGESV 454  
        CPOSV 489  
        DBSSV 524  
        DBSTRF 530  
        DBSTRS 535  
        DGESV 454  
        DPOSV 489  
        SGEF, DGEF, CGEF, and ZGEF 467  
        SGEFCD and DGEFCD 479  
        SGES, DGES, CGES, and ZGES 470  
        SGESM, DGESM, CGESM, and  
        ZGESM 474  
        SGESV 454  
        SGETRF, DGETRF, CGETRF and  
        ZGETRF 458  
        SGETRI, DGETRI, CGETRI, ZGETRI,  
        SGEICD, and DGEICD 539  
        SGETRS, DGETRS, CGETRS, and  
        ZGETRS 462  
        SPOFCD and DPOFCD 518  
        SPOSM, DPOSM, CPOSM, ZPOSM,  
        SPPTRS, DPPTRS, CPPTRS, ZPPTRS,  
        SPOTRS, DPOTRS, CPOTRS, and  
        ZPOTRS 507  
        SPOSV 489  
dense linear algebraic equation  
    subroutines (*continued*)  
        SPOTRI, DPOTRI, CPOTRI, ZPOTRI,  
        SPOICD, DPOICD, SPPTRI, DPPTRI,  
        SPPICD, and DPPICD 547  
        SPPE, DPPF, SPPTRF, DPPTRF,  
        CPPTRF, ZPPTRF, SPOF, DPOF,  
        CPOF, ZPOF, SPOTRF, DPOTRF,  
        CPOTRF, ZPOTRF 495  
        SPPFCD and DPPFCD 518  
        SPPS and DPPS 515  
        SPPSV, DPPSV, CPPSV, ZPPSV 483  
        STPSV, DTPSV, CTPSV, and  
        ZTPSV 557  
        STRSM, DTRSM, CTRSM, and  
        ZTRSM 563  
        STRSV, DTRSV, CTRSV, and  
        ZTRSV 557  
        STRTRI, DTRTRI, CTRTRI, ZTRTRI,  
        STPTRI, DTPTRI, CTPTRI,  
        ZTPTRI 570  
        ZGESV 454  
        ZPOSV 489  
dense matrix, definition 94  
descriptions, conventions used in the  
    subroutine xix  
designing your program  
    accuracy of results 47  
    choosing the ESSL library 25  
    choosing the ESSL subroutine 25  
    error considerations 50  
    performance considerations 49  
    storage considerations 33  
determinant  
    general matrix 479, 539  
    general skyline sparse matrix 627  
    matrix notation xviii  
    positive definite complex Hermitian  
    matrix 547  
    positive definite real symmetric  
    matrix 518, 547  
    symmetric skyline sparse matrix 644  
DGBF 579  
DGBMV 336  
DGBS 583  
DGEADD 377  
DGEEV 737  
DGEF 467  
DGEFCD 479  
DGEGV 764  
DGEICD 539  
DGELLS 728  
DGELS 721  
DGEMM 404  
DGEMMS 398  
DGEMTX 294  
DGEMUL 389  
DGEMV 294  
DGEMX 294  
DGEQRF 717  
DGER 305  
DGES 470  
DGESM 474  
DGESUB 383  
DGESV 454  
DGESVF 704  
DGESVS 712  
DGETMI 439  
DGETMO 442  
DGETRF 458  
DGETRI 539  
DGETRS 462  
DGHMQ 988  
DGKFS 627  
DGKTRN 1030  
DGLGQ 981  
DGLNQ 972  
DGLNQ2 975  
DGRAQ 984  
DGSF 617  
DGSS 623  
DGTf 593  
DGTHR 280  
DGTHRZ 283  
DGTNP 598  
DGTNPF 601  
DGTNPS 604  
DGTS 596  
diagnosis procedures  
    attention error messages 179  
    computational errors 178  
    ESSL messages, list of 179  
    in your program 175  
    informational error messages 179  
    initial problem diagnosis procedures  
    (symptom index) 177  
    input-argument errors 177  
    miscellaneous error messages 179  
    program exceptions 177  
    resource error messages 178  
diagnostics 179  
diagonal-out skyline storage mode 102  
dimensions of arrays  
    storage layout 112  
direct method  
    general skyline sparse matrix 627  
    general sparse matrix 617  
    symmetric skyline sparse matrix 644  
direct sparse matrix solvers  
    usage considerations 449  
distributions of Linux that support  
    ESSL 8  
DIZC 910  
DNAXPY 224  
DNDOT 229  
DNORM2 237  
DNRAND 996  
DNRM2 234  
documentation 1055  
dot product  
    notation xviii  
    of dense vectors 220  
    of sparse vectors 289  
    special (compute N times) 229  
DPBCHF 586  
DPBCHS 590  
DPBF 586  
DPBS 590  
DPINT 947  
DPOF 495  
DPOFCD 518  
DPOICD 547  
DPOLY 907  
DPOSM 507

DPOSV 489  
 DPOTRF 495  
 DPOTRI 547  
 DPOTRS 507  
 DPPF 495  
 DPPFCD 518  
 DPPICD 547  
 DPPS 515  
 DPPSV 483  
 DPPTRF 495  
 DPPTRI 547  
 DPPTRS 507  
 DPTF 607  
 DPTNQ 969  
 DPTS 609  
 DQINT 916  
 DRCFT 796  
 DRCFT2 835  
 DRCFT3 856  
 DROT 247  
 DROTG 240  
 DSBMV 343  
 DSCAL 251  
 DSCTR 277  
 DSDCG 681  
 DSDGCG 696  
 DSDMX 367  
 DSINF 820  
 DSKFS 644  
 DSKTRN 1035  
 DSLMX 312  
 DSLR1 320  
 DSLR2 327  
 DSMCG 673  
 DSMGCG 689  
 DSMMX 360  
 DSMTM 363  
 DSORT 927  
 DSORTS 932  
 DSORTX 929  
 DSPEV 748  
 DSPMV 312  
 DSPR 320  
 DSPR2 327  
 DSPSV 757  
 DSRIS 662  
 DSRSM 1026  
 DSSRCH 940  
 DSWAP 254  
 DSYGV 770  
 DSYMM 412  
 DSYMV 312  
 DSYR 320  
 DSYR2 327  
 DSYR2K 432  
 DSYRK 426  
 DTBMV 354  
 DTBSV 611  
 DTPINT 952  
 DTPMV 348  
 DTPSV 557  
 DTPTRI 570  
 DTREC 913  
 DTRMM 419  
 DTRMV 348  
 DTRSM 563  
 DTRSV 557  
 DTRTRI 570  
 DURAND 993  
 DURXOR 1000  
 DVEA 257  
 DVEM 265  
 DVES 261  
 DWLEV 920  
 DYAX 269  
 dynamic allocation of auxiliary working storage 37  
 dynamic linking versus static linking 163, 167  
 DZASUM 211  
 DZAXPY 272  
 DZNRM2 234

**E**

efficiency of your program 49  
 eigensystem analysis subroutines performance and accuracy considerations 735  
 SGEEV, DGEEV, CGEEV, and ZGEEV 737  
 SGEGV and DGEGV 764  
 SSPEV, DSPEV, CHPEV, and ZHPEV 748  
 SSPSV, DSPSV, CHPSV, and ZHPSV 757  
 SSYGV and DSYGV 770  
 eigenvalues and eigenvectors 737  
 complex Hermitian matrix 748  
 general matrix 737  
 real general matrices 764  
 real symmetric matrix 748, 770  
 real symmetric positive definite matrix 770  
 EINFO, ESSL error information-handler considerations when designing your program 51  
 diagnosis procedures using 178  
 subroutine description 1008  
 using EINFO in C programs 136  
 using EINFO in C++ programs 152  
 using EINFO in Fortran programs 119  
 element of a matrix notation xviii  
 element of a vector notation xviii  
 error conditions, conventions used in the subroutine descriptions xxi  
 error messages 179  
 error option table default values 54  
 error-handling subroutines  
 EINFO 1008  
 ERRSAV 1011  
 ERRSET 1012  
 ERRSTR 1014  
 errors  
 attention error messages, interpreting 179  
 attention messages, overview 54  
 calculating auxiliary storage 36  
 computational errors 51, 178  
 EINFO subroutine description 1008  
 extended error-handling subroutines 23

errors (*continued*)  
 handling errors in your C program 136  
 handling errors in your C++ program 152  
 handling errors in your Fortran program 118  
 how errors affect output 50  
 informational error messages, interpreting 179  
 input-argument errors 177  
 input-argument errors, overview 50  
 miscellaneous error messages, interpreting 179  
 overview of 50  
 program exceptions 50, 177  
 resource error messages, interpreting 178  
 resource errors, overview 53  
 types of errors that you can encounter 50  
 using ERRSAV and ERRSTR 56  
 values returned for EINFO error codes 1008  
 when to use ERRSET 54  
 where to find information on 50  
 ERRSAV  
 in workstation environment 23  
 subroutine description 1011  
 using with large applications 56  
 ERRSET  
 diagnosis procedures using 178  
 ESSL default values for 54  
 handling errors in C 136  
 handling errors in C++ 152  
 in workstation environment 23  
 subroutine description 1012  
 using EINFO in C programs 136  
 using EINFO in C++ programs 152  
 using EINFO in Fortran programs 119  
 using ERRSET, EINFO, and return codes in C 136  
 using ERRSET, EINFO, and return codes in C++ 152  
 using ERRSET, EINFO, and return codes in Fortran 119  
 when to use 51, 54  
 when to use ERRSAV and ERRSTR with ERRSET 56  
 ERRSTR  
 in workstation environment 23  
 subroutine description 1014  
 using with large applications 56  
 ESSL (Engineering and Scientific Subroutine Library)  
 advantages of 3  
 attention error messages, interpreting 179  
 attention messages, overview 54  
 coding your program 111  
 computational areas, overview 4  
 computational errors 51  
 computational errors, diagnosing 178  
 designing your program 25  
 diagnosis procedures for ESSL errors 175

- ESSL (Engineering and Scientific Subroutine Library) (*continued*)
  - dynamic linking versus static linking 163, 167
  - eigensystem analysis subroutines 735
  - error option table default values 54
  - extended error-handling subroutines 23
  - Fourier transform, convolutions and correlations, and related-computation subroutines 777
  - functional capability 4
  - informational error messages, interpreting 179
  - input-argument errors, diagnosing 177
  - input-argument errors, overview 50
  - installation requirements 10
  - interpolation subroutines 945
  - introduction to 3
  - languages supported 7, 8
  - linear algebra subprograms 193
  - linear algebraic equations subroutines 445
  - matrix operation subroutines 373
  - message conventions 179
  - messages, list of 179
  - migrating from one IBM hardware platform to another 172
  - migrating programs 171
  - migrating to future releases or future hardware 172
  - miscellaneous error messages, interpreting 179
  - name xiv
  - names with an underscore, interpreting xiii
  - number of subroutines in each area 4
  - numerical quadrature subroutines 965
  - ordering publications 1060
  - overview 3
  - overview of the subroutines 4
  - packaging characteristics 10
  - parallel processing subroutines on the workstations 4
  - processing your program 163
  - program exceptions 50
  - program number for 1060
  - publications overview 1060
  - random number generation subroutines 991
  - reference information
    - conventions xix
  - related publications 1060
  - resource error messages, interpreting 178
  - resource errors, overview 53
  - setting up your data structures 59
  - sorting and searching subroutines 925
  - usability of subroutines 3
  - utility subroutines 1005
  - when coding large applications 56
  - when to use ERRSET for ESSL errors 54

- ESSL libraries
  - Blue Gene 32, 167
  - serial 167
  - shared 32
  - SMP 167
- ESSL messages 179
- ESSL program number 8
- ESSL release 8
- ESSL/370, migrating from 173
- Euclidean length
  - with no scaling of input 237
  - with scaling of input 234
- Euclidean norm notation xviii
- examples of matrices 65
- examples of vectors 59
- examples, conventions used in the subroutine descriptions xxi
- exponential function notation xviii
- expressions, special usage of xviii
- extended error-handling subroutines
  - handling errors in C 136
  - handling errors in C++ 152
  - handling errors in your Fortran program 118
  - how they work 50, 56
  - in ESSL and in Fortran, list of 23
  - using them in diagnosing problems 177
- extended-error-handling subroutines, using
  - in your C program 136
  - in your C++ program 152
  - in your Fortran program 118
- extreme eigenvalues and eigenvectors 737, 757, 770
  - complex Hermitian matrix 757
  - real symmetric matrix 757

## F

- factoring
  - complex Hermitian matrix 489
  - general band matrix 579
  - general matrix 454, 458, 467, 479
  - general skyline sparse matrix 627
  - general sparse matrix 617
  - general tridiagonal matrix 593
  - positive definite
    - complex Hermitian matrix 483, 495
    - real symmetric indefinite matrix 530, 535
    - real symmetric matrix 483, 495, 518
    - symmetric band matrix 586
    - symmetric tridiagonal matrix 607
  - real symmetric matrix 489
  - symmetric skyline sparse matrix 644
  - tridiagonal matrix 598, 601
- fast Fourier transform (FFT) 783
- FFT 783
- floor notation and meaning xviii
- fonts used in this book xv
- formula for transform lengths, interpreting 43
- formulas for auxiliary storage, interpreting 37

- Fortran
  - languages required by ESSL for AIX on the workstations 8
  - languages required by ESSL for Linux on the workstations 9
  - modifying procedures for using ESSL 167
  - modifying procedures for using ESSL for AIX 163
- Fortran considerations
  - coding programs 111
  - function reference 193
  - handling errors in your program 119
- Fortran function reference 111
- Fortran program calling interface 111
- Fourier transform 783
  - one dimension
    - complex 787
    - complex-to-real 804
    - cosine transform 812
    - real-to-complex 796
    - sine transform 820
  - three dimensions
    - complex 850
    - complex-to-real 862
    - real-to-complex 856
  - two dimensions
    - complex 828
    - complex-to-real 842
    - real-to-complex 835
- fourier transform subroutines
  - SCFT and DCFT 787
  - SCFT2 and DCFT2 828
  - SCFT3 and DCFT3 850
  - SCOSF and DCOSF 812
  - SCRFT and DCRFT 804
  - SCRFT2 and DCRFT2 842
  - SCRFT3 and DCRFT3 862
  - SRCFT and DRCFT 796
  - SRCFT2 and DRCFT2 835
  - SRCFT3 and DRCFT3 856
  - SSINF and DSINF 820
- Fourier transform subroutines
  - accuracy considerations 781
  - how they achieve high performance 783
  - performance considerations 781
  - terminology used for 778
  - usage considerations 778
- Frobenius norm notation xviii
- full-matrix storage mode 94
- full-vector, definition and storage mode 64
- function
  - calling sequence in C programs 129
  - calling sequence in C++ programs 145
  - calling sequence in Fortran programs 111
  - function reference 193
- functional capability of the ESSL subroutines 4
- functional description, conventions used in the subroutine descriptions xx
- functions, ESSL 193
- future migration considerations 172

## G

- gather vector elements 280, 283
- Gaussian quadrature methods
  - Gauss-Hermite Quadrature 988
  - Gauss-Laguerre Quadrature 981
  - Gauss-Legendre Quadrature 972
  - Gauss-Rational Quadrature 984
  - two-dimensional Gauss-Legendre Quadrature 975
- general matrix 445
- general matrix subroutines, names of 445
- general tridiagonal matrix
  - definition of 92
  - storage layout 92
- general-band storage mode 81
- generalized eigensystem
  - real general matrices 764
  - real symmetric matrix 770
  - real symmetric positive definite matrix 770
- generation of random numbers 991
- Givens plane rotation, constructing 240
- greek letters notation xviii
- guide information 1
- guidelines for handling problems 175

## H

- half band width 85
- handling errors
  - in your C program 136
  - in your C++ program 152
  - in your Fortran program 118
- hardware
  - required on the workstations 8
- header file, ESSL, for C 129, 132
- header file, ESSL, for C++ 145, 148
- Hermitian band matrix
  - definition of 88
  - storage layout 88
- Hermitian matrix
  - definition of 73
  - definition of, complex 76
  - storage layout 73
- how to use this book xi, xiii
- Hypertext Markup Language, required products 11

## I

- i-th zero crossing 778, 910
- IBM products, migrating from 173
- IBM publications 1060
- IBSRCH 936
- ICAMAX 199
- IDAMAX 199
- IDAMIN 202
- identifying problems 177
- IDMAX 205
- IDMIN 208
- IESSL 1015
- industry areas 4
- infinity notation xviii
- informational error messages, interpreting 179

- informational messages, for ESSL 179
- input arguments, conventions used in the subroutine descriptions xx
- input data, conventions for 33
- input-argument errors
  - diagnosing 177
  - list of messages for 180, 188
  - overview 50, 53, 54
- int notation and meaning xviii
- integer data
  - conventions xv, 33
- integral notation xviii
- interchange elements of two vectors 254
- interface, ESSL
  - for C programs 129
  - for C++ programs 145
  - for Fortran programs 111
- interpolating
  - cubic spline 955
  - local polynomial 952
  - polynomial 947
  - quadratic 916
  - two-dimensional cubic spline 961
- interpolation subroutines
  - accuracy considerations 945
  - performance considerations 945
  - SCSIN2 and DCSIN2 961
  - SCSINT and DCSINT 955
  - SPINT and DPINT 947
  - STPINT and DTPINT 952
  - usage considerations 945
- introduction to ESSL 3
- inverse
  - general matrix 539
  - matrix notation xviii
  - positive definite complex Hermitian matrix 547
  - positive definite real symmetric matrix 547
  - triangular matrix 570
- ISAMAX 199
- ISAMIN 202
- ISMAX 205
- ISMIN 208
- ISORT 927
- ISORTS 932
- ISORTX 929
- ISSRCH 940
- italic font usage xv
- iterative linear system solver
  - general sparse matrix 662, 689, 696
  - sparse negative definite symmetric matrix 673, 681
  - sparse positive definite symmetric matrix 673, 681
  - symmetric sparse matrix 662
  - usage considerations 451
- IZAMAX 199

## L

- l(2) norm
  - with no scaling of input 237
  - with scaling of input 234
- languages supported by ESSL 7
- languages supported by ESSL for AIX 8

- LAPACK
  - ESSL subprograms 1043
- LAPACK, migrating from 173
- leading dimension for matrices
  - how it is used for matrices 67
  - how it is used in three dimensions 108
- least squares solution 712, 717
- letters, fonts of xv
- Level 1 BLAS 1041
- Level 2 BLAS 1041
- Level 3 BLAS 1042
- level of ESSL, getting 1015
- library
  - migrating from a non-IBM 173
  - migrating from another IBM 173
  - migrating from ESSL Version 3 Release 3 to Version 4 Release 1 172
  - migrating from ESSL Version 4 Release 1 to Version 4 Release 2 171
  - migrating from ESSL Version 4 Release 2 to Version 4 Release 2.1 171
  - migrating from ESSL Version 4 Release 2.1 to Version 4 Release 2.2 171
  - migrating from LAPACK 173
  - overview 4
- Licensed Program Specification, ESSL 1060
- linear algebra 445
- linear algebra subprograms 193
  - accuracy considerations 196
  - list of matrix-vector linear algebra subprograms 195
  - list of sparse matrix-vector linear algebra subprograms 196
  - list of sparse vector-scalar linear algebra subprograms 194
  - list of vector-scalar linear algebra subprograms 193
  - overview 193
  - performance considerations 196
  - usage considerations 196
- linear algebraic equations
  - accuracy considerations 449
  - list of banded linear algebraic equation subroutines 447
  - list of dense linear algebraic equations 445
  - list of linear least squares subroutines 448
  - list of sparse linear algebraic equation subroutines 447
  - overview 445
  - performance considerations 449
  - usage considerations 448
- linear least squares solution
  - preparing for 704
  - QR decomposition with column pivoting 728
  - QR factorization 721
  - singular value decomposition 712
- linear least squares subroutines 445
- DGELS 721

- linear least squares subroutines  
(*continued*)
  - DGEQRF 717
  - SGELLS and DGELLS 728
  - SGESVF and DGESVF 704
  - SGESVS and DGESVS 712
- linking 163, 167
  - C programs 164, 168
  - C++ programs 165, 168
  - dynamic versus static 163, 167
  - Fortran programs 163, 167
- linking and loading your program  
under AIX 163
- Linux distributions 8
- Linux, supported distributions 8
- logical data
  - conventions xv, 33
  - setting up for C 132
  - setting up for C++ 148
- long precision
  - accuracy statement 5
  - meaning of 47
- lower band width 80
- lower storage mode 69, 72
- lower-band-packed storage mode 87
- lower-packed storage mode 69
- lower-storage-by-rows for symmetric  
sparse matrices 100
- lower-triangular storage mode 78, 79
- lower-triangular-band-packed storage  
mode 90, 91
- lower-triangular-packed storage  
mode 78

**M**

- mailing list for ESSL customers 12
- masking underflow
  - for performance 49
  - why you should 48
- math and programming notations xviii
- math background publications 1055
- mathematical expressions, conventions  
for xviii
- mathematical functions, overview 4
- matrix
  - band matrix 80
  - complex Hermitian band matrix 88
  - complex Hermitian matrix 73, 76
  - complex Hermitian Toeplitz  
matrix 76
  - conventions for xvi
  - description of 65
  - font for xv
  - full or dense matrix 94
  - general tridiagonal matrix 92
  - leading dimension for 67
  - negative definite complex Hermitian  
matrix 75
  - negative definite symmetric  
matrix 73
  - positive definite complex Hermitian  
matrix 75
  - positive definite symmetric band  
matrix 87
  - positive definite symmetric matrix 73

- matrix (*continued*)
  - positive definite symmetric tridiagonal  
matrix 94
  - sparse matrix 94
  - storage of 66
  - symmetric band matrix 85
  - symmetric matrix 69
  - symmetric tridiagonal matrix 93
  - Toeplitz matrix 75
  - triangular band matrices 88
  - triangular matrices 77
- matrix operation subroutines
  - accuracy considerations 375
  - performance considerations 375
  - SGEADD, DGEADD, CGEADD, and  
ZGEADD 377
  - SGEMM, DGEMM, CGEMM, and  
ZGEMM 404
  - SGEMMS, DGEMMS, CGEMMS, and  
ZGEMMS 398
  - SGEMUL, DGEMUL, CGEMUL, and  
ZGEMUL 389
  - SGESUB, DGESUB, CGESUB, and  
ZGESUB 383
  - SGETMI, DGETMI, CGETMI, and  
ZGETMI 439
  - SGETMO, DGETMO, CGETMO, and  
ZGETMO 442
  - SSYMM, DSYMM, CSYMM, ZSYMM,  
CHEMM, and ZHEMM 412
  - SSYR2K, DSYR2K, CSYR2K, ZSYR2K,  
CHER2K, and ZHER2K 432
  - SSYRK, DSYRK, CSYRK, ZSYRK,  
CHERK, and ZHERK 426
  - STRMM, DTRMM, CTRMM, and  
ZTRMM 419
  - usage considerations 374
- matrix-matrix product
  - complex Hermitian matrix 412
  - complex symmetric matrix 412
  - general matrices, their transposes, or  
their conjugate transposes 404
  - real symmetric matrix 412
  - triangular matrix 419
- matrix-vector linear algebra subprograms
  - SGBMV, DGBMV, CGBMV, and  
ZGBMV 336
  - SGEMX, DGEMX, SGEMTX,  
DGEMTX, SGEMV, DGEMV,  
CGEMV, and ZGEMV 294
  - SGER, DGER, CGERU, ZGERU,  
CGERC, and ZGERC 305
  - SSBMV, DSBMV, CHBMV, and  
ZHBMV 343
  - SSPMV, DSPMV, CHPMV, ZHPMV,  
SSYMV, DSYMV, CHEMV, ZHEMV,  
SSLMX and DSLMX 312
  - SSPR, DSPR, CHPR, ZHPR, SSYR,  
DSYR, CHER, ZHER, SSLR1, and  
DSLR1 320
  - SSPR2, DSPR2, CHPR2, ZHPR2,  
SSYR2, DSYR2, CHER2, ZHER2,  
SSLR2, and DSLR2 327
  - STBMV, DTBMV, CTBMV, and  
ZTBMV 354

- matrix-vector linear algebra  
subprograms (*continued*)
  - STPMV, DTPMV, CTPMV, ZTPMV,  
STRMV, DTRMV, CTRMV, and  
ZTRMV 348
- matrix-vector product
  - complex Hermitian band matrix 343
  - complex Hermitian matrix 312
  - general band matrix, its transpose, or  
its conjugate transpose 336
  - general matrix, its transpose, or its  
conjugate transpose 294
  - real symmetric band matrix 343
  - real symmetric matrix 312
  - sparse matrix 360
  - sparse matrix or its transpose 367
  - triangular band matrix, its transpose,  
or its conjugate transpose 354
  - triangular matrix, its transpose, or its  
conjugate transpose 348
- max notation and meaning xviii
- maximum
  - absolute value 199
  - value 205
- messages
  - ESSL and attention messages,  
interpreting 179
  - ESSL informational messages,  
interpreting 179
  - ESSL miscellaneous messages,  
interpreting 179
  - ESSL resource messages,  
interpreting 178
  - list of ESSL messages 180, 188
  - message conventions 179
- migrating
  - from ESSL Version 3 Release 3 to  
Version 4 Release 1 172
  - from ESSL Version 4 Release 1 to  
Version 4 Release 2 171
  - from ESSL Version 4 Release 2 to  
Version 4 Release 2.1 171
  - from ESSL Version 4 Release 2.1 to  
Version 4 Release 2.2 171
  - from ESSL/370 173
  - from LAPACK 173
  - from non-IBM libraries 173
  - from one IBM hardware platform to  
another 172
  - from other IBM subroutine  
libraries 173
  - future migration considerations 172
  - programs to ESSL 171
- min notation and meaning xviii
- minimum
  - absolute value 202
  - value 208
- miscellaneous error messages,  
interpreting 179
- mod notation and meaning xviii
- modification level of ESSL, getting 1015
- modifying
  - C programs, for using ESSL for  
AIX 164
  - C programs, for using ESSL for  
Linux 168

- modifying (*continued*)
  - C++ programs, for using ESSL for AIX 165
  - C++ programs, for using ESSL for Linux 168
  - Fortran programs, for using ESSL 167
  - Fortran programs, for using ESSL for AIX 163
- modulo notation xviii
- multiplying
  - compute SAXPY or DAXPY N times 224
  - general matrices using Strassen's algorithm 398
  - general matrices, their transposes, or their conjugate transposes 389
  - notation xviii
  - sparse vector x by a scalar, add sparse vector y, and store in vector y 286
  - vector x by a scalar and store in vector x 251
  - vector x by a scalar and store in vector y 269
  - vector x by a scalar, add to vector y, and store in vector y 214
  - vector x by a scalar, add to vector y, and store in vector z 272
  - vector x by vector y, and store in vector z 265
- multithreaded
  - ESSL subroutines 25

## N

- name usage restrictions 32
- names in ESSL with an underscore (\_)
  - prefix, how to interpret xiii
- names of
  - products and acronyms xiv
  - the eigensystem analysis subroutines 735
  - the Fourier transform, convolution and correlation, and related-computation subroutines 777
  - the interpolation subroutines 945
  - the linear algebra subprograms 193
  - the linear algebraic equations subroutines 445
  - the matrix operations subroutines 373
  - the numerical quadrature subroutines 965
  - the random number generation subroutines 991
  - the sorting and searching subroutines 925
  - the utility subroutines 1005
- National Language Support 176
- negative definite complex Hermitian matrix
  - definition of 75
- negative definite complex Hermitian Toeplitz matrix
  - definition of 76

- negative definite Hermitian matrix
  - storage layout 75
- negative definite symmetric matrix
  - definition of 73
  - storage layout 73
- negative definite symmetric Toeplitz matrix
  - definition of 75
- negative stride, for vectors 63
- NLS, National Language Support 176
- non-IBM library, migrating from 173
- norm notation xviii
- normally distributed random numbers, generate 996
- notations and conventions xv
- notes, conventions used in the subroutine descriptions xx
- number of subroutines in each area 4
- numbers 23
  - accuracy of computations 48
  - accuracy of computations, for ESSL 5
- numerical quadrature
  - accuracy considerations 965
  - performance considerations 965
  - programming considerations for SUBF 966
  - usage considerations 965
- numerical quadrature performed
  - on a function
    - using Gauss-Hermite Quadrature 988
    - using Gauss-Laguerre Quadrature 981
    - using Gauss-Legendre Quadrature 972
    - using Gauss-Rational Quadrature 984
    - using two-dimensional Gauss-Legendre Quadrature 975
  - on a set of points 969
- numerical quadrature subroutines
  - SGHMQ and DGHMQ 988
  - SGLGQ and DGLGQ 981
  - SGLNQ and DGLNQ 972
  - SGLNQ2 and DGLNQ2 975
  - SGRAQ and DGRAQ 984
  - SPTNQ and DPTNQ 969

## O

- one norm notation xviii
- online documentation
  - required Hypertext Markup Language products 11
- operating systems that support ESSL 8
- option table, default values for ESSL errors 54
- order numbers of the publications 1060
- ordering IBM publications 1060
- output
  - accuracy on different processors 5
  - how errors affect output 50
- output arguments, conventions used in the subroutine descriptions xx
- overflow, avoiding 234
- overview
  - of eigensystem analysis 735

- overview (*continued*)
  - of ESSL 3
  - of Fourier transforms, convolutions and correlations, and related computations 777
  - of interpolation 945
  - of linear algebra subprograms 193
  - of linear algebraic equations 445
  - of matrix operations 373
  - of numerical quadrature 965
  - of random number generation 991
  - of sorting and searching 925
  - of the documentation 1060
  - of utility subroutines 1005

## P

- packed band storage mode 81
- packed-Hermitian-Toeplitz storage mode 77
- packed-symmetric-Toeplitz storage mode 76
- parallel processing
  - introduction to 4
- performance
  - achieving better performance in your program 49
  - aspects of parallel processing on the workstations 4
  - coding techniques that affect performance 49
  - considerations for dense and banded linear algebraic equations 449
  - considerations for eigensystem analysis 735
  - considerations for Fourier transforms, convolutions, and correlations 781
  - considerations for interpolation 945
  - considerations for linear algebra subprograms 196
  - considerations for matrix operations 375
  - considerations for numerical quadrature 965
  - considerations for related computations 785
  - considerations for sorting and searching 925
  - how the Fourier transforms achieve high performance 783
  - information on ESSL run-time performance 50
  - tradeoffs for convolution and correlation subroutines 783
  - where to find information on 50
- pi notation xviii
- PL/I (Programming Language/I)
  - handling errors in your program 136, 152
- plane rotation
  - applying a 247
  - constructing a Givens 240
- planning your program 25
- polynomial
  - evaluating 907
  - interpolating 947, 952

- positive definite complex Hermitian matrix
  - definition of 75
- positive definite complex Hermitian Toeplitz matrix
  - definition of 76
- positive definite Hermitian matrix
  - storage layout 75
- positive definite symmetric band matrix
  - definition of 87
  - storage layout 88
- positive definite symmetric band matrix subroutines, names of 445
- positive definite symmetric matrix
  - definition of 73
  - storage layout 73
- positive definite symmetric matrix subroutines, names of 445
- positive definite symmetric Toeplitz matrix
  - definition of 75
- positive definite symmetric tridiagonal matrix 94
  - definition of 94
  - storage layout 94
- positive stride, for vectors 62
- precision, meaning of 47
- precision, short and long 5
- problems, handling 175
- problems, IBM support for 175
- processing your program
  - requirements for ESSL for AIX on the workstations 8
  - requirements for ESSL for Linux on the workstations 8
  - steps involved in 163
  - using parallel subroutines on the workstations 4
- processor-independent formulas for auxiliary storage, interpreting 37
- product 214
  - matrix-matrix
    - complex Hermitian matrix 412
    - complex symmetric matrix 412
    - general matrices, their transposes, or their conjugate transposes 404
    - real symmetric matrix 412
    - triangular matrix 419
  - matrix-vector
    - complex Hermitian band matrix 343
    - complex Hermitian matrix 312
    - general band matrix, its transpose, or its conjugate transpose 336
    - general matrix, its transpose, or its conjugate transpose 294
    - real symmetric band matrix 343
    - real symmetric matrix 312
    - sparse matrix 360
    - sparse matrix or its transpose 367
    - triangular band matrix, its transpose, or its conjugate transpose 354
    - triangular matrix, its transpose, or its conjugate transpose 348
- product names, acronyms for xiv

- products, programming
  - migrating from LAPACK 173
  - migrating from other IBM 173
  - required by ESSL for AIX on the workstations, programming 8
  - required by ESSL for Linux on the workstations, programming 9
- profile-in skyline storage mode 104
- program
  - attention messages, overview 54
  - coding 111
  - computational errors 51
  - design 25
  - errors 50
  - handling errors in your C program 136
  - handling errors in your C++ program 152
  - handling errors in your Fortran program 118
  - input-argument errors, overview 50
  - interface for C programs 129
  - interface for C++ programs 145
  - interface for Fortran programs 111
  - migrated to ESSL 171
  - performance, achieving high 49
  - processing your program 163
  - resource errors, overview 53
  - setting up your data structures 59
  - types of data in your program 33
  - when coding large applications 56
- program exceptions
  - description of ESSL 50
- program exceptions, diagnosing 177
- program number for ESSL 1060
- program number of ESSL 8
- programming considerations for SUBF in numerical quadrature 966
- programming items, font for xv
- programming products
  - required by ESSL for Linux on the workstations 9
  - required by ESSL for AIX on the workstations 8
- programming publications 1060
- PTF
  - getting the most recent level applied 1015
- publications
  - list of ESSL 1060
  - math background 1055
  - related 1060

## Q

- QR decomposition with column pivoting 728
- QR factorization 721
- quadratic interpolation 22, 916

## R

- random number generation
  - long period uniformly distributed 1000
  - normally distributed 996

- random number generation (*continued*)
  - uniformly distributed 993
  - usage considerations 991
- random number generation subroutines
  - SNRAND and DNRAND 996
  - SURAND and DURAND 993
  - SURXOR and DURXOR 1000
- rank-2k update
  - complex Hermitian matrix 432
  - complex symmetric matrix 432
  - real symmetric matrix 432
- rank-k update
  - complex Hermitian matrix 426
  - complex symmetric matrix 426
  - real symmetric matrix 426
- rank-one update
  - complex Hermitian matrix 320
  - general matrix 305
  - real symmetric matrix 320
- rank-two update
  - complex Hermitian matrix 327
  - real symmetric matrix 327
- real and complex array elements 112
- real data
  - conventions xv, 33
- real general matrix eigensystem analysis subroutine 735
- real symmetric matrix eigensystem analysis subroutine 735
- reciprocal of the condition number
  - general matrix 479, 539
  - positive definite complex Hermitian matrix 547
  - positive definite real symmetric matrix 518, 547
- reference information
  - math background texts and reports 1055
  - organization of 191
  - what is in each subroutine description and the conventions used xix
- related publications 1060
- related-computation subroutines
  - accuracy considerations 785
  - CWLEV and ZWLEV 920
  - performance considerations 785
  - SIZC and DIZC 910
  - SPOLY and DPOLY 907
  - SQINT and DQINT 916
  - STREC and DTREC 913
  - SWLEV and DWLEV 920
- release of ESSL 8
- release of ESSL, getting 1015
- reporting problems to IBM 175
- required publications 1060
- required software products 9
- requirements
  - auxiliary working storage 37
  - for ESSL for AIX workstation product 8
  - for ESSL for Linux workstation product 8
  - software products on the workstations 8, 9
  - transforms in storage, lengths of 42
  - workstation hardware 8

resource error messages,  
 interpreting 178  
 restrictions, ESSL coding 32  
 results  
   accuracy on different processors 5  
   how accuracy is affected by the nature  
   of the computation 48  
   in C programs 129  
   in C++ programs 145  
   in Fortran programs 111  
   multiplication of NaN 48  
 results transposed and conjugate  
 transposed for matrix  
 multiplication 392, 402, 407  
 results transposed for matrix  
 addition 379  
 results transposed for matrix  
 subtraction 385  
 return code  
   in C programs 136  
   in C++ programs 152  
   in Fortran programs 119  
   using during diagnosis 178  
 rotation  
   applying a plane 247  
   constructing a Givens plane 240  
 routine names 32  
 row vector 59  
 Run-Time Environment, XL Fortran 9  
 run-time performance  
   optimizing in your program 49  
 run-time problems, diagnosing  
   attention error messages,  
   interpreting 179  
   computational errors 178  
   informational error messages,  
   interpreting 179  
   input-argument errors 177  
   miscellaneous error messages,  
   interpreting 179  
   resource error messages,  
   interpreting 178  
 running your program  
   C programs 164, 168  
   C++ programs 165, 168  
   Fortran programs 163, 167

## S

SACOR 896  
 SACORF 900  
 SASUM 211  
 SAXPY 214  
 SAXPYI 286  
 SBSRCH 936  
 scalar data  
   conventions xv, 33  
 scalar items, font for xv  
 scale argument used for Fourier  
 transform subroutines 782  
 scaling, when to use 49  
 SCASUM 211  
 scatter vector elements 277  
 SCFT 787  
 SCFT2 828  
 SCFT3 850  
 SCNRM2 234

SCON 869  
 SCOND 875  
 SCONF 881  
 SCOPY 217  
 SCOR 869  
 SCORD 875  
 SCORF 881  
 SCOSF 812  
 SCOSFT, no documentation provided  
   for 777  
 SCRFT 804  
 SCRFT2 842  
 SCRFT3 862  
 SCSIN2 961  
 SCSINT 955  
 SDCON 891  
 SDCOR 891  
 SDOT 220  
 SDOTI 289  
 searching  
   binary 936  
   sequential 940  
 selecting an ESSL library 25  
 selecting an ESSL subroutine 25  
 sequences  
   conventions for xvi  
   description of 106  
   storage layout 106  
 sequential search 940  
 service, IBM 175  
 setting up  
   AIX procedures 163  
 setting up your data 33  
 SGBF 579  
 SGBMV 336  
 SGBS 583  
 SGEADD 377  
 SGEEV 737  
 SGEF 467  
 SGEFCD 479  
 SGEGV 764  
 SGEICD 539  
 SGELLS 728  
 SGEMM 404  
 SGEMMS 398  
 SGEMTX 294  
 SGEMUL 389  
 SGEMV 294  
 SGEMX 294  
 SGER 305  
 SGES 470  
 SGESM 474  
 SGESUB 383  
 SGEV 454  
 SGEVSV 704  
 SGEVSV 712  
 SGETMI 439  
 SGETMO 442  
 SGETRF 458  
 SGETRI 539  
 SGETRS 462  
 SGHMQ 988  
 SGLGQ 981  
 SGLNQ 972  
 SGLNQ2 975  
 SGRAQ 984  
 SGTf 593

SGTHR 280  
 SGTHRZ 283  
 SGTNP 598  
 SGTNPF 601  
 SGTNPS 604  
 SGTS 596  
 short precision  
   accuracy statement 5  
   meaning of 47  
 SIGN notation and meaning xviii  
 signal processing subroutines 778  
 simple formulas for auxiliary storage,  
 interpreting 37  
 sin notation xviii  
 sine transform 820  
 singular value decomposition for a  
 general matrix 704, 712  
 SIZC 910  
 size of array  
   required for a vector 61  
 skyline solvers  
   usage considerations 450  
 skyline storage mode for sparse matrices,  
 diagonal-out 102  
 skyline storage mode for sparse matrices,  
 profile-in 104  
 SL MATH (Subroutine  
 Library—Mathematics)  
   migrating from 173  
 SLSS (Subscription Library Services  
 System) 1060  
 SMP  
   ESSL Library, why use it 25  
   ESSL multithreaded subroutines 25  
   performance 6  
 SNAXPY 224  
 SNDOT 229  
 SNORM2 237  
 SNRAND 996  
 SNRM2 234  
 software for linking, loading, or  
 running 10  
 software products  
   required by ESSL for Linux on the  
   workstations 9  
   required by ESSL for AIX on the  
   workstations 8  
   required by Hypertext Markup  
   Language 11  
 software products required 9  
 solving  
   general band matrix 583  
   general matrix or its transpose 462,  
   470  
   general skyline sparse matrix 627  
   general sparse matrix or its  
   transpose 623  
   general tridiagonal matrix 596, 598,  
   604  
   iterative linear system solver  
     general sparse matrix 662, 689,  
     696  
     sparse negative definite symmetric  
     matrix 673, 681  
     sparse positive definite symmetric  
     matrix 673, 681  
     symmetric sparse matrix 662



- solving (*continued*)
  - multiple right-hand sides
    - general matrix, its transpose, or its conjugate transpose 462, 474
    - positive definite complex Hermitian matrix 507
    - positive definite real symmetric matrix 507
    - triangular matrix 563
  - positive definite
    - real symmetric matrix 515
    - symmetric band matrix 590
    - symmetric tridiagonal matrix 609
    - symmetric skyline sparse matrix 644
    - triangular band matrix 611
    - triangular matrix 557
  - some eigenvalues and eigenvectors 757
  - sorting
    - elements of a sequence 927
    - index 929
    - stable sort 932
  - sorting and searching subroutines
    - accuracy considerations 925
    - IBSRCH, SBSRCH, and DBSRCH 936
    - ISORT, SSORT, and DSORT 927
    - ISORTS, SSORTS, and DSORTS 932
    - ISORTX, SSORTX, and DSORTX 929
    - ISSRCH, SSSRCH, and DSSRCH 940
    - performance considerations 925
    - usage considerations 925
  - sparse linear algebraic equation
    - subroutines 445
      - DGKFS 627
      - DGSF 617
      - DGSS 623
      - DSDCG 681
      - DSDGCG 696
      - DSKFS 644
      - DSMCG 673
      - DSMGCG 689
      - DSRIS 662
  - sparse matrix subroutines
    - direct solvers 449
    - iterative linear system solvers 451
    - performance and accuracy considerations 449, 450, 451
    - skyline solvers 450
  - sparse matrix-vector linear algebra
    - subprograms
      - DSDMX 367
      - DSMMX 360
      - DSMTM 363
  - sparse matrix, definition and storage
    - modes 94
  - sparse vector-scalar linear algebra
    - subprograms
      - SAXPYI, DAXPYI, CAXPYI, and ZAXPYI 286
      - SDOTI, DDOTI, CDOTUI, ZDOTUI, CDOTCI, and, ZDOTCI 289
      - SGTHR, DGTHR, CGTHR, and ZGTHR 280
      - SGTHRZ, DGTHRZ, CGTHRZ, and ZGTHRZ 283
      - SSCTR, DSCTR, CSCTR, and ZSCTR 277
  - sparse vector, definition and storage
    - modes 64
    - SPBCHF 586
    - SPBCHS 590
    - SPBF 586
    - SPBS 590
    - special usage
      - of matrix addition 379
      - of matrix multiplication 392, 402, 407
      - of matrix subtraction 385
    - spectral norm notation xviii
    - SPINT 947
    - SPOF 495
    - SPOFCD 518
    - SPOICD 547
    - SPOLY 907
    - SPOSM 507
    - SPOSV 489
    - SPOTRF 495
    - SPOTRI 547
    - SPOTRS 507
    - SPPF 495
    - SPPFCD 518
    - SPPICD 547
    - SPPS 515
    - SPPSV 483
    - SPPTRF 495
    - SPPTRI 547
    - SPPTRS 507
    - SPTF 607
    - SPTNQ 969
    - SPTS 609
    - SQINT 916
    - square root notation xviii
    - SRCFT 796
    - SRCFT2 835
    - SRCFT3 856
    - SROT 247
    - SROTG 240
    - SSBMV 343
    - SSCAL 251
    - SSCTR 277
    - SSINF 820
    - SSLMX 312
    - SSLR1 320
    - SSLR2 327
    - SSORT 927
    - SSORTS 932
    - SSORTX 929
    - SSP (Scientific Subroutine Package)
      - migrating from 173
    - SSPEV 748
    - SSPMV 312
    - SSPR 320
    - SSPR2 327
    - SSPSV 757
    - SSSRCH 940
    - SSWAP 254
    - SSYGV 770
    - SSYMM 412
    - SSYMV 312
    - SSYR 320
    - SSYR2 327
    - SSYR2K 432
    - SSYRK 426
    - stable sort 932
    - STBMV 354
  - STBSV 611
  - stepping through storage, for matrices 66
  - stepping through storage, for vectors 62
  - storage
    - array storage techniques overview 33
    - auxiliary working storage
      - requirements 37
    - compressed-diagonal storage mode for sparse matrices 96
    - compressed-matrix storage mode for sparse matrices 95
    - considerations when designing your program 33
    - diagonal-out skyline storage mode for sparse matrices 102
    - for matrices 66
    - for vectors 61
    - layout for a complex Hermitian band matrix 88
    - layout for a complex Hermitian matrix 73
    - layout for a general tridiagonal matrix 92
    - layout for a negative definite Hermitian matrix 75
    - layout for a negative definite symmetric matrix 73
    - layout for a positive definite Hermitian matrix 75
    - layout for a positive definite symmetric matrix 73
    - layout for a positive definite symmetric tridiagonal matrix 94
    - layout for a sequence 106, 107
    - layout for a symmetric indefinite matrix 73
    - layout for a symmetric tridiagonal matrix 93
    - layout for a Toeplitz matrix 76, 77
    - layout for band matrices 81, 83
    - layout for positive definite symmetric band matrices 88
    - layout for sparse matrices 94
    - layout for sparse vectors 64
    - layout for symmetric band matrices 85
    - layout for symmetric matrices 69
    - layout for triangular band matrices 90, 91
    - layout for triangular matrices 78
    - list of subroutines using auxiliary storage 36
    - list of subroutines using transforms 42
    - of arrays in Fortran 112
    - profile-in skyline storage mode for sparse matrices 104
    - storage-by-columns for sparse matrices 99
    - storage-by-indices for sparse matrices 98
    - storage-by-rows for sparse matrices 100
    - tradeoffs for input 49
    - transform length requirements 42

storage conversion subroutine	subroutines, ESSL ( <i>continued</i> )	subroutines, ESSL ( <i>continued</i> )
general skyline sparse matrix 1030	CGEMUL 389	CZAXPY 272
sparse matrix 1026	CGEMV 294	DASUM 211
symmetric skyline sparse	CGERC 305	DAXPY 214
matrix 1035	CGERU 305	DAXPYI 286
storage-by-columns for sparse	CGES 470	DBSRCH 936
matrices 99	CGESM 474	DBSSV 524
storage-by-indices for sparse matrices 98	CGESUB 383	DBSTRF 530
storage-by-rows for sparse matrices 100	CGESV 454	DBSTRS 535
STPINT 952	CGETMI 439	DCFT 787
STPMV 348	CGETMO 442	DCFT2 828
STPSV 557	CGETRF 458	DCFT3 850
STPTRI 570	CGETRI 539	DCOPY 217
Strassen's algorithm, multiplying general	CGETRS 462	DCOSF 812
matrices 398	CGTHR 280	DCRFT 804
STREC 913	CGTHRZ 283	DCRFT2 842
stride	CGTNP 598	DCRFT3 862
defining vectors in arrays 62	CGTNPF 601	DCSIN2 961
how it is used in three	CGTNPS 604	DCSINT 955
dimensions 108	CHBMV 343	DDCON 891
negative 63	CHEMM 412	DDCOR 891
optimizing for your Fourier	CHEMV 312	DDOT 220
transforms 782	CHER 320	DDOTI 289
positive 62	CHER2 327	DGBF 579
subroutine for optimizing Fourier	CHER2K 432	DGBMV 336
transforms 1017	CHERK 426	DGBS 583
zero 63	CHPEV 748	DGEADD 377
STRIDE 1017	CHPMV 312	DGEEV 737
STRMM 419	CHPR 320	DGEF 467
STRMV 348	CHPR2 327	DGEFCD 479
STRSM 563	CHPSV 757	DGEGV 764
STRSV 557	CNORM2 237	DGEICD 539
STRTRI 570	CPOF 495	DGELLS 728
structures, data (vectors and	CPOSM 507	DGELS 721
matrices) 59	CPQSV 489	DGEMM 404
subject code for ESSL	CPOTRF 495	DGEMMS 398
documentation 1060	CPOTRI 547	DGEMTX 294
subprogram	CPOTRS 507	DGEMUL 389
linear algebra 193	CPPSV 483	DGEMV 294
meaning of xiii, 193	CPPTRF 495	DGEMX 294
subprogram, definition xiii	CPPTRS 507	DGEQRF 717
subroutine	CROT 247	DGER 305
calling sequence format for C	CROTG 240	DGES 470
programs 129	CSCAL 251	DGESM 474
calling sequence format for C++	CSCTR 277	DGESUB 383
programs 145	CSROT 247	DGESV 454
calling sequence format for Fortran	CSSCAL 251	DGESVF 704
programs 111	CSWAP 254	DGESVS 712
choose of 25	CSYAX 269	DGETMI 439
conventions used in the description	CSYMM 412	DGETMO 442
of xix	CSYR2K 432	DGETRF 458
overview of ESSL 4	CSYRK 426	DGETRI 539
subroutine, definition xiii	CTBMV 354	DGETRS 462
subroutines, ESSL	CTBSV 611	DGHMQ 988
CAXPY 214	CTPMV 348	DGKFS 627
CAXPYI 286	CTPSV 557	DGKTRN 1030
CCOPY 217	CTPTRI 570	DGLGQ 981
CDOTC 220	CTRMM 419	DGLNQ 972
CDOTCI 289	CTRMV 348	DGLNQ2 975
CDOTU 220	CTRSM 563	DGRAQ 984
CDOTUI 289	CTRSV 557	DGSF 617
CGBMV 336	CTRTRI 570	DGSS 623
CGEADD 377	CVEA 257	DGTF 593
CGEEV 737	CVEM 265	DGTHR 280
CGEF 467	CVES 261	DGTHRZ 283
CGEMM 404	CWLEV 920	DGTNP 598
CGEMMS 398	CYAX 269	DGTNPF 601

subroutines, ESSL (*continued*)

DGTNPS 604  
 DGTS 596  
 DIZC 910  
 DNAXPY 224  
 DNDOT 229  
 DNORM2 237  
 DNRAND 996  
 DNRM2 234  
 DPBCHF 586  
 DPBCHS 590  
 DPBF 586  
 DPBS 590  
 DPINT 947  
 DPOF 495  
 DPOFCD 518  
 DPOICD 547  
 DPOLY 907  
 DPOSM 507  
 DPOSV 489  
 DPOTRF 495  
 DPOTRI 547  
 DPOTRS 507  
 DPPF 495  
 DPPFCD 518  
 DPPICD 547  
 DPPS 515  
 DPPSV 483  
 DPPTRF 495  
 DPPTRI 547  
 DPPTRS 507  
 DPTF 607  
 DPTNQ 969  
 DPTS 609  
 DQINT 916  
 DRCFT 796  
 DRCFT2 835  
 DRCFT3 856  
 DROT 247  
 DROTG 240  
 DSBMV 343  
 DSCAL 251  
 DSCTR 277  
 DSDCG 681  
 DSDGCG 696  
 DSDMX 367  
 DSINF 820  
 DSKFS 644  
 DSKTRN 1035  
 DSLMX 312  
 DSLR1 320  
 DSLR2 327  
 DSMCG 673  
 DSMGCG 689  
 DSMMX 360  
 DSMTM 363  
 DSORT 927  
 DSORTS 932  
 DSORTX 929  
 DSPEV 748  
 DSPMV 312  
 DSPR 320  
 DSPR2 327  
 DSPSV 757  
 DSRIS 662  
 DSRSM 1026  
 DSSRCH 940

subroutines, ESSL (*continued*)

DSWAP 254  
 DSYGV 770  
 DSYMM 412  
 DSYMV 312  
 DSZR 320  
 DSZR2 327  
 DSZR2K 432  
 DSYRK 426  
 DTBMV 354  
 DTBSV 611  
 DTPINT 952  
 DTPMV 348  
 DTPSV 557  
 DTPTRI 570  
 DTREC 913  
 DTRMM 419  
 DTRMV 348  
 DTRSM 563  
 DTRSV 557  
 DTRTRI 570  
 DURAND 993  
 DURXOR 1000  
 DVEA 257  
 DVEM 265  
 DVES 261  
 DWLEV 920  
 DYAX 269  
 DZASUM 211  
 DZAXPY 272  
 DZNRM2 234  
 EINFO 1008  
 ERRSAV 1011  
 ERRSET 1012  
 ERRSTR 1014  
 IBSRCH 936  
 ICAMAX 199  
 IDAMAX 199  
 IDAMIN 202  
 IDMAX 205  
 IDMIN 208  
 IESSL 1015  
 ISAMAX 199  
 ISAMIN 202  
 ISMAX 205  
 ISMIN 208  
 ISORT 927  
 ISORTS 932  
 ISORTX 929  
 ISSRCH 940  
 IZAMAX 199  
 SACOR 896  
 SACORF 900  
 SASUM 211  
 SAXPY 214  
 SAXPYI 286  
 SBSRCH 936  
 SCASUM 211  
 SCFT 787  
 SCFT2 828  
 SCFT3 850  
 SCNRM2 234  
 SCON 869  
 SCOND 875  
 SCONF 881  
 SCOPY 217  
 SCOR 869

subroutines, ESSL (*continued*)

SCORD 875  
 SCORF 881  
 SCOSF 812  
 SCRFT 804  
 SCRFT2 842  
 SCRFT3 862  
 SCSIN2 961  
 SCSINT 955  
 SDCON 891  
 SDCOR 891  
 SDOT 220  
 SDOTI 289  
 SGBF 579  
 SGBMV 336  
 SGBS 583  
 SGEADD 377  
 SGEEV 737  
 SGEF 467  
 SGEFCD 479  
 SGEGV 764  
 SGEICD 539  
 SGELLS 728  
 SGEMM 404  
 SGEMMS 398  
 SGEMTX 294  
 SGEMUL 389  
 SGEMV 294  
 SGEMX 294  
 SGER 305  
 SGES 470  
 SGESM 474  
 SGESUB 383  
 SGESV 454  
 SGESVF 704  
 SGESVS 712  
 SGETMI 439  
 SGETMO 442  
 SGETRF 458  
 SGETRI 539  
 SGETRS 462  
 SGHMQ 988  
 SGLGQ 981  
 SGLNQ 972  
 SGLNQ2 975  
 SGRAQ 984  
 SGTf 593  
 SGTHR 280  
 SGTHRZ 283  
 SGTNP 598  
 SGTNPF 601  
 SGTNPS 604  
 SGTs 596  
 SIZC 910  
 SNAXPY 224  
 SNDOT 229  
 SNORM2 237  
 SNRAND 996  
 SNRM2 234  
 SPBCHF 586  
 SPBCHS 590  
 SPBF 586  
 SPBS 590  
 SPINT 947  
 SPOF 495  
 SPOFCD 518  
 SPOICD 547

subroutines, ESSL (*continued*)

SPOLY 907  
 SPOSM 507  
 SPOSV 489  
 SPOTRF 495  
 SPOTRI 547  
 SPOTRS 507  
 SPPF 495  
 SPPFCD 518  
 SPPICD 547  
 SPPS 515  
 SPPSV 483  
 SPPTRF 495  
 SPPTRI 547  
 SPPTRS 507  
 SPTF 607  
 SPTNQ 969  
 SPTS 609  
 SQINT 916  
 SRCFT 796  
 SRCFT2 835  
 SRCFT3 856  
 SROT 247  
 SROTG 240  
 SSBMV 343  
 SSCAL 251  
 SSCTR 277  
 SSINF 820  
 SSLMX 312  
 SSLR1 320  
 SSLR2 327  
 SSORT 927  
 SSORTS 932  
 SSORTX 929  
 SSPEV 748  
 SSPMV 312  
 SSPR 320  
 SSPR2 327  
 SSPSV 757  
 SSSRCH 940  
 SSWAP 254  
 SSYGV 770  
 SSYMM 412  
 SSYMV 312  
 SSYR 320  
 SSYR2 327  
 SSYR2K 432  
 SSYRK 426  
 STBMV 354  
 STBSV 611  
 STPINT 952  
 STPMV 348  
 STPSV 557  
 STPTRI 570  
 STREC 913  
 STRIDE 1017  
 STRMM 419  
 STRMV 348  
 STRSM 563  
 STRSV 557  
 STRTRI 570  
 SURAND 993  
 SURXOR 1000  
 SVEA 257  
 SVEM 265  
 SVES 261  
 SWLEV 920

subroutines, ESSL (*continued*)

SYAX 269  
 SZAXPY 272  
 ZAXPY 214  
 ZAXPYI 286  
 ZCOPY 217  
 ZDOTC 220  
 ZDOTCI 289  
 ZDOTU 220  
 ZDOTUI 289  
 ZDROT 247  
 ZDSCAL 251  
 ZDYAX 269  
 ZGBMV 336  
 ZGEADD 377  
 ZGEEV 737  
 ZGEF 467  
 ZGEMM 404  
 ZGEMMS 398  
 ZGEMUL 389  
 ZGEMV 294  
 ZGERC 305  
 ZGERU 305  
 ZGES 470  
 ZGESM 474  
 ZGESUB 383  
 ZGESV 454  
 ZGETMI 439  
 ZGETMO 442  
 ZGETRF 458  
 ZGETRI 539  
 ZGETRS 462  
 ZGTHR 280  
 ZGTHRZ 283  
 ZGTNP 598  
 ZGTNPF 601  
 ZGTNPS 604  
 ZHBMV 343  
 ZHEMM 412  
 ZHEMV 312  
 ZHER 320  
 ZHER2 327  
 ZHER2K 432  
 ZHERK 426  
 ZHPEV 748  
 ZHPMV 312  
 ZHPR 320  
 ZHPR2 327  
 ZHPSV 757  
 ZNORM2 237  
 ZPOF 495  
 ZPOSM 507  
 ZPOSV 489  
 ZPOTRF 495  
 ZPOTRI 547  
 ZPOTRS 507  
 ZPPSV 483  
 ZPPTRF 495  
 ZPPTRS 507  
 ZROT 247  
 ZROTG 240  
 ZSCAL 251  
 ZSCTR 277  
 ZSWAP 254  
 ZSYMM 412  
 ZSYR2K 432  
 ZSYRK 426

subroutines, ESSL (*continued*)

ZTBMV 354  
 ZTBSV 611  
 ZTPMV 348  
 ZTPSV 557  
 ZTPTRI 570  
 ZTRMM 419  
 ZTRMV 348  
 ZTRSM 563  
 ZTRSV 557  
 ZTRTRI 570  
 ZVEA 257  
 ZVEM 265  
 ZVES 261  
 ZWLEV 920  
 ZYAX 269  
 ZZAXPY 272

subscript notation, what it means xviii

subtracting

general matrices or their  
 transposes 383  
 vector *y* from vector *x* and store in  
 vector *z* 261

sum, calculating  
absolute values 211

summ xviii

superscript notation, what it means xviii

support, IBM 175

SURAND 993

SURXOR 1000

SVEA 257

SVEM 265

SVES 261

swap elements of two vectors 254

SWLEV 920

SYAX 269

symbols, special usage of xviii

symmetric band matrix

definition of 85  
 storage layout 85

symmetric indefinite matrix

definition of 73  
 storage layout 73  
 symmetric indefinite matrix 73  
 real symmetric indefinite  
 matrix 524

symmetric matrix

definition of 69  
 storage layout 69

symmetric tridiagonal matrix 93

definition of 93  
 storage layout 93

symmetric-tridiagonal storage mode 93

symptoms, identifying problem 177

syntax rules for call statements and  
data 34syntax, conventions used in the  
subroutine descriptions xx

SZAXPY 272

**T**table, default values for ESSL error  
option 54

termination, program

attention messages 54  
 computational errors 51

termination, program (*continued*)  
   input-argument errors 50  
   resource errors 53  
 terminology used for Fourier transforms,  
   convolutions, and correlations 778  
 terminology, names of products xiv  
 textbooks cited 1055  
 thread-safe  
   ESSL Library, why use it 25  
 three-dimensional data structures, how  
   stride is used for 108  
 time-varying recursive filter 22, 913  
 times notation, multiply xviii  
 timings, achieving high performance in  
   your program 49  
 Toeplitz matrix 75  
   definition of 75, 76  
   storage layout 76, 77  
 traceback map, using during  
   diagnosis 178  
 trademarks 1046  
 transform lengths, calculating 42  
 transpose  
   conjugate, of a matrix 66  
   conjugate, of a vector 60  
   notation xviii  
   of a matrix 66  
   of a matrix inverse notation xviii  
   of a vector 60, 61  
   of a vector or matrix notation xviii  
   of matrix operation results for  
     add 379  
   of matrix operation results for  
     multiply 392, 402, 407  
   of matrix operation results for  
     subtract 385  
 transposing  
   general matrix (In-Place) 439  
   general matrix (Out-of-Place) 442  
   sparse matrix 363  
 triangular band matrices  
   storage layout 90  
 triangular band matrices, upper and  
   lower  
   definition of 88  
 triangular matrices  
   storage layout 78  
 triangular matrices, upper and lower  
   definition of 77  
 tridiagonal matrix  
   definition of 92  
   storage layout 92  
 tridiagonal storage mode 92  
 truncation  
   how truncation affects output 48  
 type font usage xv

## U

underflow  
   avoiding underflow 234  
   why mask it 48  
 uniformly distributed random numbers,  
   generate 993, 1000  
 upper band width 80  
 upper storage mode 69, 72  
 upper-band-packed storage mode 86

upper-packed storage mode 69, 71  
 upper-storage-by-rows for symmetric  
   sparse matrices 100  
 upper-triangular storage mode 78, 79  
 upper-triangular-band-packed storage  
   mode 90  
 upper-triangular-packed storage  
   mode 78  
 usability of subroutines 3  
 usability of the ESSL subroutines 3  
 usage considerations  
   direct sparse matrix solvers 449  
   for Fourier transforms, convolutions,  
     and correlations 778  
   for interpolation 945  
   for linear algebra subprograms 196  
   for linear algebraic equations 448  
   for matrix operations 374  
   for numerical quadrature 965  
   for random number generation 991  
   for sorting and searching 925  
   for utility subroutines 1005  
   sparse matrix subroutines (iterative  
     linear system solvers) 451  
   sparse matrix subroutines (skyline  
     solvers) 450  
 usage, special  
   conventions used in the subroutine  
     description xxi  
   for matrix addition 379  
   for matrix multiplication 392, 402,  
     407  
   for matrix subtraction 385  
 user applications 4  
 using this book xi, xiii  
 utility subroutines  
   DGKTRN 1030  
   DSKTRN 1035  
   DSRSM 1026  
   EINFO 1008  
   ERRSAV 1011  
   ERRSET 1012  
   ERRSTR 1014  
   IESSL 1015  
   STRIDE 1017  
   usage considerations 1005

## V

vector  
   compressed vector 64  
   conventions for xv  
   description of 59  
   font for xv  
   full vector 64  
   number of array elements needed  
     for 61  
   sparse vector 64  
   storage of 61  
   stride for 62  
 vector-scalar linear algebra subprograms  
   ISAMAX, ICAMAX, IDAMAX, and  
     IZAMAX 199  
   ISAMIN and IDAMIN 202  
   ISMAX and IDMAX 205  
   ISMIN and IDMIN 208

vector-scalar linear algebra subprograms  
   (*continued*)  
   SASUM, DASUM, SCASUM, and  
     DZASUM 211  
   SAXPY, DAXPY, CAXPY, and  
     ZAXPY 214  
   SCOPY, DCOPY, CCOPY, and  
     ZCOPY 217  
   SDOT, DDOT, CDOTU, ZDOTU,  
     CDOTC, and ZDOTC 220  
   SNAXPY and DNAXPY 224  
   SNDOT and DNDOT 229  
   SNORM2, DNORM2, CNORM2, and  
     ZNORM2 237  
   SNRM2, DNRM2, SCNRM2, and  
     DZNRM2 234  
   SROT, DROT, CROT, ZROT, CSROT,  
     and ZDROT 247  
   SROTG, DROTG, CROTG, and  
     ZROTG 240  
   SSCAL, DSCAL, CSCAL, ZSCAL,  
     CSSCAL, and ZDSCAL 251  
   SSWAP, DSWAP, CSWAP, and  
     ZSWAP 254  
   SVEA, DVEA, CVEA, and ZVEA 257  
   SVEM, DVEM, CVEM, and  
     ZVEM 265  
   SVES, DVES, CVES, and ZVES 261  
   SYAX, DYAX, CYAX, ZYAX, CSYAX,  
     and ZDYAX 269  
   SZAXPY, DZAXPY, CZAXPY, and  
     ZZAXPY 272  
 version of ESSL, getting 1015  
 versions of subroutines 4

## W

Wiener-Levinson filter coefficients 920  
 Wiener-Levinson filter coefficients  
   subroutine 22  
 working auxiliary storage, list of  
   subroutines using 36  
 working storage for band matrix 81  
 workstations  
   migrating from one IBM hardware  
     platform to another 172  
   required for ESSL for AIX 8  
   required for ESSL for Linux 8

## X

XL C/C++ 9  
 XL Fortran 9  
 XL Fortran Run-Time Environment 9

## Z

ZAXPY 214  
 ZAXPYI 286  
 ZCOPY 217  
 ZDOTC 220  
 ZDOTCI 289  
 ZDOTU 220  
 ZDOTUI 289  
 ZDROT 247  
 ZDSCAL 251

ZDYAX	269	ZVEM	265
zero stride, for vectors	63	ZVES	261
ZGBMV	336	ZWLEV	920
ZGEADD	377	ZYAX	269
ZGEEV	737	ZZAXPY	272
ZGEF	467		
ZGEMM	404		
ZGEMMS	398		
ZGEMUL	389		
ZGEMV	294		
ZGERC	305		
ZGERU	305		
ZGES	470		
ZGESM	474		
ZGESUB	383		
ZGESV	454		
ZGETMI	439		
ZGETMO	442		
ZGETRF	458		
ZGETRI	539		
ZGETRS	462		
ZGTHR	280		
ZGTHRZ	283		
ZGTNP	598		
ZGTNPF	601		
ZGTNPS	604		
ZHBMV	343		
ZHEMM	412		
ZHEMV	312		
ZHER	320		
ZHER2	327		
ZHER2K	432		
ZHERK	426		
ZHPEV	748		
ZHPMV	312		
ZHPR	320		
ZHPR2	327		
ZHPSV	757		
ZNORM2	237		
ZPOF	495		
ZPOSM	507		
ZPOSV	489		
ZPOTRF	495		
ZPOTRI	547		
ZPOTRS	507		
ZPPSV	483		
ZPPTRF	495		
ZPPTRS	507		
ZROT	247		
ZROTG	240		
ZSCAL	251		
ZSCTR	277		
ZSWAP	254		
ZSYMM	412		
ZSYR2K	432		
ZSYRK	426		
ZTBMV	354		
ZTBSV	611		
ZTPMV	348		
ZTPSV	557		
ZTPTRI	570		
ZTRMM	419		
ZTRMV	348		
ZTRSM	563		
ZTRSV	557		
ZTRTRI	570		
ZVEA	257		





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