Compaq Extended Math Library

Reference Guide

January 2001

This document describes the Compaq® Extended Math Library (CXML). CXML is a set of high-performance mathematical routines designed for use in numerically intensive scientific and engineering applications. This document is a guide to using CXML and provides reference information about CXML routines.

Revision/Update Information: This document has been revised for this release of CXML.

Compaq Computer Corporation
Houston, Texas

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This document prepared using DECdocument, Version 3.3-1b.

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Preface

The Compaq Extended Math Library (CXML) is a collection of high performance mathematical routines optimized for Alpha systems. CXML routines perform numerically intensive operations that occur frequently in engineering and scientific computing, such as linear algebra and signal processing. CXML can help reduce the cost of computation, enhance portability, and improve productivity.

Although optimized for Alpha, CXML is supported on most common hardware architectures. CXML can be used on most popular operating systems, such as Tru64 Unix, OpenVMS, LINUX, and Windows NT. CXML is primarily used with Fortran programs, but is also recommended for use with many other languages as well, such as C or C++ for example. This documentation uses Fortran for most examples and explanations of CXML routines.

CXML documentation is intended for a user who has an advanced understanding of computer concepts, strong knowledge and experience in computer programming and languages, and a solid knowledge of mathematics in the areas of CXML computations.

Using CXML Documentation

Information about CXML is available in several ways, and in many forms and formats.

CXML documentation is available as hardcopy (.ps), Adobe Acrobat format (.pdf), web browser readable format (.html), and UNIX/LINUX manpages.

All CXML documentation can be downloaded from the CXML website, located at: *www.compaq.com/math*.

- The *CXML Reference Guide* is the complete reference manual for CXML. In addition to a complete reference section of CXML routines, it also fully describes all aspects of using CXML. This guide is available in both Postscript and Adobe PDF format (see Adobe PDF Format of CXML Documentation). It is included with Compaq products that make use of the CXML library. It also available for downloading or viewing at the CXML website at: *www.compaq.com/math*.
- Online CXML reference information contains descriptions of all the CXML routines. Routine descriptions are are available in HTML format, UNIX/LINUX manpage format (see About CXML Manpages), and OpenVMS Help format. Online reference information is included with the CXML kit, and can be installed in the appropriate format for your operating system.
- CXML reference information can be accessed and viewed directly on the internet by means of a web browser. Or it can be downloaded and viewed locally. It is available on the CXML website at: *www.compaq.com/math*. Follow the links to obtain the reference documentation you want.

- CXML installation infomation, release notes, and readme files are included with the CXML software kit. When CXML is obtained with another product, such as Fortran, this information is also available with that product. This information is also separately available from the CXML website at: *www.compaq.com/math*.

Related Documentation

Additionally, depending upon your operating system, the following related documentation is recommended:

- *Compaq Fortran 90 User Manual for Tru64 UNIX Systems*
- *Compaq Fortran Language Reference Manual*
- *LAPACK Users' Guide* (see About LAPACK)
- Compaq Visual Fortran online and printed documentation:
  - *Getting Started*
  - *Programmer's Guide*
  - *Language Reference*
  - *Error Messages*

About LAPACK

To make use of the LAPACK library, Compaq recommends the use of the major documentation for LAPACK, the LAPACK Users' Guide, 3rd Edition, by E. Anderson et al. This documentation is published by the Society for Industrial and Applied Math (SIAM). It is available for purchase in hardcopy form at the SIAM website at: *http://www.siam.org*

The LAPACK Users' Guide is also available on the internet in a format viewable by a web browser. It is located at the *Netlib Repository at UTK and ORNL* website. To view this book on the internet, use the following URL:

http://www.netlib.org/lapack/lug/lapack_lug.html

About CXML Manpages

For the Tru64 UNIX and LINUX platforms, CXML provides the following online manpages.

- A top-level manpage consisting of a product overview and a list of the manpages that describe CXML subcomponents.
- A manpage for each CXML subcomponent that describes its functionality and lists the manpages that describe its routines.
- A manpage for each routine that provides details of its use and the operations it implements.

Refer to the section of this Preface titled "Using Manpages" if you need information about accessing or using these manpages.

Adobe PDF Format of CXML Documentation

The Adobe PDF version of CXML documentation is identical to the Postscript version. Both of these formats are especially suitable for depicting the complex mathematical figures and equations that are described in CXML documentation.

Adobe PDF format can be displayed by your web browser using the free Adobe Acrobat Reader. This requires that you download and install the Acrobat Reader on your system if it is not already installed. It you do not have the Acrobat Reader, you can obtain it from the Adobe website at: *www.adobe.com*.

About Code Examples

CXML contains several working code examples which are installed along with the software. These examples can be executed, and are included to illustrate various aspects of CXML. Many of these examples are also reproduced in the documentation as text examples to supplement the explanatory material.

When an example printed in the documentation is also present in the online examples directory, its file name is specified so that you can correlate it with the working example.

CXML Documentation Conventions

In this book, unless otherwise stated, the following conventions are used:

- All references to OpenVMS mean the Compaq OpenVMS Alpha operating system.
- All references to UNIX mean Compaq's Tru64 UNIX operating system.
- All references to Windows NT mean both Windows NT for Intel and Windows NT for Alpha.
- All references to Fortran include both Compaq Fortran and Compaq Visual Fortran.
- The terms *subprogram*, *subroutine*, *routine*, and *function*, are used interchangably to generically refer to CXML routines and functions. When a discussion is specific to either a routine or a function, the more specific term is used.

This book also uses the conventions summarized in the following tables and sections. Please take note of these conventions to facilitate your use of this book.

Table 1 General Conventions

Convention	Meaning
Ctrl/*x*	A sequence such as Ctrl/*x* indicates that you must hold down the key labeled Ctrl while you press another key or a pointing device button.
PF1 *x* or GOLD *x*	A sequence such as PF1 *x* or GOLD *x* indicates that you must first press and release the key labeled PF1 or GOLD and then press and release another key or a pointing device button. GOLD key sequences can also have a slash (/), dash (–), or underscore (_) as a delimiter in EVE commands.
Return	In examples, a key name enclosed in a box indicates that you press a key on the keyboard. (In text, a key name is not enclosed in a box.)

(continued on next page)

Table 1 (Cont.) General Conventions

Convention	Meaning
`...`	A horizontal ellipsis in examples indicates one of the following possibilities: • Additional optional arguments in a statement have been omitted. • The preceding item or items can be repeated one or more times. • Additional parameters, values, or other information can be entered.
. . .	A vertical ellipsis indicates the omission of items from a code example or command format; the items are omitted because they are not important to the topic being discussed.
( )	In command format descriptions, parentheses indicate that, if you choose more than one option, you must enclose the choices in parentheses.
[ ]	In command format descriptions, brackets indicate optional elements. You can choose one, none, or all of the options. (Brackets are not optional in the syntax of a substring specification in an assignment statement.)
{ }	In command format descriptions, braces indicate a required choice of options; you must choose one of the options listed.
bold	Bold type is used to emphasize a word or phrase or to indicate math variables. In text, it represents the introduction of a new term or the name of an argument, an attribute, or a reason. In examples, it shows user input.
italic text	Italic text indicates important information, complete titles of manuals, or variables. Variables include information that varies in system output (Internal error *number*), in command lines (/PRODUCER=*name*), and in command parameters in text (where *device-name* contains up to five alphanumeric characters).
UPPERCASE TEXT	Uppercase text indicates a command, the name of a routine, the name of a file, or the abbreviation for a system privilege.
`Monospace type`	Monospace type indicates code examples and interactive screen displays. In the C programming language, monospace type in text identifies the following elements: keywords, the names of independently compiled external functions and files, syntax summaries, and references to variables or identifiers introduced in an example.
`MONOSPACE TYPE`	Monospaced uppercase characters are used for lines of code, commands, and command qualifiers.
-	A hyphen at the end of a command format description, command line, or code line indicates that the command or statement continues on the following line.
numbers	All numbers in text are assumed to be decimal unless otherwise noted. Nondecimal radixes—binary, octal, or hexadecimal—are explicitly indicated.

(continued on next page)

Table 1 (Cont.) General Conventions

Convention	Meaning
*	An asterisk means that no value is stored at that location in the array.

Table 2 How Progamming and Math Items are Represented in Text

Item	Example	Description	Usage
Vector	x	Lowercase italic	The vector x has six elements.
Vector element	x_2	Lowercase italic with one subscript indicating position	The second element of the vector x is x_2.
Matrix	A	Uppercase italic	The matrix A has three rows and four columns.
Matrix element	a_{23}	Lowercase italic with two subscripts indicating position	Element a_{23} is in the second row and third column of A.
Scalar quantity specifying length or count	m by n	Lowercase italic	A is an m by n band matrix with *kl* subdiagonals and *ku* superdiagonals.
Array	A or X	Uppercase	The matrix A is stored in the array A, and the vector x is stored in the array X.
Array element	A(1,2) or X(3)	Uppercase with numbers in parentheses indicating position	A(1,2) is the element in the first row and second column of the array A. X(3) is the third element in the array X.
Arguments mentioned in text	**n** or **A**	Bold	The data length is specified by the **n** argument.

Table 3 How Math Symbols and Expressions are Represented in Text

Symbol or Expression	Description
α, β, a	Greek and English letters denoting scalar values
$\|incx\|$	Absolute value of $incx$
$A \leftarrow B$	Matrix A is replaced by matrix B
B^T y^T	Transpose of the matrix B; transpose of the vector y
B^{-1}	Inverse of the matrix B
B^{-T}	Inverse of the transpose of matrix B
B^m	Product of matrix B, m times
$\overline{B}$ $\overline{y}$	Complex conjugate of the matrix B; complex conjugate of the vector y
$B^H y^H$	Complex conjugate transpose of the matrix B; complex conjugate transpose of the vector y
$\overline{b}_{ij}$ $\overline{y}_i$	Complex conjugate of the matrix element b_{ij}; complex conjugate of the vector element y_i
$\sum_{i=1}^{n} x_i$	Sum of the elements x_1 to x_n
$\min\{x_j\}$	Minimum element in the vector x
$\max\{x_j\}$	Maximum element in the vector x

Using the Reference Sections

The following information may be helpful when using the reference sections contained in this book.

CXML reference material is documented in sections - one section for each of CXML's routine libraries. For example, all of the BLAS1 routines are described in the *BLAS1 Reference* section.

Each reference section consists of reference material that describes the functionality, calling sequences, and parameters of each routine.

Many CXML routines have variations to accomodate different data types. These routines are differentiated from each other by a letter prefixed to the name, indicating the data type that the routine uses. This naming convention is discussed in more detail in the next section.

The description of each routine in the reference section combines the purpose and attributes of all its variations. The letter prefix is used with the routine's name when a specific variation is discussed. When the discussion applies to all versions, a leading underscore character (_) is used instead of the letter prefix.

CXML Routine Naming Conventions

There is a relationship between CXML routine names and Fortran datatypes. This relationship is explained in this section.

Each CXML routine deals principally with data from one *real* or one *complex* data type. CXML uses the symbol of the data type (i.e. I, S, D, C, Z) as the first letter of the routine's name to identify the data type upon which it operates (or returns).

If the CXML routine name begins with this letter:	The CXML routine uses this data type:
I	Integer
S	Single precision
D	Double precision
C	Complex
Z	Double Complex

For example, consider the CXML routines called SAXPY, DAXPY, CAXPY, ZAXPY. It is easy to determine what data type each routine uses by reading its name. The SAXPY routine is used for single precision data. The DAXPY routine is used for double precision data. The CAXPY routine is used for complex data. The ZAXPY routine is used for double complex data.

When a routine is generically referenced in text, a leading underscore (_) is used in place of the first letter to indicate that all versions of the routine are being discussed.

In the case of SAXPY, DAXPY, CAXPY, ZAXPY, _AXPY would be used to generically refer to this group of routines.

Use of REAL and COMPLEX

In this book, references to REAL*4, REAL*8, COMPLEX*8, and COMPLEX*16 refer to single precision, double precision, complex, and double complex, as follows:

- REAL*4 = single precision
- REAL*8 = double precision
- COMPLEX*8 = complex
- COMPLEX*16 = double complex

Other Reference Section Conventions

The following conventions indicate any differences among the four variations:

- Data types
  If a parameter's data type is the same for all variations of the routine, the data type is listed once:

  integer*4

  If a parameter has a different data type when used with each of the variations, the parameter's data type is documented in the following way:

  real*4 | real*8 | complex*8 | complex*16

  This indicates that the parameter must be single-precision when calling routines with the prefix S, double-precision when calling routines with the prefix D, complex when calling routines with the prefix C, and double complex when calling routines with the prefix Z.

- Parameters

  For some routines, a variation requires additional parameters. This is indicated in the calling sequence in the following way:

  {S,D}xxxx(..., ..., ...)

  {C,Z}xxxx(..., rwork, ...)

- Ordering of routines

  In general, the BLAS routines are sorted alphabetically, However, some routines that have the same logical function are documented together even though they have different names. This occurs when the real version of the routine deals with a symmetric matrix (and so has SY in its name) and the complex version deals with a Hermitian matrix (HE). The signal processing, iterative solver, and direct solver routines are grouped according to the type of mathematical task.

Using Manpages

Online reference information for CXML on the Tru64 UNIX platform is available in the form of manpages. Symbolic links to the manpages are installed in the */usr/share/man/man3* directory at installation time.

Use the *man* command, with the manpage name, to display a CXML manpage. For example, to display the product overview - which gives a brief summary of the contents of CXML, a list of subcomponents, and pointers to related information - enter the following command:

```
man dxml
```

To display the manpage that describes a subcomponent, such as BLAS 3, and its list of associated routines, use the name of the subcomponent, as follows:

```
man blas3
```

To display the manpage that provides a description of a routine, such as SAXPY, use the name of the routine, as follows:

```
man saxpy
```

Note About LAPACK Manpages

To display the manpage that gives an overview of LAPACK, and lists LAPACK routines and the operations they perform, use the following command:

```
man lapack
```

LAPACK routines have a separate manpage for each data type. When you use the *man* command for an LAPACK routine, the routine name should have the correct data type. For example, to display the manpage for the DGETRF routine, use the command:

```
man dgetrf
```

To display the CGETRF routine, use the command:

```
man cgetrf
```

Sending Compaq Your Comments

Compaq welcomes your comments on this product and on its documentation. You can send comments to us in the following ways:

- By email: *cxml@compaq.com*
- By accessing the support page on the Math Group website: *www.compaq.com/math/support*

- By a letter sent to the following address:

  Compaq Computer Corporation
  High Performance Computing Group (CXML), ZK02-3/Q18
  110 Spit Brook Road
  Nashua, N.H. 03062-2698
  USA

If you have suggestions for improving particular sections, or find errors, please indicate the title, order number, and section number.

Getting Help from Compaq

If you have a customer support contract and have comments or questions about CXML software, you contact Compaq's Customer Support Center (CSC), preferably using electronic means such as DSNlink. In the United States, customers can call the CSC at 1-800-354-9000.

Introduction to CXML

The Compaq Extended Math Library (CXML) is a collection of high-performance, computationally-intensive mathematical subprograms designed for use in many different types of scientific and engineering applications. CXML subprograms are callable from any programming language.

CXML's subprograms cover the areas of Basic Linear Algebra, Linear System and Eigenproblem Solvers, Sparse Linear System Solvers, Sorting, Random Number Generation, and Signal Processing.

- **Basic Linear Algebra Subprograms** - The Basic Linear Algebra Subprograms (BLAS) library includes the industry-standard Basic Linear Algebra Subprograms for Level 1 (vector-vector (BLAS1)), Level 2 (matrix-vector (BLAS2)), and Level 3 (matrix-matrix (BLAS3)). Also included are subprograms for BLAS Level 1 Extensions, Sparse BLAS Level 1, and Array Math Functions (VLIB).
- **Signal Processing Subprograms** - The Signal Processing library provides a basic set of signal processing functions. Included are one-, two-, and three-dimensional Fast Fourier Transforms (FFT), group FFTs, Cosine/Sine Transforms (FCT/FST), Convolution, Correlation, and Digital Filters.
- **Sparse Linear System Subprograms** - The Sparse Linear System library provides both direct and iterative sparse linear system solvers. The direct solver package supports both symmetric and nonsymmetric sparse matrices stored using the skyline storage scheme. The iterative solver package contains a basic set of storage schemes, preconditioners, and iterative solvers. The design of this package is modular and matrix-free, allowing future expansion and easy modification by users.
- **LAPACK subprograms** - The Linear System and Eigenproblem Solver library provides the complete LAPACK package developed by a consortium of university and government laboratories. LAPACK is an industry-standard subprogram package offering an extensive set of linear system and eigenproblem solvers. LAPACK uses blocked algorithms that are better suited to most modern architectures, particularly ones with memory hierarchies. LAPACK will supersede LINPACK and EISPACK for most users.

Where appropriate, each subprogram has a version to support each combination of real or complex arithmetic and single or double precision. The supported floating point format is IEEE, and additionally VAX float on the OpenVMS platform.

1 Parallel Library Support for Symmetric Multiprocessing

CXML supports symmetric multiprocessing (SMP) for improved performance on the Tru64 UNIX platform. Key BLAS Level 2 and 3 routines, the LAPACK GETRF and POTRF routines, the sparse iterative solvers, the skyline solvers, and the FFT routines have been modified to execute in parallel if run on SMP hardware. These parallel routines along with the other serial routines are supplied in an alternative library.

The user may choose to link with either the parallel (" -lcxmlp ") library, or the serial (" -lcxml ") library, depending on whether SMP support is required, since each library contains the complete set of routines. The parallel CXML library achieves its parallelization using OpenMP.

2 Cray SciLib Support (SCIPORT)

SCIPORT is Compaq Computer Corporation's implementation of the Cray Reasearch scientific numerical library, SciLib. SCIPORT provides 64-bit single-precision and 64-bit integer interfaces to underlying CXML routines for Cray users porting programs to Alpha systems running the Compaq Tru64 UNIX operating system. SCIPORT also provides an equivalent version of almost all Cray Math Library and CF77 (Cray Fortran 77) Math intrinsic routines.

In order to be completely source code compatible with SciLib, the SCIPORT library calling sequence supports 64-bit integers passed by reference. However, internally, SCIPORT used 32 bit integers. Consequently, some run-time uses of SciLib are not supported by SCIPORT.

SCIPORT provides the following:

- 64-bit versions of all Cray SciLib single-precision BLAS Level 1, Level 2, and Level 3 routines
- All Cray SciLib LAPACK routines
- All Cray SciLib Special Linear System Solver routines
- All Cray SciLib Signal Processing routines
- All Cray SciLib Sorting and Searching routines

These routines are completely interchangeable with their Cray SciLib counterparts, up to the runtime limit on integer size - and with the exception of the ORDERS routine, require no program changes to function correctly. Due to endian differences of machine architecture, special considerations must be given when the ORDERS routine is used to sort multi-byte character strings.

3 Calling CXML from Programming Languages

CXML subprograms are callable from any programming language. However, CXML subprograms follow Fortran conventions and assume a Fortran standard for the passing of arguments and for the storing of data. Unless specifically noted, all non-character arguments are passed by reference. Data in arrays is stored column by column.

If you are programming in a language other than Fortran, consult the specific language's user guide and reference manual for information about how that language stores and passes data. You may be required to set up your data differently from the way you normally would when using that language.

4 How CXML Achieves High Performance

CXML relies on the following design techniques to achieve high performance:

- Computational constructs maximize the use of available instructions and promote pipelined use of functional units.
- Where appropriate, selected routines are available in parallel and serial, to offer additional performance on multiprocessor (SMP) systems.
- The hierarchical memory system is efficiently managed by enhancing the data locality of reference:
  - Data in registers is often reused to minimize load and store operations.
  - The cache is managed efficiently to maximize the locality of reference and data reuse. For example, the algorithms are structured to operate on sub-blocks of arrays that are sized to remain in the cache until all operations involving the data in the sub-block are complete.
  - The algorithms minimize Translation Buffer misses and page faults.
- Unity increment (or stride) is used wherever possible.

5 CXML's Accuracy

To obtain the highest performance from processors, the operations in CXML subprograms have been reordered to take advantage of processor-level parallelism.

As a result of this reordering, some subprograms may have an arithmetic evaluation order different from the conventional evaluation order. This difference in the order of floating point operations introduces round-off errors that imply the subprograms can return results that are not bit-for-bit identical to the results obtained when the computation is in the conventional order. However, for well-conditioned problems, these round-off errors should be insignificant.

Significant round-off errors in application code that is otherwise correct indicates that the problem is most likely not correctly conditioned. The errors could be the result of inappropriate scaling during the mathematical formulation of the problem or an unstable solution algorithm. Re-examine the mathematical analysis of the problem and the stability characteristics of the solution algorithm.

Part 1—Programming Considerations

This section discusses what you need to know when preparing application programs that utilize CXML.

The following major topics are addressed:

- Preparing and storing data - Chapter 1
- Coding your program - Chapter 2
- Compiling and linking - Chapter 3

1
Preparing and Storing Program Data

This chapter discusses some of the things you need to know about handling program data in relation to using CXML.

1.1 Data and Data Types

The data your program uses can be broadly classified as one of two kinds: *scalar* or *array* data.

A single data item, having one value, is known as scalar data. A scalar can be passed to a subprogram as input, or returned as output. Several scalars grouped together into a single unit is referred to as an array. Each piece of data in an array is an element of that array. All elements of an array are of the same *data type*.

CXML Data Types in Relation to Programming Languages

Programming languages such as Fortran and C, among others, have several data types that are used to pass data to CXML subprograms. Fortran is used for most of the examples and explanations in this book, and is used here in explaining data types.

Data can be one of several different data types, such as character, integer, single-precision real, double-precision real, single-precision complex, and double-precision complex.

Data types have language-specific equivalents. For example, some of the relevant Fortran equivalents to the above data types are:

- Integer data - called INTEGER (or INTEGER*4, or sometimes INTEGER*8)
- Real data - called SINGLE PRECISION (or REAL*4), DOUBLE PRECISION (or REAL*8), COMPLEX (or COMPLEX*8), DOUBLE COMPLEX (or COMPLEX*16)
- Characters - called CHAR (or CHAR*1)

The following section outlines the Fortran data types that CXML uses.

Fortran Data Types Used in CXML

The following table (Table 1–1) defines the Fortran data types that can be passed to CXML subprograms.

Table 1–1 Fortran Data Types

Data Type	Fortran Equivalent	Definition
Character	CHARACTER*1	A single character such as “n”, “t”, or “C”.
Character string	CHARACTER*(*)	A sequence of one or more characters.
Logical	LOGICAL*4	A logical value: TRUE or FALSE.
Integer	INTEGER*4	A number such as $+8$ or -136.
Single-precision real	REAL*4	A single-precision floating-point number.
Double-precision real	REAL*8	A double-precision floating-point number.
Single-precision complex	COMPLEX*8	Two floating-point numbers that together represent a complex number. Each number is REAL*4.
Double-precision complex	COMPLEX*16	Two floating-point numbers that together represent a complex number. Each number is REAL*8.

1.2 Platforms and Number Formats

CXML can be used on a variety of platforms, such as Tru64 UNIX Alpha, Windows NT Alpha, Windows NT Intel, and OpenVMS Alpha. For each platform, it is required that data (i.e. numbers) be in the correct format for that platform.

Integers

CXML routines accept integer data in 4 byte (32 bit) format.

Floating Point Numbers

Floating point numbers are in IEEE format for Tru64 UNIX Alpha, Windows NT Alpha, Windows NT Intel, and OpenVMS Alpha platforms. However, the OpenVMS Alpha platform also supports a second format called VAX floating point format.

- **IEEE Format** - Uses single precision (S) and double precision (T) floating point numbers.

  Single precision (S) - The range of single precision numbers is approximately $1.18 * 10^{-38}$ to $3.4 * 10^{38}$. The precision is approximately one part in 2^{23} or seven decimal digits.
  Double precision (T) - The range of double precision numbers is approximately $2.23 * 10^{-308}$ to $1.8 * 10^{308}$. The precision is approximately one part in 2^{52} or 15 decimal digits.

- **VAX Format** - Uses single precision (F) and double precision (G) floating point numbers.

  Single precision (F) - The range of single precision numbers is approximately $.29 * 10^{-38}$ to $1.7 * 10^{38}$. The precision is approximately one part in 2^{23} or seven decimal digits.
  Double precision (G) - The range of double precision numbers is approximately $.56 * 10^{-308}$ to $.9 * 10^{308}$. The precision is approximately one part in 2^{52} or 15 decimal digits.

1.3 Storing Data

CXML handles data in data structures called arrays, vectors, and matrices. This document uses the term "array" to refer to the mathematical concept, and the terms "vector" and "matrix" to refer to the data structures upon which CXML subprograms perform operations.

The following sections descibe these data structures in relation to CXML.

1.3.1 Arrays

An array can be thought of as many pieces of data grouped together into one unit. Each piece of data is called an element of the array. Each element is a scalar and all elements are of the same data type.

In CXML, an array can be either one-dimensional or two-dimensional.

1.3.1.1 One-dimensional arrays

A single column or row of numbers is a one-dimensional array. A one-dimensional array is usually represented as a column or row of elements within parentheses. For example:

$$(3.1,\ 2.2,\ 1.3,\ 2.2,\ 3.1)$$

To locate a value in this array, you specify its position within the column or row.

1.3.1.2 Two-dimensional Arrays

A table with two or more rows and columns of figures is a two-dimensional array. A two-dimensional array is usually represented as rows and columns enclosed in square brackets:

$$\begin{bmatrix} 3.1 & 4.3 & 9.0 \\ 1.1 & 4.0 & 11.7 \end{bmatrix}$$

To locate a value in this array, you specify its position within the brackets by specifying its row number and then its column number.

1.3.1.3 Storing Values in an Array

From the user’s perspective, an array is a group of contiguous storage locations associated with a single symbolic name, such as A, the array name. The individual storage locations (the array elements) are referred to by a number or a series of numbers in parentheses after the array name. A(1) is the first element of a one-dimensional array A. A(3,2) is the element in the third row and second column of a two-dimensional array A.

An array can contain data structures such as vectors and matrices. The way vector or matrix elements are separated in array storage is defined by stride and leading dimension arguments passed to CXML subprograms. See Section 1.3.2 for detailed information on array storage techniques.

An array can be passed to a CXML subprogram as input, it can be returned as output to your application program, or it can be used by the subprogram as both input and output. In the latter case, some input data would be overwritten and therefore lost.

1.3.1.4 Array Storage Requirements

Not all programming languages use the same storage techniques to store arrays. Some programming languages, such as Fortran, store arrays in memory in column-major order, storing the first column, then the second column, and so on. Other languages, such as C, store arrays in row-major order, storing the first row, then the second row, and so on.

CXML assumes that array elements are stored in column-major order when processing data. Use Fortran conventions as described in Section 1.3.2 for arrays passed to a CXML subprogram.

If you are calling CXML subprograms from languages other than Fortran, you must set up your data so that Fortran conventions for array storage can be applied. For information about calling subprograms from other languages, see Chapter 2.

1.3.2 Fortran Arrays

A Fortran array can have from one to seven dimensions. An array is specified by the name of the array, the number of dimensions in the array, and the number of elements in each dimension. CXML can operate on either one- or two-dimensional arrays.

You must state the size of each array explicitly in your Fortran program. Use a DIMENSION statement, or preferably, a specific data type statement (such as REAL*4 or COMPLEX*8) for each array. Fortran arrays are always stored in memory as a linear sequence of values.

1.3.2.1 One-Dimensional Fortran Array Storage

A one-dimensional Fortran array is stored with its first element in the first storage location, the second element in the second storage location, and so on until the last element is in the last storage location.

For example, consider the one-dimensional array A with 4 elements shown in (1–1):

$$A = (A(1), A(2), A(3), A(4)) \tag{1–1}$$

The array A has its elements stored as shown in Table 1–2.

Table 1–2 One-Dimensional Fortran Array Storage

Storage Location	Array Element
1	A(1)
2	A(2)
3	A(3)
4	A(4)

1.3.2.2 Two-Dimensional Fortran Array Storage

The elements of a two-dimensional array are stored column by column, so that the left subscripts vary most rapidly and the right subscripts vary least rapidly. The elements of the first column are stored, then the elements of suceeding columns are stored, until the elements in the last column are stored. This mode of storage is called column-major order.

For example, consider the two-dimensional array A with 12 elements shown in Table 1–3:

$$A = \begin{bmatrix} A(1,1) & A(1,2) & A(1,3) \\ A(2,1) & A(2,2) & A(2,3) \\ A(3,1) & A(3,2) & A(3,3) \\ A(4,1) & A(4,2) & A(4,3) \end{bmatrix}$$

The array A has its elements stored as shown in Table 1–3.

Table 1–3 Two-Dimensional Fortran Array Storage

Storage Location	Array Element
1	A(1,1) (column 1 starts)
2	A(2,1)
3	A(3,1)
4	A(4,1)
5	A(1,2) (column 2 starts)
6	A(2,2)
7	A(3,2)
8	A(4,2)
9	A(1,3) (column 3 starts)
10	A(2,3)
11	A(3,3)
12	A(4,3)

1.3.2.3 Array Elements

All the elements of an array have the same data type: real or complex, single- or double-precision. The size of the storage locations for the elements depends on the data type of the array. Single-precision real (REAL*4, S_floating) data requires 4 bytes of storage; double-precision real (REAL*8, T_floating) data requires 8 bytes of storage.

Because a complex number is an ordered pair of two real numbers, (a, b) or $a + ib$, where $i = \sqrt{-1}$, storing a complex number requires two storage locations, one location for each part of the complex number. Single-precision complex (COMPLEX*8, S_floating complex) data requires 8 bytes of storage; double-precision complex (COMPLEX*16, T_floating complex) data requires 16 bytes of storage.

1.3.3 Vectors

CXML subprograms perform operations on two particular kinds of data structures: vectors and matrices. This section defines and describes vectors, and discusses the various ways of storing vectors in arrays.

A vector is a one-dimensional ordered collection of numbers, either real or complex. A real vector contains real numbers, and a complex vector contains complex numbers.

A complex number has the form $a + bi$ where a is a real number called the real part, b is a real number called the imaginary part, and $i = \sqrt{-1}$.

A vector can be represented symbolically as a column of numbers, or as a row of numbers.

For a column of numbers, use the following vector notation for a vector x with n elements:

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

For a row of numbers, use the following vector notation for a vector y with n elements:

$$y = \begin{bmatrix} y_1 & y_2 & y_3 & \dots & y_n \end{bmatrix}$$

1.3.3.1 Transpose and Conjugate Transpose of a Vector

The transpose of a vector changes a column vector to a row vector or a row vector to a column vector. Use the following notation for a vector x and its transpose x^T:

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \qquad x^T = \begin{bmatrix} x_1 & x_2 & x_3 & \dots & x_n \end{bmatrix}$$

A complex number c is defined as $c = a + bi$, where a and b are real and $i = \sqrt{-1}$.

The complex conjugate $\overline{c}$ is obtained by replacing i by $-i$:

$$\overline{c} = a - bi$$

If a vector x has elements that are complex numbers, the conjugate transpose (or Hermite) of the vector x, denoted by x^H, is the vector that changes each element of $x_j = a_j + b_j i$ to its complex conjugate $\overline{x}_j = a_j - b_j i$ and then transposes it:

$$x^H = \begin{bmatrix} \overline{x}_1 & \overline{x}_2 & \overline{x}_3 & \dots & \overline{x}_n \end{bmatrix}$$

1.3.3.2 Defining a Vector in an Array

A vector is a set of numbers that is given in order (i.e. $a_1, a_2, ..., a_n$. A vector is usually stored in a one- or two-dimensional array. When a CXML subroutine is called, the array is passed as an argument to the subroutine, with the vector inside of it. The elements of the vector are stored in order inside the array, but are not necessarily contiguous. The separation between the vector elements is called the *stride*.

In a vector of complex type, each vector element has the form $a + bi$. Two storage locations are needed to store a and b. Therefore, storing a complex vector requires twice the number of storage locations as storing a real vector of the same precision.

An array can be much larger than the vector that it contains. The storage of a vector is defined using three arguments in a CXML subprogram argument list:

- Vector length: Number of elements in the vector
- Vector location: Base address of the vector in the array
- Stride: Space, or increment, between consecutive elements in the array

These three arguments together specify which elements of an array are selected to become the vector.

1.3.3.2.1 Vector Length To specify the length n of a vector, you specify an integer value for a length argument, such as the argument **n**. The length of a vector can be less than the length of the array that contains the vector.

Vector length can also be thought of as the number of elements of the associated array that a subroutine will process. Processing continues until n elements have been processed.

1.3.3.2.2 Vector Location The location of the first element of a vector inside an array is specified by the argument in the call to the CXML subprogram. The program that calls the CXML subroutine usually declares the array. For example, an array such as X is declared, X(1:20) or X(20).

In this case, if you want to specify vector x as starting at the first element of an array X, the argument is specified as X(1) or X. If you want to specify vector x as starting at the fifth element of X, the argument is specified as X(5).

However, in an array X that is declared as X(3:20), with a lower bound and an upper bound given for the dimension, specifying vector x as starting at the fifth element of X means that the argument is specified as X(7).

For a two-dimensional array X that is declared as X(1:10,1:20) or X(10,20), specifying the vector x as starting at the seventh row and eleventh column of X means that the argument is specified as X(7,11).

Most of the examples shown in this manual assume that the lower bound in each dimension of an array is 1. Therefore, the lower bound is not specified, and the value of the upper bound is the number of elements in that dimension. So, a declaration of X(50) means X has 50 elements.

When vector elements are selected by the CXML subprogram, the starting point for the selection of vector elements is not always the location of the vector as specified by the argument passed to the CXML subroutine. Which element is the starting point for processing depends on whether the spacing parameter is positive, negative, or zero.

1.3.3.2.3 Stride of a Vector The spacing parameter, called the increment or stride, indicates how to move from the starting point through the array to select the vector elements from the array. The increment is specified by an argument in the CXML subprogram argument list, such as the argument **incx**. Because one vector element does not necessarily immediately follow another, the increment specifies the size of the step (or stride) between elements.

The sign (+ or −) of the stride indicates the direction in which the vector elements are selected:

- Forward indexing

  The stride is positive. Vector elements are stored forward in the array in the order $x_1, x_2, ..., x_n$. As the vector element index increases, the array element index increases.

- Backward indexing

  The stride is negative. Vector elements are stored backward in the array, in the reverse order $x_n, x_{n-1}, ..., x_1$. As the vector element index increases, the array element index decreases.

The absolute value of the stride is the spacing between each element. An increment of 1 indicates that the vector elements are contiguous. An increment of 0 indicates that all the elements of a vector are selected from the same location in the array.

1.3.3.2.4 Selecting Vector Elements from an Array CXML uses the stride to select elements from the array to construct the vector composed of these elements. The stride associates consecutive elements of the vector with equally spaced elements of the array.

When the stride is positive:

- The location specified by the argument for the vector is the location of the first element in the vector, x_1.
- The starting point for the selection of elements is at the first vector element.
- The indexing is forward, with the vector elements stored forward in the array.

For example, consider the array X declared as X(10) with X defined as shown in (1–2):

$$\mathrm{X} = (10.0,\ 9.1,\ 8.2,\ 7.3,\ 6.4,\ 5.5,\ 4.6,\ 3.7,\ 2.8,\ 1.9) \qquad (1\text{–}2)$$

If you specify X, which means X(1), for the vector x, the first element processed is the first element of X, which is 10.0. If you specify X(3) for the vector x, the first element processed is the third element of X, which is 8.2.

To select the vector from the array, CXML adds the stride to the starting point and processes the number of elements you specify. For example, if the location of the vector is X(2), the stride is 2, and the vector length is 4, the vector is

$$x = (9.1,\ 7.3,\ 5.5,\ 3.7)$$

Processing begins at array element X(2), which is 9.1, and processing ends at array element X(8), which is 3.7.

If you are using a two-dimensional array for vector storage, remember that array elements are selected as they are stored, column by column. See Section 1.3.2.2, for this storage information.

For example, consider the array X declared as X(4,4) with X defined as shown in (1–3):

$$\mathrm{X} = \begin{bmatrix} 1.1 & 1.2 & 1.3 & 1.4 \\ 2.1 & 2.2 & 2.3 & 2.4 \\ 3.1 & 3.2 & 3.3 & 3.4 \\ 4.1 & 4.2 & 4.3 & 4.4 \end{bmatrix} \qquad (1\text{–}3)$$

If the location of the vector x is X(4,1), the stride is 3, and the vector length is 5, the vector is

$$x = (4.1,\ 3.2,\ 2.3,\ 1.4,\ 4.4)$$

When the increment is negative, vector elements are selected as follows:

- The location specified by the argument for the vector is the location of the last element in the vector, x_n.
- CXML calculates the starting point for the selection of elements by considering the location of the vector, the increment, and the number of elements to process.
- The indexing is backward. Vector elements are stored backwards in the array.

For example, consider the array X declared as X(12) with X defined as shown in (1–4):

$$\mathrm{X} = (1.0,\ 2.0,\ 3.0,\ 4.0,\ 5.0,\ 6.0,\ 7.0,\ 8.0,\ 9.0,\ 10.0,\ 11.0,\ 12.0) \qquad (1\text{–}4)$$

If the location of the vector is X(3), the increment is -2, and the vector length is 5, the vector is

$$x = (11.0,\ 9.0,\ 7.0,\ 5.0,\ 3.0)$$

In this case, processing begins at array element X(11), which is 11.0, and processing ends at array element X(3), which is 3.0.

When the increment is 0, the location specified by the argument such as the **x** argument, is the only array element used in the selection of the vector. Each element of the vector has the same value.

For example, consider the array X declared as X(6) with X defined as shown in (1–5):

$$\mathrm{X} = (1.0,\ 2.0,\ 3.0,\ 4.0,\ 5.0,\ 6.0) \qquad (1\text{–}5)$$

If the location of the vector is X(3), the increment is 0, and the number of elements to process is 5, the vector is

$$x = (3.0,\ 3.0,\ 3.0,\ 3.0,\ 3.0)$$

1.3.3.3 Storing a Vector in an Array

CXML provides various storage schemes to store vectors in arrays. The general storage scheme which applies to all CXML subprograms is described in this section. You can find further information about vector storage schemes that relate to specific types of vectors in the following sections:

- Storing a sparse vector (See Section 5.2.1 and Section 5.2.2).
- Storing vectors for signal processing subprograms (See Section 9.1.2).

Suppose X is a real one-dimensional array of k elements. Let vector x have length n and let $incx$ be the increment used to access the elements of vector x whose components $x_i,\ i = 1, \ldots, n$, are stored in X.

If $incx \geq 0$, and if the location of the vector is specified at the first element of the array, then x_i is stored in the array location as shown in (1–6):

$$\mathrm{X}(1 + (i-1) * incx) \qquad (1\text{–}6)$$

If $incx = 0$, and if the location of the vector is specified at the first element of the array, all the elements of the vector x are at the same array location, X(1).

If $incx < 0$, and if the location of the vector is specified at the first element of the array, then x_i is stored in the array location as shown in (1–7):

$$\mathrm{X}(1 + (n-i) * |incx|) \qquad (1\text{–}7)$$

Therefore, k, the number of elements in the array, must be as shown in (1–8):

$$ndim \geq 1 + (n-1) * |incx| \qquad (1\text{–}8)$$

For the general case where the location of the vector in the array is at the point X(BP) rather than at the first element of the array, (1–9) or (1–10) can be used to find the position of each vector element x_i in a one-dimensional array.

For $incx \geq 0$,

$$X(\mathrm{BP} + (i-1) * incx) \qquad (1\text{–}9)$$

For $incx < 0$,

$$X(\mathrm{BP} + (n - i) * |incx|) \tag{1–10}$$

For example, suppose that $\mathrm{BP} = 3$, $k = 20$, and $n = 5$. Then a value of $incx = 2$ implies that x_1, x_2, x_3, x_4, and x_5 are stored in array elements X(3), X(5), X(7), X(9), and X(11). However, if $incx = -2$, then x_1, x_2, x_3, x_4, and x_5 are stored in array elements X(11), X(9), X(7), X(5), and X(3).

With a suitable choice for the location of a vector, you can operate on vectors that are embedded in other vectors or matrices. For example, consider an m by n matrix A, stored in an md by nd array.

The *j*th column of the matrix is a vector represented by:

base address:	A(1,*j*)
increment:	1
length:	*m*

The *i*th row of the matrix is a vector represented by:

base address:	A(*i*,1)
increment:	*md*
length:	*n*

The main diagonal of the matrix is a vector represented by:

base address:	A(1,1)
increment:	*md* + 1
length:	min(*m*,*n*)

1.3.4 Matrices

CXML subprograms perform operations on two particular kinds of data structures: vectors and matrices. This section defines and describes matrices, and discusses the various ways of storing matrices in arrays.

A matrix is a two-dimensional ordered collection of numbers, either real or complex. For example, the matrix A with m rows and n columns, an m by n matrix, is represented in the following way:

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

The elements of the matrix are represented as a_{ij} where $i = 1, ..., m$ and $j = 1, ..., n$. A square matrix with n rows and n columns is called a matrix of order n.

1.3.4.1 Transpose and Conjugate Transpose of a Matrix

The transpose of a matrix A, denoted by A^T, is formed by taking the ith row of A and making it the ith column of A^T. The columns of A become the rows of A^T. If A is an m by n matrix, A^T is an n by m matrix. Use the following notation for a matrix A and its transpose:

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

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

The effect of transposing a matrix is to flip the matrix across its main diagonal. The element in row i, column j of A^T comes from row j, column i of A:

$$A^T_{ij} = A_{ji}$$

Taking the conjugate transpose of a matrix A that contains complex numbers is an operation on the matrix that changes each element of the matrix to its complex conjugate and then transposes the matrix:

$$A^H = \begin{bmatrix} \overline{a}_{11} & \cdots & \overline{a}_{n1} \\ \vdots & \vdots & \vdots \\ \overline{a}_{1n} & \cdots & \overline{a}_{mn} \end{bmatrix}$$

The effect of finding the complex conjugate of a matrix is to get the complex conjugate of each element of the matrix and then flip the matrix across its main diagonal. The element in row i, column j of A^H is the complex conjugate of the element in row j, column i of A:

$$A^H_{ij} = \overline{A}_{ji}$$

1.3.4.2 Storing a Matrix in an Array

CXML provides various storage schemes to store matrices in arrays. The general storage scheme which applies to most CXML subprograms is described in the following sections:

- Defining and storing a matrix in an array (see Section 1.3.4.3)
- Symmetric and Hermitian matrices (see Section 1.3.4.4 and Section 1.3.4.5)
- Triangular matrix (see Section 1.3.4.6 and Section 1.3.4.7)
- General band matrices (see Section 1.3.4.8 and Section 1.3.4.9)
- Real symmetric band matrices and complex hermitian band matrices (see Section 1.3.4.10 and Section 1.3.4.11)
- Upper and lower triangular band matrices (see Section 1.3.4.12 and Section 1.3.4.13)

Further information about matrix storage schemes that relate to CXML is located in the following places:

- Sparse matrices for iterative solvers (see Section 10.3 and Section 10.3.1)
- Sparse matrices for direct solvers (see Section 11.4)

1.3.4.3 Defining a Matrix in an Array

A matrix is usually stored in a two-dimensional array. When every element of a matrix is stored, the storage scheme is called full matrix storage. If the matrix itself is a special kind of matrix such as a triangular matrix or a band matrix, a large number of storage locations are wasted using full matrix storage, and other storage methods can be used.

If a matrix is complex, each matrix element has the form $a + bi$. For each complex element, two storage locations in succession are needed to store a and b. Storing a complex matrix requires twice the number of storage locations as storing a real matrix of the same precision.

The columns of the matrix are stored one after the other in the array. The array can be much larger than the matrix that is stored in the array.

The storage of a matrix is defined using four arguments in a CXML subprogram argument list:

- Matrix location: Base address of the matrix in the array. It also tells where processing begins.
- The first, or leading, dimension of the array: Space, or increment, between consecutive elements of a row in an array.
- The number of rows m of the matrix.
- The number of columns n of the matrix.

These four quantities together specify which elements of an array are selected to become the matrix.

1.3.4.3.1 Matrix Location The location given by the matrix argument in a CXML subroutine argument list is the starting point for selecting matrix elements. For example, consider the array A declared as A(5,7).

$$\mathrm{A} = \begin{bmatrix} 1.0 & 6.0 & 11.0 & 16.0 & 21.0 & 26.0 & 31.0 \\ 2.0 & 7.0 & 12.0 & 17.0 & 22.0 & 27.0 & 32.0 \\ 3.0 & 8.0 & 13.0 & 18.0 & 23.0 & 28.0 & 33.0 \\ 4.0 & 9.0 & 14.0 & 19.0 & 24.0 & 29.0 & 34.0 \\ 5.0 & 10.0 & 15.0 & 20.0 & 25.0 & 30.0 & 35.0 \end{bmatrix} \quad (1\text{–}11)$$

If you specify A(2,3) as the starting point for the selection of matrix elements, then processing begins at the element in row 2 and column 3, which is the element 12.0.

1.3.4.3.2 First Dimension of the Array The first (or leading) dimension of an array, which is specified by an argument such as **lda** in the CXML subprogram argument list, is the number of rows in the array from which the matrix elements are being selected. The first dimension of the array is used as an increment to select matrix elements from successive columns of the array.

The first dimension must be greater than or equal to m, the number of rows of the matrix. If the first dimension were less than m, then elements from one column of a matrix would be stored in more than one column of the array. This storage mechanism would lead to access of incorrect elements.

For the array A shown in (1–11), the first dimension is 5. More generally, for an array A declared as A(FL:FU,SL:SU), the first dimension of the array is as follows:

$$\mathrm{FU} - \mathrm{FL} + 1$$

1.3.4.3.3 Number of Rows and Columns of the Matrix You specify the number of rows m of the matrix and the number of columns n of the matrix by specifying an integer value for the row and column arguments, such as **m** and **n**.

You can think about the matrix as the number of rows and columns of the array that you want to process. After processing the first element, the subprogram continues until m elements in each of n columns have been processed.

1.3.4.3.4 Selecting Matrix Elements from an Array Again, consider the array A declared as A(5,7), with A(2,3) specified as the location of the matrix, which is also the starting point for the selection of matrix elements.

$$\mathrm{A} = \begin{bmatrix} 1.0 & 6.0 & 11.0 & 16.0 & 21.0 & 26.0 & 31.0 \\ 2.0 & 7.0 & 12.0 & 17.0 & 22.0 & 27.0 & 32.0 \\ 3.0 & 8.0 & 13.0 & 18.0 & 23.0 & 28.0 & 33.0 \\ 4.0 & 9.0 & 14.0 & 19.0 & 24.0 & 29.0 & 34.0 \\ 5.0 & 10.0 & 15.0 & 20.0 & 25.0 & 30.0 & 35.0 \end{bmatrix} \tag{1–12}$$

Processing begins at element 12.0. If the number of rows m to be processed is 3, and the number of columns n to be processed is 4, CXML adds the value of the first dimension of the array, which is 5, to find the starting point in the next column, which is element 17.0. CXML continues this until the number of columns processed is 4. The starting points of the columns are elements 12.0, 17.0, 22.0, and 27.0. Then, to find the matrix elements in each column of A, CXML repeatedly adds the value 1 to the starting point in a column until 3 elements in each column have been processed. The matrix elements selected in this example specify the matrix A shown in (1–13):

$$A = \begin{bmatrix} 12.0 & 17.0 & 22.0 & 27.0 \\ 13.0 & 18.0 & 23.0 & 28.0 \\ 14.0 & 19.0 & 24.0 & 29.0 \end{bmatrix} \tag{1–13}$$

The matrix does not have elements from all the rows and columns of the array. No elements are selected from rows 1 or 5 or from columns 1, 2, or 7. However, the matrix formed is a rectangular block in the array.

1.3.4.4 Symmetric and Hermitian Matrices

A matrix is symmetric if it is equal to its transpose:

$$A = A^T$$

A symmetric matrix A has the following properties:

- A has the same number of rows as columns; symmetric matrices are square.
- $a_{ij} = a_{ji}$ for all i and j. Each element of A on one side of the diagonal equals its mirror on the other side of the diagonal.

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

$$A = A^H$$

A Hermitian matrix has the same number of rows as columns; Hermitian matrices are square. However, in general, a Hermitian matrix is not symmetric, as shown by looking at a complex Hermitian matrix B of order 3, its transpose B^T and its conjugate transpose B^H: $B = B^H$, but $B \neq B^T$:

$$B = \begin{bmatrix} (2,0) & (8,-9) & (27,26) \\ (8,9) & (12,0) & (1,-7) \\ (27,-26) & (1,7) & (-3,0) \end{bmatrix}$$

$$B^T = \begin{bmatrix} (2,0) & (8,9) & (27,-26) \\ (8,-9) & (12,0) & (1,7) \\ (27,26) & (1,-7) & (-3,0) \end{bmatrix}$$

$$B^H = \begin{bmatrix} (2,0) & (8,-9) & (27,26) \\ (8,9) & (12,0) & (1,-7) \\ (27,-26) & (1,7) & (-3,0) \end{bmatrix}$$

In a Hermitian matrix, the imaginary part of each of the diagonal elements must be 0.

The symmetry properties of symmetric matrices and Hermitian matrices enable storage of only the upper-triangular part of the matrix (the diagonal and above) or the lower-triangular part of the matrix (the diagonal and below).

1.3.4.5 Storage of Symmetric and Hermitian Matrices

All n by n symmetric or Hermitian matrices are stored in one of two ways:

- In either the upper or lower triangle of a two-dimensional array
- Packed in a one-dimensional array

1.3.4.5.1 Two-Dimensional Upper- or Lower-Triangular Storage When the upper-triangular part of the matrix is stored in the upper triangle of the array, the strictly lower-triangular part of the array is not referenced. Conversely, when the lower-triangular part of the matrix is stored in the lower triangle of the array, the strictly upper-triangular part of the array is not referenced.

As an example, consider a 4 by 4 real symmetric matrix A:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

Upper-triangular storage in a two-dimensional array A is shown in (1–14):

$$\mathrm{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ * & a_{22} & a_{23} & a_{24} \\ * & * & a_{33} & a_{34} \\ * & * & * & a_{44} \end{bmatrix} \quad (1\text{–}14)$$

Lower-triangular storage in a two-dimensional array A is shown in (1–15):

$$\mathrm{A} = \begin{bmatrix} a_{11} & * & * & * \\ a_{21} & a_{22} & * & * \\ a_{31} & a_{32} & a_{33} & * \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \quad (1\text{–}15)$$

1.3.4.5.2 One-Dimensional Packed Storage The total number of elements in any n by n matrix is n^2. The total number of elements in the upper or lower triangle is as follows:

$$1 + 2 + ... + n = \frac{n(n+1)}{2}$$

Therefore, when an n by n symmetric or complex Hermitian matrix is stored in a one-dimensional array, $n(n+1)/2$ memory locations are used. The amount of memory saved is as follows:

$$n^2 - \frac{n(n+1)}{2} = \frac{n(n-1)}{2}$$

Such an arrangement is called packed storage. Either the upper triangle of the matrix can be packed sequentially, column by column, or the lower triangle of the matrix can be packed sequentially, column by column.

As an example, consider a 4 by 4 real symmetric matrix A:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

Upper triangle packing for A in a one-dimensional array AP is shown in (1–16):

$$\text{AP} = \begin{bmatrix} a_{11} \\ a_{12} \\ a_{22} \\ a_{13} \\ a_{23} \\ a_{33} \\ a_{14} \\ a_{24} \\ a_{34} \\ a_{44} \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{21} \\ a_{22} \\ a_{31} \\ a_{32} \\ a_{33} \\ a_{41} \\ a_{42} \\ a_{43} \\ a_{44} \end{bmatrix} \qquad (1\text{–}16)$$

For symmetric matrices, packing the upper triangle by columns is equivalent to packing the lower triangle by rows. For Hermitian matrices, the only difference is that the off-diagonal elements are conjugated.

In this packed storage scheme, the ijth element in the upper triangle of the real symmetric matrix is stored in position k of the array, where:

$$k = i + (j(j-1)/2), \quad \text{for} \quad 1 \le i \le j \quad \text{and} \quad 1 \le j \le n$$

For example, element a_{13} is in position $1 + (3(3-1)/2) = 4$ of the array, and element a_{24} is in position $2 + (4(4-1)/2) = 8$ of the array.

The following Fortran program segment transfers the upper triangle of a symmetric matrix from conventional full matrix storage in a two-dimensional array A to upper-triangle packed storage in a one-dimensional array AP:

```
      K=0
      DO 20 J=1,N
         DO 10 I=1,J
            K=K+1
            AP(K)=A(I,J)
10       CONTINUE
20    CONTINUE
```

Lower triangle packing for A in a one-dimensional array AP is shown in (1–17):

$$\mathrm{AP} = \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \\ a_{22} \\ a_{32} \\ a_{42} \\ a_{33} \\ a_{43} \\ a_{44} \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{12} \\ a_{13} \\ a_{14} \\ \cdots \\ a_{22} \\ a_{23} \\ a_{24} \\ \cdots \\ a_{33} \\ a_{34} \\ \cdots \\ a_{44} \end{bmatrix} \qquad (1\text{–}17)$$

For symmetric matrices, packing the lower triangle by columns is equivalent to packing the upper triangle by rows. For Hermitian matrices, the only difference is that the off-diagonal elements are conjugated.

In this packed storage scheme, the ijth element in the lower triangle of the real symmetric matrix is stored in position k of the array where:

$$k = i - (j(j-1)/2) + n(j-1), \ \text{ for } \ j \le i \le n \ \text{ and } \ 1 \le j \le n$$

For example, element a_{31} is in position $3 - 1(1-1)/2 + 4(1-1) = 3$ of the array, and element a_{43} is in position $4 - 3(3-1)/2 + 4(3-1) = 9$ of the array.

The following Fortran program segment transfers the lower triangle of a symmetric matrix from conventional full matrix storage in a two-dimensional array A to lower-triangle packed storage in a one-dimensional array AP:

```
      K=0
      DO 20 J=1,N
         DO 10 I=J,N
            K=K+1
            AP(K)=A(I,J)
10       CONTINUE
20    CONTINUE
```

1.3.4.6 Triangular Matrices

A triangular matrix is a square matrix whose nonzero elements are all either in the upper-triangular part of the matrix or in the lower-triangular part of the matrix.

In an n by n upper-triangular matrix, $u_{ij} = 0$ for all $i > j$.

The matrix U shown in (1–18) is a 4 by 4 upper-triangular matrix:

$$U = \begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{bmatrix} \qquad (1\text{–}18)$$

In an n by n lower-triangular matrix, $l_{ij} = 0$ for all $i < j$.

The matrix L shown in (1–19) is a 4 by 4 lower-triangular matrix:

$$L = \begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \qquad (1\text{–}19)$$

A unit upper triangular matrix has 1's on the diagonal for $u_{ii} = 1$ and $l_{ii} = 1$.

1.3.4.7 Storage of Triangular Matrices

When an n by n upper- or lower-triangular matrix is stored conventionally in a two-dimensional array, the $(n - 1)$ by $(n - 1)$ strictly lower- or upper-triangular part of the array is not referenced by the subroutine. In the case of a unit upper- or lower-triangular matrix, the main diagonal elements of the array are also not referenced, because these elements are assumed to be unity.

As in the case of symmetric and Hermitian matrices, upper- and lower-triangular matrices can be packed in a one-dimensional array. The upper or lower triangle is packed sequentially, column by column. For packed triangular matrices, the same storage layout is used whether or not the diagonal elements are assumed to have the value 1. That is, space is left for the diagonal elements even if those array elements are not referenced.

1.3.4.8 General Band Matrices

A general band matrix, or band matrix, is a matrix whose nonzero elements are all near the main diagonal such that:

$$a_{ij} = 0 \quad \text{for} \quad (i - j) > k_l \quad \text{or} \quad (j - i) > k_u$$

The lower bandwidth is kl, the upper bandwidth is ku, and the total bandwidth is $kt = (kl + ku + 1)$. The matrix is said to have kl subdiagonals and ku superdiagonals.

The m by n matrix B shown in (1–20) is a general band matrix where the lower bandwidth is $kl = (g - 1)$ and the upper bandwidth is $ku = (p - 1)$:

$$B = \begin{bmatrix}
b_{11} & b_{12} & b_{13} & \cdot & b_{1p} & 0 & \cdot & \cdot & 0 \\
b_{21} & b_{22} & b_{23} & & & \cdot & & \cdot & \cdot \\
b_{31} & b_{32} & b_{33} & & & & \cdot & & \cdot \\
\cdot & & & \cdot & & & & \cdot & 0 \\
\cdot & & & & \cdot & & & & b_{n-p+1,n} \\
b_{g1} & & & & & & & & \cdot \\
 & & & & & \cdot & & & \\
0 & \cdot & & & & & & & \cdot \\
\cdot & & \cdot & & & & \cdot & & \cdot \\
\cdot & \cdot & & \cdot & & & & \cdot & \cdot \\
\cdot & \cdot & \cdot & & \cdot & & & & \\
0 & \cdot & \cdot & \cdot & 0 & b_{m,m-g+1} & \cdot & \cdot & b_{mn}
\end{bmatrix} \qquad (1\text{–}20)$$

In matrix B, the number ku is the number $(p - 1)$ of diagonals above the main diagonal. The number kl is the number $(g - 1)$ of diagonals below the main diagonal. Including the main diagonal, the total bandwidth (or the total number of diagonals) is $(kl + ku + 1)$.

The matrix B shown in (1–21) is a 7 by 8 band matrix with bandwidths $kl = 2$ and $ku = 1$ and total bandwidth of 4:

$$L = \begin{bmatrix}
1 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & 4 & 5 & 0 & 0 & 0 & 0 & 0 \\
6 & 7 & 8 & 9 & 0 & 0 & 0 & 0 \\
0 & 10 & 11 & 12 & 13 & 0 & 0 & 0 \\
0 & 0 & 14 & 15 & 16 & 17 & 0 & 0 \\
0 & 0 & 0 & 18 & 19 & 20 & 21 & 0 \\
0 & 0 & 0 & 0 & 22 & 23 & 24 & 25
\end{bmatrix} \qquad (1\text{–}21)$$

1.3.4.9 Storage of General Band Matrices

When stored in band storage mode, an m by n band matrix with kl subdiagonals and ku superdiagonals is stored in a two-dimensional $(kl + ku + 1)$ by n array. The matrix is stored columnwise so that the nonzero elements of the jth column of the matrix are stored in the jth column of the Fortran array. Consequently, the zero elements of the matrix are not stored in the array.

The main diagonal of the matrix is stored in row $ku + 1$ of the array. The first superdiagonal is stored in row ku starting at column 2. The first subdiagonal is stored in row $ku + 2$ starting at column 1, and so on. Elements of the array that do not correspond to elements in the band matrix, specifically those in the top left ku by ku triangle and those in the bottom right $(n - m + kl)$ by $(n - m + kl)$ triangle, are not referenced by the subroutine.

For example, consider the 5 by 6 band matrix A shown in (1–22) with 1 subdiagonal and 2 superdiagonals. Here, $kl = 1$, $ku = 2$, $m = 5$, and $n = 7$:

$$A = \begin{bmatrix}
a_{11} & a_{12} & a_{13} & 0 & 0 & 0 \\
a_{21} & a_{22} & a_{23} & a_{24} & 0 & 0 \\
0 & a_{32} & a_{33} & a_{34} & a_{35} & 0 \\
0 & 0 & a_{43} & a_{44} & a_{45} & a_{46} \\
0 & 0 & 0 & a_{54} & a_{55} & a_{56}
\end{bmatrix} \qquad (1\text{–}22)$$

The band matrix A is stored in array ABD as shown in (1–23). Array ABD is 4 by 6. The main diagonal of A is stored in row 3 of ABD. The first superdiagonal is stored in row 3 starting at column 2. The top left 2 by 2 triangle and the bottom right 2 by 2 triangle is not referenced.

$$\text{ABD} = \begin{bmatrix} * & * & a_{13} & a_{24} & a_{35} & a_{46} \\ * & a_{12} & a_{23} & a_{34} & a_{45} & a_{56} \\ a_{11} & a_{22} & a_{33} & a_{44} & a_{55} & * \\ a_{21} & a_{32} & a_{43} & a_{54} & * & * \end{bmatrix} \qquad (1–23)$$

In this storage scheme, the ijth element of the band matrix is stored in position $(k,\ j)$ of the array, where $k = (i - j + ku + 1)$.

The following Fortran program segment transfers a band matrix from conventional Fortran full matrix storage in A to band storage in array ABD:

```
      DO 20 J=1,N
         K=KU+1-J
         DO 10 I=MAX(1,J-KU),MIN(M,J+KL)
            ABD(K+I,J)=A(I,J)
10       CONTINUE
20    CONTINUE
```

1.3.4.10 Real Symmetric Band Matrices and Complex Hermitian Band Matrices

A real symmetric band matrix is a real band matrix that is equal to its transpose.

$$B = B^T$$

A real symmetric band matrix is square. It has all its nonzero elements near the main diagonal.

In an n by n real symmetric band matrix B,

$$b_{ij} = b_{ji} \quad \text{for all } i \text{ and } j$$

and

$$b_{ij} = 0 \quad \text{for} \quad (i - j) > k \quad \text{or} \quad (j - i) > k$$

where k is the lower or upper bandwidth. For example, matrix B, shown in (1–24), is a real symmetric band matrix:

$$B = \begin{bmatrix} 2.0 & 3.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 3.0 & 3.0 & -4.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & -4.0 & 4.0 & 5.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 5.0 & 5.0 & -6.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & -6.0 & 6.0 & 7.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 7.0 & 7.0 & -8.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -8.0 & 8.0 \end{bmatrix} \qquad (1–24)$$

A complex Hermitian band matrix is a square complex band matrix that is equal to its conjugate transpose. It has all its nonzero elements near the main diagonal, but, in general, it is not symmetric. The imaginary part of each of the diagonal elements is 0.

For example, matrix H shown in (1–25) is a complex Hermitian band matrix:

$$H = \begin{bmatrix} (2,0) & (3,1) & (0,0) & (0,0) & (0,0) \\ (3,-1) & (3,0) & (-4,1) & (0,0) & (0,0) \\ (0,0) & (-4,-1) & (4,0) & (5,-1) & (0,0) \\ (0,0) & (0,0) & (5,1) & (5,0) & (-6,1) \\ (0,0) & (0,0) & (0,0) & (-6,-1) & (6,0) \end{bmatrix} \qquad (1–25)$$

1.3.4.11 Storage of Real Symmetric Band Matrices or Complex Hermitian Band Matrices

When stored in band storage mode, an n by n real symmetric or complex Hermitian band matrix with k subdiagonals and k superdiagonals is stored in a two-dimensional $(k+1)$ by n array. Either the upper-triangular band part or the lower-triangular band part of the matrix can be stored.

When the upper-triangle storage mode is used, the nonzero elements of the upper-triangular part of the jth column of the matrix are stored in the jth column of the array. The main diagonal of the matrix is stored in row $(k+1)$ of the array. The first superdiagonal is stored in row k, starting at column 2, and so on. Elements of the array that do not correspond to elements in the band matrix, specifically those in the top left k by k triangle, are not referenced.

As an example, a 6 by 6 real symmetric band matrix A is shown in (1–26). The matrix A has two superdiagonals and two subdiagonals.

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & 0 & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & 0 \\ 0 & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ 0 & 0 & a_{53} & a_{54} & a_{55} & a_{56} \\ 0 & 0 & 0 & a_{64} & a_{65} & a_{66} \end{bmatrix} \qquad (1\text{–}26)$$

The matrix A would be stored in upper-triangle storage mode in array ABD as shown in (1–27):

$$\mathrm{ABD} = \begin{bmatrix} * & * & a_{13} & a_{24} & a_{35} & a_{46} \\ * & a_{12} & a_{23} & a_{34} & a_{45} & a_{56} \\ a_{11} & a_{22} & a_{33} & a_{44} & a_{55} & a_{66} \end{bmatrix} \qquad (1\text{–}27)$$

In this storage scheme, the nonzero element in the ijth position of the upper triangular part of the symmetric band matrix is stored in position (m, j) of the array, where:

$$m = (i - j + k + 1), \quad \max(1,\ j-k) \le i \le j \quad \text{and} \quad 1 \le j \le n$$

The following Fortran program segment transfers the upper-triangular part of a symmetric band matrix from conventional Fortran full matrix storage in A to band storage in array ABD:

```
      DO 20 J=1,N
         M=K+1-J
         DO 10 I=MAX(1,J-K),J
            ABD(M+I,J)=A(I,J)
10       CONTINUE
20    CONTINUE
```

When the lower-triangle storage mode is used, the nonzero elements of the lower-triangular part of the jth column of the matrix are stored in the jth column of the array. The main diagonal of the matrix is stored in row 1 of the array. The first subdiagonal is stored in row 2 starting at column 1, and so on. Elements of the array that do not correspond to elements in the band matrix, specifically those in the bottom right k by k triangle, are not referenced.

As an example, consider the 7 by 7 real symmetric band matrix A, with two superdiagonals and two subdiagonals shown in (1–28):

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & 0 & 0 & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & 0 & 0 \\ 0 & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} & 0 \\ 0 & 0 & a_{53} & a_{54} & a_{55} & a_{56} & a_{57} \\ 0 & 0 & 0 & a_{64} & a_{65} & a_{66} & a_{67} \\ 0 & 0 & 0 & 0 & a_{75} & a_{76} & a_{77} \end{bmatrix} \quad (1\text{–}28)$$

The matrix A would be stored in array ABD in lower-triangle storage mode as shown in (1–29):

$$\text{ABD} = \begin{bmatrix} a_{11} & a_{22} & a_{33} & a_{44} & a_{55} & a_{66} & a_{77} \\ a_{21} & a_{32} & a_{43} & a_{54} & a_{65} & a_{76} & * \\ a_{31} & a_{42} & a_{53} & a_{64} & a_{75} & * & * \end{bmatrix} \quad (1\text{–}29)$$

In this storage scheme, the nonzero element in the ijth position of the lower-triangular part of the symmetric band matrix is stored in position (m, j) of the array, where:

$$m = (i - j + 1), \quad j \leq i \leq \min(n,\ j + k) \ \text{ and } \ 1 \leq j \leq n$$

The following Fortran program segment transfers the lower-triangular part of a symmetric band matrix A from conventional Fortran full matrix storage to band storage in array ABD:

```
      DO 20 J=1,N
         M=1-J
         DO 10 I=J,MIN(N,J+K)
            ABD(M+I,J)=A(I,J)
10       CONTINUE
20    CONTINUE
```

For a complex Hermitian band matrix, the imaginary parts of the main diagonal are by definition, 0. Therefore, the imaginary parts of the corresponding array elements need not be set, and are assumed to be 0.

1.3.4.12 Upper- and Lower-Triangular Band Matrices

A triangular band matrix is a square matrix whose nonzero elements are all near the main diagonal and are in either the upper-triangular part of the matrix or the lower-triangular part of the matrix.

In an n by n upper-triangular band matrix U,

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

and

$$u_{ij} = 0 \ \text{ for } \ (j - i) > ku$$

where ku is the upper bandwidth.

The matrix U shown in (1–30) is a 4 by 4 upper-triangular band matrix:

$$U = \begin{bmatrix} 1.0 & 2.0 & 0.0 & 0.0 \\ 0.0 & 3.0 & 4.0 & 0.0 \\ 0.0 & 0.0 & 5.0 & 6.0 \\ 0.0 & 0.0 & 0.0 & 7.0 \end{bmatrix} \quad (1\text{–}30)$$

In an n by n lower-triangular band matrix L,

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

and

$$l_{ij} = 0 \quad \text{for} \quad (i - j) > kl$$

where kl is the lower bandwidth.

The matrix L shown in (1–31) is a 4 by 4 lower-triangular band matrix:

$$L = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 \\ 2.0 & 3.0 & 0.0 & 0.0 \\ 0.0 & 4.0 & 5.0 & 0.0 \\ 0.0 & 0.0 & 6.0 & 7.0 \end{bmatrix} \tag{1–31}$$

1.3.4.13 Storage of Upper- and Lower-Triangular Band Matrices

Similar to the case of real symmetric band matrices and complex Hermitian band matrices, upper- and lower-triangular band matrices can also be stored in band storage mode.

Upper-triangle storage mode is used for an upper-triangular band matrix. An n by n upper-triangular band matrix with k superdiagonals is stored in a two-dimensional $(k + 1)$ by n array.

When upper-triangle storage mode is used, the nonzero elements of the upper-triangular part of the jth column of the matrix are stored in the jth column of the array. The main diagonal of the matrix is stored in row $(k + 1)$ of the array. The first superdiagonal is stored in row k starting at column 2; and so on. Elements of the array that do not correspond to elements in the band matrix, specifically those in the top left k by k triangle, are not referenced.

As an example, a 6 by 6 upper-triangular band matrix A is shown in (1–32). The matrix A has two superdiagonals.

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 & 0 & 0 \\ 0 & a_{22} & a_{23} & a_{24} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} & a_{35} & 0 \\ 0 & 0 & 0 & a_{44} & a_{45} & a_{46} \\ 0 & 0 & 0 & 0 & a_{55} & a_{56} \\ 0 & 0 & 0 & 0 & 0 & a_{66} \end{bmatrix} \tag{1–32}$$

The matrix A would be stored in upper-triangle storage mode in array ABD as shown in (1–33):

$$\text{ABD} = \begin{bmatrix} * & * & a_{13} & a_{24} & a_{35} & a_{46} \\ * & a_{12} & a_{23} & a_{34} & a_{45} & a_{56} \\ a_{11} & a_{22} & a_{33} & a_{44} & a_{55} & a_{66} \end{bmatrix} \tag{1–33}$$

In this storage scheme, the nonzero element in the ijth position of the upper triangular part of the upper-triangular band matrix is stored in position (m, j) of the array, where:

$$m = (i - j + k + 1), \quad \max(1,\ j - k) \le i \le j \quad \text{and} \quad 1 \le j \le n$$

The following Fortran program segment transfers the upper-triangular part of an upper-triangular band matrix from conventional Fortran full matrix storage in A to band storage in array ABD:

```
      DO 20 J=1,N
         M=K+1-J
         DO 10 I=MAX(1,J-K),J
            ABD(M+I,J)=A(I,J)
10       CONTINUE
20    CONTINUE
```

Lower-triangle storage mode is used for a lower-triangular band matrix. An n by n lower-triangular band matrix with k subdiagonals is stored in a two-dimensional $(k+1)$ by n array.

When lower-triangle storage mode is used, the nonzero elements of the lower-triangular part of the jth column of the matrix are stored in the jth column of the array. The main diagonal of the matrix is stored in row 1 of the array; the first subdiagonal in row 2 starting at column 1; and so on. Elements of the array that do not correspond to elements in the band matrix, specifically those in the bottom right k by k triangle, are not referenced.

As an example, consider the 7 by 7 lower-triangular band matrix A, with two subdiagonals, shown in (1–34):

$$A = \begin{bmatrix} a_{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 & 0 & 0 & 0 \\ a_{31} & a_{32} & a_{33} & 0 & 0 & 0 & 0 \\ 0 & a_{42} & a_{43} & a_{44} & 0 & 0 & 0 \\ 0 & 0 & a_{53} & a_{54} & a_{55} & 0 & 0 \\ 0 & 0 & 0 & a_{64} & a_{65} & a_{66} & 0 \\ 0 & 0 & 0 & 0 & a_{75} & a_{76} & a_{77} \end{bmatrix} \quad (1\text{–}34)$$

The matrix A would be stored in array ABD in lower-triangle storage mode as shown in (1–35):

$$\text{ABD} = \begin{bmatrix} a_{11} & a_{22} & a_{33} & a_{44} & a_{55} & a_{66} & a_{77} \\ a_{21} & a_{32} & a_{43} & a_{54} & a_{65} & a_{76} & * \\ a_{31} & a_{42} & a_{53} & a_{64} & a_{75} & * & * \end{bmatrix} \quad (1\text{–}35)$$

In this storage scheme, the nonzero element in the ijth position of the lower-triangular part of the lower-triangular band matrix is stored in position (m, j) of the array, where:

$$m = (i - j + 1), \quad j \le i \le \min(n,\ j + k) \ \text{ and } \ 1 \le j \le n$$

The following Fortran program segment transfers the lower-triangular part of a lower-triangular band matrix A from conventional Fortran full matrix storage to band storage in array ABD:

```
      DO 20 J=1,N
         M=1-J
         DO 10 I=J,MIN(N,J+K)
            ABD(M+I,J)=A(I,J)
10       CONTINUE
20    CONTINUE
```

2
Coding an Application Program

This chapter provides information that you need to know as you code your application program.

2.1 Selecting the Appropriate Data Type

CXML supports integer data, single-precision real, double-precision real, single-precision complex, and double-precision complex data. For each datatype, CXML provides a corresponding version of each of its subprograms. The type of data your program uses determines which version of a subprogram that you should use. When coding your program, you must use the CXML subprogram that operates on the type of data your program is using.

CXML uses a naming convention for subprograms that identifies the type of data that it can use. This is discussed in detail in the Preface, in *Using the Reference Sections*.

2.2 Data Structure and Storage Methods

CXML subprograms operate on vectors and matrices. For the subprograms that operate on matrices, different kinds of matrices use different storage schemes. When you use a CXML subprogram, consider the type of matrix used in your application and the data structure used to store it.

General information about data structure and storage methods for CXML is provided in Chapter 1. Vectors are discussed in Section 1.3.3. Matrices are discussed in Section 1.3.4. Information about data structure and storage methods that pertains to a specific group of subprograms is included with the discussion of that group.

The storage methods described in Chapter 1 apply to Fortran and other languages that store arrays in column-major order. See Section 2.6 for techniques to use for languages that store arrays in row-major order.

2.3 Improving Performance

You have several options for improving the performance of your application:

- Use higher level BLAS subprograms where applicable. For example, use a Level 3 BLAS subprogram rather than a sequence of calls to Level 2 BLAS subprograms.
- Use subprograms that perform more than one computation rather than subprograms that perform a single computation.
- Use an increment or stride of 1. Performance is better if the elements of a vector are stored close to each other.

- In a few cases, the difference between two subprograms is that one performs scaling. Since performance is better when no scaling is done, use the subprogram without scaling whenever possible.

2.4 Calling Sequences

Each of the CXML subprograms has a specific calling sequence. The calling sequences for each subprogram are described in this manual.

These descriptions specify the correct syntax for the argument list; whether an argument is an input argument, an output argument, or both; required numerical values for arguments; and specific actions that might be taken by the subprogram.

Each subprogram is described using a structured format:

Name
Overview
Format
Function Value (if applicable)
Arguments
Description
Example

The **Arguments** section provides detailed information about each subprogram argument, such as the argument name, the Fortran data type, the information the argument passes to or returns from the subprogram, and the acceptable values of the argument. All arguments in the calling sequences are required arguments.

The terms *On entry* and *On exit* are used in each argument description to show whether the argument is an input argument, an output argument, or both:

- An input argument has a value on entry and is unchanged on exit.
  An input argument passes information from the application program to the subprogram.
- An output argument has no value on entry and is overwritten on exit.
  An output argument passes information from the subprogram back to the application program.
- An argument that is used for both input and output has a value on entry that is overwritten on exit by the output value. An argument used for both input and output passes information both to the subprogram and back to the application program. If you want to keep the input data, save it before calling the subprogram.

To avoid errors and the possible termination of a program's execution, be sure input data is of the correct type. Do not mix single-precision data and double-precision data. Also, character values must be one of the allowed characters and numeric values have to be within the specified range.

2.4.1 Passing of Arguments

In Fortran, a character argument can be longer than its corresponding dummy argument. For example, some BLAS subroutines have the arguments with the data type CHARACTER*1. One such argument is the **trans** argument, which is used to select the form of the input matrix. The value 'T' can be passed as 'TRANSPOSE'.

Some signal processing subroutines have arguments with the data type CHARACTER*(*). For example, the value 'F' for the argument **direction** can be passed as 'FORWARD'.

2.4.2 Implicit and Explicit Arguments

Arguments can be coded either implicitly or explicitly. For example, consider the Level 3 subprogram SSYMM. The following programs are equivalent.

```
REAL*4 A(20,20), B(30,40), C(30,50), ALPHA, BETA
SIDE = 'L'
UPLO = 'U'
M = 10
N = 20
ALPHA = 2.0
BETA = 3.0
LDA = 20
LDB = 30
LDC = 30
CALL SSYMM(SIDE,UPLO,M,N,ALPHA,A,LDA,B,LDB,BETA,C,LDC)
```

```
REAL*4 A(20,20), B(30,40), C(30,50)
CALL SSYMM('L','U',10,20,2.0,A,20,B,30,3.0,C,30)
```

2.4.3 Expanding Argument Lists

CXML provides the ability to expand the argument lists of each CXML subprogram from within some text editors. This capability is convenient when creating or modifying code that frequently calls CXML subprograms.

EMACS Editor

If your system has an EMACS editor available, you can access this capability to expand the parameter list of a subroutine. Do this as follows:

1. At the EMACS command line, load one of the following files:

   OpenVMS Alpha - `SYS$LIBRARY:DXML$EMACS.ML`
   Tru64 UNIX - `/usr/share/dxml.ml`
   Windows NT - `directory-spec/dxml.ml`

2. Enter ABBREV mode.
3. Enter the subroutine name and then press the SPACE bar.

Note that on Windows NT systems, the *directory-spec* will vary according to the directory specified at installation time.

TPU Editors: EVE and LSE

If you are using an OpenVMS system, you can also use a TPU editor to expand the parameter list of a subroutine. Do this as follows:

1. Invoke the TPU editor at the DCL command line with either of the following commands, depending upon whether you are using EVE or LSE:

   ```
   $ EDIT/TPU/COMMAND=SYS$LIBRARY:DXML$EVE.TPU filename
   ```

   ```
   $ LSEDIT/COMMAND=SYS$LIBRARY:DXML$EVE.TPU filename
   ```

   You will still be able to expand the components of the language you are using.

2. In the editor, type the subroutine name and then press Ctrl/E.

If you prefer, you can edit the TPU file to change the key that expands the argument list.

2.5 Calling Subroutines and Functions in Fortran

A few CXML subprograms return a scalar. These subprograms are functions, and they are called as functions by coding a function reference. First, declare the data type of the returned value and the subprogram name, and then code the function reference, as shown in the following generic example:

```
INTEGER*4 function_value, subprogram_name
function_value = subprogram_name (argument_1,argument_2, . . .  ,argument_n)
```

For example, the Level 1 BLAS subprogram ISAMAX returns the index of the element of vector x having the largest absolute value:

```
   .
   .
   .
INTEGER*4 IAMAX, ISAMAX
   .
   .
   .
IAMAX=ISAMAX(N,X,INCX)
```

For the signal processing routines, the declaration of function type is done by including either "dxmldef.h" or "DXMLDEF.FOR" in your code. All arguments of function subprograms are input arguments, which are unchanged on exit. The value is returned to the function value.

Most subprograms return a vector or a matrix. These subprograms are subroutines and they are called as subroutines with a CALL statement.

```
CALL subroutine_name (argument_1,argument_2, . . .  ,argument_n)
```

For example, the call statement for the subroutine SSET looks like the following:

```
CALL SSET(N,A,X,INCX)
```

Each subroutine has an output argument that is overwritten on exit and contains the output information.

2.5.1 Fortran Program Example

The following is an example of a Fortran program that makes a call to SAXPY:

```
integer n,incx,incy
real x(5),y(5),alpha

DATA  x /2.0,4.0,6.0,8.0,10.0/
DATA  y /5*1.0/
incx = 1
incy = 1
alpha = 2.0
n = 5

call saxpy (n,alpha,x,incx,y,incy)

write (6,*) y

stop
end
```

2.6 Using CXML from Non-Fortran Programming Languages

If your application involves only one-dimensional arrays (for example, one-dimensional FFTs), call CXML routines as described in the calling standard. However, two-dimensional (and higher) arrays are not covered by most calling standards. High-level languages have different ways of storing the elements of a two-dimensional matrix in a two-dimensional array.

CXML requires that arrays be stored in column-major order the way Fortran does. If you are writing applications in languages such as ADA or C, and you want to call CXML routines, you must consider how to ensure that array data is passed and processed correctly to obtain the highest performance.

The most direct and least error-prone method of calling CXML routines from another language, is to write a matrix transpose routine in that language, and to use transposed (column-stored) matrices in calls to CXML routines. The application program can subsequently transpose the results of calls to CXML when appropriate, to return to the row-major format of the calling language.

In some cases, using matrix identities is a shortcut, at a small cost in program complexity, as shown in the following two cases of the same operation (to compute the row-stored product of two matrices):

A and B are n by n matrices, stored in row-major order. To compute their product, $C = AB$:

1. Transpose A. Store it in the array AT.
2. Transpose B. Store it in the array BT.
3. Invoke the matrix-multiply routine to compute $D = AB$, column-stored.

   ```
   CALL SGEMM('N','N',N,N,N,1.0,AT,N,BT,N,0.0,D,N)
   ```

4. Transpose D to get C, the row-stored version of the result.

The shortcut uses the matrix identity, as in (2–1):

$$(B^T A^T)^T = AB \tag{2–1}$$

From a Fortran point of view, row-major storage of the matrices A and B is simply the matrices A^T and B^T. Therefore, the same row-major product can be computed using the following procedure:

1. Invoke the matrix-multiply routine.

```
SGEMM('N','N',N,N,N,1.0,B,N,A,N,0.0,C,N)
```

This routine computes $B^T A^T$, column-stored, that is $C = (B^T A^T)^T = AB$, the row-stored result.

A third way to achieve the same product is somewhat slower because of the way memory is accessed:

1. Invoke the matrix-multiply routine to compute $(A^T)^T(B^T)^T$, column-stored, that is $D = C^T$.

```
SGEMM('T','T',N,N,N,1.0,A,N,B,N,0.0,D,N)
```

2. Transpose D to get C, the row-stored version of the result.

2.6.1 Calling CXML from C Programs

In addition to the differences in storage of multi-dimensional arrays between Fortran and C, the following changes may also be required for a C program that calls CXML subroutines.

- In Fortran, a two-dimensional array declared as:

  ```
  DOUBLE PRECISION A(LDA,N)
  ```

  is a contiguous piece of LDA $\times$ N double precision words in memory stored in a column major order. However, a similar declaration in C:

  ```
  double A[LDA][N]);
  ```

  is LDA pointers to rows of length N. As these pointers can be anywhere, there is no guarantee that the rows of the array are contiguous. To interface a C program with a CXML routine that expects the memory locations to be contiguous, the array A should be declared as

  ```
  double A[LDA*N];
  ```

  or allocated as contiguous memory locations using `malloc`.

- On Tru64 UNIX, you must append an underscore at the end of each subroutine or function subprogram name.

2.6.2 C Program Example

The following example works on the Compaq Tru64 UNIX platform, but can be modified for other platforms. It illustrates the calculation of a matrix-vector product using the CXML routine DGEMV. The matrix is stored using the row-major storage of C. The column-major storage of the CXML Fortran routine is implicitly taken into account by calculating $A^T * x$, instead of $A * x$.

```
#include <stdio.h>
#include <stdlib.h>

#define dgemv dgemv_
#define max_size  10

extern void dgemv(char *, int *, int*, double *,
    double [], int *, double[], int *, double *,
    double[], int *);
```

```
int main()
{
    double *a, *b, *x;
    double alpha, beta;

    int length, lda, incx, i, j;

    length = 3;
    lda = max_size;
    incx = 1;

    alpha = 1.0;
    beta = 0.0;

    a = (double *)malloc(max_size*max_size*sizeof(double));
    b = (double *)malloc(max_size*sizeof(double));
    x = (double *)malloc(max_size*sizeof(double));

    for (i=0; i<length; i++)
    {
        for (j=0; j<length; j++)
            a[max_size*i+j] = (double)(2*i+j);
        x[i] = 1.0;
    }

    printf("  matrix:\n");
    for (i=0; i<length; i++)
    {
        for (j=0; j<length; j++)
            printf("   %6.2f  ", a[i*max_size+j]);
        printf("\n");
    }

    printf("\n  vector:\n");
    for (j=0; j<length; j++)
        printf("   %6.2f  \n", x[j]);

    dgemv("T", &length, &length, &alpha, a, &lda, x, &incx,
          &beta, b, &incx);

    printf("\n  matrix times vector: \n");
    for (i = 0; i < length; i++)
        printf ("    %.2f\n",b[i]);

    free (a);
    free (b);
    free (x);

}  /* end of main() */
```

Additional examples illustrating the use of CXML routines from a C program can be found online in the examples directory that is created when CXML is installed. The location of this directory depends upon your operating system. For instance, on a Tru64 UNIX system, the online examples are located in /usr/examples/dxml.

2.7 Error Handling

Some errors are common to all portions of the CXML library. Other errors are unique to a particular library within CXML. This section describes general information about how errors are handled. See the appropriate chapters for more details about error handling for specific subprograms.

2.7.1 Internal Exceptions

Under certain extreme conditions, such as passing numbers on the verge of underflow or overflow, you can receive an internal exception error message. If this happens, you should check arguments for valid range.

When underflow occurs, the number is replaced by a zero, and execution continues. No error message is provided.

When overflow occurs, execution terminates and you receive a message directed to the devices or files that are defined as: *stdout* and *stderr* on Tru64 UNIX or Windows NT, and SYS$OUTPUT and SYS$ERROR on OpenVMS. Check the subprogram arguments for valid range.

Internal exceptions also occur if you have a shorter array than that specified by a data length argument. In this case, you receive an error message, since you are trying to address a location outside the bounds of the array. Check the length of the arrays used, or the value denoting the length of the arrays.

3 Compiling and Linking an Application Program

This chapter discusses compiling and linking an application program with CXML. This process is somewhat different for each platform, so each is discussed in a separate section. Please refer to the section appropriate for your platform.

3.1 Tru64 UNIX Platform

Compiling and linking your application program with CXML on the Tru64 UNIX platform is usually performed by a single command:

- the `f77` command for Fortran 77
- the `f90` command for Fortran 90
- the `cc` command for C

You can take advantage of the DEC C compilation environment by using the `-migrate` compilation flag, as shown in the examples in this chapter.

3.1.1 CXML Libraries

The CXML kit for Tru64 UNIX contains three libraries:

- Serial shared - called libdxml.so - normally installed at /usr/shlib/
- Parallel shared - called libdxmlp.so - normally installed at /usr/shlib/
- Serial archive - called libdxml.a - normally installed at /usr/lib/

The serial and the parallel shared libraries each contain a complete set of CXML routines; routine names are identical in these libraries. In the parallel library some of the core routines are parallelized to take advantage of additional CPUs in shared memory configurations (SMP). See Section A.1.2 for a complete list of CXML routines that have been parallelized.

The following sections show how to compile and link an application program to each of the CXML libraries. For more details about compiling and linking your application, see the reference pages of `f77`, `f90`, and `cc`.

3.1.2 Compiling and Linking to the Serial Library

The following examples show how to compile and link to the serial shared library.

Fortran examples:

```
f77 program.f -ldxml
```

```
f90 program.f90 -ldxml
```

C example:

```
cc -migrate program.c -ldxml
```

3.1.3 Compiling and Linking to the Parallel Library

The following examples show how to compile and link to the parallel shared library.

Fortran examples:

```
f77 program.f -ldxmlp
```

```
f90 program.f90 -ldxmlp
```

C example:

```
cc -migrate program.c -ldxmlp
```

The following Fortran 90 example shows how to compile and link to the parallel static (non-shared) library.

```
f90 program.f90 -non_shared -ldxmlp -omp
```

3.1.4 Compiling and Linking to the Archive Library

The following examples show how to compile and link to the archive library.

Fortran examples:

```
f77 program.f /usr/lib/libdxml.a
```

```
f90 program.f90 /usr/lib/libdxml.a
```

C example:

```
cc -migrate program.c /usr/lib/libdxml.a  -lfor -lm
```

3.2 Windows NT Platform

Compiling and linking your program on the Windows NT platform can be performed either by using the Developer Studio, or by using the command console. This section discusses both methods.

3.2.1 CXML Libraries

The CXML kit for Windows NT contains a shared library and an object serial library:

- the serial shared library name ends with `dll.dll`
- the serial object library name ends with `.lib`

3.2.2 Using the Libraries from the Command Console

This section discusses discuss how to compile and link your program using the command console. Please note that it is assumed that the environment variables required by the CXML have already been set. Refer to Section B.1 "Setting Environment Variables" for information about doing this.

To compile/link and run your Fortran 77 application from the command console (MS/DOS prompt), use the following commands:

```
DF MAIN.FOR %LINK_F90%
MAIN
```

To compile and link your Fortran 90 application from the command console (MS/DOS prompt), use the following commands:

```
DF MAIN.F90 %LINK_F90%
MAIN
```

Fortran 77 programs have the .FOR filename extension and Fortran 90 programs have the .F90 filename extension.

3.2.3 Using the Libraries from Developer Studio

This section discusses discuss how to compile and link your program using the Developer Studio.

During the installation, the paths to the location of the object libraries and include files are automatically defined. However, before attempting to build an application that accesses the libraries, the names of the libraries must be specified for the linker. You can do this by performing the following steps:

1. Start the Developer Studio.
2. If you have not already defined a Project Workspace for your application, you must do so before proceeding. If you have defined a Project Workspace, open it by selecting "Open Workspace..." from the File pull-down menu.
3. Bring up the Project Settings dialog box by selecting "Settings..." from the Project pull-down menu.
4. Click on the "Link" tab.
5. From the Category pull-down menu, select "Input".
6. Add the names of the CXML libraries. under "Object/Library Modules" (separated by spaces).
7. Click on "OK" to exit the dialog and save the settings.

The Microsoft Developer Studio is now set up to use the CXML libraries. For further information about compiling and linking with Developer Studio, refer to the "Building Programs and Libraries" section of the *Compaq Visual Fortran* online documentation.

3.3 OpenVMS Alpha Platform

This section discusses compiling and linking on the OpenVMS Alpha platform.

3.3.1 Compiling

The OpenVMS Alpha platform provides 2 formats: IEEE Standard floating point format and VAX floating point format. The IEEE format has single precision (S) and double precision (T) floating point numbers. The VAX format has single precision (F) and double precision (G) floating point numbers.

When you compile your program, you must specify that floating point numbers are in either IEEE float or VAX float.

VAX float is the default. If you want to compile for IEEE, you must specify `/float=IEEE_floating`. Be sure to compile your program for the format that is appropriate for your application.

After you compile your application program, you need to link it to the corresponding CXML image library. The next section discusses this topic.

3.3.2 CXML Image Libraries

As mentioned in the previous section, CXML supports two different families of floating point data formats for the OpenVMS Alpha platform, IEEE and VAX.

An image library is provided for each format - one compiled for IEEE, and one for VAX. These two libraries come as "shared", rather than "object", libraries.

These libraries are:

SYS$SHARE:DXML$IMAGELIB_GS	for G_floating format
SYS$SHARE:DXML$IMAGELIB_TS	for IEEE format

Each of these libraries contain the shareable images for all of the CXML components. Only one of these libraries is the default library. You can specify the default library at installation time.

Before linking, you should find out which library has been identified as the default - you will need to know this when you link.

Use the following command to display the name of the default library:

```
$ SHOW LOGICAL LNK$LIBRARY*
```

3.3.3 Linking to a CXML Library

As discussed in the previous section, a CXML shared library is provided for both IEEE and VAX floating point formats. Entrynames are independent of format, so when you link your program it can be linked with either the IEEE or VAX version of the CXML library. However, you must link your compiled program with the CXML image library that matches the format you used when you compiled the program. If the default library is not the correct one, you need to link to the correct one by explicitly naming the image library, or by invoking a command procedure that changes the default to the correct library. This is discussed in the following sections.

Using the default library

If you are linking your program with the default library, you do not have to specify an image library. For example, if the image library for G_floating data is the default and you want to link to it, you would issue the LINK command as follows:

```
$ LINK MY_FILE
```

Using another library

If you want to use a library other than the default, you can specify it in the LINK command. In OpenVMS Alpha, for example, if the default is the G_floating data type, and you want to use the IEEE floating point library, you would issue the following command:

```
$ LINK MY_FILE, SYS$SHARE:DXML$IMAGELIB_TS/LIB
```

Changing the default library

You can identify another library as the default for the current process by invoking the DXML$SET_LIB command procedure, which is provided by CXML.

The following example changes the current default library to the one for IEEE data format:

```
$ @SYS$SHARE:DXML$SET_LIB TS
```

If you usually link to a library other than the system's default, it is recommended that you invoke the command procedure within your login command procedure.

3.3.4 Linking Errors

If you compile your program for one type of data (IEEE, for example), and you do not link the compiled program to the corresponding image library (IEEE, in this case), *you will not get an error message - however, your results will be incorrect*.

Part 2—Using CXML Subprograms

This section discusses what you need to know to use CXML subroutines and functions.

The following groups of subprograms are discussed:

- Chapter 4 describes how to use the Level 1 BLAS subprograms and extensions.
- Chapter 5 describes how to use the Sparse Level 1 BLAS subprograms.
- Chapter 6 describes how to use the Level 2 BLAS subprograms.
- Chapter 7 describes how to use the Level 3 BLAS subprograms.
- Chapter 8 provides an overview of the LAPACK library of subroutines.
- Chapter 9 describes how to use the signal processing subprograms.
- Chapter 10 describes how to use the Iterative Solvers for Sparse Linear Systems.
- Chapter 11 describes how to use Direct Sparse Solvers.
- Chapter 12 describes how to use the VLIB subprograms.
- Chapter 13 describes how to use the random number generator subprograms.
- Chapter 14 describes how to use the sort subprograms.
- Chapter 15 describes how to use the Sciport subprograms.

4 Using the Level 1 BLAS Subprograms and Extensions

The Level 1 BLAS (Basic Linear Algebra Subprograms) Subprograms and Extensions to the Level 1 BLAS subprograms perform vector-vector operations commonly occurring in many computational problems in linear algebra. This chapter provides information about the following topics:

- Operations performed by the Level 1 BLAS subprograms and their Extensions (Section 4.1)
- Vector storage (Section 4.2)
- Subprogram naming conventions (Section 4.3)
- Subprogram summaries (Section 4.4)
- Calling Level 1 BLAS subprograms (Section 4.5)
- Arguments and definitions used in the subprograms (Sections 4.6 and 4.8)
- Error handling (Section 4.7)
- A look at a Level 1 Extensions subprogram and its use (Section 4.9)

4.1 Level 1 BLAS Operations

BLAS Level 1 operations work with vectors. The Level 1 BLAS subprograms and the Extensions usually operate on only one vector, but a few of the subprograms involve operations on two vectors. The subprograms can be classified into two types:

- Vector output is returned from a vector input.
  The results of these operations are independent of the order in which the elements of the vector are processed.
- Scalar output is returned from a vector input.
  The results of these reduction operations usually depend on the order in which the elements of the vector are processed.

4.2 Vector Storage

For the Level 1 BLAS and the Extensions subprograms, a vector is stored in a one-dimensional array.

For general information about how CXML stores data, refer to Section 1.3. Arrays are discussed in Section 1.3.1. For specific information about vector storage, refer to Section 1.3.3.

4.3 Naming Conventions

Table 4–1 shows the characters used in the names of the Level 1 BLAS and the Extensions and what the characters mean.

Table 4–1 Naming Conventions: Level 1 BLAS Subprograms

Character Group	Mnemonic	Length	Meaning
First group	I	1	Computes the index of a particular vector element.
	No mnemonic	0	Computes the value of a particular vector element or performs an operation on one or more vectors.
Second group	S	1	Single-precision real data.
	D	1	Double-precision real data.
	C	1	Single-precision complex data.
	Z	1	Double-precision complex data.
Third group	A combination of letters at the end such as AMIN or AXPY		Type of computation such as Absolute (A) Minimum (MIN) or Scalar (A) Times a Vector (X) Plus (P) a Vector (Y).

For example, the name ICAMIN is the subprogram for computing the index of the element of a single-precision complex vector having the minimum absolute value.

4.4 Summary of Level 1 BLAS Subprograms

Tables 4–2 and 4–3 summarize the BLAS Level 1 subprograms and the extension subprograms.

Table 4–2 Summary of Level 1 BLAS Subprograms

Subprogram Name	Operation
ISAMAX	Calculates, in single-precision arithmetic, the index of the element of a real vector with maximum absolute value.
IDAMAX	Calculates, in double-precision arithmetic, the index of the element of a real vector with maximum absolute value.
ICAMAX	Calculates, in single-precision arithmetic, the index of the element of a complex vector with maximum absolute value.
IZAMAX	Calculates, in double-precision arithmetic, the index of the element of a complex vector with maximum absolute value.
SASUM	Calculates, in single-precision arithmetic, the sum of the absolute values of the elements of a real vector.

(continued on next page)

Table 4–2 (Cont.) Summary of Level 1 BLAS Subprograms

Subprogram Name	Operation
DASUM	Calculates, in double-precision arithmetic, the sum of the absolute values of the elements of a real vector.
SCASUM	Calculates, in single-precision arithmetic, the sum of the absolute values of the elements of a complex vector.
DZASUM	Calculates, in double-precision arithmetic, the sum of the absolute values of the elements of a complex vector.
SAXPY	Calculates, in single-precision arithmetic, the product of a real scalar and a real vector and adds the result to a real vector.
DAXPY	Calculates, in double-precision arithmetic, the product of a real scalar and a real vector and adds the result to a real vector.
CAXPY	Calculates, in single-precision arithmetic, the product of a complex scalar and a complex vector and adds the result to a complex vector.
ZAXPY	Calculates, in double-precision arithmetic, the product of a complex scalar and a complex vector and adds the result to a complex vector.
SCOPY	Copies a real, single-precision vector.
DCOPY	Copies a real, double-precision vector.
CCOPY	Copies a complex, single-precision vector.
ZCOPY	Copies a complex, double-precision vector.
SDOT	Calculates the inner product of two real, single-precision vectors.
DDOT	Calculates the inner product of two real, double-precision vectors.
DSDOT	Calculates the inner product of two real, single-precision vectors using double precision arithmetic operations and returns a double-precision result.
CDOTC	Calculates the conjugated inner product of two complex, single-precision vectors.
ZDOTC	Calculates the conjugated inner product of two complex, double-precision vectors.
CDOTU	Calculates the unconjugated inner product of two complex, single-precision vectors.
ZDOTU	Calculates the unconjugated inner product of two complex, double-precision vectors.
SDSDOT	Calculates the inner product of two real, single-precision vectors using double-precision arithmetic operations, adds the inner product result to a real single-precision scalar, and returns a single-precision value.
SNRM2	Calculates, in single-precision arithmetic, the square root of the sum of the squares of the elements of a real vector.
DNRM2	Calculates, in double-precision arithmetic, the square root of the sum of the squares of the elements of a real vector.

(continued on next page)

Table 4–2 (Cont.) Summary of Level 1 BLAS Subprograms

Subprogram Name	Operation
SCNRM2	Calculates, in single-precision arithmetic, the square root of the sum of the squares of the elements of a complex vector.
DZNRM2	Calculates, in double-precision arithmetic, the square root of the sum of the squares of the elements of a complex vector.
SROT	Applies a real Givens plane rotation to two real, single-precision vectors.
DROT	Applies a real Givens plane rotation to two real, double-precision vectors.
CROT	Applies a complex Givens plane rotation to two single-precision complex vectors.
ZROT	Applies a complex Givens plane rotation to two double-precision complex vectors.
CSROT	Applies a real Givens plane rotation to two complex, single-precision vectors.
ZDROT	Applies a real Givens plane rotation to two complex, double-precision vectors.
SROTM	Applies a modified Givens transformation to two real, single-precision vectors.
DROTM	Applies a modified Givens transformation to two real, double-precision vectors.
SROTG	Generates the real elements for a real, single-precision Givens plane rotation.
DROTG	Generates the elements for a real, double-precision Givens plane rotation.
CROTG	Generates the elements for a complex, single-precision Givens plane rotation.
ZROTG	Generates the real elements for a complex, double-precision Givens plane rotation.
SROTMG	Generates the real elements for a real, single-precision Givens transform.
DROTMG	Generates the real elements for a real, double-precision Givens transform.
SSCAL	Calculates, in single-precision arithmetic, the product of a real scalar and a real vector.
DSCAL	Calculates, in double-precision arithmetic, the product of a real scalar and a real vector.
CSCAL	Calculates, in single-precision arithmetic, the product of a complex scalar and a complex vector.

(continued on next page)

Table 4–2 (Cont.) Summary of Level 1 BLAS Subprograms

Subprogram Name	Operation
ZSCAL	Calculates, in double-precision arithmetic, the product of a complex scalar and a complex vector.
CSSCAL	Calculates, in single-precision arithmetic, the product of a real scalar and a complex vector.
ZDSCAL	Calculates, in double-precision arithmetic, the product of a real scalar and a complex vector.
SSWAP	Swaps the elements of two real, single-precision vectors.
DSWAP	Swaps the elements of two real, double-precision vectors.
CSWAP	Swaps the elements of two complex, single-precision vectors.
ZSWAP	Swaps the elements of two complex, double-precision vectors.

Table 4–3 Summary of Extensions to Level 1 BLAS Subprograms

Subprogram Name	Operation
ISAMIN	Calculates, in single-precision arithmetic, the index of the element of a real vector with minimum absolute value.
IDAMIN	Calculates, in double-precision arithmetic, the index of the element of a real vector with minimum absolute value.
ICAMIN	Calculates, in single-precision arithmetic, the index of the element of a complex vector with minimum absolute value.
IZAMIN	Calculates, in double-precision arithmetic, the index of the element of a complex vector with minimum absolute value.
ISMAX	Calculates, in single-precision arithmetic, the index of the real vector element with maximum value.
IDMAX	Calculates, in double-precision arithmetic, the index of the real vector element with maximum value.
ISMIN	Calculates, in single-precision arithmetic, the index of the real vector element with minimum value.
IDMIN	Calculates, in double-precision arithmetic, the index of the real vector element with minimum value.
SAMAX	Calculates, in single-precision arithmetic, the largest absolute value of the elements of a real vector.
DAMAX	Calculates, in double-precision arithmetic, the largest absolute value of the elements of a real vector.
SCAMAX	Calculates, in single-precision arithmetic, the largest absolute value of the elements of a complex vector.
DZAMAX	Calculates, in double-precision arithmetic, the largest absolute value of the elements of a complex vector.

(continued on next page)

Table 4–3 (Cont.) Summary of Extensions to Level 1 BLAS Subprograms

Subprogram Name	Operation
SAMIN	Calculates, in single-precision arithmetic, the smallest absolute value of the elements of a real vector.
DAMIN	Calculates, in double-precision arithmetic, the smallest absolute value of the elements of a real vector.
SCAMIN	Calculates, in single-precision arithmetic, the smallest absolute value of the elements of a complex vector.
DZAMIN	Calculates, in double-precision arithmetic, the smallest absolute value of the elements of a complex vector.
SMAX	Calculates, in single-precision arithmetic, the largest value of the elements of a real vector.
DMAX	Calculates, in double-precision arithmetic, the largest value of the elements of a real vector.
SMIN	Calculates, in single-precision arithmetic, the smallest value of the elements of a real vector.
DMIN	Calculates, in double-precision arithmetic, the smallest value of the elements of a real vector.
SNORM2	Calculates, in single-precision arithmetic, the square root of the sum of the squares of the elements of a real vector.
DNORM2	Calculates, in double-precision arithmetic, the square root of the sum of the squares of the elements of a real vector.
SCNORM2	Calculates, in single-precision arithmetic, the square root of the sum of the squares of the absolute value of the elements of a complex vector.
DZNORM2	Calculates, in double-precision arithmetic, the square root of the sum of the squares of the absolute value of the elements of a complex vector.
SNRSQ	Calculates, in single-precision arithmetic, the sum of the squares of the elements of a real vector.
DNRSQ	Calculates, in double-precision arithmetic, the sum of the squares of the elements of a real vector.
SCNRSQ	Calculates, in single-precision arithmetic, the sum of the squares of the absolute value of the elements of a complex vector.
DZNRSQ	Calculates, in double-precision arithmetic, the sum of the squares of the absolute value of the elements of a complex vector.
SSET	For single-precision data, sets all the elements of a real vector equal to a real scalar.
DSET	For double-precision data, sets all the elements of a real vector equal to a real scalar.

(continued on next page)

Table 4–3 (Cont.) Summary of Extensions to Level 1 BLAS Subprograms

Subprogram Name	Operation
CSET	For single-precision data, sets all the elements of a complex vector equal to a complex scalar.
ZSET	For double-precision data, sets all the elements of a complex vector equal to a complex scalar.
SSUM	Calculates, in single-precision arithmetic, the sum of the values of the elements of a real vector.
DSUM	Calculates, in double-precision arithmetic, the sum of the values of the elements of a real vector.
CSUM	Calculates, in single-precision arithmetic, the sum of the values of the elements of a complex vector.
ZSUM	Calculates, in double-precision arithmetic, the sum of the values of the elements of a complex vector.
SVCAL	Calculates, in single-precision arithmetic, the product of a real scalar and a real vector.
DVCAL	Calculates, in double-precision arithmetic, the product of a real scalar and a real vector.
CVCAL	Calculates, in single-precision arithmetic, the product of a complex scalar and a complex vector.
ZVCAL	Calculates, in double-precision arithmetic, the product of a complex scalar and a complex vector.
CSVCAL	Calculates, in single-precision arithmetic, the product of a real scalar and a complex vector.
ZDVCAL	Calculates, in double-precision arithmetic, the product of a real scalar and a complex vector.
SZAXPY	Calculates, in single-precision arithmetic, the product of a real scalar and a real vector and adds the result to a real vector.
DZAXPY	Calculates, in double-precision arithmetic, the product of a real scalar and a real vector and adds the result to a real vector.
CZAXPY	Calculates, in single-precision arithmetic, the product of a complex scalar and a complex vector and adds the result to a complex vector.
ZZAXPY	Calculates, in double-precision arithmetic, the product of a complex scalar and a complex vector and adds the result to a complex vector.

4.5 Calling Subprograms

The BLAS Level 1 and Extensions subprograms consist of both functions and subroutines:

- Functions

  Return a scalar
  Require a function reference from a program
  Processing does not change arguments
  Documented with a **Function Value** section

- Subroutines

  Return a vector
  Require a CALL statement from a program
  Processing overwrites an output argument with the output vector
  No **Function Value** section

4.6 Argument Conventions

Subprograms use a list of *arguments* to specify requirements and control results. All arguments are required. The argument list is specified in the same order for each subprogram. The following are typical arguments for the BLAS Level 1 and Extensions subprograms.

- Arguments that define the length of the input vectors
  The argument **n** specifies the length of the input vectors. The values $n < 0$, $n = 0$, and $n > 0$ are all allowed. However, for $n \leq 0$, either the output vector is unchanged or the function value is immediately set equal to a value specified previously.
- Arguments that specify the input scalar
  The argument **alpha** defines the input scalar.
- Arguments that describe the input and output vectors
  In addition to the argument **n**, the following arguments describe a vector:
  - The arguments **x**, **y**, and **z** define the location of the vectors x, y, and z in the array. In the usual case, the argument **x** specifies the location in the array as X(1), but the location can be specified at any other element of the array. An array can be much larger than the vector that it contains.
  - The arguments **incx**, **incy**, and **incz** provide the increment between the elements of the vector x, vector y, and vector z, respectively. The increment can be positive, negative, or zero. The vector can be stored forward or backward in the array.

Not every type of argument is used by every subprogram.

4.7 Error Handling

The Level 1 BLAS subprograms assume that input parameters are correct and provide no feedback when problems occur. You must ensure that all input data for these subprograms is correct.

4.8 Definition of Absolute Value

Real subprograms define the absolute value in the following way:

$|x_j| = x_j$ if x_j is non-negative
$|x_j| = -x_j$ if x_j is negative

Complex subprograms define the absolute value in a way that depends on the subprogram and its operations. The definitions are consistent with the definitions used in the BLAS Level 1 subprograms.

In some cases, the definition is the strict definition of the absolute value of a complex number, that is, the square root of the sum of the squares of the real part and the imaginary part:

$$|x_j| = \sqrt{a_j^2 + b_j^2} = \sqrt{\text{real}^2 + \text{imaginary}^2}$$

In other cases, the definition for the absolute value of a complex number is the absolute value of the real part plus the absolute value of the imaginary part:

$$|x_j| = |a_j| + |b_j| = |\text{real}| + |\text{imaginary}|$$

The subprogram name does not specify the definition used. Check the **Description** section of the subprogram reference description for the definition used for that subprogram.

4.9 A Look at a Level 1 Extensions Subprogram

To understand the meaning of the arguments, consider the subroutine SVCAL. SVCAL computes the product of a real scalar α and a real (n-element) vector x, and the result is returned in the vector y. SVCAL has the arguments **n**, **alpha**, **x**, **incx**, **y**, and **incy** as shown in the following code:

```
REAL*4 X(100), Y(200), ALPHA
INCX = 1
INCY = 2
ALPHA = 3.2
N = 100
CALL SVCAL(N,ALPHA,X,INCX,Y,INCY)
```

The argument **x** specifies the array X with 100 elements and specifies X(1) as the location of the vector x whose elements are embedded in X. Since **n** = 100, the vector also has 100 elements. The length of the array X is the same as the length of the vector x. The **incx** is positive, indicating the vector starts at the first array element. Because **incx** = 1, the vector elements are contiguous in the array. Each element of the array X is multiplied by 3.2 and stored in array Y, beginning at Y(1), in the locations Y(1), Y(3), Y(5), and so on, since **incy** is 2.

As another example, if vector x has 20 elements, the starting point of the vector is X(1), and the elements are selected from the array X with an increment of 3, then the array X must have at least $(1 + (n - 1)|incx|)$ or 58 elements to store the vector. The following code shows this case:

```
REAL*4 X(58), Y(200), ALPHA
INCX = 3
INCY = 2
ALPHA = 3.2
N = 20
CALL SVCAL(N,ALPHA,X,INCX,Y,INCY)
```

In this case, elements X(1), X(4), X(7), . . . , X(58) of the array are multiplied by 3.2 and are stored in array Y, beginning at Y(1), in the locations Y(1), Y(3), Y(5), . . . , Y(39).

When the increment is negative, the starting point for the vector selection is at the last element of the vector. Consider the following code where the increment is −2 and the starting point is specified as X(20):

```
REAL*4 X(100), Y(200), ALPHA
INCX = -2
INCY = 2
ALPHA = 3.2
N = 6
CALL SVCAL(N,ALPHA,X(20),INCX,Y,INCY)
```

The vector x has 6 elements. The elements selected to form the vector are X(30), X(28), X(26), X(24), X(22), and X(20). Each of these elements is multiplied by 3.2 and the results are stored in Y(1), Y(3), Y(5), Y(7), Y(9), and Y(11), respectively.

5

Using the Sparse Level 1 BLAS Subprograms

The Sparse Level 1 BLAS subprograms perform vector-vector operations commonly occuring in many computational problems in sparse linear algebra. In contrast to the subprograms in Level 1 BLAS Subprograms and Level I BLAS Extensions, these subprograms operate on sparse vectors. This chapter provides information on the following topics:

- Operations performed by the Sparse Level 1 BLAS subprograms (Section 5.1)
- Sparse Level 1 vector storage (Section 5.2)
- Naming conventions (Section 5.3)
- Subprogram summary (Section 5.4)
- Calling Sparse Level 1 BLAS subprograms (Section 5.5)
- Argument conventions (Section 5.6)
- Error handling (Section 5.7)
- A look at a Sparse Level 1 BLAS subprogram (Section 5.8)

5.1 Sparse Level 1 BLAS Operations

The Sparse Level 1 BLAS subprograms are sparse extensions of the Level 1 BLAS subprograms. While similar in functionality to the Level 1 BLAS subprograms, the sparse subprograms operate on sparse vectors stored in a compressed form.

CXML enhances the functionality of the Sparse Level 1 BLAS outlined in [Dodson, Grimes, and Lewis 1991], by the addition of three subprograms that also operate on sparse vectors.

The sparse extensions of Level 1 BLAS subprograms that are of interest involve two vectors. The standard approach in sparse vector computation is to expand one vector into its full form and perform the numerical operations between that uncompressed vector and the remaining compressed vector. The Sparse Level 1 BLAS subprograms can be classified into two types:

- A vector in uncompressed form is returned as output.
  In order for these operations to give correct and consistent results on a vector or parallel machine, the values in the index vector, associated with the vector stored in compressed form, must be distinct.
- A scalar or a vector in compressed form is returned as output.

5.2 Sparse Vector Storage

For the Sparse Level 1 BLAS subprograms, a vector is stored in one of two ways:

- In a one-dimensional array in full form
- In two one-dimensional arrays in compressed form

5.2.1 Sparse Vectors

A sparse vector is a vector that has a large number of zeros. In such cases, substantial savings in computation and memory requirements can be achieved by storing and operating on only the nonzero elements. For example, consider the vector x, of length 9, as shown in the following example:

$$\mathrm{X} = \begin{bmatrix} 2.0 \\ 0.0 \\ 0.0 \\ 3.5 \\ 0.0 \\ 9.8 \\ 0.0 \\ 0.0 \\ 0.0 \end{bmatrix}$$

Only three of the nine elements in this vector are nonzero and by storing just these elements, the memory requirements for storing x can be reduced by a factor of three. This transformation converts the original vector from its full form to a vector in compressed form. Additional storage is, however, required for storing information that enables the original vector to be reconstructed from the vector stored in the compressed form. This implies that in addition to the vector of nonzero elements and the number of nonzero elements, there should be a companion array of indices that map the stored elements into their proper places in the original vector. Thus, the vector x is stored in compressed form as two separate arrays, XC and INDXC:

$$\mathrm{XC} = \begin{bmatrix} 2.0 \\ 3.5 \\ 9.8 \end{bmatrix}$$

$$\mathrm{INDXC} = \begin{bmatrix} 1 \\ 4 \\ 6 \end{bmatrix}$$

where XC is the array of nonzero elements and INDXC is an array of indices that is used to reconstruct the original vector. For example, since the second element in INDXC is 4, it implies that the second element in XC, 3.5, is the fourth element in the original array X. Both XC and INDXC are of length n = 3, where nz is the number of nonzero elements in X.

Operations on sparse vectors are performed only on the nonzero elements of the vector. As a result, it is the number of nonzero elements that is important, not the length of the original vector x. Moreover, as the elements of the vector stored in compressed form are contiguous, there is no need for an increment parameter; it is always 1.

5.2.2 Storing a Sparse Vector

Suppose X is a sparse one-dimensional array of length n, with nz nonzero elements. As x is a sparse vector, nz is much smaller than n, that is, a large number of elements of the vector x are zero.

Let XC be the vector x stored in compressed form, that is, XC contains only the nonzero elements of x. Let INDXC be the array of indices that map each element of XC into its proper position in the array X. Then X(INDXC(i)) = XC(i). It follows that:

$$\max(\mathrm{INDXC}(i),\ i = 1, nz) \leq n$$

That is, if the original vector has length n, then the values of the elements in array INDXC can be at most n.

A sparse vector, stored in a compressed form, is thus defined by three quantities:

- Number of nonzero elements: nz
- Array of length at least nz, containing the nonzero elements of array X: XC
- Array of length at least nz containing the indices of the nonzero elements in the original uncompressed form: INDXC

5.3 Naming Conventions

Table 5–1 shows the characters used in the names of the Sparse Level 1 BLAS, and their meaning.

Table 5–1 Naming Conventions: Sparse Level 1 BLAS Subprogram

Character Group	Mnemonic	Meaning
First group	S	Single-precision real
	D	Double-precision real
	C	Single-precision complex
	Z	Double-precision complex
Second group	A combination of letters such as DOT or SCTR	Type of computation such as dot product or a vector scatter
Third group	I	Refers to indexed computation used in sparse vectors
	S or Z	Scale or zero
	No mnemonic	-

For example, the name SSCTRS refers to the single precision real subprogram for scaling and then scattering the elements of a sparse vector stored in compressed form.

5.4 Summary of Sparse Level 1 BLAS Subprograms

Table 5–2 summarizes the Sparse Level 1 BLAS subprograms provided by CXML.

Table 5–2 Summary of Sparse Level 1 BLAS Subprograms

Subprogram Name	Operation
SAXPYI	Calculates, in single-precision arithmetic, the product of a real scalar and a real sparse vector in compressed form and adds the result to a real vector in full form.
DAXPYI	Calculates, in double-precision arithmetic, the product of a real scalar and a real sparse vector in compressed form and adds the result to a real vector in full form.
CAXPYI	Calculates, in single-precision arithmetic, the product of a complex scalar and a complex sparse vector in compressed form and adds the result to a complex vector in full form.
ZAXPYI	Calculates, in double-precision arithmetic, the product of a complex scalar and a complex sparse vector in compressed form and adds the result to a complex vector in full form.
SSUMI	Calculates, in single-precision arithmetic, the sum of a real sparse vector stored in compressed form and a real vector stored in full form.
DSUMI	Calculates, in double-precision arithmetic, the sum of a real sparse vector stored in compressed form and a real vector stored in full form.
CSUMI	Calculates, in single-precision arithmetic, the sum of a complex sparse vector stored in compressed form and a complex vector stored in full form.
ZSUMI	Calculates, in double-precision arithmetic, the sum of a complex sparse vector stored in compressed form and a complex vector stored in full form.
SDOTI	Calculates, in single-precision arithmetic, the product of a real vector and a real sparse vector stored in compressed form.
DDOTI	Calculates, in double-precision arithmetic, the product of a real vector and a real sparse vector stored in compressed form.
CDOTUI	Calculates, in single-precision arithmetic, the product of a complex vector and an unconjugated complex sparse vector stored in compressed form.
ZDOTUI	Calculates, in double-precision arithmetic, the product of a complex vector and an unconjugated complex sparse vector stored in compressed form.
CDOTCI	Calculates, in single-precision arithmetic, the product of a complex vector and a conjugated complex sparse vector stored in compressed form.
ZDOTCI	Calculates, in double-precision arithmetic, the product of a complex vector and a conjugated complex sparse vector stored in compressed form.

(continued on next page)

Table 5–2 (Cont.) Summary of Sparse Level 1 BLAS Subprograms

Subprogram Name	Operation
SGTHR	Constructs, in single-precision arithmetic, a real sparse vector in compressed form from the specified elements of a real vector in full form.
DGTHR	Constructs, in double-precision arithmetic, a real sparse vector in compressed form from the specified elements of a real vector in full form.
CGTHR	Constructs, in single-precision arithmetic, a complex sparse vector in compressed form from the specified elements of a complex vector in full form.
ZGTHR	Constructs, in double-precision arithmetic, a complex sparse vector in compressed form from the specified elements of a complex vector in full form.
SGTHRS	Constructs, in single-precision arithmetic, a real sparse vector in compressed form from the specified scaled elements of a real vector in full form.
DGTHRS	Constructs, in double-precision arithmetic, a real sparse vector in compressed form from the specified scaled elements of a real vector in full form.
CGTHRS	Constructs, in single-precision arithmetic, a complex sparse vector in compressed form from the specified scaled elements of a complex vector in full form.
ZGTHRS	Constructs, in double-precision arithmetic, a complex sparse vector in compressed form from the specified scaled elements of a complex vector in full form.
SGTHRZ	Constructs, in single-precision arithmetic, a real sparse vector in compressed form from the specified elements of a real vector in full form and sets the elements to zero.
DGTHRZ	Constructs, in double-precision arithmetic, a real sparse vector in compressed form from the specified elements of a real vector in full form and sets the elements to zero.
CGTHRZ	Constructs, in single-precision arithmetic, a complex sparse vector in compressed form from the specified elements of a complex vector in full form and sets the elements to zero.
ZGTHRZ	Constructs, in double-precision arithmetic, a complex sparse vector in compressed form from the specified elements of a complex vector in full form and sets the elements to zero.
SROTI	Applies, in single-precision arithmetic, a Givens rotation for a real sparse vector stored in compressed form and another vector stored in full form.
DROTI	Applies, in double-precision arithmetic, a Givens rotation for a real sparse vector stored in compressed form and another vector stored in full form.

(continued on next page)

Table 5–2 (Cont.) Summary of Sparse Level 1 BLAS Subprograms

Subprogram Name	Operation
SSCTR	Scatters, in single-precision arithmetic, the components of a sparse real vector in compressed form into the specified components of a real vector in full form.
DSCTR	Scatters, in double-precision arithmetic, the components of a sparse real vector in compressed form into the specified elements a real vector in full form.
CSCTR	Scatters, in single-precision arithmetic, the components of a sparse complex vector in compressed form into the specified elements of a complex vector in full form.
ZSCTR	Scatters, in double-precision arithmetic, the components of a sparse complex vector in compressed form into the specified elements of a complex vector in full form.
SSCTRS	Scales and then scatters, in single-precision arithmetic, the components of a sparse real vector in compressed form into the specified components of a real vector in full form.
DSCTRS	Scales and then scatters, in double-precision arithmetic, the components of a sparse real vector in compressed form into the specified elements a real vector in full form.
CSCTRS	Scales and then scatters, in single-precision arithmetic, the components of a sparse complex vector in compressed form into the specified elements of a complex vector in full form.
ZSCTRS	Scales and then scatters, in double-precision arithmetic, the components of a sparse complex vector in compressed form into the specified elements of a complex vector in full form.

5.5 Calling Subprograms

Some of the subprograms return a scalar. These subprograms are functions and are called as functions by coding a function reference.

In the reference section at the end of this chapter, a reference description for a function includes a **Function Value** section. For all the subprograms that are functions, all of the arguments are input arguments, which are unchanged on exit. The example at the end of each function reference description shows the function call.

Some of the subprograms return a vector. These subprograms are subroutines and are called as subroutines with a CALL statement.

A reference description for a subroutine does not have a **Function Value** section. Each subroutine has an output argument that is overwritten on exit and contains the output vector information. The example at the end of each subroutine reference description shows the subroutine call.

5.6 Argument Conventions

Each Sparse Level 1 BLAS subprogram has arguments that specify the nature and requirements of the subprogram. There are no optional arguments.

The arguments are ordered by category, but not every argument category is needed in each of the subprograms:

- Argument defining the number of nonzero elements
- Argument defining the input scalar
- Arguments describing the input and output vectors

5.6.1 Defining the Number of Nonzero Elements

The Sparse Level 1 BLAS subprograms operate only on the nonzero elements of the sparse vector. Thus in contrast to the Level 1 BLAS subprograms, it is the number of nonzero elements that is input to the subprogram, not the length of the vector. The number of nonzero elements is defined by the argument **nz**.

The values **nz**< 0, **nz** $= 0$ and **nz** > 0 are all allowed. For **nz**≤ 0, the routines return zero function values (if applicable) and make no references to their vector arguments.

5.6.2 Defining the Input Scalar

The input scalar α is always defined by the argument **alpha**.

5.6.3 Describing the Input/Output Vectors

Sparse Level 1 BLAS subprograms operate on two types of vectors: compressed and uncompressed. The elements of the full uncompressed vector y, specified by the argument **y** are stored contiguously, that is, with increment equal to 1. As a result, there is no input parameter for the increment of the vector y as it is always assumed to be 1.

The sparse vector x is stored in compressed form as array X, containing nz elements. The companion array of indices, array INDX, also of length nz, replaces the increment argument of the Level 1 BLAS subprograms.

5.7 Error Handling

The Sparse Level 1 BLAS subprograms assume that input parameters are correct and provide no feedback when problems occur. You must ensure that all input data for these subprograms is correct.

5.8 A Look at a Sparse Level 1 BLAS Subprogram

To understand the differences between a Level 1 BLAS subprogram and its sparse counterpart, consider the routines SAXPY and SAXPYI. They perform essentially the same operation, but SAXPY operates on full vectors and SAXPYI operates on sparse vectors.

Consider two arrays: array Y of length n = 9, stored in full uncompressed form and the sparse array X, also of length n = 9 and also stored in full form.

$$Y = \begin{bmatrix} 1.0 \\ 2.0 \\ 3.0 \\ 4.0 \\ 5.0 \\ 6.0 \\ 7.0 \\ 8.0 \\ 9.0 \end{bmatrix} \qquad X = \begin{bmatrix} 2.0 \\ 0.0 \\ 1.0 \\ 0.0 \\ 0.0 \\ 3.0 \\ 0.0 \\ 0.0 \\ 0.0 \end{bmatrix}$$

As the array X is sparse, it can be stored in the compressed form as an array XC of length 3 and a companion integer array INDXC, also of length 3.

$$XC = \begin{bmatrix} 2.0 \\ 1.0 \\ 3.0 \end{bmatrix} \qquad INDXC = \begin{bmatrix} 1 \\ 3 \\ 6 \end{bmatrix}$$

The routine SAXPY, from Level 1 BLAS, operates on the arrays X and Y as shown in the following code:

```
REAL*4   X(9), Y(9), ALPHA
INTEGER INCX, INCY, N
ALPHA = 2.0
INCX = 1
INCY = 1
N = 9
CALL SAXPY(N,ALPHA,X,INCX,Y,INCY)
```

The routine SAXPYI, from Sparse Level 1 BLAS, operates on the arrays XC and Y as shown in the following code:

```
REAL*4   XC(3), Y(9), ALPHA
INTEGER INDXC(3), NZ
ALPHA = 2.0
NZ = 3
CALL SAXPYI(NZ,ALPHA,XC,INDXC,Y)
```

With α = 2.0, both calls result in the updated vector y:

$$Y = \begin{bmatrix} 5.0 \\ 2.0 \\ 5.0 \\ 4.0 \\ 5.0 \\ 12.0 \\ 7.0 \\ 8.0 \\ 9.0 \end{bmatrix}$$

In SAXPY, all the elements of the array X and Y are operated on, resulting in 18 arithmetic operations (additions and multiplications). In contrast, SAXPYI operates only on the nonzero elements, resulting in 6 arithmetic operations. Storing both the vectors in uncompressed form requires 18 memory locations for real operands. Storing array X in a compressed form and array Y in an uncompressed form requires 12 memory locations for real operands and 3 for integer operands.

The savings in compute time and memory requirements can be substantial, when the array X is very sparse.

6 Using the Level 2 BLAS Subprograms

The Level 2 BLAS subprograms perform matrix-vector operations commonly occurring in many computational problems in linear algebra. This chapter provides information about the following topics:

- Operations performed by the Level 2 BLAS subprograms (Section 6.1)
- Vector and matrix storage (Section 6.2)
- Subprogram naming conventions (Section 6.3)
- Subprogram summary (Section 6.4)
- Calling Level 2 BLAS subprograms (Section 6.5)
- Arguments used in the subprograms and invalid arguments (Sections 6.6 and 6.6.6)
- Performing rank-one and rank-two updates to band matrices (Section 6.7)
- Error handling (Section 6.8)
- A look at a Level 2 subprogram and its use (Section 6.9)

A key Level 2 BLAS subprogram, {C,D,S,Z}GEMV, has been parallelized for improved peformance on multiprocessor systems. For information about using the parallel library, see Section A.1.

6.1 Level 2 BLAS Operations

Level 2 BLAS subprograms perform operations that involve only one matrix. Some Level 2 BLAS subprograms combine several possible operations, such as matrix times, vector, or transpose times vector.

Level 2 BLAS subprograms perform three types of basic matrix-vector operations: matrix-vector products, rank-one and rank-two updates, and triangular system solvers.

- Matrix-vector products

$$y \leftarrow \alpha Ax + \beta y$$

$$y \leftarrow \alpha A^T x + \beta y$$

$$y \leftarrow \alpha A^H x + \beta y$$

$$x \leftarrow Tx$$

$$x \leftarrow T^T x$$

- Rank-one and rank-two updates

$$A \leftarrow A + \alpha x y^T$$

$$A \leftarrow A + \alpha x y^H$$

$$A \leftarrow A + \alpha x y^T + \alpha y x^T$$

$$A \leftarrow A + \alpha x y^H + \overline{\alpha} y x^H$$

- Triangular system solvers

$$Tx = b$$

$$T^T x = b$$

$$T^H x = b$$

α and β are scalars, x, y, and b are vectors, A is a matrix, and T is an upper- or lower-triangular matrix. For the triangular system solvers, T must also be non-singular; that is, $\det(T)$ is not equal to zero. Where appropriate, these operations are applied to different types of matrices:

- General matrix
- General band matrix
- Symmetric matrix
- Symmetric band matrix
- Hermitian matrix
- Hermitian band matrix
- Triangular matrix
- Triangular band matrix

6.2 Vector and Matrix Storage

Level 2 BLAS subprograms manipulate a single matrix and one or two vectors. Each vector is stored in a one-dimensional array.

The matrix A is stored in one of two ways:

- A is stored in a two-dimensional array.
- A is stored in packed form in a one-dimensional array.

For information about how Level 2 BLAS subprograms store vectors and matrices, refer to Chapter 1.

6.3 Naming Conventions for Level 2 BLAS Subprograms

Each Level 2 BLAS subprogram has a name consisting of four or five characters. The first character of the name denotes the Fortran data type of the matrix. The second and third characters denote the type of matrix operated on by the subprogram. The fourth and fifth characters denote the type of operation.

Table 6–1 shows the characters used in the Level 2 BLAS subprogram names and what the characters mean.

Table 6–1 Naming Conventions: Level 2 BLAS Subprograms

Character	Mnemonic	Meaning
First character	S	Single-precision real data
	D	Double-precision real data
	C	Single-precision complex data
	Z	Double-precision complex data
Second and third characters	GE	General matrix
	GB	General band matrix
	HE	Hermitian matrix
	SY	Symmetric matrix
	HP	Hermitian matrix stored in packed form
	SP	Symmetric matrix stored in packed form
	HB	Hermitian band matrix
	SB	Symmetric band matrix
	TR	Triangular matrix
	TP	Triangular matrix stored in packed form
	TB	Triangular band matrix
Fourth and fifth characters	MV	Matrix-vector product
	R	Rank-one update
	RU	Rank-one unconjugated update
	RC	Rank-one conjugated update
	R2	Rank-two update
	SV	Solution of a system of linear equations

For example, the name SGEMV is the subprogram for performing matrix-vector multiplication, where the matrix is a general matrix with single-precision real elements, and the matrix is stored using full matrix storage.

6.4 Summary of Level 2 BLAS Subprograms

Table 6–2 summarizes the Level 2 BLAS subprograms. For the general rank-one update (_GER) operations, two complex subprograms are provided, CGERC and CGERU. This is the only exception to the one-to-one correspondence between real and complex subprograms.

Subprograms for rank-one and rank-two updates applied to band matrices are not provided because these can be obtained by calls to the rank-one and rank-two full matrix subprogram. See Section 6.7 for information about how to make these calls.

Table 6–2 Summary of Level 2 BLAS Subprograms

Subprogram Name	Operation
SGBMV	Calculates, in single-precision arithmetic, a matrix-vector product for either a real general band matrix or its transpose.
DGBMV	Calculates, in double-precision arithmetic, a matrix-vector product for either a real general band matrix or its transpose.
CGBMV	Calculates, in single-precision arithmetic, a matrix-vector product for either a complex general band matrix, its transpose, or its conjugate transpose.
ZGBMV	Calculates, in double-precision arithmetic, a matrix-vector product for either a complex general band matrix, its transpose, or its conjugate transpose.
SGEMV	Calculates, in single-precision arithmetic, a matrix-vector product for either a real general matrix or its transpose.
DGEMV	Calculates, in double-precision arithmetic, a matrix-vector product for either a real general matrix or its transpose.
CGEMV	Calculates, in single-precision arithmetic, a matrix-vector product for either a complex general matrix, its transpose, or its conjugate transpose.
ZGEMV	Calculates, in double-precision arithmetic, a matrix-vector product for either a complex general matrix, its transpose, or its conjugate transpose.
SGER	Calculates, in single-precision arithmetic, a rank-one update of a real general matrix.
DGER	Calculates, in double-precision arithmetic, a rank-one update of a real general matrix.
CGERC	Calculates, in single-precision arithmetic, a rank-one conjugated update of a complex general matrix.
ZGERC	Calculates, in double-precision arithmetic, a rank-one conjugated update of a complex general matrix.
CGERU	Calculates, in single-precision arithmetic, a rank-one unconjugated update of a complex general matrix.
ZGERU	Calculates, in double-precision arithmetic, a rank-one unconjugated update of a complex general matrix.

(continued on next page)

Table 6–2 (Cont.) Summary of Level 2 BLAS Subprograms

Subprogram Name	Operation
SSBMV	Calculates, in single-precision arithmetic, a matrix-vector product for a real symmetric band matrix.
DSBMV	Calculates, in double-precision arithmetic, a matrix-vector product for a real symmetric band matrix.
CHBMV	Calculates, in single-precision arithmetic, a matrix-vector product for a complex Hermitian band matrix.
ZHBMV	Calculates, in double-precision arithmetic, a matrix-vector product for a complex Hermitian band matrix.
SSPMV	Calculates, in single-precision arithmetic, a matrix-vector product for a real symmetric matrix stored in packed form.
DSPMV	Calculates, in double-precision arithmetic, a matrix-vector product for a real symmetric matrix stored in packed form.
CHPMV	Calculates, in single-precision arithmetic, a matrix-vector product for a complex Hermitian matrix stored in packed form.
ZHPMV	Calculates, in double-precision arithmetic, a matrix-vector product for a complex Hermitian matrix stored in packed form.
SSPR	Calculates, in single-precision arithmetic, a rank-one update of a real symmetric matrix stored in packed form.
DSPR	Calculates, in double-precision arithmetic, a rank-one update of a real symmetric matrix stored in packed form.
CHPR	Calculates, in single-precision arithmetic, a rank-one update of a complex Hermitian matrix stored in packed form.
ZHPR	Calculates, in double-precision arithmetic, a rank-one update of a complex Hermitian matrix stored in packed form.
SSPR2	Calculates, in single-precision arithmetic, a rank-two update of a real symmetric matrix stored in packed form.
DSPR2	Calculates, in double-precision arithmetic, a rank-two update of a real symmetric matrix stored in packed form.
CHPR2	Calculates, in single-precision arithmetic, a rank-two update of a complex Hermitian matrix stored in packed form.
ZHPR2	Calculates, in double-precision arithmetic, a rank-two update of a complex Hermitian matrix stored in packed form.
SSYMV	Calculates, in single-precision arithmetic, a matrix-vector product for a real symmetric matrix.
DSYMV	Calculates, in double-precision arithmetic, a matrix-vector product for a real symmetric matrix.
CHEMV	Calculates, in single-precision arithmetic, a matrix-vector product for a complex Hermitian matrix.
ZHEMV	Calculates, in double-precision arithmetic, a matrix-vector product for a complex Hermitian matrix.

(continued on next page)

Table 6–2 (Cont.) Summary of Level 2 BLAS Subprograms

Subprogram Name	Operation
SSYR	Calculates, in single-precision arithmetic, a rank-one update of a real symmetric matrix.
DSYR	Calculates, in double-precision arithmetic, a rank-one update of a real symmetric matrix.
CHER	Calculates, in single-precision arithmetic, a rank-one update of a complex Hermitian matrix.
ZHER	Calculates, in double-precision arithmetic, a rank-one update of a complex Hermitian matrix.
SSYR2	Calculates, in single-precision arithmetic, a rank-two update of a real symmetric matrix.
DSYR2	Calculates, in double-precision arithmetic, a rank-two update of a real symmetric matrix.
CHER2	Calculates, in single-precision arithmetic, a rank-two update of a complex Hermitian matrix.
ZHER2	Calculates, in double-precision arithmetic, a rank-two update of a complex Hermitian matrix.
STBMV	Calculates, in single-precision arithmetic, a matrix-vector product for either a real triangular band matrix or its transpose.
DTBMV	Calculates, in double-precision arithmetic, a matrix-vector product for either a real triangular band matrix or its transpose.
CTBMV	Calculates, in single-precision arithmetic, a matrix-vector product for a complex triangular band matrix, its transpose, or its conjugate transpose.
ZTBMV	Calculates, in double-precision arithmetic, a matrix-vector product for a complex triangular band matrix, its transpose, or its conjugate transpose.
STBSV	Solves, in single-precision arithmetic, a system of linear equations where the coefficient matrix is a real triangular band matrix.
DTBSV	Solves, in double-precision arithmetic, a system of linear equations where the coefficient matrix is a real triangular band matrix.
CTBSV	Solves, in single-precision arithmetic, a system of linear equations where the coefficient matrix is a complex triangular band matrix.
ZTBSV	Solves, in double-precision arithmetic, a system of linear equations where the coefficient matrix is a complex triangular band matrix.
STPMV	Calculates, in single-precision arithmetic, a matrix-vector product for either a real triangular matrix stored in packed form or its transpose.
DTPMV	Calculates, in double-precision arithmetic, a matrix-vector product for either a real triangular matrix stored in packed form or its transpose.
CTPMV	Calculates, in single-precision arithmetic, a matrix-vector product for a complex triangular matrix stored in packed form, its transpose, or its conjugate transpose.

(continued on next page)

Table 6–2 (Cont.) Summary of Level 2 BLAS Subprograms

Subprogram Name	Operation
ZTPMV	Calculates, in double-precision arithmetic, a matrix-vector product for a complex triangular matrix stored in packed form, its transpose, or its conjugate transpose.
STPSV	Solves, in single-precision arithmetic, a system of linear equations where the coefficient matrix is a real triangular matrix stored in packed form.
DTPSV	Solves, in double-precision arithmetic, a system of linear equations where the coefficient matrix is a real triangular matrix stored in packed form.
CTPSV	Solves, in single-precision arithmetic, a system of linear equations where the coefficient matrix is a complex triangular matrix stored in packed form.
ZTPSV	Solves, in double-precision arithmetic, a system of linear equations where the coefficient matrix is a complex triangular matrix stored in packed form.
STRMV	Calculates, in single-precision arithmetic, a matrix-vector product for either a real triangular matrix or its transpose.
DTRMV	Calculates, in double-precision arithmetic, a matrix-vector product for either a real triangular matrix or its transpose.
CTRMV	Calculates, in single-precision arithmetic, a matrix-vector product for a complex triangular matrix, its transpose, or its conjugate transpose.
ZTRMV	Calculates, in double-precision arithmetic, a matrix-vector product for a complex triangular matrix, its transpose, or its conjugate transpose.
STRSV	Solves, in single-precision arithmetic, a system of linear equations where the coefficient matrix is a real triangular matrix.
DTRSV	Solves, in double-precision arithmetic, a system of linear equations where the coefficient matrix is a real triangular matrix.
CTRSV	Solves, in single-precision arithmetic, a system of linear equations where the coefficient matrix is a complex triangular matrix.
ZTRSV	Solves, in double-precision arithmetic, a system of linear equations where the coefficient matrix is a complex triangular matrix.

6.5 Calling Subprograms

All of the Level 2 subprograms are subroutines, and have the following characteristics:

Return a vector or a matrix
Require a CALL statement from a program
Processing overwrites an output argument with the output vector
No **Function Value** section

6.6 Argument Conventions

The subroutines use a list of arguments to specify the requirements and control the result of the subroutine. All arguments are required. The argument list is in the same order for each subprogram:

- Arguments specifying matrix options
- Arguments defining the size of the matrix
- Arguments specifying the input scalar
- Arguments describing the input matrix
- Arguments describing the input vector or vectors
- Arguments specifying the input scalar associated with the input-output vector
- Arguments describing the input-output vector
- Arguments describing the input-output matrix

Not every type of argument is needed by every subprogram.

6.6.1 Specifying Matrix Options

The arguments that specify matrix options are character arguments:

- **trans**
- **uplo**
- **diag**

In Fortran, a character argument can be longer than its corresponding dummy argument. For example, the value 'T' for the argument **trans** can be passed as 'TRANSPOSE'.

trans

In some subroutines, the argument **trans** is used to select the form of the input matrix to use in an operation. You do not change the form of the input matrix in your application program. CXML selects the proper elements, depending on the value of the **trans** argument.

For example, if A is the input matrix, and you want to use it in the operation, set the **trans** argument to 'N'. If you want to use A^T in the operation, set the **trans** argument to 'T'. The subroutine makes the changes and selects the proper elements from the matrix, so that A^T is used. Table 6–3 shows the meaning of the values for the argument **trans**.

Table 6–3 Values for the Argument TRANS

Value of trans	Meaning
'N' or 'n'	Operate with the matrix
'T' or 't'	Operate with the transpose of the matrix
'C' or 'c'	Operate with the conjugate transpose of the matrix

When the operation is performed on a real matrix, the values 'T' and 't' or 'C' and 'c' all have the same meaning.

uplo

The Hermitian, symmetric, and triangular matrix subroutines (HE, SY, and TR subroutines) use the argument **uplo** to specify either the upper or lower triangle. Because of the structure of these matrices, the subroutines do not refer to all of the matrix values. Table 6–4 shows the meaning of the values for the argument **uplo**.

Table 6–4 Values for the Argument UPLO

Value of uplo	Meaning
'U' or 'u'	Refers to the upper triangle
'L' or 'l'	Refers to the lower triangle

diag

The triangular matrix (TR) subroutines use the argument **diag** to specify whether or not the triangular matrix is unit-triangular. Table 6–5 shows the meaning of the values for the argument **diag**.

Table 6–5 Values for the Argument DIAG

Value of diag	Meaning
'U' or 'u'	Unit-triangular
'N' or 'n'	Not unit-triangular

When **diag** is specified as 'U' or 'u', the diagonal elements are not referenced by the subroutine. These elements are assumed to be unity.

6.6.2 Defining the Size of the Matrix

The following arguments define the size of the input-output matrix:

- For a rectangular matrix, m rows by n columns: arguments **m** and **n**
- For a symmetric, Hermitian, or triangular matrix: argument **n**
- For a rectangular band matrix: arguments **m** and **n** for the rows and columns, **kl** for the subdiagonals, and **ku** for the superdiagonals
- For a symmetric, Hermitian, or triangular band matrix: arguments **n** for the dimensions and **k** for the diagonal

You can call a subroutine with arguments **m** or **n** equal to 0 but the subroutine exits immediately without referencing its other arguments.

6.6.3 Describing the Matrix

The description of the matrix depends on how the matrix is stored. The matrix can be stored in one of the following ways:

- Two-dimensional array
- Packed form of a one-dimensional array

Two-Dimensional Array

When the matrix is stored in a two-dimensional array, the subroutine requires the following arguments in addition to the size arguments:

- Argument **a** specifies the array A in which the matrix is stored
- Argument **lda** specifies the leading dimension of the array A

To store the matrix, the array must contain at least the number of elements as described:

$$(n-1)d+l$$

n is the number of columns of the matrix
d is the leading dimension of the array with $d \geq 1$; and
$l = m$ for the GE subroutines,
$l = n$ for the SY, HE, and TR subroutines,
$l = (kl + ku + 1)$ for the GB subroutines, and
$l = (k + 1)$ for the SB, HB, and TB subroutines.

One-Dimensional Array

When the matrix is stored packed in a one-dimensional array, the matrix is described by only one argument, **ap**, which specifies the one-dimensional array in which the matrix is stored.

To store the packed matrix, the array AP must contain at least $n(n+1)/2$ elements.

6.6.4 Describing the Input Scalars

The input scalars, α and β, are always described by the dummy argument names **alpha** and **beta**.

6.6.5 Describing the Vectors

A vector is described by three arguments:

- The length of the vector: **n**

  When the vector x consists of n elements, the corresponding array X must be of length at least $(1 + (n-1)|incx|)$.

- The location of the vector in the array: **x** for the vector X, **y** for the vector y

  The location is the base address of the vector. If the argument is the name of the array, such as X, the location of the vector is specified at X(1), but the location can be specified at any other element of the array. The array can be much larger than the vector that it contains.

- The spacing increment for selecting the vector elements from the array: **incx** for vector x, argument **incy** for vector y

  The increment can be positive or negative, but, unlike the Level 1 Extensions, it cannot be equal to zero.

If you supply an input scalar **beta** of zero, you do not need to set the array Y. This means that an operation such as $y \leftarrow \alpha Ax$ can be performed without having to set y to zero in the calling program.

6.6.6 Invalid Arguments

The following values of the arguments are invalid:

- Any value of the arguments **trans**, **uplo**, or **diag** that is not defined
- **m** < 0 for GE and GB subroutines
- **n** < 0 for all subroutines
- **kl** < 0 for the GB subroutines
- **ku** < 0 for the GB subroutines
- **k** < 0 for the HB, SB, and TB subroutines
- **lda** < **m** for the GE subroutines
- **lda** < **kl** + **ku** + 1 for the GB subroutines
- **lda** < **n** for the HE, SY, and TR subroutines
- **lda** < **k** + 1 for the HB, SB, and TB subroutines
- **incx** = 0
- **incy** = 0

6.7 Rank-One and Rank-Two Updates to Band Matrices

The BLAS 2 subroutines for full matrix updates can be used to perform rank-one and rank-two updates to band matrices. The following operation is the rank-one update to the band matrix A:

$$A \leftarrow A + xy^T$$

Vectors x and y are such that no fill-in occurs outside the band. In this case, the update affects only a full $(kl + 1)$ by $(ku + 1)$) rectangle within the band matrix A.

The operation is shown in (6–1) for the case where $m = n = 9$, $kl = 2$, and $ku = 3$. The update begins in row l and column l where $l = 3$ and affects only the 12 elements within A that are in the full 3 by 4 rectangle starting at $a_{ll} = a_{33}$.

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

$$+$$

$$\begin{bmatrix} 0 \\ 0 \\ x_3 \\ x_4 \\ x_5 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & y_3 & y_4 & y_5 & y_6 & 0 & 0 & 0 \end{bmatrix} \qquad (6–1)$$

For real data, SGER with $\alpha = 1$ provides this operation, as shown in the following code fragment:

```
KM=MIN(KL+1,M-L+1)
KN=MIN(KU+1,N-L+1)
CALL SGER (KM, KN, 1., X, 1, Y, 1, A(KU+1,L), MAX(KM,LDA-1))
```

L denotes the starting row and column for the update. The elements x_l and y_l of the vectors x and y are in elements X(l) and Y(l) of the arrays X and Y.

For the case where A is a symmetric band matrix of n by n with k subdiagonals and k superdiagonals, the operation can be achieved by a call to the subroutine SSYR, referring to either the upper or lower triangle of A. To refer to the upper-triangular part of A, use the following call to SSYR:

```
KN=MIN(K+1,N-L+1)
CALL SSYR ('U', KN, 1., X, 1, A(K+1,L), MAX(1,LDA-1))
```

To refer to the lower-triangular part of A, use the following call to SSYR:

```
KN=MIN(K+1,N-L+1)
CALL SSYR ('L', KN, 1., X, 1, A(1,L), MAX(1,LDA-1))
```

If the data is complex, the same operations can be achieved by calls to the subroutines CGER and CHER.

Rank-two updates for real symmetric band matrices and complex Hermitian band matrices can be achieved by calls to the subroutines SSYR2 and CHER2.

6.8 Error Handling

The BLAS Level 2 subroutines provide a check of the input arguments. If you call a Level 2 subroutine with an invalid value for any of its arguments, CXML reports the message and terminates execution of the program.

The code for BLAS Level 2 subroutines has calls to an input argument error handler, the XERBLA routine. When a subroutine detects an error, it passes the name of the subroutine and the number of the first argument that is in error to the XERBLA routine. CXML directs this information to a device or file:

- For OpenVMS, the device or file is defined as *SYS$OUTPUT*.
- For Tru64 UNIX or Windows NT, the device or file is defined as *stdout*.

6.9 A Look at a Level 2 BLAS Subroutine

SGEMV computes a matrix-vector product for either a real general matrix or its transpose:

$$y \leftarrow \alpha A x + \beta y$$

or

$$y \leftarrow \alpha A^T x + \beta y$$

where α and β are scalars, x and y are vectors, and A is an m by n matrix.

Let A be the following 6 by 6 matrix:

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 \\ 7.0 & 8.0 & 9.0 & 10.0 & 11.0 & 12.0 \\ 13.0 & 14.0 & 15.0 & 16.0 & 17.0 & 18.0 \\ 19.0 & 20.0 & 21.0 & 22.0 & 23.0 & 24.0 \\ 25.0 & 26.0 & 27.0 & 28.0 & 29.0 & 30.0 \\ 31.0 & 32.0 & 33.0 & 34.0 & 35.0 & 36.0 \end{bmatrix}$$

Let x be the vector:

$$x = \begin{bmatrix} 2.0 & 4.0 & 6.0 & 8.0 & 10.0 & 12.0 & 14.0 & 16.0 \end{bmatrix}^T$$

Let y be the vector:

$$y = \begin{bmatrix} 1.0 & 3.0 & 5.0 & 7.0 & 9.0 & 11.0 & 13.0 & 15.0 & 17.0 \end{bmatrix}^T$$

The subroutine SGEMV has the following format:

```
CALL SGEMV(trans,m,n,alpha,a,lda,x,incx,beta,y,incy)
```

The following code calls SGEMV:

```
REAL      A(6,6), ALPHA, BETA, X(8), Y(9)
INTEGER   LDA,INCY,INCX,M,N
CHARACTER TRANS

CALL SGEMV('n', 2, 3, 1.0, a(2,2), 6, x(1), 2, 0.0, y(1), 1)
```

This code multiplies the submatrix

$$\begin{bmatrix} 8.0 & 9.0 & 10.0 \\ 14.0 & 15.0 & 16.0 \end{bmatrix}$$

by the vector $\begin{bmatrix} 2.0 & 6.0 & 10.0 \end{bmatrix}$ to give the new vector y:

$$\begin{bmatrix} 170.0 & 278.0 & 5.0 & 7.0 & 9.0 & 11.0 & 13.0 & 15.0 & 17.0 \end{bmatrix}^T$$

The vector x and the matrix A are unchanged.

The following code uses the transpose:

```
SGEMV('t', 2, 2, 2.0, a, 6, x(3), 1, 1.0, y(1), 1)
```

This code multiplies the transpose of the submatrix

$$\begin{bmatrix} 1.0 & 2.0 \\ 7.0 & 8.0 \end{bmatrix}$$

by the vector

$$\alpha \begin{bmatrix} 6.0 \\ 8.0 \end{bmatrix}$$

where α is 2.0, and then adds the result to β where β is equal to 1.0 times the first two elements of the vector y to produce the new vector y:

$$\begin{bmatrix} 125.0 & 155.0 & 5.0 & 7.0 & 9.0 & 11.0 & 13.0 & 15.0 & 17.0 \end{bmatrix}^T$$

The vector x and the matrix A remain unchanged.

7

Using the Level 3 BLAS Subprograms

The Level 3 BLAS subprograms perform matrix-matrix operations commonly occurring in many computational problems in linear algebra. This chapter provides information about the following topics:

- Operations performed by the Level 3 BLAS subprograms (Section 7.1)

  7 types of basic operations (Section 7.1.1)
  How Level 3 matrices are stored (Section 7.1.2)
  Subprogram naming conventions (Section 7.1.3)

- Subprogram summary (Section 7.2)
- Calling Level 3 BLAS subprograms (Section 7.3)
- Arguments used in the subprograms and invalid arguments (Sections 7.4 and 7.4.5)
- Error handling (Section 7.5)
- A look at some Level 3 subprograms and their use (Section 7.6)
- Some examples (Section 7.7 and Section 7.8)

A key Level 3 BLAS subprogram, {C,D,S,Z}GEMM, has been parallelized for improved peformance on Tru64 UNIX multiprocessor systems. For information about using the parallel library, see Section A.1.

7.1 Level 3 BLAS Operations

The BLAS Level 3 subprograms perform operations that involve one, two, or three matrices. Operations performed by BLAS Level 3 subprograms do not involve vectors.

7.1.1 Types of Operations

BLAS Level 3 subprograms perform seven types of basic matrix-matrix operations, which are described in this section. In these descriptions, α and β are scalars, A, B and C are rectangular matrices (sometimes symmetric or Hermitian), and T is an upper- or lower-triangular matrix.

- Matrix addition operations

$$C \leftarrow \alpha \mathrm{op}(A) + \beta \mathrm{op}(B)$$

  where $\mathrm{op}(X) = X, X^T, \overline{X}, or X^H$

- Matrix multiply-and-add operations

$$C \leftarrow \alpha \mathrm{op}(A) \mathrm{op}(B) + \beta C$$

  where $\mathrm{op}(X) = X, X^T, \overline{X}, or X^H$

- Matrix subtraction operations

$$C \leftarrow \alpha \mathrm{op}(A) - \beta \mathrm{op}(B)$$

where $\mathrm{op}(X) = X, X^T, \overline{X}, or X^H$

- Miscellaneous matrix operations

$$C \leftarrow \alpha \mathrm{op}(A)$$

where $\mathrm{op}(X) = X, X^T, \overline{X}, or X^H$

- Rank-k and rank-2k updates of a symmetric matrix

$$C \leftarrow \alpha AA^T + \beta C$$

$$C \leftarrow \alpha A^T A + \beta C$$

$$C \leftarrow \alpha AB^T + \alpha BA^T + \beta C$$

$$C \leftarrow \alpha A^T B + \alpha B^T A + \beta C$$

- Full matrix-triangular matrix multiply operations

$$B \leftarrow TB$$

$$B \leftarrow T^T B$$

$$B \leftarrow BT$$

$$B \leftarrow BT^T$$

- Solution of triangular systems of equations

$$TX = \alpha B$$

$$T^T X = \alpha B$$

$$XT = \alpha B$$

$$XT^T = \alpha B$$

Many Level 3 subprograms apply to special types of matrices with the following characteristics:

- Only one of the matrices is symmetric.
- Only one of the matrices is Hermitian.
- Only one of the matrices is triangular.

All Level 3 subprograms have corresponding versions that apply to general rectangular matrices.

7.1.2 Matrix Storage

For the Level 3 BLAS subroutines, all matrices are stored in a two-dimensional array.

There is no provision for packed storage of symmetric, Hermitian, or triangular matrices. For these matrices, only the upper triangle or the lower triangle is stored. Since the imaginary parts of the diagonal elements of a Hermitian matrix are zero, you do not have to set the imaginary parts of the corresponding Fortran array. They are assumed to be zero.

7.1.3 Naming Conventions

Each Level 3 BLAS subroutine has a name consisting of five or six characters. The first character of the name denotes the Fortran data type of the elements of the matrix. The second and third characters denote the type of matrices involved in the operation. The fourth, fifth, and sixth characters denote types of operations.

Table 7–1 shows the characters used in the Level 3 BLAS subroutine names and what the characters mean.

Table 7–1 Naming Conventions: Level 3 BLAS Subprograms

Character	Mnemonic	Meaning
First character	S	Single-precision real data
	D	Double-precision real data
	C	Single-precision complex data
	Z	Double-precision complex data
Second and third characters	GE	General matrices
	HE	One Hermitian matrix
	SY	One symmetric matrix
	TR	One triangular matrix
Fourth, fifth, and sixth characters	MM	Matrix-matrix product
	MA	Matrix addition
	MS	Matrix subtraction
	MT	Matrix transposition
	RK	Rank-k update
	R2K	Rank-2k update
	SM	Solution of a system of linear equations

For example, the name SGEMM is the subroutine for performing matrix-matrix multiplication (and addition if desired), where the matrices are general matrices with single-precision real elements.

7.2 Summary of Level 3 BLAS Subprograms

Table 7–2 summarizes the Level 3 BLAS subroutines provided by CXML. The rank-k updates of general matrices are provided by the _GEMM subroutines.

Table 7–2 Summary of Level 3 BLAS Subprograms

Routine Name	Operation
SGEMA	Calculates, in single-precision arithmetic, the sum of two real general matrices or their transposes.

(continued on next page)

Table 7–2 (Cont.) Summary of Level 3 BLAS Subprograms

Routine Name	Operation
DGEMA	Calculates, in double-precision arithmetic, the sum of two real general matrices or their transposes.
CGEMA	Calculates, in single-precision arithmetic, the sum of two complex general matrices, their transposes, their conjugates, or their conjugate transposes.
ZGEMA	Calculates, in double-precision arithmetic, the sum of two complex general matrices, their transposes, their conjugates, or their conjugate transposes.
SGEMM	Calculates, in single-precision arithmetic, a matrix-matrix product and addition for real general matrices or their transposes.
DGEMM	Calculates, in double-precision arithmetic, a matrix-matrix product and addition for real general matrices or their transposes.
CGEMM	Calculates, in single-precision arithmetic, a matrix-matrix product and addition for complex general matrices, their transposes, their conjugates, or their conjugate transposes.
ZGEMM	Calculates, in double-precision arithmetic, a matrix-matrix product and addition for complex general matrices, their transposes, their conjugates, or their conjugate transposes.
SGEMS	Calculates, in single-precision arithmetic, the difference of two real general matrices or their transposes.
DGEMS	Calculates, in double-precision arithmetic, the difference of two real general matrices or their transposes.
CGEMS	Calculates, in single-precision arithmetic, the difference of two complex general matrices, their transposes, their conjugates, or their conjugate transposes.
ZGEMS	Calculates, in double-precision arithmetic, the difference of two complex general matrices, their transposes, their conjugates, or their conjugate transposes.
SGEMT	Copies a single-precision, real general matrix or its transpose.
DGEMT	Copies a double-precision, real general matrix or its transpose.
CGEMT	Copies a single-precision, complex general matrix, its transpose, its conjugate, or its conjugate transpose.
ZGEMT	Copies a double-precision, complex general matrix, its transpose, its conjugate, or its conjugate transpose.
SSYMM	Calculates, in single-precision arithmetic, a matrix-matrix product and addition where one matrix multiplier is a real symmetric matrix.
DSYMM	Calculates, in double-precision arithmetic, a matrix-matrix product and addition where one matrix multiplier is a real symmetric matrix.
CSYMM	Calculates, in single-precision arithmetic, a matrix-matrix product and addition where one matrix multiplier is a complex symmetric matrix.

(continued on next page)

Table 7–2 (Cont.) Summary of Level 3 BLAS Subprograms

Routine Name	Operation
ZSYMM	Calculates, in double-precision arithmetic, a matrix-matrix product and addition where one matrix multiplier is a complex symmetric matrix.
CHEMM	Calculates, in single-precision arithmetic, a matrix-matrix product and addition where one matrix multiplier is a complex Hermitian matrix.
ZHEMM	Calculates, in double-precision arithmetic, a matrix-matrix product and addition where one matrix multiplier is a complex Hermitian matrix.
SSYRK	Calculates, in single-precision arithmetic, the rank-k update of a real symmetric matrix.
DSYRK	Calculates, in double-precision arithmetic, the rank-k update of a real symmetric matrix.
CSYRK	Calculates, in single-precision arithmetic, the rank-k update of a complex symmetric matrix.
ZSYRK	Calculates, in double-precision arithmetic, the rank-k update of a complex symmetric matrix.
CHERK	Calculates, in single-precision arithmetic, the rank-k update of a complex Hermitian matrix.
ZHERK	Calculates, in double-precision arithmetic, the rank-k update of a complex Hermitian matrix.
SSYR2K	Calculates, in single-precision arithmetic, the rank-2k update of a real symmetric matrix.
DSYR2K	Calculates, in double-precision arithmetic, the rank-2k update of a real symmetric matrix.
CSYR2K	Calculates, in single-precision arithmetic, the rank-2k update of a complex symmetric matrix.
ZSYR2K	Calculates, in double-precision arithmetic, the rank-2k update of a complex symmetric matrix.
CHER2K	Calculates, in single-precision arithmetic, the rank-2k update of a complex Hermitian matrix.
ZHER2K	Calculates, in double-precision arithmetic, the rank-2k update of a complex Hermitian matrix.
STRMM	Calculates, in single-precision arithmetic, a matrix-matrix product for a real triangular matrix or its transpose.
DTRMM	Calculates, in double-precision arithmetic, a matrix-matrix product for a real triangular matrix or its transpose.
CTRMM	Calculates, in single-precision arithmetic, a matrix-matrix product for a complex triangular matrix, its transpose, or its conjugate transpose.
ZTRMM	Calculates, in double-precision arithmetic, a matrix-matrix product for a complex triangular matrix, its transpose, or its conjugate transpose.

(continued on next page)

Table 7–2 (Cont.) Summary of Level 3 BLAS Subprograms

Routine Name	Operation
STRSM	Solves, in single-precision arithmetic, a triangular system of equations where the coefficient matrix is a real triangular matrix.
DTRSM	Solves, in double-precision arithmetic, a triangular system of equations where the coefficient matrix is a real triangular matrix.
CTRSM	Solves, in single-precision arithmetic, a triangular system of equations where the coefficient matrix is a complex triangular matrix.
ZTRSM	Solves, in double-precision arithmetic, a triangular system of equations where the coefficient matrix is a complex triangular matrix.

7.3 Calling the Subprograms

Each of the BLAS Level 3 subprograms returns a matrix. All the subprograms are subroutines. They are called as subroutines with a CALL statement. The example at the end of each subroutine reference description shows the subroutine call.

7.4 Argument Conventions

Each Level 3 BLAS subroutine has arguments that specify the nature and requirements of the subroutine. There are no optional arguments.

The arguments are ordered. Not every argument category is used in all cases in each of the subroutines. In some cases, the user must specify "dummy" (placeholder) arguments.

- Arguments specifying matrix options
- Arguments defining the size of the matrices
- Argument specifying the input scalar
- Arguments describing the input matrices
- Argument specifying the input scalar associated with the input-output matrix
- Arguments describing the input-output matrix

7.4.1 Specifying Matrix Options

The arguments that specify matrix options are character arguments:

- **side**
- **trans**
- **transa**
- **transb**
- **uplo**
- **diag**

Note that the subroutine requires a single character, but the user can supply a longer character string. For example, the value 'T' for **trans** can be passed as 'TRANSPOSE'.

side

The argument **side** is used in some subroutines to specify whether the matrix multiplier is on the left or the right. Table 7–3 shows the meaning of the values for the argument **side**.

Table 7–3 Values for the Argument SIDE

Value of side	Meaning
'L' or 'l'	Multiply the general matrix by the symmetric or triangular matrix on the left
'R' or 'r'	Multiply the general matrix by the symmetric or triangular matrix on the right

trans, transa, transb

Arguments **transa** and **transb** define the form of the input matrices to use in an operation. You do not change the form of an input matrix in your application program. CXML selects the proper elements, depending on the value of the **transa** and **transb** arguments.

For example, if A is the input matrix, and you want to use A in the operation, set the **transa** argument to 'N'. If you want to use A^T in the operation, pass in argument A and set the **trans** argument to 'T'. The subroutine makes the changes and selects the proper elements from the matrix, so that A^T is used. Table 7–4 shows the meaning of the values for the arguments **transa** and **transb**.

Table 7–4 Values for the Arguments transa and transb

Value of transa and transb	Meaning for transa	Meaning for transb
'N' or 'n'	Operate with the matrix A.	Operate with the matrix B.
'T' or 't'	Operate with the transpose of matrix A.	Operate with the transpose of matrix B.
'R' or 'r'	Operate with the conjugate of matrix A.	Operate with the conjugate of matrix B.
'C' or 'c'	Operate with the conjugate transpose of matrix A.	Operate with the conjugate transpose of matrix B.

When an operation is performed with real matrices, the values 'C' and 'c' have the same meaning as 'T' or 't'. And, the values 'R' and 'r' have the same meaning as 'N' or 'n'.

uplo

The Hermitian, symmetric, and triangular matrix subroutines (HE, SY, and TR subroutines) use the argument **uplo** to specify either the upper or lower triangle. Because of the structure of these matrices, the subroutines do not refer to all of the matrix values. Table 7–5 shows the meaning of the values for the argument **uplo**.

Table 7–5 Values for the Argument uplo

Value of uplo	Meaning
'U' or 'u'	Refers to the upper triangle
'L' or 'l'	Refers to the lower triangle

diag

The triangular matrix (TR) subroutines use the argument **diag** to specify whether or not the triangular matrix is unit-triangular. Table 7–6 shows the meaning of the values for the argument **diag**.

Table 7–6 Values for the Argument diag

Value of diag	Meaning
'U' or 'u'	Unit-triangular
'N' or 'n'	Not unit-triangular

When **diag** is specified as 'U' or 'u', the diagonal elements are not referenced by the subroutine. These elements are assumed to be unity (value 1).

7.4.2 Defining the Size of the Matrices

The sizes of the matrices are defined by the arguments **m**, **n**, and **k**. These arguments specify the number of rows or columns, m, n, or k of particular matrices.

You can call a subroutine with arguments **m** or **n** equal to 0 but the subroutine exits immediately without referencing its other arguments. For the _GEMM, _SYRK, and _HERK subroutines, if **k** = 0, the operations are reduced to $C \leftarrow \beta C$.

7.4.3 Describing the Matrices

In addition to their size, the description of each matrix is given by two arguments:

- Arguments that specify the array that stores the matrix: **a**, **b**, and **c** specify the arrays A, B, and C that store the matrices A, B, and C.
- Arguments that specify the leading dimension of each array: **lda**, **ldb**, and **ldc** specify the leading dimension of the arrays A, B, and C.

7.4.4 Specifying the Input Scalar

The input scalars α and β are always specified by the dummy argument names **alpha** and **beta**.

The input scalar associated with the input-output matrix is normally β and is specified by the dummy argument name **beta**.

If you supply an input scalar **beta** of zero, you do not need to initialize the array C. This means that an operation such as $C \leftarrow \alpha AB$ can be performed without having to set C to zero in the calling program.

7.4.5 Invalid Arguments

The following values of Level 3 subroutine arguments are invalid:

- Any value of the arguments **side**, **trans**, **transa**, **transb**, **uplo**, or **diag** that is not specified for the routine
- **m** < 0
- **n** < 0
- **k** < 0
- **lda** < the number of rows in the matrix A
- **ldb** < the number of rows in the matrix B
- **ldc** < the number of rows in the matrix C

7.5 Error Handling

The BLAS Level 3 subroutines do provide a check of the input arguments. If you call a Level 3 subroutine with an invalid value for any of its arguments, CXML reports the message and terminates execution of the program.

The code for BLAS Level 3 subroutines has calls to an input argument error handler, the XERBLA routine. When a subroutine detects an error, it passes the name of the subroutine and the number of the first argument that is in error to the XERBLA routine. CXML directs this information to a device or file:

- For OpenVMS, the device or file is defined as *SYS$OUTPUT*.
- For Tru64 UNIX or Windows NT, the device or file is defined as *stdout*.

7.6 A Look at a Level 3 BLAS Subroutine

The _TRMM subroutines compute a matrix-matrix product for either a triangular matrix, its transpose, or its conjugate transpose:

$$B \leftarrow \alpha AB \qquad B \leftarrow \alpha A^T B \qquad B \leftarrow \alpha A^H B$$

$$B \leftarrow \alpha BA \qquad B \leftarrow \alpha BA^T \qquad B \leftarrow \alpha BA^H$$

The triangular matrix multiply subroutines DTRMM (REAL*8 matrices) and ZTRMM (COMPLEX*16 matrices) have the following call format:

```
CALL DTRMM(side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb)
CALL ZTRMM(side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb)
```

The matrix B is an arbitrary rectangular matrix of size m by n, embedded in a possibly larger ldb by q matrix. The matrix A is a triangular matrix embedded in a larger matrix of size lda by p. The triangular part of A is n by n or m by m, depending on whether A multiplies B on the left side or the right. The user determines this by setting the argument **side**.

The lower or upper triangle of A is accessed by setting the argument **uplo**. The other triangle of A is ignored. The diagonal of A can be used, or it can be assumed to be unity by setting the argument **diag** to `'u'`. Either A, A^T, or A^H can be used by setting the argument **transa**. The scalar α has the same data type as the matrices A and B.

7.7 Examples of REAL*8 Matrices

For the following REAL*8 examples, assume A is a 7 by 7 matrix and B is a 6 by 5 matrix: $lda = 7$, $p = 7$, $ldb = 6$, and $q = 5$, as shown below.

$$A = \begin{bmatrix} -10.00 & -7.00 & -6.00 & 3.00 & 6.00 & -9.00 & 8.00 \\ -4.00 & 5.00 & -6.00 & 2.00 & 3.00 & 5.00 & 1.00 \\ -1.00 & -5.00 & -4.00 & -5.00 & -8.00 & -9.00 & 8.00 \\ -5.00 & 1.00 & -7.00 & -1.00 & 3.00 & 1.00 & -8.00 \\ 6.00 & -2.00 & -6.00 & -4.00 & 9.00 & 2.00 & 3.00 \\ 10.00 & 0.00 & -7.00 & -4.00 & -1.00 & -10.00 & 3.00 \\ 1.00 & 10.00 & 6.00 & 2.00 & -4.00 & -3.00 & 2.00 \end{bmatrix}$$

For matrix B, only the leading 4 by 3 rectangle of B will be used: $m = 4$ and $n = 3$:

$$B = \begin{bmatrix} 4.00 & 9.00 & 2.00 & 5.00 & 0.00 \\ -8.00 & 3.00 & 9.00 & 3.00 & 4.00 \\ 4.00 & -8.00 & 0.00 & 4.00 & -9.00 \\ 7.00 & 4.00 & 8.00 & -2.00 & 0.00 \\ 2.00 & 10.00 & -7.00 & 4.00 & 5.00 \\ 2.00 & 4.00 & -7.00 & 5.00 & -3.00 \end{bmatrix}$$

Example 1: Compute $B \leftarrow \alpha AB$ with $\alpha = 1.0$

For this example, we will use the upper 4 by 4 triangle of A and the original diagonal. The matrix A essentially becomes:

$$\begin{bmatrix} -10.00 & -7.00 & -6.00 & 3.00 \\ 0.00 & 5.00 & -6.00 & 2.00 \\ 0.00 & 0.00 & -4.00 & -5.00 \\ 0.00 & 0.00 & 0.00 & -1.00 \end{bmatrix}$$

The call is shown in the following code:

```
SIDE = 'L'
UPLO = 'U'
TRANSA = 'N'
DIAG = 'N'
CALL DTRMM(SIDE, UPLO, TRANSA, DIAG, 4, 3, 1.0D0, A, LDA, B, LDB)
```

The product matrix B is as follows:

$$\begin{bmatrix} 13.00 & -51.00 & -59.00 \\ -50.00 & 71.00 & 61.00 \\ -51.00 & 12.00 & -40.00 \\ -7.00 & -4.00 & -8.00 \end{bmatrix}$$

Example 2: Compute $B \leftarrow \alpha A^T B$ with $\alpha = -2.0$

For this example, we will use the lower 4 by 4 triangle of A, the original diagonal, and take the transpose. On entry, the matrix A looks like the following:

$$\begin{bmatrix} -10.00 & 0.00 & 0.00 & 0.00 \\ -4.00 & 5.00 & 0.00 & 0.00 \\ -1.00 & -5.00 & -4.00 & 0.00 \\ -5.00 & 1.00 & -7.00 & -1.00 \end{bmatrix}$$

But after the transpose, A becomes:

$$\begin{bmatrix} -10.00 & -4.00 & -1.00 & -5.00 \\ 0.00 & 5.00 & -5.00 & 1.00 \\ 0.00 & 0.00 & -4.00 & -7.00 \\ 0.00 & 0.00 & 0.00 & -1.00 \end{bmatrix}$$

The call is shown in the following code:

```
SIDE = 'L'
UPLO = 'L'
TRANSA = 'T'
DIAG = 'N'
CALL DTRMM(SIDE, UPLO, TRANSA, DIAG, 4, 3, -2.0D0, A, LDA, B, LDB)
```

The product matrix B is as follows:

$$\begin{bmatrix} 94.00 & 228.00 & 192.00 \\ 106.00 & -118.00 & -106.00 \\ 130.00 & -8.00 & 112.00 \\ 14.00 & 8.00 & 16.00 \end{bmatrix}$$

Example 3: Compute $B \leftarrow \alpha BA$ with $\alpha = 3.0$

In this example, matrix A multiplies matrix B on the right, so that A must be 3 by 3. We take the lower triangle of A, and we also assume A has unit diagonal. On entry, A is treated as the following:

$$\begin{bmatrix} 1.00 & 0.00 & 0.00 \\ -4.00 & 1.00 & 0.00 \\ -1.00 & -5.00 & 1.00 \end{bmatrix}$$

The call is shown in the following code:

```
SIDE = 'R'
UPLO = 'L'
TRANSA = 'N'
DIAG = 'U'
CALL DTRMM(SIDE, UPLO, TRANSA, DIAG, 4, 3, 3.0D0, A, LDA, B, LDB)
```

The product matrix B is as follows:

$$\begin{bmatrix} -102.00 & -3.00 & 6.00 \\ -87.00 & -126.00 & 27.00 \\ 108.00 & -24.00 & 0.00 \\ -51.00 & -108.00 & 24.00 \end{bmatrix}$$

7.8 Example of COMPLEX*16 Matrices

In the following COMPLEX*16 example, assume that on entry, A is the following 3 by 3 complex matrix:

$$\begin{bmatrix} (-7.0,-6.0) & (2.0,6.0) & (-4.0,9.0) \\ (-5.0,4.0) & (-6.0,-4.0) & (-10.0,-6.0) \\ (6.0,8.0) & (-3.0,8.0) & (1.0,-8.0) \end{bmatrix}$$

B is the following 4 by 3 complex matrix:

$$\begin{bmatrix} (8.0,-2.0) & (8.0,-9.0) & (10.0,-8.0) \\ (-3.0,8.0) & (3.0,-5.0) & (3.0,4.0) \\ (-2.0,-6.0) & (-6.0,-2.0) & (6.0,2.0) \\ (0.0,10.0) & (10.0,0.0) & (-6.0,-5.0) \end{bmatrix}$$

Example 1: Compute $B \leftarrow \alpha BA^H$ with $\alpha = (1.0,-2.0)$

Where A and B are COMPLEX*16 matrices.

We will use the upper triangle of A and the original diagonal. The triangular A effectively looks like the following:

$$\begin{bmatrix} (-7.0,-6.0) & (2.0,6.0) & (-4.0,9.0) \\ (0.0,0.0) & (-6.0,-4.0) & (-10.0,-6.0) \\ (0.0,0.0) & (0.0,0.0) & (1.0,-8.0) \end{bmatrix}$$

After the conjugate transpose, A becomes the following:

$$\begin{bmatrix} (-7.0,6.0) & (0.0,0.0) & (0.0,0.0) \\ (2.0,-6.0) & (-6.0,-4.0) & (0.0,0.0) \\ (-4.0,-9.0) & (-10.0,6.0) & (1.0,8.0) \end{bmatrix}$$

The call is shown in the following code:

```
SIDE = 'R'
UPLO = 'U'
TRANSA = 'C'
DIAG = 'N'
ALPHA = (1.0D0, -2.0D0)
CALL ZTRMM(SIDE, UPLO, TRANSA, DIAG, 4, 3, ALPHA, A, LDA, B, LDB)
```

The product matrix B is as follows:

$$\begin{bmatrix} (-318.0,326.0) & (388.0,354.0) & (218.0,-76.0) \\ (-317.0,-91.0) & (-12.0,124.0) & (27.0,86.0) \\ (20.0,-40.0) & (-20.0,60.0) & (90.0,70.0) \\ (-173.0,66.0) & (138.0,-6.0) & (-72.0,-121.0) \end{bmatrix}$$

8 Using LAPACK Subprograms

LAPACK is a collection of Fortran 77 routines written to solve a wide array of problems in applied linear algebra. These routines provide CXML users with state of the art tools for linear equation solutions, eigenvalue problems, and linear least squares problems.

LAPACK subprograms are the result of a large, publicly-funded project at major government labs and research universities. These subprograms are intended by their developers to replace and expand the functionality of the famous LINPACK and EISPACK routines.

LAPACK provides enhancements in speed, primarily by utilizing blocked algorithms and the highly optimized CXML BLAS Level 3 and other BLAS routines. The collection also provides better accuracy and robustness than the LINPACK and EISPACK packages. Additionally, two LAPACK computational routines, {C,D,S,Z}GETRF and {C,D,S,Z}POTRF, have been parallelized for improved performance on Tru64 UNIX multiprocessor systems. See Section A.1 for information about using the CXML parallel library. The first public release of LAPACK, Version 1.0, was on February 29, 1992. LAPACK Version 2.0 was released on September 30, 1994 and is part of CXML.

This chapter provides information about the following topics:

- Overview of LAPACK (Section 8.1)
- Naming conventions and mnemonics (Section 8.2)
- A summary of LAPACK driver routines (Section 8.3)
- An example of how LAPACK is used (Section 8.4)
- How to experiment with performance parameters (Section F.1)

To use LAPACK, you must purchase the LAPACK documentation, published in book form, by the Society for Industrial and Applied Math (SIAM) in 1995:

> LAPACK Users' Guide, 2nd Edition, by E. Anderson et al
> SIAM
> 3600 University City Science Center
> Philadelphia PA 19104-2688
> ISBN 0-89871-345-5
> Tel: 1-800-447-SIAM
> FAX: 1-215-386-7999
> email: service@siam.org

Information on ordering SIAM books, including the *LAPACK Users' Guide*, is available on the internet at "http://www.siam.org."

You can also display the html version of the *LAPACK Users' Guide* at the following url:

```
http://www.netlib.org/lapack/lug/lapack_lug.html
```

A quick reference card for all the driver routines is included with SIAM's *LAPACK Users' Guide*.

The LAPACK project is currently based at the University of Tennessee. Information on software releases, corrections to the user guide, and other information can be obtained by sending the following one-line message to `netlib@ornl.gov`:

```
send release_notes from lapack
```

The CXML release notes indicate the version of LAPACK included in the CXML product.

8.1 Overview

The computational tasks carried out by the LAPACK routines play an essential role in solving problems arising in virtually every area of scientific computation, simulation, or mathematical modeling. Optimal performance of the LAPACK routines is assured by the inclusion of high performance BLAS (particularly BLAS Level 3) as part of the CXML library, and the automatic choice of suitable blocking parameters.

The major capabilities provided by LAPACK include:

- Solution of linear systems of equations, that is, solving:

  $$Ax = b$$

  where A is a square matrix, and x and b are vectors.
- Solution of eigenvalue/eigenvector problems, that is, solving:

  $$Ax = \lambda * x$$

  or

  $$Ax = \lambda * B * x$$

  for either λ and/or x. Routines for more general eigenproblems and matrix factorizations involving eigenproblems are also provided.
- Solution of overdetermined systems by means of modern least squares methods including singular value decomposition. These problems involve linear systems of equations where A typically has many more rows than columns (so there are many more equations than unknowns).

Most of the capabilities in LAPACK are provided for several storage formats (full matrix, banded, packed symmetric, and so on). Consult SIAM's LAPACK Users' Guide for a complete description of LAPACK capabilities, including algorithm descriptions and further references.

8.2 Naming Conventions

LAPACK routine names have single letter prefixes indicating the precision (data type) of the input and/or output data:

Mnemonic	Meaning
S	real*4, single-precision
D	real*8, double-precision
C	complex*8, single-precision
Z	complex*16, double-precision

The LAPACK driver and computational (top level) routines always have names of the form:

```
_MMFF
_MMFFX
```

The underscore character (_) is one of the prefixes {S,D,C,Z}. `MM` is a two-letter code indicating the matrix type, that is, its storage and/or mathematical property. `FF` is a code of two or three letters indicating the type of mathematical task being performed. The letter *X* as the last letter on a routine name, indicates an **expert driver** routine, that is, a more sophisticated version of an existing routine which either uses or computes additional information about the problem, for example, condition numbers or error estimates.

Table 8–1 lists the mnemonics and their meaning used for the `mm` code.

Table 8–1 Naming Conventions: Mnemonics for MM

Mnemonic	Meaning
GB	General band matrix
GE	General matrix
GG	General matrices, generalized problems (i.e. a pair of general matrices)
GT	General tridiagonal
HB	(Complex) Hermitian band
HE	Hermitian indefinite (C, Z prefixes only)
HP	Hermitian indefinite, packed storage (C,Z prefixes only)
PB	Positive definite, either symmetric or Hermitian, banded storage
PO	Positive definite, either symmetric or Hermitian
PP	Positive definite, either symmetric or Hermitian, packed storage
PT	Positive definite, either symmetric or Hermitian, tridiagonal
SB	(Real) symmetric band
SP	Symmetric indefinite, packed storage (S, D prefixes only)
ST	Symmetric tridiagonal
SY	Symmetric indefinite (S, D prefixes), or complex symmetric (C, Z prefixes)

Table 8–2 lists the mnemonics for the driver routines and their meaning.

Table 8–2 Naming Conventions: Mnemonics for FF

Mnemonic	Meaning
ES	Eigenvalues and Schur decomposition
EV	Eigenvalues and/or vectors
GLM	Generalized linear regression model
GS	Generalized eigenvalues, Schur form, and/or Schur vectors
GV	Generalized eigenvalues, and/or generalized eigenvectors
LS	Least squares solution, orthogonal factorization (general matrix only)
LSS	Least squares solution, singular value decomposition (general matrix only)
LSE	Least squares solution, Eigenvalues
SV	Linear system solutions
SVD	Singular value decomposition

Subprograms that provide linear system solutions use SV in the `ff` portion of their names. Thus, the simple driver routines for this task all have names of the form:

```
{S,D,C,Z}mmSV.
```

For example, to solve a general linear system with complex input data, you need to call CGESV.

To find the eigenvalues and (optionally) eigenvectors of a general complex Hermitian matrix stored in single precision, you need to call CHEEV.

The generalized eigenvalue routines involve problems of the form:

$$A * x = \lambda * B * x$$

The mnemonics for the mathematical task are **GV** (generalized eigenvalue/vector), or **GS** (generalized Schur factorization).

8.3 Summary of LAPACK Driver Subroutines

Table 8–3 lists simple driver routines for eigenvalue and singular value problems, linear equation solvers and linear least square problems.

Table 8–3 Simple Driver Routines

Routine	Function
Eigenvalue and Singular Value Problems	
SSYEV DSYEV CHEEV ZHEEV	Computes all eigenvalues and eigenvectors of a symmetric/Hermitian matrix.
SSPEV DSPEV CHPEV ZHPEV	Computes all eigenvalues and eigenvectors of a symmetric/Hermitian matrix in packed storage.

(continued on next page)

Table 8–3 (Cont.) Simple Driver Routines

Routine	Function
Eigenvalue and Singular Value Problems	
SSBEV DSBEV CHBEV ZHBEV	Computes all eigenvalues and eigenvectors of a symmeric/Hermitian band matrix.
SSTEV DSTEV	Computes all eigenvalues and eigenvectors of a real symmetric tridiagonal matrix.
SGEES DGEES CGEES ZGEES	Computes the eigenvalues and Schur factorization of a general matrix, and orders the factorization so that selected eigenvalues are at the top left of the Schur form.
SGEEV DGEEV CGEEV ZGEEV	Computes the eigenvalues and left and right eigenvectors of a general matrix.
SGESVD DGESVD CGESVD ZGESVD	Computes the singular value decomposition (SVD) of a general rectangular matrix.
SSYGV DSYGV CHEGV ZHEGV	Computes all eigenvalues and the eigenvectors of a generalized symmetric/Hermitian-definite generalized eigenproblem, $Ax = \lambda Bx$, or $BAx = \lambda x$.
SSPGV DSPGV CHPGV ZHPGV	Computes all eigenvalues and eigenvectors of a generalized symmetric/Hermitian-definite generalized eigenproblem, $Ax = \lambda Bx$, or $BAx = \lambda x$, where A and B are in packed storage.
SSBGV CHBGV	Computes all eigenvalues and eigenvectors of a generalized symmetric/Hermitian-definite and banded eigenproblem, $Ax = \lambda Bx$, or $BAx = \lambda x$.
SGEGS DGEGS CGEGV ZGEGV	Computes the generalized eigenvalues, Schur form, and left and/or right Schur vectors for a pair of nonsymmetric matrices.
SGGSVD DGGSVD CGGSVD ZGGSVD	Computes the generalized singular value decomposition.

(continued on next page)

Table 8–3 (Cont.) Simple Driver Routines

Routine	Function
Linear Equation Problems	
SGESV DGESV CGESV ZGESV	Solves a general system of linear equations AX=B.
SGBSV DGBSV CGBSV ZGBSV	Solves a general banded system of linear equations AX=B.
SGTSV DGTSV CGTSV ZGTSV	Solves a general tridiagonal system of linear equations AX=B.
SPOSV DPOSV CPOSV ZPOSV	Solves a symmetric/Hermitian positive definite system of linear equations AX=B.
SPPSV DPPSV CPPSV ZPPSV	Solves a symmetric/Hermitian positive definite system of linear equations AX=B, where A is held in packed storage.
SPBSV DPBSV CPBSV ZPBSV	Solves a symmetric/Hermitian positive definite banded system of linear equations AX=B.
SPTSV DPTSV CPTSV ZPTSV	Solves a symmetric/Hermitian positive definite tridiagonal system of linear equations AX=B.
SSYSV DSYSV CSYSV ZSYSV CHESV ZHESV	Solves a real/complex/complex symmetric/symmetric/Hermitian indefinite system of linear equations AX=B.
SSPSV DSPSV CSPSV ZSPSV CHPSV ZHPSV	Solves a real/complex/complex symmetric/symmetric/Hermitian indefinite system of linear equations AX=B, where A is held in packed storage.

(continued on next page)

Table 8–3 (Cont.) Simple Driver Routines

Routine	Function
Linear Least Squares Problems	
SGELS DGELS CGELS ZGELS	Computes the least squares solution to an over-determined system of linear equations, AX=B or A**H X=B, or the minimum norm solution of an under-determined system, where A is a general rectangular matrix of full rank, using a QR or LQ factorization of A.
SGELSS DGELSS CGELSS ZGELSS	Computes the minimum norm least squares solution to an over-determined or under-determined system of linear equations AX=B, using the singular value decomposition of A.
SGGGLM DGGGLM CGGGLM ZGGGLM	Solves the GLM (Generalized Linear Regression Model) using the GQR (Generalized QR) factorization.
SGGLSE DGGLSE CGGLSE ZGGLSE	Solves the LSE (Constrained Linear Least Squares Problem) using the GRQ (Generalized RQ) factorization.

Table 8–4 lists the following expert driver routines: linear equation, least square, and eigenvalue.

Table 8–4 Expert Driver Routines

Routine	Function
Linear Equation Problems	
SGESVX DGESVX CGESVX ZGESVX	Solves a general system of linear equations AX=B, A**T X=B or A**H X=B, and provides an estimate of the condition number and error bounds on the solution.
SGBSVX DGBSVX CGBSVX ZGBSVX	Solves a general banded system of linear equations AX=B, A**T X=B or A**H X=B, and provides an estimate of the condition number and the error bounds on the solution.
SGTSVX DGTSVX CGTSVX ZGTSVX	Solves a general tridiagonal system of linear equations AX=B, A**T X=B or A**H X=B, and provides an estimate of the condition number and the error bounds on the solution.
SPOSVX DPOSVX CPOSVX ZGOSVX	Solves a symmetric/Hermitian positive definite system of linear equations AX=B, and provides an estimate of the condition number and error bounds on the solution.
SPPSVX DPPSVX CPPSVX ZPPSVX	Solves a symmetric/Hermitian positive definite system of linear equations AX=B, where A is held in packed storage, and provides an estimate of the condition number and error bounds on the solution.
SPBSVX DPBSVX CPBSVX ZPBSVX	Solves a symmetric/Hermitian positive definite banded system of linear equations AX=B, and provides an estimate of the condition number and error bounds on the solution.

(continued on next page)

Table 8–4 (Cont.) Expert Driver Routines

Routine	Function
Linear Equation Problems	
SPTSVX DPTSVX CPTSVX ZPTSVX	Solves a symmetric/Hermitian positive tridiagonal system of linear equations AX=B, and provides an estimate of the condition number and error bounds on the solution.
SSYSVX DSYSVX CSYSVX ZSYSVX CHESVX ZHESVX	Solves a real/complex/complex symmetric/symmetric/Hermitian indefinite system of linear equations AX=B, and provides an estimate of the condition number and error bounds on the solution.
SSPSVX DSPSVX CSPSVX ZSPSVX CHPSVX ZHPSVX	Solves a real/complex/complex symmetric/symmetric/Hermitian indefinite system of linear equations AX=B, where A is held in packed storage, and provides an estimate of the condition number and error bounds on the solution.
Least Squares Problems	
SGELSX DGELSX CGELSX ZGELSX	Computes the minimum norm least squares solution to an over-determined or under-determined system of linear equations AX=B, using a complete orthogonal factorization of A.
Eigenvalue Problems	
SSYEVX DSYEVX CHEEVX ZHEEVX	Computes selected eigenvalues and eigenvectors of a symmetric/Hermitian matrix.
SSPEVX DSPEVX CHPEVX ZHPEVX	Computes selected eigenvalues and eigenvectors of a symmetric/Hermitian matrix in packed storage.
SSBEVX DSBEVX CHBEVX ZHBEVX	Computes selected eigenvalues and eigenvectors of a symmetric/Hermitian band matrix.
SSTEVX DSTEVX	Computes selected eigenvalues and eigenvectors of a real symmetric tridiagonal matrix.
SGEESX DGEESX CGEESX ZGEESX	Computes the eigenvalues and Schur factorization of a general matrix, orders the factorization so that selected eigenvalues are at the top left of the Schur form, and computes reciprocal condition numbers for the average of the selected eigenvalues, and for the associated right invariant subspace.
SGEEVX DGEEVX CGEEVX ZGEEVX	Computes the eigenvalues and left and right eigenvectors of a general matrix, with preliminary balancing of the matrix, and computes reciprocal condition numbers for the eigenvalues and right eigenvectors.

The remaining routines are either computational or auxiliary. The computational routines solve a lower level of problem than the driver routines and the auxiliary routines solve an even lower level problem.

8.4 Example of LAPACK Use and Design

One of the most common uses for LAPACK is solving linear systems. If you are using the old LINPACK routines to solve $Ax = b$, you first call the subroutine `dgefa` to factor A, and then call `dgesl` to solve the system using the factored A.

In the above case, you can replace the two LINPACK calls with one call to LAPACK. The corresponding LAPACK call is as follows:

```
CALL DGESV(N,NRHS,A,LDA,IPIV,B,LDB,INFO)
```

The routine DGESV calls DGETRF to factor and overwrite A, and DGETRS to solve (overwriting B) using the LU factors computed by DGETRF.

Blocked BLAS Level 3 algorithms come into the picture because DGETRF calls the LAPACK routine ILAENV to obtain an optimal blocksize, and then DGETRF uses blocked algorithms (for example, DTRSM) to complete its task. All of this is invisible to normal top-level use because only the above call to the driver routine DGESV need be made.

8.5 Equivalence Between LAPACK and LINPACK/EISPACK Routines

The LAPACK equivalence utility provides the names and parameter lists of LAPACK routines that are equivalent to the LINPACK and EISPACK routines you specify. The utility command is as follows:

```
directory-spec equivalence_lapack routine_name [routine_name...]
```

where you replace `directory-spec` with the proper directory information, and `routine_name` with the LINPACK and/or EISPACK routine names.

For example, on a UNIX system you would enter:

```
/usr/share/equivalence_lapack dgesl imtql1
```

This returns:

```
DGESL:
      SUBROUTINE SGETRS( TRANS, N, NRHS, A, LDA, IPIV, B, LDB, INFO )
      SUBROUTINE DGETRS( TRANS, N, NRHS, A, LDA, IPIV, B, LDB, INFO )
IMTQL1:
      SUBROUTINE SSTEQR( COMPZ, N, D, E, Z, LDZ, WORK, INFO )
      SUBROUTINE DSTEQR( COMPZ, N, D, E, Z, LDZ, WORK, INFO )
```

The LINPACK or EISPACK routine names are to the left of the colons. The equivalent LAPACK routines and calling sequences are to the right of the colons.

This utility helps you to convert LINPACK and EISPACK routine calls to equivalent LAPACK routine calls. The utility has limitations in that the argument lists of the LAPACK routines are generally different from those of the corresponding LINPACK and EISPACK routines, and the workspace requirements are often different as well.

On Tru64 UNIX systems, the LAPACK equivalence utility is installed in the following location:

```
/usr/opt/XMDLOAnnn/dxml/equivalence_lapack.c  (source code)
/usr/opt/XMDLOAnnn/dxml/equivalence_lapack    (executable)
```

where *nnn* refers to the version number for the release.

On Windows NT systems, the LAPACK equivalence utility is installed in a subdirectory located with the CXML software. This location can vary, depending upon what is specified at installation time. The LAPACK equivalence utility can easily be located by searching for the following files:

```
equivalence_lapack.c  (source code)
equivalence_lapack    (executable)
```

On OpenVMS systems, only the source code for the LAPACK equivalence utility is provided.

9 Using the Signal Processing Subprograms

CXML provides functions that perform signal processing operations for Fast Fourier transforms (FFT), Cosine (DCT) and Sine (DST) transforms, Convolutions and Correlations, and Digital Filters.

This chapter provides information about these functions in the following sections:

- Fast Fourier transforms (FFT) Section 9.1

    Mathematical definitions of FFT (Section 9.1.1)
    Storing the Fourier coefficients (Section 9.1.2)
    Fourier transform functions (Section 9.1.3)

- Cosine (DCT) and Sine (DST) transforms Section 9.2

    Mathematical definitions of DCT and DST (Section 9.2.1)
    Cosine and Sine transform functions (Section 9.2.2.4)

- Convolutions and correlations Section 9.3

    Mathematical description of convolution and correlation (Section 9.3.1)
    Convolution and correlation functions (Section 9.3.2)

- Digital filters Section 9.4

    Mathematical description of a digital filter (Section 9.4.1)
    Controlling a digital filter (Sections 9.4.2 and 9.4.3)
    Filtering routines (Section 9.4.4)

- Error handling (Section 9.5)

For information about using CXML subprograms with non-Fortran programming languages, see Section 2.6 and Section 2.6.2.

Examples are included online in the following locations:

- For Tru64 UNIX: `/usr/examples/dxml`. See `*.c` and `*.cxx`.
- For OpenVMS: `SYS$COMMON:[SYSHLP.EXAMPLES.DXML]`. See `*.c`.
- For Windows NT: Look in the `/examples` subdirectory, located in the directory where CXML is installed. See `*.c` and `*.cxx`.

Key Fast Fourier subprograms have been parallelized for improved peformance on Tru64 UNIX multiprocessor systems. For a list of these subprograms and information about using the parallel library, see Section A.1.

9.1 Fourier Transform

A finite or discrete Fourier transform converts (i.e. transforms) a collection of data into component sine and cosine representation. A continuous Fourier transform of a function converts the function into a generalized sum of sinusoids of different frequencies. A continuous Fourier transform is represented graphically by a diagram that shows the amplitude and frequency of each of the sinusoids.

9.1.1 Mathematical Definition of FFT

The forward Fourier transform is a mathematical operation that converts numbers typically in the time domain to numbers typically in the frequency domain. The inverse Fourier transform performs the reverse operation, converting numbers in the frequency domain to numbers in the time domain.

This section reviews the mathematical definition of the various Fourier transforms.

9.1.1.1 One-Dimensional Continuous Fourier Transform

The analytical expression for the one-dimensional forward Fourier transform for continuous functions is commonly given as:

$$H(f) = \int_{-\infty}^{\infty} h(t)e^{-i2\pi ft}dt \qquad (9–1)$$

where $H(f)$, a function in the frequency domain, is the Fourier transform of $h(t)$; $h(t)$, a function in the time domain, is the waveform to be converted into a sum of sinusoids; and $i = \sqrt{-1}$.

The one-dimensional inverse operation is given as:

$$h(t) = \int_{-\infty}^{\infty} H(f)e^{i2\pi tf}df \qquad (9–2)$$

Variations on the definitions given in Equations (9–1) and (9–2) do exist. Sometimes a weighting function of $1/2\pi$ is found in front of the integral sign, and 2π is removed from the exponential term. See the references given in Appendix G for information on the various definitions of the continuous forward and inverse Fourier transforms.

9.1.1.2 One-Dimensional Discrete Fourier Transform

A digital computer cannot perform the integration indicated by the mathematical expressions for the continuous Fourier transform. Since a digital computer can only deal with discrete data points, the integration can only be approximated.

The Fourier transform functions must use a method known as the discrete Fourier transform (DFT) to approximate the continuous Fourier transform at discrete frequencies. The discrete Fourier transform does not process a continuous function. Instead, it processes discrete points or samples that give only an approximation of the continuous function. The continuous function might not be known analytically.

The simplest interpretation of the one-dimensional discrete Fourier transform results from interpreting a finite sequence as one period of a periodic sequence.

The mathematical expression for the one-dimensional discrete Fourier transform is given as:

$$H(k) = \sum_{m=0}^{n-1} h(m) e^{-i2\pi km/n} \tag{9–3}$$

where m and k are indices, $k = 0, 1, 2, \ldots, n - 1$; $H(k)$ and $h(m)$ represent discrete functions of uniformly spaced data in the time and frequency domains respectively; n is the data length, and $i = \sqrt{-1}$.

The one-dimensional inverse operation is given as:

$$h(m) = \frac{1}{n} \sum_{k=0}^{n-1} H(k) e^{i2\pi mk/n} \tag{9–4}$$

where $m = 0, 1, 2, \ldots, n - 1$

9.1.1.3 Two-Dimensional Discrete Fourier Transform

The simplest interpretation of the two-dimensional discrete Fourier transform results from interpreting a two-dimensional sequence as one period of a doubly periodic sequence.

Thus, with $H(j, k)$ denoting the discrete Fourier transform of $h(m_x, m_y)$, the mathematical expression for the discrete Fourier transform in two dimensions is given as:

$$H(j, k) = \sum_{m_x=0}^{n_x-1} \sum_{m_y=0}^{n_y-1} h(m_x, m_y) e^{(-i2\pi j m_x)/n_x} e^{(-i2\pi k m_y)/n_y} \tag{9–5}$$

where:

$j = 0, 1, 2, \ldots, n_x - 1$
$k = 0, 1, 2, \ldots, n_y - 1$
$i = \sqrt{-1}$

The inverse transform operation in two dimensions is given as:

$$h(m_x, m_y) = \frac{1}{n_x n_y} \sum_{j=0}^{n_x-1} \sum_{k=0}^{n_y-1} H(j, k) e^{(i2\pi j m_x)/n_x} e^{(i2\pi k m_y)/n_y} \tag{9–6}$$

The two-dimensional discrete Fourier transform given by Equation (9–5) can be rewritten as:

$$H(j, k) = \sum_{m_x=0}^{n_x-1} \{ \sum_{m_y=0}^{n_y-1} h(m_x, m_y) e^{(-i2\pi k m_y)/n_y} \} e^{(-i2\pi j m_x)/n_x} \tag{9–7}$$

The quantity in braces, which we now call $G(m_x, k)$, is a two-dimensional sequence which allows $H(j, k)$ to be rewritten as:

$$G(m_x, k) = \sum_{m_y=0}^{n_y-1} h(m_x, m_y) e^{(-i2\pi k m_y)/n_y} \tag{9–8}$$

$$H(j, k) = \sum_{m_x=0}^{n_x-1} G(m_x, k) e^{(-i2\pi m_x j)/n_x} \tag{9–9}$$

Each row of G is the one-dimensional discrete Fourier transform of the corresponding row of h. Each column of H is the one-dimensional discrete Fourier transform of the corresponding column of G.

9.1.1.4 Three-Dimensional Discrete Fourier Transform

For three dimensions, the definition of the forward transform can be written as:

$$H(j,k,l) = \sum_{m_x=0}^{n_x-1} \sum_{m_y=0}^{n_y-1} \sum_{m_z=0}^{n_z-1} h(m_x, m_y, m_z) e^{(-i2\pi j m_x)/n_x} e^{(-i2\pi k m_y)/n_y} e^{(-i2\pi l m_z)/n_z} \qquad (9\text{–}10)$$

where:

$j = 0, 1, 2, \ldots, n_x - 1$
$k = 0, 1, 2, \ldots, n_y - 1$
$l = 0, 1, 2, \ldots, n_z - 1$
$i = \sqrt{-1}$

The three-dimensional inverse operation can be written as:

$$h(m_x, m_y, m_z) = \frac{1}{n_x n_y n_z} \sum_{j=0}^{n_x-1} \sum_{k=0}^{n_y-1} \sum_{l=0}^{n_z-1} H(j,k,l) e^{(i2\pi j m_x)/n_x} e^{(i2\pi k m_y)/n_y} e^{(i2\pi l m_z)/n_z} \qquad (9\text{–}11)$$

where:

$m_x = 0, 1, 2, \ldots, n_x - 1$
$m_y = 0, 1, 2, \ldots, n_y - 1$
$m_z = 0, 1, 2, \ldots, n_z - 1$

9.1.1.5 Size of Fourier Transform

Table 9–1 shows the restrictions on the size of FFT.

Table 9–1 FFT Size

Complex FFT	1D	$n > 0$
	2D	$n_x > 0$
		$n_y > 0$
	3D	$n_x > 0$
		$n_y > 0$
		$n_z > 0$
Real FFT	1D	$n > 0$, n is even
	2D	$n_x > 0$, n_x is even
		$n_y > 0$
	3D	$n_x > 0$, n_x is even
		$n_y > 0$
		$n_z > 0$

9.1.2 Data Storage

The output of Fourier transforms can be stored in several ways, depending on the format of the data, and its symmetry. This section describes the efficiencies of the data storage method.

9.1.2.1 Storing the Fourier Coefficients of a 1D-FFT

When the Fourier transform of a real data sequence is performed, the transformed data is complex, and the identity shown in Equation (9–12) results from symmetry considerations:

$$H(n-k) = H^*(k) \qquad (9\text{–}12)$$

where $H^*(k)$ is the complex conjugate of $H(k)$, and $k = 0, 1, 2, \ldots, \frac{n}{2}$.

Note that $H(0) = H^*(n) = H^*(0)$ and $H(\frac{n}{2}) = H^*(\frac{n}{2})$. Therefore, $H(0)$ and $H(\frac{n}{2})$ are real. So, to specify the Fourier transform of a real sequence, only $(\frac{n}{2} - 1)$ complex values and 2 real values are needed. The storage of the Fourier coefficient takes advantage of this.

When the Fourier transform of a complex data sequence is performed, the transformed data does not usually exhibit symmetry properties. The elements of the resulting output array are usually unique. As a result, all of the output data needs to be stored. CXML stores all the output data, and the length of the output array is the same as the length of the input array.

In the following, let X be the Fourier transform of x.

Storing the 1D-FFT in Real Data Format (R,R)

$$\begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{pmatrix} \longleftrightarrow \begin{pmatrix} X_r(0) \\ X_r(1) \\ \vdots \\ X_r(\frac{n}{2}) \\ X_i(\frac{n}{2}-1) \\ X_i(\frac{n}{2}-2) \\ \vdots \\ X_i(1) \end{pmatrix}$$

In each type of transform, the resulting array has the size described in Table 9–2.

Table 9–2 Size of Output Array for SFFT and DFFT

Direction	Input Format	Output Format	Input Values		Output Values	
			Complex	Real	Complex	Real
F	R	C	0	n	$\frac{n}{2}+1$	0
B	C	R	$\frac{n}{2}+1$	0	0	n
F	R	R	0	n	$\frac{n}{2}-1$	2
B	R	R	$\frac{n}{2}-1$	2	0	n

Storing the 1D-FFT in Complex Data Format (R,C)

$$\begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{pmatrix} \longleftrightarrow \begin{pmatrix} X_r(0) \\ X_i(0) \\ \vdots \\ X_r(\frac{n}{2}) \\ X_i(\frac{n}{2}) \end{pmatrix}$$

In each type of transform, the resulting array has the size described in Table 9–3.

Table 9–3 Size of Output Array from CFFT and ZFFT

Direction	Input Format	Output Format	Input Values		Output Values	
			Complex	Real	Complex	Real
F/B	R	R	n	0	n	0
F/B	C	C	n	0	n	0

Storing the 1D-FFT in Complex Data Format (C,C)

$$\begin{pmatrix} (x_r(0), x_i(0)) \\ \vdots \\ (x_r(N-1), x_i(N-1)) \end{pmatrix} \longleftrightarrow \begin{pmatrix} (X_r(0), X_i(0)) \\ \vdots \\ (X_r(N-1), X_i(N-1)) \end{pmatrix}$$

Storing the Transform of a Complex Sequence in Real Data Format (C,R)

$$\begin{pmatrix} x_r(0) \\ \vdots \\ x_r(N-1) \end{pmatrix} \begin{pmatrix} x_i(0) \\ \vdots \\ x_i(N-1) \end{pmatrix} \longleftrightarrow \begin{pmatrix} X_r(0) \\ \vdots \\ X_r(N-1) \end{pmatrix} \begin{pmatrix} X_i(0) \\ \vdots \\ X_i(N-1) \end{pmatrix}$$

9.1.2.2 Storing the Fourier Coefficients of 2D-FFT

When the 2D FFT of a real data sequence is performed, the transformed data is complex with the following symmetry:

$$H(j,k) = H^*(n_x - j, n_y - k) \qquad (9\text{–}13)$$

for:

$0 \leq j \leq n_x$-1
$0 \leq k \leq n_y$-1

where $H_i(j,k) = 0$ for $(0,0), (\frac{n_x}{2}, 0)(0, \frac{n_y}{2}), \text{and}(\frac{n_x}{2}, \frac{n_y}{2})$. The storage of FFT takes advantage of this.

When the Fourier transform of a complex data sequence is performed, the transformed data does not usually exhibit symmetry properties. As a result, all of the output data needs to be stored. CXML stores all the output data, and the length of the output array is the same as the length of the input array.

Storing a Real Sequence and its Transform in Real Data Format

The following cases show how the value of X is stored in a location in array A. The index of array A starts at zero. When n_y is odd, cases 2 and 4 do not apply.

1. $X_r(0,0) \rightarrow A(0,0)$
2. $X_r(0, \frac{n_y}{2}) \rightarrow A(0, \frac{n_y}{2})$
3. $X_r(\frac{n_x}{2}, 0) \rightarrow A(\frac{n_x}{2}, 0)$
4. $X_r(\frac{n_x}{2}, \frac{n_y}{2}) \rightarrow A(\frac{n_x}{2}, \frac{n_y}{2})$
5. $X_r(j,k) \rightarrow A(j,k), X_i(j,k) \rightarrow A(j, n_y - k)$ for $j = 0, \frac{n_x}{2}, 0 < k < \frac{n_y}{2}$

6. $X_r(j,k) \rightarrow A(j,k), X_i(j,k) \rightarrow A(n_x - j, k)$ for $1 \leq j \leq \frac{n_x}{2} - 1, 0 \leq k \leq n_y - 1$

The following is an example of $n_x = 8$ and $n_y = 4$:

$$\begin{pmatrix} x(0,0) & x(0,1) & x(0,2) & x(0,3) \\ x(1,0) & x(1,1) & x(1,2) & x(1,3) \\ x(2,0) & x(2,1) & x(2,2) & x(2,3) \\ x(3,0) & x(3,1) & x(3,2) & x(3,3) \\ x(4,0) & x(4,1) & x(4,2) & x(4,3) \\ x(5,0) & x(5,1) & x(5,2) & x(5,3) \\ x(6,0) & x(6,1) & x(6,2) & x(6,3) \\ x(7,0) & x(7,1) & x(7,2) & x(7,3) \end{pmatrix} \longleftrightarrow \begin{pmatrix} X_r(0,0) & X_r(0,1) & X_r(0,2) & X_i(0,1) \\ X_r(1,0) & X_r(1,1) & X_r(1,2) & X_r(1,3) \\ X_r(2,0) & X_r(2,1) & X_r(2,2) & X_r(2,3) \\ X_r(3,0) & X_r(3,1) & X_r(3,2) & X_r(3,3) \\ X_r(4,0) & X_r(4,1) & X_r(4,2) & X_i(4,1) \\ X_i(3,0) & X_i(3,1) & X_i(3,2) & X_i(3,3) \\ X_i(2,0) & X_i(2,1) & X_i(2,2) & X_i(2,3) \\ X_i(1,0) & X_i(1,1) & X_i(1,2) & X_i(1,3) \end{pmatrix}$$

Storing a Real Sequence and its Transform in Complex Data Format

$$X_r(j,k) \rightarrow A(2j,k) \qquad 0 \leq j \leq \frac{n_x}{2},\ 0 \leq k \leq n_y - 1$$

$$X_i(j,k) \rightarrow A(2j+1,k) \qquad 0 \leq j \leq \frac{n_x}{2},\ 0 \leq k \leq n_y - 1$$

$$\begin{pmatrix} x(0,0) & x(0,1) & x(0,2) & x(0,3) \\ x(1,0) & x(1,1) & x(1,2) & x(1,3) \\ x(2,0) & x(2,1) & x(2,2) & x(2,3) \\ x(3,0) & x(3,1) & x(3,2) & x(3,3) \\ x(4,0) & x(4,1) & x(4,2) & x(4,3) \\ x(5,0) & x(5,1) & x(5,2) & x(5,3) \\ x(6,0) & x(6,1) & x(6,2) & x(6,3) \\ x(7,0) & x(7,1) & x(7,2) & x(7,3) \end{pmatrix} \longleftrightarrow \begin{pmatrix} X_r(0,0) & X_r(0,1) & X_r(0,2) & X_r(0,3) \\ X_i(0,0) & X_i(0,1) & X_i(0,2) & X_i(0,3) \\ X_r(1,0) & X_r(1,1) & X_r(1,2) & X_r(1,3) \\ X_i(1,0) & X_i(1,1) & X_i(1,2) & X_i(1,3) \\ X_r(2,0) & X_r(2,1) & X_r(2,2) & X_r(2,3) \\ X_i(2,0) & X_i(2,1) & X_i(2,2) & X_i(2,3) \\ X_r(3,0) & X_r(3,1) & X_r(3,2) & X_r(3,3) \\ X_i(3,0) & X_i(3,1) & X_i(3,2) & X_i(3,3) \\ X_r(4,0) & X_r(4,1) & X_r(4,2) & X_r(4,3) \\ X_i(4,0) & X_i(4,1) & X_i(4,2) & X_i(4,3) \end{pmatrix}$$

Storing a Complex Sequence and its Transform in Complex Data Format

$$\begin{pmatrix} (x_r(0,0), x_i(0,0)) & (x_r(0,1), x_i(0,1)) & \dots & (x_r(n_y-1,0), x_i(n_y-1,0)) \\ \vdots & & & \\ (x_r(n_x-1,0), x_i(n_x-1,0)) & \dots & \dots & (x_r(n_x-1,n_y-1), x_i(n_x-1,n_y-1)) \end{pmatrix}$$

$$\updownarrow$$

$$\begin{pmatrix} (X_r(0,0), X_i(0,0)) & (X_r(0,1), X_i(0,1)) & \dots & (X_r(n_y-1,0), X_i(n_y-1,0)) \\ \vdots & & & \\ (X_r(n_x-1,0), X_i(n_x-1,0)) & \dots & \dots & (X_r(n_x-1,n_y-1), X_i(n_x-1,n_y-1)) \end{pmatrix}$$

Storing Complex Sequence in Real Data Format

$$\begin{pmatrix} x_r(0,0) & x_r(0,1) & \dots & x_r(0,n_y-1) \\ x_r(1,0) & x_r(1,1) & \dots & x_r(1,n_y-1) \\ \vdots & & & \\ x_r(n_x-1,0) & \dots & \dots & x_r(n_x-1,n_y-1) \end{pmatrix} \quad \begin{pmatrix} x_i(0,0) & x_i(0,1) & \dots & x_i(0,n_y-1) \\ x_i(1,0) & x_i(1,1) & \dots & x_i(1,n_y-1) \\ \vdots & & & \\ x_i(n_x-1,0) & \dots & \dots & x_i(n_x-1,n_y-1) \end{pmatrix}$$

$$\updownarrow$$

$$\begin{pmatrix} X_r(0,0) & X_r(0,1) & \dots & X_r(0,n_y-1) \\ X_r(1,0) & X_r(1,1) & \dots & X_r(1,n_y-1) \\ \vdots & & & \\ X_r(n_x-1,0) & \dots & \dots & X_r(n_x-1,n_y-1) \end{pmatrix} \quad \begin{pmatrix} X_i(0,0) & X_i(0,1) & \dots & X_i(0,n_y-1) \\ X_i(1,0) & X_i(1,1) & \dots & X_i(1,n_y-1) \\ \vdots & & & \\ X_i(n_x-1,0) & \dots & \dots & X_i(n_x-1,n_y-1) \end{pmatrix}$$

9.1.2.3 Storing the Fourier Coefficients of 3D-FFT

When the Fourier transform of a real data sequence is performed, the transformed data is complex, and the identity shown in Equation (9–14) results from symmetry considerations:

$$H(j,k,l) = H^*(n_x - j, n_y - k, n_z - l) \tag{9–14}$$

for:

$0 \le j \le n_x - 1$
$0 \le k \le n_y - 1$
$0 \le l \le n_z - 1$

where H^* is the complex conjugate of H.

When the Fourier transform of a complex data sequence is performed, the transformed data does not usually exhibit symmetry properties. The elements of the resulting output array are usually unique. As a result, all of the output data needs to be stored. CXML stores all the output data, and the length of the output array is the same as the length of the input array.

Storing Real Sequence in Real Data Format

$$X(j,k,l) = X(n_x - j, n_y - k, n_z - l)$$

For $l = 0$, $x(j,k,0)$ is stored in 2D format.
For $l = \frac{n_z}{2}$, and n_z is even, $x(j,k,\frac{n_z}{2})$ is stored in 2D format.
For $1 \le l \le \frac{n_z}{2} - 1$ is stored in 2D format.

This example is $(8,4,l)$.

$$\begin{pmatrix} x(0,0,l) & x(0,1,l) & x(0,2,l) & x(0,3,l) \\ x(1,0,l) & x(1,1,l) & x(1,2,l) & x(1,3,l) \\ x(2,0,l) & x(2,1,l) & x(2,2,l) & x(2,3,l) \\ x(3,0,l) & x(3,1,l) & x(3,2,l) & x(3,3,l) \\ x(4,0,l) & x(4,1,l) & x(4,2,l) & x(4,3,l) \\ x(5,0,l) & x(5,1,l) & x(5,2,l) & x(5,3,l) \\ x(6,0,l) & x(6,1,l) & x(6,2,l) & x(6,3,l) \\ x(7,0,l) & x(7,1,l) & x(7,2,l) & x(7,3,l) \end{pmatrix} \quad \begin{pmatrix} x(0,0,n_z-l) & x(0,1,n_z-l) & x(0,2,n_z-l) & x(0,3,n_z-l) \\ x(1,0,n_z-l) & x(1,1,n_z-l) & x(1,2,n_z-l) & x(1,3,n_z-l) \\ x(2,0,n_z-l) & x(2,1,n_z-l) & x(2,2,n_z-l) & x(2,3,n_z-l) \\ x(3,0,n_z-l) & x(3,1,n_z-l) & x(3,2,n_z-l) & x(3,3,n_z-l) \\ x(4,0,n_z-l) & x(4,1,n_z-l) & x(4,2,n_z-l) & x(4,3,n_z-l) \\ x(5,0,n_z-l) & x(5,1,n_z-l) & x(5,2,n_z-l) & x(5,3,n_z-l) \\ x(6,0,n_z-l) & x(6,1,n_z-l) & x(6,2,n_z-l) & x(6,3,n_z-l) \\ x(7,0,n_z-l) & x(7,1,n_z-l) & x(7,2,n_z-l) & x(7,3,n_z-l) \end{pmatrix}$$

$$\updownarrow$$

$$\begin{pmatrix} X_r(0,0,l) & X_r(0,1,l) & X_r(0,2,l) & X_r(0,3,l) \\ X_r(1,0,l) & X_r(1,1,l) & X_r(1,2,l) & X_r(1,3,l) \\ X_r(2,0,l) & X_r(2,1,l) & X_r(2,2,l) & X_r(2,3,l) \\ X_r(3,0,l) & X_r(3,1,l) & X_r(3,2,l) & X_r(3,3,l) \\ X_r(4,0,l) & X_r(4,1,l) & X_r(4,2,l) & X_r(4,3,l) \\ X_i(3,0,l) & X_i(3,1,l) & X_i(3,2,l) & X_i(3,3,l) \\ X_i(2,0,l) & X_i(2,1,l) & X_i(2,2,l) & X_i(2,3,l) \\ X_i(1,0,l) & X_i(1,1,l) & X_i(1,2,l) & X_i(1,3,l) \end{pmatrix} \quad \begin{pmatrix} X_i(0,0,l) & X_i(0,3,l) & X_i(0,2,l) & X_i(0,1,l) \\ X_r(1,0,n_z-l) & X_r(1,1,n_z-l) & X_r(1,2,n_z-l) & X_r(1,3,n_z-l) \\ X_r(2,0,n_z-l) & X_r(2,1,n_z-l) & X_r(2,2,n_z-l) & X_r(2,3,n_z-l) \\ X_r(3,0,n_z-l) & X_r(3,1,n_z-l) & X_r(3,2,n_z-l) & X_r(3,3,n_z-l) \\ X_i(4,0,l) & X_i(4,3,l) & X_i(4,2,l) & X_i(4,1,l) \\ X_i(3,0,n_z-l) & X_i(3,1,n_z-l) & X_i(3,2,n_z-l) & X_i(3,3,n_z-l) \\ X_i(2,0,n_z-l) & X_i(2,1,n_z-l) & X_i(2,2,n_z-l) & X_i(2,3,n_z-l) \\ X_i(1,0,n_z-l) & X_i(1,1,n_z-l) & X_i(1,2,n_z-l) & X_i(1,3,n_z-l) \end{pmatrix}$$

The following cases show how the value of X is stored in a location in array A. The index of array A starts at zero. When n_y is odd, cases 3 and 5 do not apply.

1. $1 \le j \le \frac{n_x}{2} - 1$:

$$X_r(j,k,l) \rightarrow A(j,k,l)$$
$$X_i(j,k,l) \rightarrow A(n_x - j,k,l)$$

2. $j = 0, k = 0$:

$$X_r(0,0,l) \rightarrow A(0,0,l)$$
$$X_i(0,0,l) \rightarrow A(0,0,n_z - l)$$

3. $j = 0, k = \frac{n_y}{2}$:

$$X_r(0,\frac{n_y}{2},l) \rightarrow A(0,\frac{n_y}{2},l)$$
$$X_i(0,\frac{n_y}{2},l) \rightarrow A(0,\frac{n_y}{2},n_z - l)$$

4. $j = \frac{n_x}{2}, k = 0$:

$$X_r(\frac{n_x}{2},0,l) \rightarrow A(\frac{n_x}{2},0,l)$$
$$X_i(\frac{n_x}{2},0,l) \rightarrow A(\frac{n_x}{2},0,n_z - l)$$

5. $j = \frac{n_x}{2}, k = \frac{n_y}{2}$:

$$X_r(\frac{n_x}{2},\frac{n_y}{2},l) \rightarrow A(\frac{n_x}{2},\frac{n_y}{2},l)$$
$$X_i(\frac{n_x}{2},\frac{n_y}{2},l) \rightarrow A(\frac{n_x}{2},\frac{n_y}{2},n_z - l)$$

6. $j = 0, 1 \le k \le \frac{n_y}{2} - 1$ or $\frac{n_y}{2} + 1 \le k \le n_y - 1$

$$X_r(0,k,l) \rightarrow A_r(0,k,l)$$
$$X_i(0,k,l) \rightarrow A_r(0,n_y - k,n_z - l)$$

7. $j = \frac{n_x}{2}, 1 \le k \le \frac{n_y}{2} - 1$ or $\frac{n_y}{2} + 1 \le k \le n_y - 1$

$$X_r(\frac{n_x}{2}, k, l) \rightarrow A(\frac{n_x}{2}, k, l)$$

$$X_i(\frac{n_x}{2}, k, l) \rightarrow A(\frac{n_x}{2}, n_y - k, n_z - l)$$

Total memory required = $n_x n_y n_z$

Storing Real Sequence in Complex Format

$$X_r(j, k, l) \rightarrow A(2j, k, l) \quad 0 \le j \le \frac{n_x}{2}, 0 \le k \le n_y - 1, 0 \le l \le n_z - 1$$

$$X_i(j, k, l) \rightarrow A(2j + 1, k, l) \quad 0 \le j \le \frac{n_x}{2}, 0 \le k \le n_y - 1, 0 \le l \le n_z - 1$$

$$\begin{pmatrix} X_r(0,0,l) & X_r(0,1,l) & X_r(0,2,l) & X_r(0,3,l) \\ X_i(0,0,l) & X_i(0,1,l) & X_i(0,2,l) & X_i(0,3,l) \\ X_r(1,0,l) & X_r(1,1,l) & X_r(1,2,l) & X_r(1,3,l) \\ X_i(1,0,l) & X_i(1,1,l) & X_i(1,2,l) & X_i(1,3,l) \\ X_r(2,0,l) & X_r(2,1,l) & X_r(2,2,l) & X_r(2,3,l) \\ X_i(2,0,l) & X_i(2,1,l) & X_i(2,2,l) & X_i(2,3,l) \\ X_r(3,0,l) & X_r(3,1,l) & X_r(3,2,l) & X_r(3,3,l) \\ X_i(3,0,l) & X_i(3,1,l) & X_i(3,2,l) & X_i(3,3,l) \\ X_r(4,0,l) & X_r(4,1,l) & X_r(4,2,l) & X_r(4,3,l) \\ X_i(4,0,l) & X_i(4,1,l) & X_i(4,2,l) & X_i(4,3,l) \end{pmatrix}$$

Total memory required = $2(\frac{n_x}{2} + 1)(n_y n_z) = n_x n_y n_z + 2n_y n_z$

Storing Complex Sequence in Complex Data Format

$$\begin{pmatrix} (x_r(0,0,l), x_i(0,0,l)) & (x_r(0,1,l), x_i(0,1,l)) & \ldots & (x_r(n_y-1,0,l), x_i(n_y-1,0,l)) \\ \vdots & & & \\ (x_r(n_x-1,0,l), x_i(n_x-1,0,l)) & \ldots & \ldots & (x_r(n_x-1,n_y-1,l), x_i(n_x-1,n_y-1,l)) \end{pmatrix}$$

$$\updownarrow$$

$$\begin{pmatrix} (X_r(0,0,l), X_i(0,0,l)) & (X_r(0,1,l), X_i(0,1,l)) & \ldots & (X_r(n_y-1,0,l), X_i(n_y-1,0,l)) \\ \vdots & & & \\ (X_r(n_x-1,0,l), X_i(n_x-1,0,l)) & \ldots & \ldots & (X_r(n_x-1,n_y-1,l), X_i(n_x-1,n_y-1,l)) \end{pmatrix}$$

Storing Complex Sequence in Real Data Format

$$\begin{pmatrix} x_r(0,0,l) & x_r(0,1,l) & \ldots & x_r(0,n_y-1,l) \\ x_r(1,0,l) & x_r(1,1,l) & \ldots & x_r(1,n_y-1,l) \\ \vdots & & & \\ x_r(n_x-1,0,l) & \ldots & \ldots & x_r(n_x-1,n_y-1,l) \end{pmatrix} \begin{pmatrix} x_i(0,0,l) & x_i(0,1,l) & \ldots & x_i(0,n_y-1,l) \\ x_i(1,0,l) & x_i(1,1,l) & \ldots & x_i(1,n_y-1,l) \\ \vdots & & & \\ x_i(n_x-1,0,l) & \ldots & \ldots & x_i(n_x-1,n_y-1,l) \end{pmatrix}$$

$$\updownarrow$$

$$\begin{pmatrix} X_r(0,0,l) & X_r(0,1,l) & \ldots & X_r(0,n_y-1,l) \\ X_r(1,0,l) & X_r(1,1,l) & \ldots & X_r(1,n_y-1,l) \\ \vdots & & & \\ X_r(n_x-1,0,l) & \ldots & \ldots & X_r(n_x-1,n_y-1,l) \end{pmatrix} \begin{pmatrix} X_i(0,0,l) & X_i(0,1,l) & \ldots & X_i(0,n_y-1,l) \\ X_i(1,0,l) & X_i(1,1,l) & \ldots & X_i(1,n_y-1,l) \\ \vdots & & & \\ X_i(n_x-1,0,l) & \ldots & \ldots & X_i(n_x-1,n_y-1,l) \end{pmatrix}$$

9.1.2.4 Storing the Fourier Coefficient of Group FFT

Storing the output of a group FFT operation is similar to the methods used for one-dimensional FFT data storage.

Storing Real Sequence in Real Data Format

$$\begin{pmatrix} x_0 x_1 \ldots x_{n-1} \\ y_0 y_1 \cdots y_{n-1} \\ \vdots \\ z_0 z_1 \ldots z_{n-1} \end{pmatrix} \longleftrightarrow \begin{pmatrix} X_r(0) X_r(1) \ldots X_r(\frac{n}{2}) X_i(\frac{n}{2}-1) \ldots X_i(1) \\ Y_r(0) Y_r(1) \ldots Y_r(\frac{n}{2}) Y_i(\frac{n}{2}-1) \ldots Y_i(1) \\ \vdots \\ Z_r(0) Z_r(1) \ldots Z_r(\frac{n}{2}) Z_i(\frac{n}{2}-1) \ldots Z_i(1) \end{pmatrix}$$

Storing Real Sequence in Complex Data Format

$$\begin{pmatrix} x_0 x_1 \ldots x_{n-1} \\ y_0 y_1 \cdots y_{n-1} \\ \vdots \\ z_0 z_1 \ldots z_{n-1} \end{pmatrix} \longleftrightarrow \begin{pmatrix} (X_r(0) X_i(0)) \ldots (X_r(\frac{n}{2}) X_i(\frac{n}{2})) \\ (Y_r(0) Y_i(0)) \ldots (Y_r(\frac{n}{2}) Y_i(\frac{n}{2})) \\ \vdots \\ (Z_r(0) Z_i(0)) \ldots (Z_r(\frac{n}{2}) Z_i(\frac{n}{2})) \end{pmatrix}$$

Storing Complex Sequence in Complex Data Format

$$\begin{pmatrix} (x_r(0), x_i(0)) \ldots (x_r(n-1), x_i(n-1)) \\ (y_r(0), y_i(0)) \ldots (y_r(n-1), y_i(n-1)) \\ \vdots \\ (z_r(0), z_i(0)) \ldots (z_r(n-1), z_i(n-1)) \end{pmatrix}$$

$$\updownarrow$$

$$\begin{pmatrix} (X_r(0), X_i(0)) \ldots (X_r(n-1), X_i(n-1)) \\ (Y_r(0), Y_i(0)) \ldots (Y_r(n-1), Y_i(n-1)) \\ \vdots \\ (Z_r(0), Z_i(0)) \ldots (Z_r(n-1), Z_i(n-1)) \end{pmatrix}$$

Storing Complex Sequence in Real Data Format

$$\begin{pmatrix} x_r(0)x_r(1)\ldots x_r(n-1) \\ y_r(0)y_r(1)\ldots y_r(n-1) \\ \vdots \\ z_r(0)z_r(1)\ldots z_r(n-1) \end{pmatrix} \begin{pmatrix} x_i(0)x_i(1)\ldots x_i(n-1) \\ y_i(0)y_i(1)\ldots y_i(n-1) \\ \vdots \\ z_i(0)z_i(1)\ldots z_i(n-1) \end{pmatrix}$$

$$\updownarrow$$

$$\begin{pmatrix} X_r(0)X_r(1)\ldots X_r(n-1) \\ Y_r(0)Y_r(1)\ldots Y_r(n-1) \\ \vdots \\ Z_r(0)Z_r(1)\ldots Z_r(n-1) \end{pmatrix} \begin{pmatrix} X_i(0)X_i(1)\ldots X_i(n-1) \\ Y_i(0)Y_i(1)\ldots Y_i(n-1) \\ \vdots \\ Z_i(0)Z_i(1)\ldots Z_i(n-1) \end{pmatrix}$$

9.1.3 CXML's FFT Functions

The CXML provides a comprehensive set of Fourier transform functions covering the following options:

- Dimensions: one, two, or three
- Direction: forward or inverse
- Data type: real or complex
- Data format: real or complex
- Precision: single or double

This section describes the effects of these options.

9.1.3.1 Choosing Data Lengths

The data length is the number of elements being transformed. This length determines the duration and method of computation for FFT operations. To save computation time, choose a nonprime value for the data length to make use of the fast algorithm. A prime value is slower because it cannot use the FFT algorithm.

Choose a value according to the following hierarchy, arranged from best performance to worst performance:

1. The data length is a power of 2.
2. The data length is the product of the small primes 2, 3, and 5.
3. The data length is a product of primes which may be greater than 7.
4. The data length is prime.

Although the performance is best when the data length is a power of 2, none of the functions limit the data length to a power of 2 as is commonly found in other FFT libraries.

9.1.3.2 Input and Output Data Format

The permitted format of input and output data is specified by the arguments **input_format** and **output_format**. Table 9–4 shows the values you specify for these arguments for real and complex, forward and inverse transforms.

Table 9–4 Input and Output Format Argument Values

Direction	Input Format	Output Format
Real Transforms		
Forward	'R'	'C'
Backward	'C'	'R'
Either	'R'	'R'
Complex Transforms		
Either	'R'	'R'
	'C'	'C'

If you use an unsupported combination of input and output format, you receive one of the status values listed in Table 9–5.

Table 9–5 Status Values for Unsupported Input and Output Combinations

Value	Function	Meaning
16	DXML_BAD_FORMAT_STRING()	The specified combination of formats is not supported.
18	DXML_BAD_FORMAT_FOR_DIRECTION()	The specified combination of formats is not supported for the specified direction.

Use the supported combinations as shown in Table 9–4.

9.1.3.3 Using the Internal Data Structures

Every time you perform an FFT operation, the software builds an internal data structure. The data structure provides a convenient way of storing attributes of the FFT such as the data length and type of stride allowed, as well as pointers to virtual memory.

If a program performs repeated FFTs, the process is more efficient if the internal data structure is saved and reused. This saves the recalculation of the same internal data structure over and over again. For this reason, CXML provides two ways of performing fast Fourier transforms, each with its own advantage:

- One-step FFT
  If your program performs only one or a few FFT operations, use one subroutine to initialize, apply, and remove the internal data structure.
- Three-step FFT
  If your program repeats the same FFT operation, use the set of three subroutines:
  - The _INIT subroutine builds the internal data structures.

- The _APPLY subroutine uses the internal data structures to compute the FFT.
- The _EXIT subroutine deallocates the virtual memory that was allocated by the _INIT subroutine.

The internal data structures are constant for a specified length of data, the data type, and for one-, two-, or three-dimensional transforms. When you change one of these characteristics, you must reinitialize the data structure. So, after you call the _INIT routine, you can call the _APPLY routine many times, as long as your data length and data type remains the same.

The three-step subroutines each use an **fft_struct** argument to manipulate the internal data structure. You declare the **fft_struct** using the appropriate call for the data format:

```
RECORD /DXML_S_FFT_STRUCTURE/
RECORD /DXML_D_FFT_STRUCTURE/
RECORD /DXML_C_FFT_STRUCTURE/
RECORD /DXML_Z_FFT_STRUCTURE/
```

These are defined in DXMLDEF.FOR.

You must not do anything else with the **fft_struct** argument. For example, to perform a three-step, one-dimensional, single-precision complex FFT, declare the variable **fft_struct** of type **RECORD /DXML_C_FFT_STRUCTURE/**, as shown in the following code example:

```
 INCLUDE 'DXMLDEF.FOR'
 REAL*4 IN_R(N,100),IN_I(N,100),OUT_R(N,100),OUT_I(N,100)
 COMPLEX*8 IN(N,100),OUT(N,100)
 INTEGER*4 STATUS
 CHARACTER*1 DIRECTION
 RECORD /DXML_C_FFT_STRUCTURE/ FFT_STRUCT

 DIRECTION = 'F'
 STATUS = CFFT_INIT(N,FFT_STRUCT,.TRUE.)
 DO I=1,100
     STATUS = CFFT_APPLY('C','C',DIRECTION,IN(1,I),OUT(1,I),
1                   FFT_STRUCT,1)
 ENDDO
 DO I=1,100
      STATUS = CFFT_APPLY('R','R',DIRECTION,IN_R(1,I),IN_I(1,I),
1                   OUT_R(1,I),OUT_I(1,I),FFT_STRUCT,1)

 ENDDO
 STATUS = CFFT_EXIT(FFT_STRUCT)
```

9.1.3.4 Naming Conventions

A Fourier transform subroutine has a name composed of character groups that tell you about the subroutine's operation. Table 9–6 shows the character groups used in the subroutine names and what they mean.

Table 9–6 Naming Conventions: Fourier Transform Functions

Character Group	Mnemonic	Meaning
First group	S	Single-precision real data

(continued on next page)

Table 9–6 (Cont.) Naming Conventions: Fourier Transform Functions

Character Group	Mnemonic	Meaning
	D	Double-precision real data
	C	Single-precision complex data
	Z	Double-precision complex data
Second group	FFT	Fast Fourier Transform
Third group	No mnemonic	One-step operation
	_INIT	Three-step operation: building of internal data structures
	_APPLY	Three-step operation: perform FFT
	_EXIT	Three-step operation: deallocation of virtual memory in internal data structure
Fourth group	No mnemonic	One-dimensional FFT
	_2D	Two-dimensional FFT
	_3D	Three-dimensional FFT
	_GRP	FFT of grouped data

For example, DFFT_APPLY is the CXML function for calculating in double-precision arithmetic the one-dimensional FFT of real data by applying the internal data structures that were calculated in the first step, DFFT_INIT, of this three-step operation.

9.1.3.5 Summary of Fourier Transform Functions

Table 9–7 summarizes the Fourier transform functions that perform the entire transform, either forward or reverse, in one step.

Table 9–7 Summary of One-Step Fourier Transform Functions

Name	Operation
SFFT	Calculates, in single-precision arithmetic, the fast forward or inverse Fourier transform of one-dimensional, real data.
DFFT	Calculates, in double-precision arithmetic, the fast forward or inverse Fourier transform of one-dimensional, real data.
CFFT	Calculates, in single-precision arithmetic, the fast forward or inverse Fourier transform of one-dimensional, complex data.
ZFFT	Calculates, in double-precision arithmetic, the fast forward or inverse Fourier transform of one-dimensional, complex data.
SFFT_2D	Calculates, in single-precision arithmetic, the fast forward or inverse Fourier transform of two-dimensional, real data.
DFFT_2D	Calculates, in double-precision arithmetic, the fast forward or inverse Fourier transform of two-dimensional, real data.

(continued on next page)

Table 9–7 (Cont.) Summary of One-Step Fourier Transform Functions

Name	Operation
CFFT_2D	Calculates, in single-precision arithmetic, the fast forward or inverse Fourier transform of two-dimensional, complex data.
ZFFT_2D	Calculates, in double-precision arithmetic, the fast forward or inverse Fourier transform of two-dimensional, complex data.
SFFT_3D	Calculates, in single-precision arithmetic, the fast forward or inverse Fourier transform of three-dimensional, real data.
DFFT_3D	Calculates, in double-precision arithmetic, the fast forward or inverse Fourier transform of three-dimensional, real data.
CFFT_3D	Calculates, in single-precision arithmetic, the fast forward or inverse Fourier transform of three-dimensional, complex data.
ZFFT_3D	Calculates, in double-precision arithmetic, the fast forward or inverse Fourier transform of three-dimensional, complex data.
SFFT_GRP	Calculates, in single-precision arithmetic, the fast forward or inverse Fourier transform of a group of real data.
DFFT_GRP	Calculates, in double-precision arithmetic, the fast forward or inverse Fourier transform of a group of real data.
CFFT_GRP	Calculates, in single-precision arithmetic, the fast forward or inverse Fourier transform of a group of complex data.
ZFFT_GRP	Calculates, in double-precision arithmetic, the fast forward or inverse Fourier transform of a group of complex data.

Table 9–8 summarizes the three-step Fourier transform functions. Each function is either an initialization step, an application step, or an exit step.

Table 9–8 Summary of Three-Step Fourier Transform Functions

Name	Operation
SFFT_INIT	Calculates internal data structures.
SFFT_APPLY	Applies SFFT_INIT's internal data structure to calculate, in single-precision arithmetic, the fast forward or inverse Fourier transform of one-dimensional, real data.
SFFT_EXIT	Deallocates the virtual memory allocated by SFFT_INIT.
DFFT_INIT	Calculates internal data structures.
DFFT_APPLY	Applies DFFT_INIT's internal data structure to calculate, in double-precision arithmetic, the fast forward or inverse Fourier transform of one-dimensional, real data.
DFFT_EXIT	Deallocates the virtual memory allocated by DFFT_INIT.
CFFT_INIT	Calculates internal data structures.

(continued on next page)

Table 9–8 (Cont.) Summary of Three-Step Fourier Transform Functions

Name	Operation
CFFT_APPLY	Applies CFFT_INIT's internal data structure to calculate, in single-precision arithmetic, the fast forward or inverse Fourier transform of one-dimensional, complex data.
CFFT_EXIT	Deallocates the virtual memory allocated by CFFT_INIT.
ZFFT_INIT	Calculates internal data structures.
ZFFT_APPLY	Applies ZFFT_INIT's internal data structure to calculate, in double-precision arithmetic, the fast forward or inverse Fourier transform of one-dimensional, complex data.
ZFFT_EXIT	Deallocates the virtual memory allocated by ZFFT_INIT.
SFFT_INIT_2D	Calculates internal data structures.
SFFT_APPLY_2D	Applies SFFT_INIT_2D's internal data structure to calculate, in single-precision arithmetic, the fast forward or inverse Fourier transform of two-dimensional, real data.
SFFT_EXIT_2D	Deallocates the virtual memory allocated by SFFT_INIT_2D.
DFFT_INIT_2D	Calculates internal data structures.
DFFT_APPLY_2D	Applies DFFT_INIT_2D's internal data structure to calculate, in double-precision arithmetic, the fast forward or inverse Fourier transform of two-dimensional, real data.
DFFT_EXIT_2D	Deallocates the virtual memory allocated by DFFT_INIT_2D.
CFFT_INIT_2D	Calculates internal data structures.
CFFT_APPLY_2D	Applies CFFT_INIT_2D's internal data structure to calculate, in single-precision arithmetic, the fast forward or inverse Fourier transform of two-dimensional, complex data.
CFFT_EXIT_2D	Deallocates the virtual memory allocated by CFFT_INIT_2D.
ZFFT_INIT_2D	Calculates internal data structures.
ZFFT_APPLY_2D	Applies ZFFT_INIT_2D's internal data structure to calculate, in double-precision arithmetic, the fast forward or inverse Fourier transform of two-dimensional, complex data.
ZFFT_EXIT_2D	Deallocates the virtual memory allocated by ZFFT_INIT_2D.
SFFT_INIT_3D	Calculates internal data structures.
SFFT_APPLY_3D	Applies SFFT_INIT_3D's internal data structure to calculate, in single-precision arithmetic, the fast forward or inverse Fourier transform of three-dimensional, real data.
SFFT_EXIT_3D	Deallocates the virtual memory allocated by SFFT_INIT_3D.
DFFT_INIT_3D	Calculates internal data structures.

(continued on next page)

Table 9–8 (Cont.) Summary of Three-Step Fourier Transform Functions

Name	Operation
DFFT_APPLY_3D	Applies DFFT_INIT_3D's internal data structure to calculate, in double-precision arithmetic, the fast forward or inverse Fourier transform of three-dimensional, real data.
DFFT_EXIT_3D	Deallocates the virtual memory allocated by DFFT_INIT_3D.
CFFT_INIT_3D	Calculates internal data structures.
CFFT_APPLY_3D	Applies CFFT_INIT_3D's internal data structure to calculate, in single-precision arithmetic, the fast forward or inverse Fourier transform of three-dimensional, complex data.
CFFT_EXIT_3D	Deallocates the virtual memory allocated by CFFT_INIT_3D.
ZFFT_INIT_3D	Calculates internal data structures.
ZFFT_APPLY_3D	Applies ZFFT_INIT_3D's internal data structure to calculate, in double-precision arithmetic, the fast forward or inverse Fourier transform of three-dimensional, complex data.
ZFFT_EXIT_3D	Deallocates the virtual memory allocated by ZFFT_INIT_3D.
SFFT_INIT_GRP	Calculates internal data structures.
SFFT_APPLY_GRP	Applies SFFT_INIT_GRP's internal data structure to calculate, in single-precision arithmetic, the fast forward or inverse Fourier transform of grouped, real data.
SFFT_EXIT_GRP	Deallocates the virtual memory allocated by SFFT_INIT_GRP.
DFFT_INIT_GRP	Calculates internal data structures.
DFFT_APPLY_GRP	Applies DFFT_INIT_GRP's internal data structure to calculate, in double-precision arithmetic, the fast forward or inverse Fourier transform of grouped, real data.
DFFT_EXIT_GRP	Deallocates the virtual memory allocated by DFFT_INIT_GRP.
CFFT_INIT_GRP	Calculates internal data structures.
CFFT_APPLY_GRP	Applies CFFT_INIT_GRP's internal data structure to calculate, in single-precision arithmetic, the fast forward or inverse Fourier transform of grouped, complex data.
CFFT_EXIT_GRP	Deallocates the virtual memory allocated by CFFT_INIT_GRP.
ZFFT_INIT_GRP	Calculates internal data structures.
ZFFT_APPLY_GRP	Applies SFFT_INIT_GRP's internal data structure to calculate, in double-precision arithmetic, the fast forward or inverse Fourier transform of grouped, complex data.
ZFFT_EXIT_GRP	Deallocates the virtual memory allocated by ZFFT_INIT_GRP.

9.2 Cosine and Sine Transforms

Similar to the discrete Fourier transform, the Cosine and the Sine transforms decompose a collection of data into a finite sum of sinusoids of different frequencies. The differences among the three transforms are in the assumptions about the data to be transformed. For example, the Fourier transform makes no assumptions about the data as long as the existence conditions for the Fourier integral are satisfied. The Sine transform assumes that the functions to be transformed are odd. The Cosine transform assumes that the functions to be transformed are even.

9.2.1 Mathematical Definitions of DCT and DST

This section reviews the mathematical definitions of the Sine and the Cosine transforms.

9.2.1.1 One-Dimensional Continuous Cosine and Sine Transforms

The analytical expressions for the one-dimensional forward Cosine transform and the one-dimensional forward Sine transform for continuous functions are commonly given as:

$$C(\omega) = \sqrt{\frac{2}{\pi}} \int_0^\infty h(t)\ cos(\omega t)\ dt \tag{9–15}$$

and:

$$S(\omega) = \sqrt{\frac{2}{\pi}} \int_0^\infty h(t)\ sin(\omega t)\ dt \tag{9–16}$$

respectively. $C(\omega)$ and $S(\omega)$, functions in the frequency domain, are the Cosine and the Sine transforms of $h(t)$. $h(t)$, a function in the time domain, is the waveform to be decomposed into a sum of sinusoids.

Equations for reversing the Cosine and the Sine transforms are as follows:

$$h(t) = \sqrt{\frac{2}{\pi}} \int_0^\infty C(\omega)\ cos(\omega t)\ d\omega \tag{9–17}$$

and:

$$h(t) = \sqrt{\frac{2}{\pi}} \int_0^\infty S(\omega)\ sin(\omega t)\ d\omega \tag{9–18}$$

respectively.

9.2.1.2 One-Dimensional Discrete Cosine and Sine Transforms

Similar to continuous Fourier transforms, continuous Cosine and Sine transforms can be discretized. Unlike the Fourier transforms, there are multiple discretization schemes that lead to multiple definitions of the discrete Cosine and Sine transforms. The simplest discretization uses the following transforms:

Type I Cosine Transform

$$C^I(k) = \alpha_k \sum_{m=0}^{N} \alpha_m\ h(m)\ cos(\frac{\pi m k}{N}) \tag{9–19}$$

where $k = 0, ..., N$.

Type I Sine Transform

$$S^{I}(k) = \sum_{m=1}^{N-1} h(m)\ sin(\frac{\pi mk}{N}) \qquad (9\text{–}20)$$

where $k = 1, ..., N - 1$
and where

$$\alpha_k = \left\{ \begin{array}{ll} \frac{1}{\sqrt{2}} & k = 0, N \\ 1 & 1 \leq k \leq N - 1 \end{array} \right\} \qquad (9\text{–}21)$$

The inverse formulas for the Type I transforms are the following:

Inverse Type I Cosine Transform

$$h(m) = \alpha_m \frac{2}{N} \sum_{k=0}^{N} \alpha_k C^{I}(k)\ cos(\frac{\pi mk}{N}) \qquad (9\text{–}22)$$

where $m = 0, ..., N$.

Inverse Type I Sine Transform

$$h(m) = \frac{2}{N} \sum_{k=1}^{N-1} S^{I}(k)\ sin(\frac{\pi mk}{N}) \qquad (9\text{–}23)$$

where $m = 1, ..., N - 1$ and with α_k defined in (9–21).

Additionally, CXML implements the following Type II transforms:

Type II Cosine Transform

$$C^{II}(k) = \alpha_k \sum_{m=0}^{N-1} h(m)\ cos[\frac{(2m+1)k\pi}{2N}] \qquad (9\text{–}24)$$

where $k = 0, ..., N - 1$.

Type II Sine Transform

$$S^{II}(k) = \alpha_k \sum_{m=1}^{N} h(m)\ sin[\frac{(2m-1)k\pi}{2N}] \qquad (9\text{–}25)$$

where $k = 1, ..., N$.

Inverse Type II Cosine Transform

$$h(m) = \frac{2}{N} \sum_{k=0}^{N} \alpha_k\ C^{II}(k)\ cos[\frac{(2m+1)k\pi}{2N}] \qquad (9\text{–}26)$$

where $m = 0, ..., N - 1$.

Inverse Type II Sine Transform

$$h(m) = \frac{2}{N} \sum_{k=1}^{N} \alpha_k\ S^{II}(k)\ sin[\frac{(2m-1)k\pi}{2N}] \qquad (9\text{–}27)$$

where $m = 1, ..., N$ with α_k defined in (9–21). Although there are two other forms of Cosine and Sine transforms, they are not implemented in CXML. See the references given in Appendix G for information on the other forms of Cosine and Sine transforms.

9.2.1.3 Size of Cosine and Sine Transforms

N, the size of the Cosine and Sine transforms, must be greater than 0 and even.

9.2.1.4 Data Storage

The minimum size and the starting index for the input and output array for each type of Cosine and Sine transform is listed in Table 9–9.

Table 9–9 Size and Starting Index for _FCT and _FST

Transform	Type	Minimum Size	Starting Index
Cosine	I	N+1	0
Sine	I	N-1	1
Cosine	II	N	0
Sine	II	N	1

9.2.2 CXML's FCT and FST Functions

CXML provides the following set of Cosine and Sine transform functions covering the following options:

- Direction: forward or inverse
- Precision: single or double
- Type: I or II

9.2.2.1 Choosing Data Lengths

Since the Cosine and Sine transform functions are built on the FFT functions, the same considerations for choosing the data length for the Fourier transforms should be applied to the Cosine and Sine transforms. See Section 9.1.3.1 for information on choosing the data lengths for FFT.

9.2.2.2 Using the Internal Data Structures

Each time you perform an FCT or an FST operation, the software builds an internal data structure. The data structure provides a convenient way of storing attributes of the FCT or FST operation such as the data length, type of stride allowed, and pointers to virtual memory. If a program performs repeated FCTs or FSTs, the process is more efficient if the internal data structure is saved and re-used. For this reason, CXML provides two ways of performing FCT and FST transforms:

- One-step FCT or FST
  If your program performs only one or a few FCT or FST operations, use one subroutine to initialize, apply, and remove the internal data structure.
- Three-step FCT or FST
  If your program repeats the same FCT or FST operations, use the set of three subroutines:
  - The _INIT subroutine builds the internal data structures.
  - The _APPLY subroutine uses the internal data structures to compute the FCT or FST.
  - The _EXIT subroutine deallocates the virtual memory that was allocated by the _INIT subroutine.

The internal data structures are constant for a specified length of data. When you change the length of data, you must reinitialize the data structure. After you call the _INIT routine, you can call the _APPLY routine repeatedly as long as the data length and transform type remain the same.

Each three-step subroutine uses a structure argument to manipulate the internal data structure. You declare the data structure using the appropriate structure argument for the data format.

For FCT:

```
RECORD /DXML_S_FCT_STRUCTURE/
RECORD /DXML_D_FCT_STRUCTURE/
```

For FST:

```
RECORD /DXML_S_FST_STRUCTURE/
RECORD /DXML_D_FST_STRUCTURE/
```

You do not have to do anything else with this argument. For example, to perform a three-step, one-dimensional, single-precision Type I FST, declare the variable **FST_STRUCT** of type **RECORD /DXML_S_FST_STRUCTURE/**, as shown in the following code example:

```
 REAL*4 IN(N,100),OUT(N,100)
 INTEGER*4 SFST_INIT, SFST_APPLY, SFST_EXIT
 INTEGER*4 STATUS
 RECORD /DXML_S_FST_STRUCTURE/ FST_STRUCT
 CHARACTER*1 DIRECTION

 DIRECTION = 'F'
 STATUS = SFST_INIT(N,FST_STRUCT,1,.TRUE.)
 DO I=1,100
     STATUS = SFST_APPLY(DIRECTION,IN(1,I),OUT(1,I),
1                   FFT_STRUCT,1)
 ENDDO
 STATUS = SFST_EXIT(FFT_STRUCT)
```

9.2.2.3 Naming Conventions

A Cosine or a Sine transform subroutine has a name composed of character groups that tell you about the subroutine's operation. Table 9–10 shows the character groups used in the subroutine names and what they mean.

Table 9–10 Naming Conventions: Cosine and Sine Transform Functions

Character Group	Mnemonic	Meaning
First group	S	Single-precision real data
	D	Double-precision real data
Second group	FCT	Fast Cosine Transform
	FST	Fast Sine Transform
Third group	No mnemonic	One-step operation
	_INIT	Three-step operation: building of internal data structures

(continued on next page)

Table 9–10 (Cont.) Naming Conventions: Cosine and Sine Transform Functions

Character Group	Mnemonic	Meaning
	_APPLY	Three-step operation: perform FCT or FST
	_EXIT	Three-step operation: deallocation of virtual memory in internal data structure

For example, SFST_APPLY is the CXML function for calculating in single-precision arithmetic the one-dimensional FST of real data by applying the internal data structures that were calculated in the first step, SFST_INIT, of this three-step operation.

9.2.2.4 Summary of Cosine and Sine Transform Functions

Table 9–11 summarizes the Cosine and Sine transform functions that perform the entire transform in one step.

Table 9–11 Summary of One-Step Cosine and Sine Transform Functions

Name	Operation
SFCT	Calculates, in single-precision arithmetic, the fast Cosine transform of one-dimensional, real data.
DFCT	Calculates, in double-precision arithmetic, the fast Cosine transform of one-dimensional, real data.
SFST	Calculates, in single-precision arithmetic, the fast Sine transform of one-dimensional, real data.
DFST	Calculates, in double-precision arithmetic, the fast Sine transform of one-dimensional, real data.

Table 9–12 summarizes the three-step Cosine and Sine transform functions. Each function is either an initialization step, an application step, or an exit step.

Table 9–12 Summary of Three-Step Cosine and Sine Transform Functions

Name	Operation
SFCT_INIT	Sets up internal data structures.
SFCT_APPLY	Applies SFCT_INIT's internal data structure to calculate, in single-precision arithmetic, the fast Cosine transform of one-dimensional, real data.
SFCT_EXIT	Releases internal data structures set up by SFCT_INIT.
DFST_INIT	Sets up internal data structures.
DFST_APPLY	Applies DFST_INIT's internal data structure to calculate, in double-precision arithmetic, the fast Sine transform of one-dimensional, real data.
DFST_EXIT	Releases internal data structures set up by DFST_INIT.

9.3 Convolution and Correlation

Convolution and correlation are operations that complement the signal processing abilities of the Fourier transform. All number transforms (including the FFT) and most digital filters are convolution operations.

Convolution modifies a signal sequence by weighting the sequence with a function or an additional sequence of numbers. The convolution is used to obtain properties from a signal source (such as the nth derivative), to selectively enhance the signal source (in the case of a filter), or to domain transform the signal source (as in the case of a Fourier transform). Some type of convolution is the basis for most signal processing.

Correlation analyzes the similarity between two signals (as in the case of cross-correlation) or of a signal with itself (as in the case of auto-correlation).

9.3.1 Mathematical Definitions of Correlation and Convolution

Many definitions exist for convolution and correlation. CXML uses very specific definitions given in Sections 9.3.1.1, 9.3.1.2, and 9.3.1.3.

9.3.1.1 Definition of the Discrete Nonperiodic Convolution

The most common definition of a discrete nonperiodic convolution is given by:

$$h_j = \sum_{k=0}^{n_h-1} x_{(j-k)} y_k \qquad (9\text{–}28)$$

for $j = 0, 1, 2, \ldots, n_h - 1$ and $n_h = n_x + n_y - 1$.

Here, n_h is the total number of points to be output from the convolution subroutine, n_x is the number of points in the x array, and n_y is the number of points in the y array.

The y array is often called the filter array because nonrecursive digital filters are commonly made by using convolution of the x data array with special filter coefficients in the y array. For more information, consult the references given in Appendix G.

The definition of convolution given in Equation (9–28) is operational for infinitely long data sets in x and y, but because the data lengths are finite, in practice, the subscript $(j - k)$ will be out of range for the x array for certain values of j and k, and the subscript k will be out of range for the y array for certain values of k.

$$x_k = 0 \text{ when } k < 0 \text{ or } k > n_x - 1 \qquad (9\text{–}29)$$

$$y_k = 0 \text{ when } k < 0 \text{ or } k > n_y - 1 \qquad (9\text{–}30)$$

For the general case used in CXML, the definition of nonperiodic convolution can be rewritten as:

$$h_j = \sum_{k=\max\{0,j-n_x+1\}}^{\min\{n_y-1,j\}} x_{(j-k)} y_k \qquad (9\text{–}31)$$

9.3.1.2 Definition of the Discrete Nonperiodic Correlation

For correlation, a similar situation exists. For the idealized case of infinitely long data lengths, the definition of discrete nonperiodic correlation of two data sets, x and y, is given as:

$$h_j = \sum_{k=0}^{n_h-1} x_{(j+k)} y_k \qquad (9\text{–}32)$$

for $1 - n_y \leq j \leq n_x - 1$

Here, n_h is the total number of points to be output from the correlation subroutine, n_x is the number of points in the x array, and n_y is the number of points in the y array.

Because of the finite lengths of the arrays, the relationships given by Equations (9–29) and (9–30) are used:

$$x_k = 0 \text{ when } k < 0 \text{ or } k > n_x - 1$$

$$y_k = 0 \text{ when } k < 0 \text{ or } k > n_y - 1$$

For this case, the definition of nonperiodic correlation can be rewritten as:

$$h_j = \sum_{k=\max\{0,-j\}}^{\min\{n_x-j,n_y\}-1} x_{(j+k)} y_k \qquad (9\text{–}33)$$

Many variations on the definitions of convolution and correlation given in Equations (9–28) and (9–32) exist, but CXML uses the definitions given by these equations. Some definitions of convolution and correlation contain a normalization factor such as a $1/N$ term in front of the summation symbol where N is usually n_h as given in the CXML definitions. CXML subroutines do not use a normalization factor.

9.3.1.3 Periodic Convolution and Correlation

For periodic convolution, CXML uses the nonperiodic definition with a few differences. For $0 \leq j \leq n - 1$:

$$h_j = \sum_{k=0}^{n-1} x_{(j-k)} y_k \qquad (9\text{–}34)$$

For periodic correlation, CXML uses the following definition. Again, for $0 \leq j \leq n-1$:

$$h_j = \sum_{k=0}^{n-1} x_{(j+k)} y_k \qquad (9\text{–}35)$$

x and y are periodic with period n, that is, $x_{(j+n)} = x_j$, $y_{(j+n)} = y_j$. The data length of the output h array is equal to that of the x and y array.

If the subscript on either x or y is out of range, the value is that of the folded array. Folding is simply a modulus operation which implies periodicity.

As with nonperiodic convolution and correlation, no normalization factor is used in front of the summation symbol in the definition of periodic convolution and correlation.

For more information on periodic convolution and correlation, refer to the references given in Appendix G.

9.3.2 CXML's Convolution and Correlation Subroutines

CXML includes a wide variety of discrete convolution and correlation subroutines that support both periodic (circular) and nonperiodic (linear) convolution and correlation. Each subroutine is available for both real and complex data and for single-precision and double-precision arithmetic.

9.3.2.1 Using FFT Methods for Convolution and Correlation

CXML provides subroutines for calculating discrete convolutions and correlations by using a discrete summing technique. Other techniques that use fast Fourier transforms for calculating convolutions and correlations also exist, but they are not part of CXML.

When data lengths are large and there is a time-critical need for computing convolution and correlation functions, these FFT methods should be used. The data lengths must be large because the FFT methods introduce distortion near the edges of the data, unless there is true periodicity in the data, the data is well behaved near the ends, and many periods are sampled.

For more information on performing convolution and correlation with FFTs, refer to the references given in Appendix G.

9.3.2.2 Naming Conventions

A convolution or correlation subroutine has a name composed of character groups that tell you about the subroutine's operation. Table 9–13 shows the character groups used in the subroutine names and what they mean.

Table 9–13 Naming Conventions: Convolution and Correlation Subroutines

Character Group	Mnemonic	Meaning
First group	S	Single-precision real data
	D	Double-precision real data
	C	Single-precision complex data
	Z	Double-precision complex data
Second group	CONV	Convolution subroutine
	CORR	Correlation subroutine
Third group	_NONPERIODIC	Nonperiodic operation
	_PERIODIC	Periodic operation
	_NONPERIODIC_EXT	Nonperiodic operation with extension[1]
	_PERIODIC_EXT	Periodic operation with extension[1]

[1]The subroutines with extensions provide many additional arguments to control the result.

For example, SCORR_PERIODIC is the CXML subroutine for calculating in single-precision arithmetic the periodic correlation of two real arrays.

9.3.2.3 Summary of Convolution and Correlation Subroutines

Tables 9–14 and 9–15 summarize the convolution and correlation subroutines.

Table 9–14 Summary of Convolution Subroutines

Subroutine Name	Operation
SCONV_NONPERIODIC	Calculates, in single-precision arithmetic, the nonperiodic convolution of two real arrays.
DCONV_NONPERIODIC	Calculates, in double-precision arithmetic, the nonperiodic convolution of two real arrays.
CCONV_NONPERIODIC	Calculates, in single-precision arithmetic, the nonperiodic convolution of two complex arrays.
ZCONV_NONPERIODIC	Calculates, in double-precision arithmetic, the nonperiodic convolution of two complex arrays.
SCONV_PERIODIC	Calculates, in single-precision arithmetic, the periodic convolution of two real arrays.
DCONV_PERIODIC	Calculates, in double-precision arithmetic, the periodic convolution of two real arrays.
CCONV_PERIODIC	Calculates, in single-precision arithmetic, the periodic convolution of two complex arrays.
ZCONV_PERIODIC	Calculates, in double-precision arithmetic, the periodic convolution of two complex arrays.
SCONV_NONPERIODIC_EXT	Calculates, in single-precision arithmetic, the nonperiodic convolution of two real arrays.
DCONV_NONPERIODIC_EXT	Calculates, in double-precision arithmetic, the nonperiodic convolution of two real arrays.
CCONV_NONPERIODIC_EXT	Calculates, in single-precision arithmetic, the nonperiodic convolution of two complex arrays.
ZCONV_NONPERIODIC_EXT	Calculates, in double-precision arithmetic, the nonperiodic convolution of two complex arrays.
SCONV_PERIODIC_EXT	Calculates, in single-precision arithmetic, the periodic convolution of two real arrays.
DCONV_PERIODIC_EXT	Calculates, in double-precision arithmetic, the periodic convolution of two real arrays.
CCONV_PERIODIC_EXT	Calculates, in single-precision arithmetic, the periodic convolution of two complex arrays.
ZCONV_PERIODIC_EXT	Calculates, in double-precision arithmetic, the periodic convolution of two complex arrays.

Table 9–15 Summary of Correlation Subroutines

Subroutine Name	Operation
SCORR_NONPERIODIC	Calculates, in single-precision arithmetic, the nonperiodic correlation of two real arrays.
DCORR_NONPERIODIC	Calculates, in double-precision arithmetic, the nonperiodic correlation of two real arrays.
CCORR_NONPERIODIC	Calculates, in single-precision arithmetic, the nonperiodic correlation of two complex arrays.

(continued on next page)

Table 9–15 (Cont.) Summary of Correlation Subroutines

Subroutine Name	Operation
ZCORR_NONPERIODIC	Calculates, in double-precision arithmetic, the nonperiodic correlation of two complex arrays.
SCORR_PERIODIC	Calculates, in single-precision arithmetic, the periodic correlation of two real arrays.
DCORR_PERIODIC	Calculates, in double-precision arithmetic, the periodic correlation of two real arrays.
CCORR_PERIODIC	Calculates, in single-precision arithmetic, the periodic correlation of two complex arrays.
ZCORR_PERIODIC	Calculates, in double-precision arithmetic, the periodic correlation of two complex arrays.
SCORR_NONPERIODIC_EXT	Calculates, in single-precision arithmetic, the nonperiodic correlation of two real arrays.
DCORR_NONPERIODIC_EXT	Calculates, in double-precision arithmetic, the nonperiodic correlation of two real arrays.
CCORR_NONPERIODIC_EXT	Calculates, in single-precision arithmetic, the nonperiodic correlation of two complex arrays.
ZCORR_NONPERIODIC_EXT	Calculates, in double-precision arithmetic, the nonperiodic correlation of two complex arrays.
SCORR_PERIODIC_EXT	Calculates, in single-precision arithmetic, the periodic correlation of two real arrays.
DCORR_PERIODIC_EXT	Calculates, in double-precision arithmetic, the periodic correlation of two real arrays.
CCORR_PERIODIC_EXT	Calculates, in single-precision arithmetic, the periodic correlation of two complex arrays.
ZCORR_PERIODIC_EXT	Calculates, in double-precision arithmetic, the periodic correlation of two complex arrays.

9.4 Digital Filtering

Digital filters are subroutines that eliminate certain frequency components from a signal which has been corrupted with unwanted noise. CXML provides a nonrecursive filter (also known as a finite impulse response filter) which can be used in four ways:

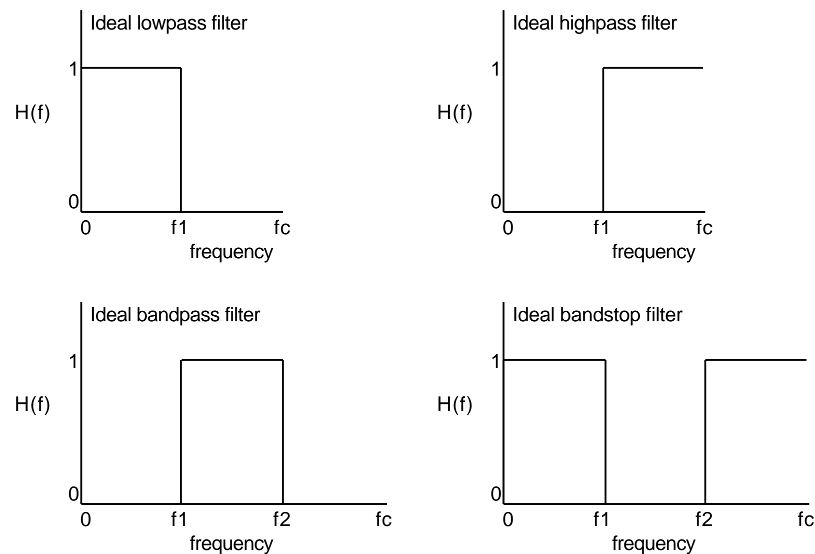
- Lowpass filter
  Eliminates frequency components above one value.
- Highpass filter
  Eliminates frequency components below one value.
- Bandpass filter
  Eliminates frequency components except those within a certain range.
- Bandstop (notch) filter
  Eliminates frequency components within a certain range.

The CXML nonrecursive filter is an adaptation of the $I_0 - sinh$ filter originally proposed by Kaiser.

9.4.1 Mathematical Definition of the Nonrecursive Filter

The transfer function of a nonrecursive digital filter, denoted as H(f), determines the range of frequencies that are eliminated by a filter. Putting a sinusoidal function of frequency f into the filter results in the output being the same as the sinusoid, except that its amplitude is multiplied by H(f). The transfer function H(f) can take on any of the forms shown in Figure 9–1.

Figure 9–1 Digital Filter Transfer Function Forms



In Figure 9–1 fc refers to the Nyquist frequency $1/(2\Delta t)$, Δt is the time between data samples, and f1 and f2 refer to the frequency values where filtering is to be applied.

These ideal filters represent an infinitely sharp band; in practice, as shown in Figure 9–2, the vertical lines are skewed.

The filtering discussed here pertains only to nonrecursive filters of the form:

$$y_n = A_0 x_n + \sum_{k=1}^{nterms} A_k \left(x_{(n+k)} + x_{(n-k)} \right) \qquad (9–36)$$

where y_n is the dependent variable synthesized by the use of previous dependent values x, A_k are the filter-dependent coefficients, and $nterms$ is the number of filter coefficients with A_0 not included.

9.4.2 Controlling Filter Type

In the filter subroutines SFILTER_NONREC and SFILTER_INIT_NONREC, you use the **flow** and **fhigh** arguments to control the type of filtering. Table 9–16 shows the **flow** and **fhigh** argument values associated with particular filtering types.

Table 9–16 Controlling Filtering Type

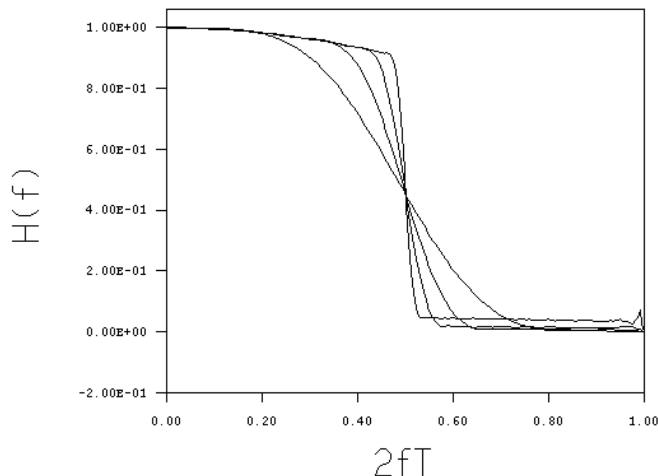
For a filter type of:	Set flow to:	Set fhigh to:
No filtering	0	1
Lowpass filter	0	0 < fhigh < 1
Highpass filter	0 < flow < 1	1
Bandpass filter	0 < flow < fhigh	flow < fhigh < 1
Bandstop filter	fhigh < flow < 1	0 < fhigh < flow

9.4.3 Controlling Filter Sharpness and Smoothness

In the filter subroutines SFILTER_NONREC and SFILTER_INIT_NONREC, you use the **nterms** and **wiggles** arguments to control the sharpness and smoothness of the filter.

Figure 9–2 shows the transfer function of a lowpass nonrecursive filter where **wiggles** = 50.0, **flow** = 0.0, and **fhigh** = 0.5, for **nterms** = 5, 10, 20, and 50.

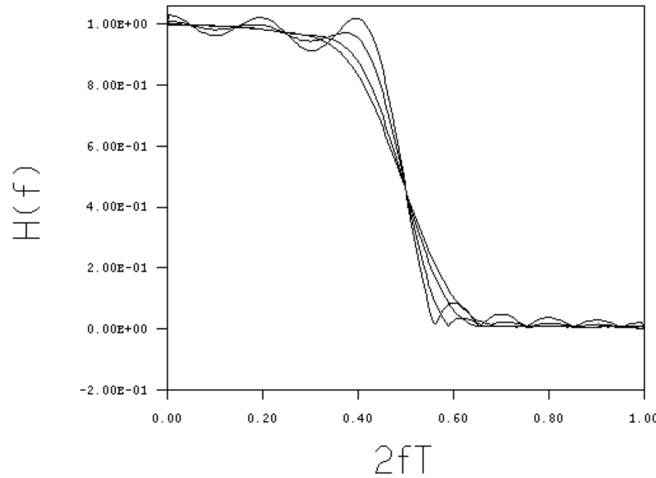
Figure 9–2 Lowpass Nonrecursive Filter for Varying Nterms



The **nterms** argument determines the sharpness of the filter. When **nterms** is increased, the filter cutoff is sharper. Though it seems that using the largest possible value for **nterms** results in a sharper filter, 2(**nterms**) number of data points from the original set are not filtered. If the data set is large, the loss of data caused by the filtering process is inconsequential. However, the loss of data can be detrimental to smaller data sets. In addition, the computational time increases proportionally to the value of **nterms**. Try to make the value of **nterms** as large as possible without losing too many end points or making the computational time too long.

Figure 9–3 shows the transfer function of a lowpass nonrecursive filter where **flow** = 0.0, **fhigh** = 0.5, and **nterms** = 10, for **wiggles** = 0, 30, 50, and 70.

Figure 9–3 Lowpass Nonrecursive Filter for Varying Wiggles



The **wiggles** argument controls the smoothness of the filter. The wiggles, which are related to the size of Gibbs Phenomenon oscillations, are most prominent when the value of the **wiggles** argument is 0.0. As the value of **wiggles** is increased, the oscillations become less noticeable; however, the sharpness of the filter decreases. A good compromise is to set **wiggles** = 50.0.

The size of the oscillations (in -dB units) is related to the value of the **wiggles** argument:

$$|\text{Magnitude of Oscillations}| = 10^{(-\text{wiggles}/20.0)} \qquad (9\text{–}37)$$

9.4.4 CXML's Digital Filter Subroutines

CXML includes three subroutines for nonrecursive filtering. These subroutines are of two types, each of which does the filter operation in a different way:

- Completes the filter operation in one step.
- Completes the filter operation in two steps.

  One subroutine initializes a working array; a second subroutine uses that working array for repeated operations so that the working array need only be calculated once.

The CXML filtering subroutines have single-precision capability; they do not have double-precision capability.

9.4.4.1 Naming Conventions

A filter subroutine has a name composed of character groups that tell you about the subroutine's operation. Table 9–17 shows the character groups used in the subroutine names and what they mean.

Table 9–17 Naming Conventions: Digital Filter Subroutines

Character Group	Mnemonic	Meaning
First group	S	Single-precision real data
Second group	FILTER	Filtering subroutine
Third group	No mnemonic _INIT _APPLY	One-step filter Two-step filter initialization Two-step filter application
Fourth group	_NONREC	Nonrecursive filter

9.4.4.2 Summary of Digital Filter Subroutines

Table 9–18 summarizes the filter subroutines.

Table 9–18 Summary of Digital Filter Subroutines

Subroutine Name	Operation
SFILTER_NONREC	Performs the filter operation in one step
SFILTER_INIT_NONREC	Initializes a working array
SFILTER_APPLY_NONREC	Uses the initialized working array for repeated filtering operations

9.5 Error Handling

The signal processing functions report success or error, using a **status** function value. To include the error code and data structure definitions in a signal processing application program, you must put the following information at the beginning of your program:

- OpenVMS:

  Fortran - `INCLUDE 'SYS$LIBRARY:DXMLDEF.FOR'`
  C - `#include "sys$library:dxmldef.h"`

- Tru64 UNIX and Windows NT:

  Fortran - `INCLUDE 'DXMLDEF.FOR'`
  C - `#include "dxmldef.h"`

A callable error routine is provided for the signal processing routines. On Tru64 UNIX and Windows NT systems, this routine is called `dxml_sig_error`. On OpenVMS systems, this routine is called `dxml$sig_error`. The following example, Example 9–1 shows how this routine is used.

Example 9–1 Example of Error Routine for Signal Processing

```
PROGRAM EXAMPLE
INCLUDE 'DXMLDEF.FOR'

COMPLEX*8 A(8),OUTA(8),B(8),OUTB(8)
COMPLEX*8 DIFF(8),W,G0,G1,AA
REAL*4 TWOPI,T0
INTEGER*4 T,K,I,NT,STATUS,N

RECORD /DXML_D_FFT_STRUCTURE/ FFT_STRUCT

N = 8
TWOPI=6.283185307
T0=TWOPI/FLOAT(8)
W=CMPLX(COS(T0),(-1.0)*SIN(T0))
AA=(0.9,0.3)

C Compute the raw data for the transform
  B(1)=(1.0,0.0)
  DO 1 T=2,8
1 B(T)=AA**(T-1)

C Calculate the analytical transform of the function
  NT=8
  G0=(1.0,0.0)-AA**NT

  DO 5 I=1,NT
  G1=(1.0,0.0)-AA*(W**(I-1))
5 OUTA(I)=G0/G1

  TYPE 100
100  FORMAT(//,3X,'FOR REAL FORWARD FFT WITH 8 POINTS ',
     1  //,3X,'POINT',T11,'ANALYTICAL RESULT',T37,'COMPUTED RESULT',
     2  T65,'DIFF.',/)

C Compute the transform of the function using CXML routines
    ISTAT = CFFT_INIT (0,FFT_STRUCT,.TRUE.)
    IF (ISTAT.NE.DXML_SUCCESS()) CALL DXML_SIG_ERROR (ISTAT)

    ISTAT = CFFT_APPLY ('C','C','F',B,OUTB,FFT_STRUCT,1)
    IF (ISTAT.NE.DXML_SUCCESS()) CALL DXML_SIG_ERROR (ISTAT)

    ISTAT = CFFT_EXIT (FFT_STRUCT)
    IF (ISTAT.NE.DXML_SUCCESS()) CALL DXML_SIG_ERROR (ISTAT)

C Calculate the difference between the computed and analytical solution
C to the transform
     DO 10 I=1,NT
10   DIFF(I)=OUTB(I)-OUTA(I)

C Print out the results
     DO 20 I=1,NT
     TYPE 130,I,OUTA(I),OUTB(I),DIFF(I)
130  FORMAT(2X,I2,2X,3(2(1X,1PE11.4)))
20   CONTINUE

     STOP
     END
```

Table 9–19 shows the status functions, the value returned, an explanation of the error associated with each value, and the appropriate user action suggested to recover from each error condition.

Table 9–19 CXML Status Functions

Function	Value	Description	User Action
DXML_SUCCESS	0	Successful execution of SIG routines	No action required.
DXML_MAND_ARG	1	Mandatory argument is missing	Check the argument list.
DXML_ILL_TEMP_ARRAY	2	temp_array is corrupted	Check code and correct the error.
DXML_IN_VERSION_SKEW	3	temp_array is from old version	Use the same version of CXML to create and use the temporary array.
DXML_ILL_N_IS_ODD	4	A value is odd	Change **n**, **n1**, or **n2** to an even value.
DXML_ILL_WIGGLES	5	Value is out of range	Change **wiggles** to a value that is in range.
DXML_ILL_FLOW	6	flow is equal to fhigh	Provide different values for the **flow** and **fhigh** arguments.
DXML_ILL_F_RANGE	7	flow or fhigh is out of range	Check values of **flow** and **fhigh** arguments and replace with a value between 0.0 and 1.0, inclusive.
DXML_ILL_N_RANGE	8	n is out of range	Check description of **n** for the allowed length.
DXML_ILL_N_NONREC	9	n is less than (2*nterms+1)	Either replace the current value of **n** with a value greater than the value of (2***nterms**)+1 or make the value of **nterms** smaller.
DXML_ILL_NTERMS	10	nterms is out of range	Replace the current value of the **nterms** argument with a value between 2 and 500, inclusive.
DXML_ILL_LDA	11	lda cannot be less than n	Change **lda** to a value greater than or equal to the number of data points in the row direction.
DXML_INS_RES	12	Virtual memory or pagefile quota is not set high enough for data length	Either change the data length to a number that is not prime or increase the allocated values of the pagefile quota and virtual memory.
DXML_BAD_STRIDE	13	Stride is incorrect	Change the value of **stride** to an integer greater than or equal to 1.
DXML_DIRECTION_NOT_ MATCH	14	APPLY/INIT directions different	Change the value of **direction** in either APPLY or INIT to match.
DXML_BAD_DIRECTION_ STRING	15	Direction string is incorrect	Change the first letter in value for **direction** to ‘F’ or ‘B’.

(continued on next page)

Table 9–19 (Cont.) CXML Status Functions

Function	Value	Description	User Action
DXML_BAD_FORMAT_STRING	16	Format string is incorrect	Change the first letter in format string to ‘R’ or ‘C’.
DXML_OPTION_NOT_ SUPPORTED	17	I/O combination not supported	Refer to description of subprogram for supported combinations.
DXML_BAD_FORMAT_ DIRECTION	18	Format/direction combination not supported	Refer to description of subprogram for supported combinations.

10 Using Iterative Solvers for Sparse Linear Systems

CXML provides subprograms for the iterative solution of sparse linear systems of equations by means of preconditioned conjugate-gradient-like methods.

This chapter covers the following topics:

- Introduction to iterative solvers (Section 10.1)
- Interface to the iterative solver, including the concepts of matrix-free formulation of an iterative method and preconditioning (Section 10.2)
- Matrix operations, including storage schemes for sparse matrices and types of preconditioners Section 10.3
- Iterative methods (Section 10.4)
- Naming conventions (Section 10.5)
- Iterative solver subroutine summary (Section 10.6)
- Error handling (Section 10.7)
- Message printing (Section 10.8)
- Hints on using the iterative solvers (Section 10.9)
- Examples of the use of iterative solvers (Section 10.10)

Many iterative solver subprograms are "parallelized" for improved peformance on Tru64 UNIX multiprocessor systems. These parallelized subprograms are discussed in CXML documentation in the "Section A.1" section. This section lists parallel subprograms, discusses the use of the parallel library, and addresses performance considerations.

Reference information for iterative solvers routines is available in Part XIV.

10.1 Introduction

Many applications in science and engineering require the solution of linear systems of equations:

$$Ax = b \tag{10–1}$$

where A is an n by n matrix and x and b are n vectors.

Often, these systems occur in the innermost loop of the application. Therefore, for good overall performance of the application, it is essential that the linear system solver is efficient. An application may solve a system of linear equations once, or many times with different right-hand sides.

The linear systems of equations that arise from science and engineering applications are usually sparse, that is, the coefficient matrix A has a large number of zero elements. Substantial savings in compute time and memory requirements can be realized by storing and operating on only the nonzero elements of A. Solution techniques that exploit this sparsity of the matrix A are referred to as sparse solvers.

10.1.1 Methods for Solutions

Methods for the solution of linear systems of equations can be broadly classified into two categories:

- Direct Methods
  These methods first factor the coefficient matrix A into its triangular factors and then perform a forward and backward solve with the triangular factors to get the required solution. The solution is obtained in a finite number of operations, usually known apriori, and is guaranteed to be as accurate as the problem definition.

  See Chapter 11 for details about direct methods.

- Iterative Methods
  These methods start with an initial guess to the solution, and proceed to calculate solution vectors that approach the exact solution with each iteration. The process is stopped when a given convergence criterion is satisfied. The number of iteration steps required for convergence varies with the coefficient matrix, the initial guess and the convergence criterion—thus an apriori estimate of the number of operations is not possible.

  The convergence of iterative techniques is often accelerated by means of a preconditioner. Instead of solving the system in equation (10–1), the iterative technique is applied to a system derived from the original system, with better convergence properties. As a result of preconditioning, the number of operations per iteration is increased, but the corresponding reduction in the number of iterations required for convergence usually leads to an overall reduction in the total time required for solution.

CXML provides iterative methods only for real double-precision data.

10.1.2 Describing the Iterative Method

Direct methods for the solution of sparse linear systems are relatively well understood and their algorithms are general purpose. However, iterative methods are not so well established and their algorithms tend to be more special purpose. It is well known that there is no general effective iterative algorithm for the solution of an arbitrary sparse linear system, only collections of algorithms each suitable for a particular class of problem. Additionally, there are no strict convergence theorems for some of the iterative methods. Selecting a good iterative technique and preconditioner - both in terms of its convergence properties and its performance on a given architecture - is more of an art than a science. This choice depends on various factors such as the problem being solved, the data structures used, the architecture of the machine, and the amount of memory available.

Despite these drawbacks, for certain classes of problems, an appropriate iterative technique can yield an approximation to the solution significantly faster than a direct method. Also, iterative methods typically require less memory than direct methods and hence can be the only means of solution for some large problems. In an attempt to compensate for the lack of robustness of any single iterative method

and preconditioner, CXML provides a variety of methods and preconditioners. All these methods belong to the class of preconditioned conjugate-gradient-type methods.

10.2 Interface to the Iterative Solver

The interface to the iterative solver requires the following as input: the matrix A, the right hand side b, and an initial guess to the solution. However, due to the large number of storage schemes in use for the storage of sparse matrices, it is not possible to provide an interface that allows all possible storage schemes. CXML resolves this issue by using the matrix-free formulation of the iterative method, as suggested in the proposed iterative standard [Ashby and Seager 1990].

All the iterative techniques provided in CXML refer to the coefficient matrix A, or matrices derived from it such as the preconditioner, only in the following three operations:

- Creation of the preconditioner
- Multiplication of the coefficient matrix by a vector
- Application of the preconditioner

The preconditioner is created from the coefficient matrix prior to a call to the iterative solver routine.

The matrix-free formulation of an iterative method separates the operations of matrix-vector product and the application of the preconditioner from the rest of the iterative solver by considering them as subroutines that are called by the iterative algorithm. These subroutines have a standard interface independent of the storage scheme used for the coefficient matrix. By writing the subroutines to provide the required functionality for the storage scheme under consideration, the same iterative solver can be used for matrices stored using different storage schemes.

While the matrix-free formulation has the advantage of making the iterative solver independent of the matrix storage format and the problem being solved, it has the disadvantage that you have to write the subroutines that perform the operations on the matrix and the preconditioner. To alleviate this disadvantage somewhat, CXML provides subroutines for the matrix-vector product, the creation of the preconditioners and the application of the preconditioners for a select set of storage schemes and preconditioners. Additionally, driver routine DITSOL_DRIVER is provided that simplifies these tasks.

Thus, you have the option of either storing the coefficient matrix in one of the storage schemes provided by CXML and using the subroutines provided, or using your own storage scheme for the matrix and writing the routines for the matrix operations. You also have the option of not storing either the coefficient matrix or the preconditioner, but instead providing the required functionality by some indirect means.

The examples in Section 10.10 illustrate the various ways in which the iterative solvers can be used. These examples, along with the hints in Section 10.9 on the use of the iterative solvers, explain the variety of options provided by CXML. If you are unfamiliar either with the issues involved in iterative methods or with the concept of matrix-free formulation of an iterative method, then the information in these sections should prove helpful.

The next sections further explain the implications of the use of a matrix-free formulation of an iterative method and describe the interface for the iterative solver and the routines that provide the matrix operations. To keep the discussion general, the iterative solver routine is referred to as SOLVER — this is a generic name and in practice you would call the iterative solver routine by a name reflective of the iterative method.

10.2.1 Matrix-Vector Product

The iterative solvers provided in CXML require the evaluation of matrix-vector products of the form:

$$v = Au$$

or:

$$v = A^T u$$

where u and v are vectors of length n. This functionality is provided to the routine SOLVER by the subroutine MATVEC, which has the following standard parameter list:

```
MATVEC (JOB, IPARAM, RPARAM, A, IA, W, U, V, N)
```

Table 10–1 describes each parameter and its data type.

Table 10–1 Parameters for the MATVEC Subroutine

Argument Data Type	Description
job integer*4	On entry, defines the operation to be performed: **job** = 0 : $v = Au$ **job** = 1 : $v = A^T u$ **job** = 2 : $v = w - Au$ **job** = 3 : $v = w - A^T u$ On exit, **job** is unchanged.
iparam integer*4	On entry, a one-dimensional array of length at least 50, containing the parameters passed to the routine SOLVER. See Table 10–4 for details. On exit, the first 50 elements of IPARAM are unchanged.
rparam real*8	On entry, a one-dimensional array of length at least 50, containing the parameters passed to the routine SOLVER. See Table 10–5 for details. On exit, the first 50 elements of RPARAM are unchanged.
a real*8	On entry, a one-dimensional array for the nonzero elements of the matrix A. If MATVEC does not require this matrix to be explicitly stored, **a** is a dummy argument. Array A can be used to provide workspace. On exit, any information related to matrix A is unchanged.
ia integer*4	On entry, a one-dimensional array for auxiliary information about the matrix A or the array A. If this information is not needed, **ia** is a dummy argument. Array IA can be used to provide workspace. On exit, ia is unchanged.
w real*8	On entry, a one-dimensional array of length at least n that contains the vector w when **job** = 2 or 3. The elements of array W are accessed with unit increment. On exit, **w** is unchanged.

(continued on next page)

Table 10–1 (Cont.) Parameters for the MATVEC Subroutine

Argument Data Type	Description
u real*8	On entry, a one-dimensional array of length at least n that contains the vector u. The elements of array U are accessed with unit increment. On exit, **u** must be unchanged.
v real*8	On entry, a one dimensional array of length at least n. On exit, array V contains the vector defined by **job**. The elements of array V are accessed with unit increment.
n integer*4	On entry, the order of the matrix A. On exit, **n** is unchanged.

The routine MATVEC is an input parameter to the routine SOLVER and should be declared external in your calling program. It could either provide the required functionality itself, or act as an interface to a routine that provides the required functionality. Suppose the iterative solver requires MATVEC to provide the functionality for **job** = 0. Then you would write the (Fortran-specific) routine MATVEC as follows:

```
SUBROUTINE MATVEC(JOB,IPARAM,RPARAM,A,IA,W,U,V,N)
        .
        .
        . (any initializations here)
        .     if necessary
        .
        .
IF (JOB.EQ.0) CALL USER_MATVEC(...)
RETURN
END
```

where USER_MATVEC is your routine for evaluating the vector Au and returning the result in vector v. This enables you to have a routine USER_MATVEC, which has a parameter list different from the parameter list of MATVEC. It also allows you to call one of the matrix-vector product routines included in CXML instead of USER_MATVEC, provided you have stored the coefficient matrix using one of CXML's sparse matrix storage schemes. In either case, you have to provide the routine MATVEC, with the required standard parameter list. If you use a storage scheme for the coefficient matrix different from those provided by CXML, or choose not to store the matrix at all, then it is your responsibility to provide the functionality required by MATVEC. If, however, you use a storage scheme provided by CXML for the coefficient matrix, then you must provide a routine MATVEC that calls the appropriate CXML routine.

The examples in Section 10.10 illustrate the different ways in which the interface provided by the routine MATVEC can be used to provide the required functionality. The reference descriptions at the end of this chapter describe the matrix-vector product routines for the various storage schemes supported by CXML.

10.2.2 Preconditioning

Preconditioning is a technique used for improving the convergence of an iterative method by applying the method to a system derived from the original with better convergence properties. The convergence of the iterative methods provided in CXML depends on the condition number and the distribution of the eigenvalues of the coefficient matrix A. A distribution where the eigenvalues are clustered is favorable for fast convergence of the iterative method.

A preconditioned iterative method applies the iterative method to an equivalent system derived from (10–2) as follows:

$$Q_L^{-1} A Q_R^{-1} * Q_R x = Q_L^{-1} b$$

that is:

$$A' x' = b' \qquad (10\text{–}2)$$

where:

$$A' = Q_L^{-1} A Q_R^{-1}$$

$$x' = Q_R x$$

and:

$$b' = Q_L^{-1} b$$

Q_L and Q_R are n by n matrices. The matrix $Q = Q_L Q_R$ is called the preconditioning matrix or the preconditioner. The matrices Q_L and Q_R are derived from the coefficient matrix A such that the matrix A' is close to the identity matrix and thus has eigenvalues clustered around unity. As a result of preconditioning, the iterative method applied to (10–2), with the coefficient matrix A', right hand side b' and solution x', usually converges faster than when it is applied to (10–1).

The implementation of the iterative method for solving (10–2) does not involve the explicit formation of A'. Instead, the matrices Q_L, Q_R and A appear in operations of the form:

$$v = Q_R^{-1} u$$

$$v = A u$$

and:

$$v = Q_L^{-1} u$$

The computation per iteration, in the preconditioned case, is more expensive than in the unpreconditioned case. This increase in the computation per iteration is usually offset by a reduction in the number of iterations required for convergence, leading to a reduction in the total computation.

The matrices Q_L and Q_R form a good preconditioner if they satisfy the following properties:

- Q is a good approximation to A so that A' is close to the identity matrix.
- Q_R and Q_L are easily obtainable.
- Solving systems of the form $Q_L u = v$ or $Q_R u = v$ is easy as the preconditioner is applied via the solution of these systems.
- The storage costs of Q_L and Q_R are not excessive.

Preconditioners can be divided into three broad classes depending on the manner in which they are applied:

- Left preconditioning:
$$(Q_L^{-1} A) x = (Q_L^{-1} b)$$
- Right preconditioning:
$$(A Q_R^{-1}) * (Q_R x) = b$$
- Split preconditioning:
$$(Q_L^{-1} A Q_R^{-1}) * (Q_R x) = (Q_L^{-1} b)$$

Left and right preconditioning can be considered as special cases of split preconditioning with Q_R and Q_L being the identity matrices, respectively.

In the case of left preconditioning, the residual of the system (10–2), evaluated by the iterative method is not the same as the residual of the original system (10–1). The unpreconditioned residual, r, and the preconditioned residual, r', are related as follows:

$$r' = Q_L^{-1}(b - Ax) = Q_L^{-1} r$$

Similarly, the solution x' evaluated using right preconditioning is related to the true solution, x, as follows:

$$x' = Q_R x$$

It follows that in the case of split preconditioning, neither the true solution nor the true residual are obtained directly from the application of the iterative technique to (10–2). Thus, the use of preconditioning implies that extra computation has to be done to recover the true residual and solution from the residual and solution of the equivalent system (10–2). However, there is a special case of split preconditioning that allows the iterative method to obtain the true residual and the true solution directly, when applied to a symmetric positive definite (SPD) matrix A. This is the case where the preconditioner is symmetric positive definite as well and hence can be written as:

$$Q = BB^T$$

for some matrix B, that is:

$$Q_L = Q_R^T = B.$$

The interface to the preconditioning operations is provided by the routines PCONDL and PCONDR for left and right preconditioning, respectively. The two routines have similar parameter lists, differing only in the matrices Q_L and Q_R:

```
SUBROUTINE PCONDR (JOB, IPARAM, RPARAM, QR, IQR, A, IA, W, U, V, N)
SUBROUTINE PCONDL (JOB, IPARAM, RPARAM, QL, IQL, A, IA, W, U, V, N)
```

Table 10–2 describes each parameter and its data type.

Table 10–2 Parameters for the PCONDR and PCONDL Subroutines

Argument Data Type	Description
job integer*4	On entry, defines the operation to be performed: **job** = 0 : $v = Q_R^{-1}u$ **job** = 1 : $v = Q_R^{-T}u$ **job** = 2 : $v = w - Q_R^{-1}u$ **job** = 3 : $v = w - Q_R^{-T}u$ On exit, **job** is unchanged.
iparam integer*4	On entry, a one-dimensional integer array of length at least 50, containing the parameters passed to the routine SOLVER. See Table 10–4 for details. On exit, the first 50 elements of IPARAM are unchanged.
rparam real*8	On entry, a one-dimensional real array of length at least 50, containing the parameters passed to the routine SOLVER. See Table 10–5 for details. On exit, the first 50 elements of RPARAM are unchanged.
qr real*8	On entry, a one-dimensional array for the nonzero elements of the matrix Q_R. If PCONDR does not require this matrix to be explicitly stored, **qr** is a dummy argument. **qr** can also be used to provide workspace for the routine PCONDR. On exit, any information related to the matrix Q_R is unchanged.
iqr integer*4	On entry, a one-dimensional array for auxiliary information about the matrix Q_R or the array QR. If no information is required, **iqr** is a dummy argument. **iqr** can also be used to provide workspace. On exit, information related to the matrix Q_R or the array QR is unchanged.
a real*8	On entry, a one-dimensional array for the nonzero elements of the matrix A. If PCONDR does not require the matrix A to be explicitly stored, **a** is a dummy argument. Array A can also be used to provide workspace. On exit, any information related to the matrix A is unchanged.
ia integer*4	On entry, a one-dimensional array for auxiliary information about the matrix A or the array A. If no information is needed, **ia** is a dummy argument. Array IA can also be used to provide workspace. On exit, any information related to the matrix A or the array A is unchanged.
w real*8	On entry, a one-dimensional array of length at least n that contains the vector w when **job** = 2 or 3. The elements of array W are accessed with unit increment. On exit, **w** is unchanged.
u real*8	On entry, a one-dimensional array of length at least n that contains the vector u. The elements of array U are accessed with unit increment. On exit, **u** must be unchanged.
v real*8	On entry, a one-dimensional array of length at least n. On exit, array V contains the vector defined by **job**. The elements of array V are accessed with unit increment.
n integer*4	On entry, the order of the matrix A. On exit, **n** is unchanged.

PCONDL and PCONDR are input parameters to SOLVER and, if used, must be declared external in your program. If only one of these preconditioning options is used, then the argument for the other is a dummy input parameter to SOLVER. If no preconditioning is used, both PCONDL and PCONDR are dummy parameters. The routines PCONDL and PCONDR are called by the iterative solver only if

you request their use by setting an appropriate parameter for preconditioning, as explained in Section 10.2.4. This implies that you do not have to provide dummy routines for either PCONDL or PCONDR if they are not being used by SOLVER.

The preconditioning routines, PCONDL and PCONDR, only apply the preconditioner; you are responsible for setting up the preconditioner before the call to the routine SOLVER. The pointers to the matrix A, that is, arrays A and IA are passed to the preconditioner for use by those routines that are dependent on A, such as polynomial preconditioners. If the preconditioning routine does not use A, both A and IA may be dummy arguments. Any workspace for use by the preconditioner can be passed through the arrays QL, QR, IQL, and IQR.

In the case of split SPD preconditioning, the iterative technique requires the solution of a system of the form $Qu = v$. An explicit split of the preconditioning matrix Q into Q_L and Q_R is not required. As a result, only one of the routines PCONDL or PCONDR is needed. CXML provides the required functionality through the routine PCONDL, that is, PCONDL provides the solution of the system $Qu = v$ when the **job** argument is set to zero and PCONDR is not used.

If the iterative solver is called with preconditioning, then you must provide the appropriate routines PCONDL and PCONDR with the standard parameter list. As in the case of MATVEC, the required functionality could be provided either by your own routines or by calls to the appropriate CXML routines from within PCONDL and PCONDR. The examples in Section 10.10 illustrate the different ways in which the interface provided by the routines PCONDL and PCONDR can be used to provide the required functionality. Section 10.3.2 and the reference descriptions at the end of this chapter describe the routines for creating and applying the preconditioners for the various storage schemes supported by CXML.

10.2.3 Stopping Criterion

An important aspect of any iterative solver is the stopping criterion, that is, the conditions that determine when the iterations are stopped. The stopping criterion has two parts: a quantity that is measured and a positive constant ϵ that the quantity is measured against to determine convergence. The choice of each is crucial as the stopping criterion should accurately reflect when a suitable approximation to the solution has been obtained.

In order for the evaluation of the stopping criterion to form a small fraction of the total computation, it should be easy to obtain the quantity that is measured from the iterative technique. Additionally, the constant ϵ must be chosen appropriately. A large value might result in a solution that does not have the required accuracy, while a small value might imply extra computation to achieve unneeded extra accuracy. Setting epsilon too small might also prevent the stopping criterion from ever being satisfied.

CXML provides you with the option of either writing your own stopping criterion or using one of the stopping criteria provided. The latter are based on the residual, r_i, of the system (10–1) at the i-th step of the iteration:

$$r_i = b - Ax_i$$

and the preconditioned residual, r'_i, of the system (10–2) at the i-th step of the iteration:

$$r'_i = Q_L^{-1} * (b - Ax_i)$$

The four stopping criteria provided by CXML are as follows:

- Stopping Criterion 1:

$$||r_i||_2 \leq \epsilon \tag{10–3}$$

- Stopping Criterion 2:

$$\frac{||r_i||_2}{||b||_2} \leq \epsilon \tag{10–4}$$

- Stopping Criterion 3:

$$||r'_i||_2 \leq \epsilon \tag{10–5}$$

- Stopping Criterion 4:

$$\frac{||r'_i||_2}{||b'||_2} \leq \epsilon \tag{10–6}$$

where:

$$r'_i = Q_L^{-1} r_i$$

$$b' = Q_L^{-1} b$$

and:

$$||r_i||_2 = \sqrt{\sum_{j=1}^{n} r_i^2(j)}$$

You can choose one of these stopping criteria by setting the value of an appropriate input parameter as explained in Section 10.2.3. In the case of an unpreconditioned iterative technique, the choice of stopping criterion (10–5) or (10–6) defaults to (10–3) or (10–4), respectively. Stopping criteria (10–4) and (10–6) require that the denominator should be nonzero to avoid a division by zero error. Some stopping criteria might require more computation than others depending on what can be easily obtained from the iterative technique. For example, the left hand side of (10–3) is calculated during the unpreconditioned conjugate gradient technique and hence very little extra computation is needed for the evaluation of (10–3) or (10–4).

CXML also provides you with the option of implementing your own stopping criterion via the routine MSTOP, which has the following standard parameter list:

```
SUBROUTINE MSTOP (IPARAM, RPARAM, X, R, Z, B, N)
```

Table 10–3 describes each parameter and its data type.

Table 10–3 Parameters for the MSTOP Subroutine

Argument Data Type	Description
iparam integer*4	On entry, a one-dimensional array of length at least 50, containing the parameters passed to the routine SOLVER. See Table 10–4 for details. On exit, the first 50 elements of IPARAM are unchanged.

(continued on next page)

Table 10–3 (Cont.) Parameters for the MSTOP Subroutine

Argument Data Type	Description
rparam real*8	On entry, a one-dimensional array of length at least 50, containing the parameters passed to the routine SOLVER. See Table 10–5 for details. On exit, the first 50 elements of RPARAM are unchanged, with the exception of RPARAM(2) that contains the left side of the stopping criterion as evaluated by MSTOP.
x real*8	On entry, a one-dimensional array of length at least n that contains the approximation to the solution obtained at the iteration number, *iters* in IPARAM(10). On exit, **x** is unchanged.
r real*8	On entry, a one-dimensional array of length at least n that contains the true residual of the system (10–1) obtained at the iteration number, *iters* in IPARAM(10). See the reference descriptions of the iterative solvers for conditions under which **r** is defined. On exit, **r** must be unchanged.
z real*8	On entry, a one-dimensional array of length at least n that contains the preconditioned residual of the system (10–2) obtained at the iteration number, *iters* in IPARAM(10). See the reference descriptions of the iterative solvers for conditions under which **z** is defined. On exit, **z** is unchanged.
b real*8	On entry, a one-dimensional real array of length at least n that contains the right-hand side of the system (10–1). On exit, **b** must be unchanged.
n integer*4	On entry, the order of the matrix A. On exit, **n** is unchanged.

By providing an interface to the routine MSTOP, CXML allows you to use a stopping criterion derived from the vectors x, r, z and b, which is different from the standard stopping criteria provided by CXML. Based on the input parameters, the routine MSTOP should evaluate the left side of the convergence test and return the value in RPARAM(2) as explained in Section 10.2.4. The iteration count parameter, iters (IPARAM(10)), allows you to evaluate quantities depending upon the iteration, such as the initial residual norm, or print out information on each iteration. MSTOP is an input parameter to the routine SOLVER and, if used, should be declared external in your calling program.

10.2.4 Parameters for the Iterative Solver

The interface to the iterative solver provided by CXML allows you to pass information to the solver - such as the maximum number of iterations allowed. It also allows you to obtain information back from the solver - such as the number of iterations required for convergence and error messages. This information is passed via two arrays - IPARAM for integer parameters and RPARAM for real parameters.

These arrays are of length at least 50, with the first 30 elements reserved for use by the proposed standard, and next 20 for use by CXML. Tables 10–4 and 10–5 describe the elements of the parameter arrays.

Table 10–4 Integer Parameters for the Iterative Solver

Parameter	Variable	Description
IPARAM(1)	*nipar*	Length of the array IPARAM, $\geq$ 50.
IPARAM(2)	*nrpar*	Length of the array RPARAM, $\geq$ 50.
IPARAM(3)	*niwk*	Length of the array IWORK, size varies with iterative solvers.
IPARAM(4)	*nrwk*	Length of the array RWORK, size varies with iterative solvers.
IPARAM(5)	*iounit*	Ignored.
IPARAM(6)	*iolevel*	Determines the kind of information output, as follows: $iolevel < 0$: Messages are not printed $iolevel = 0$: Fatal error messages only $iolevel = 1$: Warning messages and minimum output $iolevel = 2$: Short summary $iolevel \geq 3$: Detailed information
IPARAM(7)	*ipcond*	Determines the form of preconditioning: $ipcond = 0$: no preconditioning; IQR, IQL, QR, QL, PCONDL, PCONDR are dummy arguments $ipcond = 1$: left preconditioning; IQR, QR, PCONDR are dummy arguments $ipcond = 2$: right preconditioning; IQL, QL, PCONDL are dummy arguments $ipcond = 3$: split preconditioning $ipcond = 4$: SPD split preconditioning; IQR, QR, PCONDR are dummy arguments
IPARAM(8)	*istop*	Determines the stopping criterion: $istop = 0$: user-supplied routine MSTOP $istop = 1$: stopping criterion (10–3) (default) $istop = 2$: stopping criterion (10–4) $istop = 3$: stopping criterion (10–5); if no preconditioning used, defaults to $istop = 1$ $istop = 4$: stopping criterion (10–6); if no preconditioning used, defaults to $istop = 2$
IPARAM(9)	*itmax*	Maximum number of iterations allowed for convergence. If convergence is not achieved in *itmax* iterations the solver returns with error flag set. Default = 100
IPARAM(10)	*iters*	Number of iterations required to satisfy the convergence criterion.
IPARAM(31)	*nz*	Parameter related to the number of nonzeros stored for the matrix. See the storage schemes in Section 10.3.1 for more details.
IPARAM(32)	*ndim*	Leading dimension of 2 dimensional arrays. See the storage schemes in Section 10.3.1 for more details.
IPARAM(33)	*ndeg*	Degree of the polynomial used for polynomial preconditioning. Default = 1
IPARAM(34)	*kprev*	Number of previous residual vectors used in the iterative solver DITSOL_PGMRES. See the reference descriptions for details.

(continued on next page)

Table 10–4 (Cont.) Integer Parameters for the Iterative Solver

Parameter	Variable	Description
IPARAM(35)	$istore$	Storage scheme used in the driver routine: $istore = 1$: SDIA storage scheme, lower triangular part is stored (Section 10.3.1.1) $istore = 2$: SDIA storage scheme, upper triangular part is stored (Section 10.3.1.1) $istore = 3$: UDIA storage scheme (Section 10.3.1.2) $istore = 4$: GENR storage scheme (Section 10.3.1.3)
IPARAM(36)	$iprec$	Preconditioner used in the driver routine: $iprec = 1$: diagonal preconditioner (Section 10.3.2.1) $iprec = 2$: polynomial preconditioner (Section 10.3.2.2) $iprec = 3$: ILU preconditioner (Section 10.3.2.3)
IPARAM(37)	$isolve$	Iterative solver used in the driver routine: $isolve = 1$: Conjugate gradient method $isolve = 2$: Least squares conjugate gradient method $isolve = 3$: Bi-conjugate gradient method $isolve = 4$: Conjugate gradient squared method $isolve = 5$: Generalized minimum residual method $isolve = 6$: Transpose-free quasiminimal residual method

Table 10–5 Real Parameters for the Iterative Solver

Parameter	Variable	Description
RPARAM(1)	$errtol(\epsilon)$	User-supplied tolerance for convergence.
RPARAM(2)	$stptst$	Quantity that determines the convergence of the iterative technique. (lefthand side of stopping criterion)

The elements 30 through 50 of the arrays IPARAM and RPARAM are reserved for use by CXML.

The arrays IPARAM and RPARAM are passed to the routine SOLVER and all the routines called by it (MATVEC, PCONDL, PCONDR and MSTOP). If necessary, you can use these arrays to pass additional information to these routines. For example, if you declare these arrays to be of dimension 100, then the elements from 51 through 100 can be used to pass information to the routines MATVEC, PCONDL, PCONDR and MSTOP. However, the elements 30 through 50 are reserved for CXML.

CXML allows you to set the variables in the IPARAM and RPARAM arrays to their default values by a call to the routine DITSOL_DEFAULTS with the following interface:

```
SUBROUTINE DITSOL_DEFAULTS (IPARAM, RPARAM)
```

Table 10–6 defines the default values set by the routine DITSOL_DEFAULTS. You must either call DITSOL_DEFAULTS to initialize IPARAM and RPARAM, or you must initialize IPARAM(30) through IPARAM(50) to 0 in the calling program. Failing to do this can result in unpredictable behavior.

After initialization, you can change any of the parameters described in Table 10–4 as required. It is your responsibility to ensure that the variables in the arrays IPARAM and RPARAM have been assigned appropriate values before a call to the iterative solver routine. You must not change any array element between 30-50 other than the ones described in the Table 10–4. The examples in Section 10.10 illustrate the use of the DITSOL_DEFAULTS routine.

Table 10–6 Default Values for Parameters

Parameter	Variable	Default Value
iparam(1)	$nipar$	50
iparam(2)	$nrpar$	50
iparam(5)	$iounit$	6
iparam(6)	$iolevel$	0
iparam(7)	$ipcond$	0
iparam(8)	$istop$	1
iparam(9)	$itmax$	100
iparam(33)	$ndeg$	1
rparam(1)	$errtol$	1.0e-6

10.2.5 Argument List for the Iterative Solver

The matrix-free formulation of the iterative method adopted by CXML implies that the routine SOLVER has, as input parameters, the routines MATVEC, PCONDL, PCONDR, and MSTOP. Additionally, the parameter list also contains the arrays A, IA, QL, IQL, QR, and IQR for use by the routines for the matrix operations (MATVEC, PCONDL, PCONDR) as well as input parameters such as the size of the system, the right side, and the initial approximation. The approximation to the solution obtained by the solver is returned in the vector x. Real and integer workspace is provided via arrays RWORK and IWORK, respectively and real and integer parameters via arrays RPARAM and IPARAM, respectively. This results in the following interface for the routine SOLVER:

```
SUBROUTINE SOLVER (MATVEC, PCONDL, PCONDR, MSTOP, A, IA, X, B, N, QL, IQL,
                   QR, IQR, IPARAM, RPARAM, IWORK, RWORK, IERROR)
```

Table 10–7 describes each parameter and its data type.

Table 10–7 Parameters for the SOLVER Subroutine

Argument Data Type	Description
matvec procedure	On entry, the name of the routine that evaluates the matrix-vector product. **matvec** uses the standard interface and must be declared external in your calling program. See Table 10–1. On exit, **matvec** is unchanged.

(continued on next page)

Table 10–7 (Cont.) Parameters for the SOLVER Subroutine

Argument Data Type	Description
pcondl procedure	On entry, the name of the routine that applies left preconditioning. **pcondl** uses the standard interface. See Table 10–2. If left preconditioning is not used, **pcondl** is a dummy parameter. If used, **pcondl** must be declared external in your calling program. The variable $ipcond$ in IPARAM(7), must be set appropriately for access to the PCONDL routine. On exit, **pcondl** is unchanged.
pcondr procedure	On entry, the name of the routine that applies right preconditioning. **pcondr** uses the standard interface. See Table 10–2. If right preconditioning is not used, **pcondr** is a dummy parameter. If used, **pcondr** must be declared external in your calling program. The variable $ipcond$, IPARAM(7), must be set appropriately for access to the PCONDR routine. On exit, **pcondr** is unchanged.
mstop procedure	On entry, the name of the routine that evaluates a stopping criterion defined by you. **mstop** has the standard interface. See Table 10–3. If used, it must be declared external in your calling program. The variable $istop$, IPARAM(8), must be set appropriately for access to the MSTOP routine. If not used, that is, you use one of the CXML stopping criteria, **mstop** is a dummy parameter. On exit, **mstop** is unchanged.
a real*8	On entry, a one-dimensional array for the nonzero elements of matrix A. If the MATVEC, PCONDL and PCONDR routines do not require this matrix to be explicitly stored, array A may be a dummy array. Array A may also be used to provide workspace. On exit, any information related to the matrix A is unchanged.
ia integer*4	On entry, a one-dimensional array for auxiliary information about the matrix A, or the array A. If the information is not needed, array IA may be a dummy array. Array IA may also be used to provide workspace. On exit, any information related to the matrix A or the array A is unchanged.
x real*8	On entry, a one-dimensional array of length at least n that contains the initial approximation to the solution. The elements of array X are accessed with unit increment. On exit, **x** is the approximation to the solution obtained by the routine SOLVER.
b real*8	On entry, a one-dimensional array of length at least n that contains the right side of the system (10–1). The elements of array B are accessed with unit increment. On exit, **b** is unchanged.
n integer*4	On entry, the order of the matrix A. On exit, **n** is unchanged.
ql real*8	On entry, a one-dimensional array for the nonzero elements of the matrix Q_L. If PCONDL does not require this matrix to be explicitly stored, **ql** is a dummy array. Array QL may also be used to provide workspace. On exit, any information related to the matrix Q_L is unchanged.
iql integer*4	On entry, a one-dimensional array for auxiliary information about the matrix Q_L or the array QL. If no information is needed, IQL is a dummy array. Array IQL can also be used to provide workspace. On exit, any information related to the matrix Q_L or the array QL is unchanged.

(continued on next page)

Table 10–7 (Cont.) Parameters for the SOLVER Subroutine

Argument Data Type	Description
qr real*8	On entry, a one-dimensional array for the nonzero elements of the matrix Q_R. If PCONDR does not require this matrix to be explicitly stored, QR is a dummy array. QR can also be used to provide workspace. On exit, any information related to matrix Q_R is unchanged.
iqr integer*4	On entry, a one-dimensional array for auxiliary information about the matrix Q_R or the array QR. If no information is needed, IQR is a dummy array. Array IQR can also be used to provide workspace. On exit, any information related to the matrix Q_R or the array QR is unchanged.
iparam integer*4	On entry, a one-dimensional array of length at least 50, containing the parameters passed to the routine SOLVER. On exit, the elements of IPARAM (described in Table 10–4) are unchanged, with the exception of $iters$ (IPARAM(10)), which is then equal to the number of iterations required for convergence.
rparam real*8	On entry, a one-dimensional array of length at least 50, containing the parameters passed to the routine SOLVER. On exit, the first 50 elements of rparam are unchanged, with the exception of RPARAM(2) that is equal to the left side of the stopping criterion.
iwork integer*4	On entry, a one-dimensional array of length $niwk$, IPARAM(3), used as an integer workspace. On exit, the data in IWORK is overwritten.
rwork real*8	On entry, a one-dimensional array of length $nrwk$, IPARAM(4), used as a real workspace. On exit, the data in RWORK is overwritten.
ierror integer*4	On entry, a scalar value that receives the value of the error flag. On exit, the error flag returned by the routine SOLVER.

In addition to the error messages output by the iterative solver, based on the variable, **iolevel** (IPARAM(6)), the routine SOLVER also returns an error flag, ierror. It is your responsibility to check the error flag on exit from SOLVER and ensure that the solution procedure ended normally. This is especially true if you have disabled all error messages by setting a negative value for **iolevel**.

10.3 Matrix Operations

The matrix-free formulation of the iterative method adopted by CXML isolates the operations involving the coefficient matrix, A, and the preconditioning matrices, Q_L and Q_R, by separating them into subroutines that form the matrix-vector product, create the preconditioner and apply the preconditioner. This formulation allows you to use any storage scheme for storing the coefficient matrix and the preconditioner. However, it has the drawback that you must provide the routines MATVEC, PCONDL, PCONDR, and the routine for the creation of the preconditioner.

As an alternative, CXML provides you with the option of using routines written to implement the matrix operations for three matrix storage schemes. In addition to the matrix-vector product operations, CXML provides routines for the creation and application of three preconditioners for each of the three storage schemes. Calls to these CXML routines can be used in the routines MATVEC, PCONDL, and PCONDR to implement the desired operation. The only restriction is that the coefficient matrix be stored in one of the storage schemes provided by CXML.

10.3.1 Storage Schemes for Sparse Matrices

A sparse matrix is a matrix that has very few nonzero elements. By storing and operating on only the nonzero elements, it is possible to achieve substantial savings in memory requirements and computation. In addition to the nonzero elements, storage is also required for information that determines the position of each nonzero element in the matrix.

Sparse matrices can be broadly classified as either structured or unstructured matrices. A structured sparse matrix is one where the distribution of nonzero elements in the matrix has a specific structure. For example, the matrix A shown in (10–7) has its nonzero elements along the diagonals of the matrix:

$$A = \begin{bmatrix} a_{11} & a_{12} & 0 & 0 & 0 & 0 \\ 0 & a_{22} & a_{23} & 0 & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} & 0 & 0 \\ a_{41} & 0 & 0 & a_{44} & a_{45} & 0 \\ 0 & a_{52} & 0 & 0 & a_{55} & a_{56} \\ 0 & 0 & a_{63} & 0 & 0 & a_{66} \end{bmatrix} \qquad (10\text{–}7)$$

This structure can be exploited to reduce the amount of additional information that is necessary for the determination of the position of the nonzero elements within the matrix. For example, consider the elements in the superdiagonal of the matrix A:

$$\begin{pmatrix} a_{12} & a_{23} & a_{34} & a_{45} & a_{56} \end{pmatrix}$$

As the elements all lie on a diagonal, the position of each element relative to the previous element is known (that is, the row and column indices of an element on the diagonal are one higher than the row and column indices of the preceding element in the diagonal). If the row and column indices of the first element a_{12} are known, the positions of the other elements in the diagonal are also known. Thus, substantial savings in the storage requirements can be achieved by storing only the position of the first element in each diagonal.

Unstructured sparse matrices, such as the matrix A in (10–8), do not have a structure to the distribution of the nonzero elements:

$$A = \begin{bmatrix} a_{11} & 0 & a_{13} & 0 & 0 \\ 0 & a_{22} & a_{23} & 0 & 0 \\ 0 & 0 & a_{33} & 0 & 0 \\ a_{41} & 0 & 0 & a_{44} & a_{45} \\ 0 & 0 & a_{53} & 0 & a_{55} \end{bmatrix} \qquad (10\text{–}8)$$

In such cases, each nonzero element is stored along with its row and column indices. Some savings in storage is possible if the elements in a row (or column) are stored contiguously. In such cases, only the row (or column) index for the first nonzero element of the row (or column) is stored.

CXML subprograms that operate on sparse matrices store them in one of three ways:

- Symmetric diagonal storage
- Unsymmetric diagonal storage
- General storage by rows

10.3.1.1 SDIA: Symmetric Diagonal Storage Scheme

Symmetric matrices whose nonzero elements lie along a few diagonals can be stored using a scheme that stores only the diagonals and the distance of each diagonal from the main diagonal. Each diagonal is stored in its entirety, along with any zeros. The distance of a diagonal from the main diagonal is positive if the diagonal is above the main diagonal and negative if the diagonal is below the main diagonal. The main diagonal itself has a distance of zero.

An n by n matrix is stored in a two dimensional array with at least n rows and as many columns as the number of nonzero diagonals in the strict upper (or lower) triangular part plus 1 (for the main diagonal). As the matrix is symmetric, either the upper or lower triangular part can be stored. Both the elements above the main diagonal and those below the main diagonal retain the row corresponding to the row in the original matrix. Thus, the matrix A in (10–9) can be stored in the upper triangular form as shown in (10–10):

$$A = \begin{bmatrix} a_{11} & 0 & 0 & a_{14} & a_{15} & 0 \\ 0 & a_{22} & 0 & 0 & a_{25} & a_{26} \\ 0 & 0 & a_{33} & 0 & 0 & a_{36} \\ a_{14} & 0 & 0 & a_{44} & 0 & 0 \\ a_{15} & a_{25} & 0 & 0 & a_{55} & 0 \\ 0 & a_{26} & a_{36} & 0 & 0 & a_{66} \end{bmatrix} \tag{10–9}$$

$$AD = \begin{bmatrix} a_{11} & a_{14} & a_{15} \\ a_{22} & a_{25} & a_{26} \\ a_{33} & a_{36} & * \\ a_{44} & * & * \\ a_{55} & * & * \\ a_{66} & * & * \end{bmatrix} \tag{10–10}$$

$$\text{INDEX} = (0, 3, 4)$$

The first element of INDEX corresponds to the main diagonal of A, which is stored in AD(*,1). The second element of INDEX implies that the superdiagonal that is 3 away from the main diagonal is stored in AD(*,2) and so on. The positive elements in INDEX indicate that the upper triangular part is being stored.

The matrix A can also be stored in the lower triangular form as shown in (10–11):

$$AD = \begin{bmatrix} a_{11} & * & * \\ a_{22} & * & * \\ a_{33} & * & * \\ a_{44} & a_{14} & * \\ a_{55} & a_{25} & a_{15} \\ a_{66} & a_{36} & a_{26} \end{bmatrix} \tag{10–11}$$

$$\text{INDEX} = (0, -3, -4)$$

The asterisk (*) indicates that the element does not belong to the matrix A. These elements should be set to zero in the array AD. The negative elements in INDEX indicate that the lower triangular part is being stored.

The array AD is dimensioned as $ndim$ by nz, where nz is the number of diagonals stored and $ndim$ is the declared leading dimension of AD as given in the calling program. The INDEX array has dimension nz. Note that nz can be at most n for an n by n system.

The characteristics of this storage scheme are as follows:

- The diagonals can be stored in any order.
- Either the upper or the lower triangular part is stored. Thus the elements in INDEX after the first element, are all positive or all negative.
- Elements which are part of AD, but not part of A, should be set equal to zero. These are the elements denoted by the asterisk (*).

10.3.1.2 UDIA: Unsymmetric Diagonal Storage Scheme

This storage scheme follows the same principle as the symmetric diagonal storage scheme, but both the upper and the lower triangular halves of the matrix are stored. Thus, the matrix A in (10–12) is stored as shown in (10–13):

$$A = \begin{bmatrix} a_{11} & 0 & 0 & a_{14} & a_{15} & 0 \\ 0 & a_{22} & 0 & 0 & a_{25} & a_{26} \\ a_{31} & 0 & a_{33} & 0 & 0 & a_{36} \\ 0 & a_{42} & 0 & a_{44} & 0 & 0 \\ a_{51} & 0 & a_{53} & 0 & a_{55} & 0 \\ 0 & a_{62} & 0 & a_{64} & 0 & a_{66} \end{bmatrix} \qquad (10\text{–}12)$$

$$AD = \begin{bmatrix} a_{11} & a_{14} & a_{15} & * & * \\ a_{22} & a_{25} & a_{26} & * & * \\ a_{33} & a_{36} & * & a_{31} & * \\ a_{44} & * & * & a_{42} & * \\ a_{55} & * & * & a_{53} & a_{51} \\ a_{66} & * & * & a_{64} & a_{62} \end{bmatrix} \qquad (10\text{–}13)$$

$$INDEX = (0, 3, 4, -2, -4)$$

The array AD is dimensioned $ndim$ by nz, where nz is the number of diagonals stored and $ndim$ is the leading dimension of the matrix, as given in the calling program. The array INDEX has dimension nz. For an n by n system, nz can be at most $2n - 1$.

The characteristics of this storage scheme are as follows:

- The diagonals can be stored in any order.
- Elements which are part of AD, but not part of A, should be set equal to zero. These are the elements denoted by the asterisk (*).

10.3.1.3 GENR: General Storage Scheme by Rows

This storage scheme can be used for storing general unstructured matrices. Each nonzero element is stored along with its row and column indices. Thus there is a single array of matrix elements, AR, along with an array of row indices, IA, and an array of the corresponding column indices, JA.

As the matrix is stored by rows, the row index for all the nonzero elements in a row is stored only once. The i-th element of array IA points to the start of the i-th row in arrays JA and AR. For example if IA(3) = 6, then the third row is stored starting from the 6-th element in AR and JA. As IA(4) points to the start of the

fourth row, the number of elements in the third row is given by IA(4)-IA(3). Thus the matrix A in (10–14) is stored using three vectors as shown in (10–15):

$$A = \begin{bmatrix} a_{11} & 0 & 0 & a_{14} & a_{15} & 0 \\ 0 & a_{22} & a_{23} & 0 & 0 & a_{26} \\ a_{31} & 0 & a_{33} & 0 & a_{35} & a_{36} \\ 0 & a_{42} & 0 & a_{44} & 0 & 0 \\ a_{51} & 0 & 0 & 0 & a_{55} & 0 \\ 0 & 0 & a_{63} & a_{64} & 0 & a_{66} \end{bmatrix} \qquad (10\text{–}14)$$

$$\begin{aligned} \mathrm{AR} &= (a_{11}, a_{14}, a_{15}, a_{22}, a_{23}, a_{26}, a_{31}, a_{33}, a_{35}, a_{36}, a_{42}, a_{44}, a_{51}, a_{55}, a_{63}, a_{64}, a_{66}) \\ \mathrm{JA} &= (1, 4, 5, 2, 3, 6, 1, 3, 5, 6, 2, 4, 1, 5, 3, 4, 6) \\ \mathrm{IA} &= (1, 4, 7, 11, 13, 15, 18) \end{aligned} \qquad (10\text{–}15)$$

The dimension of AR and JA is at least nz, where nz is the number of nonzero elements in the matrix. IA is of length $n + 1$ (for an n by n matrix), and the last element is $nz + 1$. This helps in determining the end of the last row of the matrix and the number of nonzero elements in the last row. To store all the indices in one array, both IA and JA are stored in an array INDEX, with the first $n + 1$ location used for IA and the rest of the vector used for JA. The length of INDEX is at least $nz + n + 1$. Thus, for the previous example, the array INDEX is as follows:

$$\mathrm{INDEX} = (1, 4, 7, 11, 13, 15, 18, 1, 4, 5, 2, 3, 6, 1, 3, 5, 6, 2, 4, 1, 5, 3, 4, 6)$$

where the first 7 elements form IA and the rest form JA.

10.3.2 Types of Preconditioners

For each of the three storage schemes for sparse matrices, CXML provides the routines to create and apply the following three preconditioners:

- Diagonal preconditioner
- Neumann polynomial preconditioner
- Incomplete LU preconditioner

10.3.2.1 DIAG: Diagonal Preconditioner

This is the simplest of the three preconditioners, with the preconditioning matrix Q chosen as the diagonal of the coefficient matrix A. There is no explicit split of Q into Q_L and Q_R. As the diagonal preconditioner approximates the matrix A by just its diagonal, it is usually not a good preconditioner for a general system (10–1).

10.3.2.2 POLY: Polynomial Preconditioner

The polynomial preconditioner is derived from the matrix A by first splitting it into its diagonal and off-diagonal parts and then considering the inverse of A as a truncated version of a polynomial series expansion. Let the coefficient matrix A be written as:

$$\begin{aligned} A &= D - C \\ &= (I - CD^{-1})D \\ &= (I - B)D \end{aligned}$$

where D is the diagonal of A, $-C$ is the matrix of off-diagonal elements, and $B = CD^{-1}$. By a polynomial series expansion, the inverse of A can be written as:

$$A^{-1} = D^{-1}(I - B)^{-1} = D^{-1}(I + B + B^2 + B^3 + ...).$$

A polynomial preconditioner of degree m essentially considers Q^{-1} to be a truncated version of the series expansion, that is:

$$Q^{-1} = D^{-1}(I + B + B^2 + B^3 + ... + B^m).$$

This polynomial expansion of the inverse of A is called the Neumann polynomial. The preconditioner is obtained in the form Q^{-1}, not Q, and there is no explicit split into the matrices Q_L and Q_R.

The effectiveness of polynomial preconditioners depends on how closely Q^{-1} approximates A^{-1}. This is determined by the matrix A itself as well as the degree of the polynomial. While a higher degree polynomial usually indicates a better approximation, it also involves extra computation per iteration. For preconditioning with a higher degree polynomial to be effective, the reduction in iterations must be sufficient to offset the extra computation per iteration.

10.3.2.3 ILU: Incomplete LU Preconditioner

The incomplete LU preconditioner obtains a factorization of A into lower and upper triangular factors, the matrices L and U, respectively, such that the following conditions are satisfied:

- Matrices L and U have the same nonzero structure as the matrix A.
- Nonzero elements of matrix A are equal to the corresponding element of the product LU.

Thus $A \approx LU = Q$ and $Q^{-1} = U^{-1}L^{-1}$.

The factorization is referred to as 'incomplete' as the product LU has nonzeros in locations where the matrix A has zeros, that is, the product LU is not identical to the matrix A as in the case of a 'complete' LU factorization.

If A is a symmetric matrix, as in the SDIA storage scheme, an incomplete Cholesky decomposition is computed with:

$$U = L^T$$

Incomplete factorizations usually form good preconditioners especially if the extra nonzero elements in the product LU are relatively small.

10.4 Iterative Solvers

CXML provides six iterative solvers based on the conjugate-gradient and conjugate-gradient-like techniques:

- DITSOL_PCG: Conjugate gradient method
- DITSOL_PLSCG: Least squares conjugate gradient method
- DITSOL_PBCG: Biconjugate gradient method
- DITSOL_PCGS: Conjugate gradient squared method
- DITSOL_PGMRES: Generalized minimum residual method
- DITSOL_PTFQMR: Transpose-free quasiminimal residual method

Each solver is applicable to a class of problems determined by the properties of the coefficient matrix A in (10–1) or the preconditioned matrix A' in (10–2) if preconditioning is used. The reference descriptions of the iterative solver subprograms at the end of this chapter outline the conditions under which each method can be applied.

CXML provides you with the option of using each iterative method without preconditioning as well as with right, left and split preconditioning. Table 10–8 indicates which forms of preconditioning are available for each method.

Table 10–8 Preconditioners for the Iterative Methods

Method	None	Left	Right	Split	SPD Split
DITSOL_PCG	X				X
DITSOL_PLSCG	X	X	X	X	
DITSOL_PBCG	X	X	X	X	
DITSOL_PCGS	X	X	X	X	
DITSOL_PGMRES	X	X	X	X	
DITSOL_PTFQMR	X	X	X	X	

10.4.1 Driver Routine

CXML includes a driver routine, DITSOL_DRIVER, that incorporates the calls to the MATVEC, PCONDL, and PCONDR routines so that you do not have to write these routines. The parameter list of the driver routine is identical to the parameter list of SOLVER, with the exception of the external routines MATVEC, PCONDL and PCONDR, which now refer to routines provided by CXML.

By setting values of appropriate parameters in the array IPARAM, you can choose a solver, a storage scheme and a preconditioner. The preconditioner must be created prior to the call to the driver routine. The driver routine does not allow the use of the matrix-free formulation of the iterative solver. The reference description of the driver routine at the end of this chapter provides further details.

10.5 Naming Conventions

The CXML routines can be broadly classified into two: routines related to the iterative solver and independent of the matrix, and routines that perform the matrix operations and are thus identified with a storage scheme.

Each routine name starts with the character D to indicate double-precision real routines. The next character group determines the operation being performed, namely, iterative solver, matrix-vector product, creation of the preconditioner and application of the preconditioner. Depending on the operation, the third, fourth and fifth character groups are chosen to reflect the iterative method, the storage scheme or the preconditioner.

Table 10–9 shows the naming conventions used for the iterative solver subroutines. Each routine name is obtained by concatenating the appropriate options from a character group, each character group separated by an underscore character.

Table 10–9 Naming Conventions: Iterative Solver Routines

Character Group	Mnemonic	Meaning
first	D	double precision
second	ITSOL MATVEC CREATE APPLY	function of the routine - iterative solver, matrix vector product, creation of preconditioner, or application of preconditioner.
third	DEFAULTS DRIVER PCG PLSCG PBCG PCGS PGMRES PTFQMR	options for the iterative solver
	SDIA UDIA GENR	storage scheme options for matrix vector product
	DIAG POLY ILU	preconditioner options for creation and application of preconditioners
fourth	ALL[1] SDIA UDIA GENR	storage scheme options for creation and application of preconditioners
fifth	L U	application of ILU preconditioner for UDIA and GENR storage schemes

[1]This option is for the application of the diagonal preconditioner only.

For example, DMATVEC_UDIA is the routine that obtains the matrix-vector product for the matrix stored using the unsymmetric diagonal (UDIA) storage scheme. Similarly, DAPPLY_ILU_GENR_L applies the incomplete LU (ILU) preconditioner for a matrix stored using the general storage by rows (GENR) scheme. The L indicates that the lower triangular part of the LU preconditioner is being considered.

10.6 Summary of Iterative Solver Subroutines

Tables 10–10, 10–11, 10–12, and 10–13 summarize the subroutines for the iterative solvers and the matrix operations.

Table 10–10 Summary of Iterative Solver Routines

Routine	Operation
DITSOL_DEFAULTS	Set the default values in the arrays IPARAM and RPARAM
DITSOL_DRIVER	Driver routine for the iterative solvers
DITSOL_PCG	Apply the preconditioned conjugate gradient method

(continued on next page)

Table 10–10 (Cont.) Summary of Iterative Solver Routines

Routine	Operation
DITSOL_PLSCG	Apply the preconditioned least squares conjugate gradient method
DITSOL_PBCG	Apply the preconditioned biconjugate gradient method
DITSOL_PCGS	Apply the preconditioned conjugate gradient squared method
DITSOL_PGMRES	Apply the preconditioned generalized minimum residual method
DITSOL_PTFQMR	Apply the preconditioned transpose-free quasiminimal residual method

Table 10–11 Summary of Matrix-Vector Product Routines

Routine	Operation
DMATVEC_SDIA	Matrix vector product for the symmetric diagonal storage scheme
DMATVEC_UDIA	Matrix vector product for the unsymmetric diagonal storage scheme
DMATVEC_GENR	Matrix vector product for the general storage by rows scheme

Table 10–12 Summary of Preconditioner Creation Routines

Routine	Operation
DCREATE_DIAG_SDIA	Create the diagonal preconditioner for the symmetric diagonal storage scheme
DCREATE_DIAG_UDIA	Create the diagonal preconditioner for the unsymmetric diagonal storage scheme
DCREATE_DIAG_GENR	Create the diagonal preconditioner for the general storage by rows scheme
DCREATE_POLY_SDIA	Create the polynomial preconditioner for the symmetric diagonal storage scheme
DCREATE_POLY_UDIA	Create the polynomial preconditioner for the unsymmetric diagonal storage scheme
DCREATE_POLY_GENR	Create the polynomial preconditioner for the general storage by rows scheme
DCREATE_ILU_SDIA	Create the incomplete LU preconditioner for the symmetric diagonal storage scheme
DCREATE_ILU_UDIA	Create the incomplete LU preconditioner for the unsymmetric diagonal storage scheme
DCREATE_ILU_GENR	Create the incomplete LU preconditioner for the general storage by rows scheme

Table 10–13 Summary of Preconditioner Application Routines

Routine	Operation
DAPPLY_DIAG_ALL	Apply the diagonal preconditioner for all storage schemes
DAPPLY_POLY_SDIA	Apply the polynomial preconditioner for the symmetric diagonal storage scheme
DAPPLY_POLY_UDIA	Apply the polynomial preconditioner for the unsymmetric diagonal storage scheme
DAPPLY_POLY_GENR	Apply the polynomial preconditioner for the general storage by rows scheme
DAPPLY_ILU_SDIA	Apply the incomplete LU preconditioner for the symmetric diagonal storage scheme
DAPPLY_ILU_UDIA_L	Apply the incomplete LU preconditioner for the unsymmetric diagonal storage scheme (operates on the L part)
DAPPLY_ILU_UDIA_U	Apply the incomplete LU preconditioner for the unsymmetric diagonal storage scheme (operates on the U part)
DAPPLY_ILU_GENR_L	Apply the incomplete LU preconditioner for the general storage by rows scheme (operates on the L part)
DAPPLY_ILU_GENR_U	Apply the incomplete LU preconditioner for the general storage by rows scheme (operates on the U part)

10.7 Error Handling

The six iterative solver subroutines include an error flag in the argument list. This is not an optional argument. On exit from the iterative solver routine, check its value to ensure that the solver converged normally.

The error flag can have various values. A return value of 0 indicates a normal return from the solver, with the iterations converging under the specified conditions. A negative return value implies a fatal error such as incorrect input, insufficient workspace, or use of a method inapplicable to the problem being solved. In such cases, a fatal error message is printed out describing the problem and control is returned to the calling routine. A positive return value of the error flag indicates a warning, such as a method terminating after reaching the maximum number of iterations. This is a correctable error if the maximum number of iterations is set to a low value. However, it could also signal a more fatal error such as the stagnation of the quantity being measured for convergence.

In addition to the solvers, CXML provides routines for the creation and application of various preconditioners for matrices stored using various storage schemes. The preconditioner is created by a call to the appropriate routine prior to calling the iterative solver. You must ensure that the preconditioner routine used does indeed exist. For example, in the case of diagonal preconditioning, the elements along the diagonal of the matrix must be nonzero. The routines that generate the preconditioners do not explicitly check for the existence of the preconditioner routine. Therefore, you could get an internal exception error, such as division by zero or square-root of a negative number, that terminates the execution of the program. In contrast, an error in the iterative solver does not terminate the execution. Instead, the error flag is set and control returned to the calling program.

Table 10–14 shows the values of the error flags, an explanation of each value and the action needed to recover from each error. The values –2100 through –2104 indicate a breakdown in the iterative process caused by either an inappropriate input parameter or the use of an inappropriate method for the problem. The remaining values, all negative, indicate that input data to the solver is invalid.

Table 10–14 Error Flags for Sparse Iterative Solver Subprograms

Error Flag	Description	User Action
0	Normal exit	No action required.
2001	Method did not converge	Increase value of **itmax**; check that **rparam(2)** is not stagnating.
–2001	Invalid **ipcond**	Refer to subprogram description for valid values and rerun with acceptable value.
–2003	Invalid **nipar**	"
–2004	Invalid **nrwrk**	"
–2005	Invalid **istop**	"
–2006	Invalid **errtol**	"
–2007	Invalid **n**	"
–2008	Invalid **nrpar**	"
–2009	Zero denominator in the stopping criterion	Rerun with a different stopping criterion.
–2010	Invalid **isolve**	Refer to Table 10–4 for valid values and rerun with acceptable value.
–2011	Invalid **iprec**	Refer to Table 10–4 for valid values and rerun with acceptable value.
–2012	Invalid **istore**	Refer to Table 10–4 for valid values and rerun with acceptable value.
–2100	Preconditioner is not positive-definite	Rerun with a different preconditioner or solver.
–2101	Matrix is not positive-definite	Rerun with a different solver.
–2102	Breakdown in generation of direction vector	Rerun with a different solver, preconditioner, or starting guess.
–2103	Breakdown in update to solution vector	Rerun with a different solver, preconditioner, or starting guess.
–2104	Breakdown in *gmres* iteration	Rerun with a different solver, preconditioner, starting guess, or **kprev**.
–2200	*Tru64 UNIX only* Memory allocation routine in the parallel version failed	Increase allocated values of pagefile quota and virtual memory, or reduce the number of processors, or use serial version of the solver.

10.8 Message Printing

In cases of the return value not being 0, all the I/O is done by means of a user-supplied print routine. For convenience, it is called "USER_PRINT_ROUTINE" in this description. Iterative solvers pass a null-terminated string to the USER_PRINT_ROUTINE to do the printing. If USER_PRINT_ROUTINE is not supplied, messages are printed to the standard output.

If USER_PRINT_ROUTINE is supplied, CXML_ITSOL_SET_PRINT_ROUTINE must be called to provide the address of USER_PRINT_ROUTINE to the iterative solvers. USER_PRINT_ROUTINE must also be declared as external in the calling program.

```
SUBROUTINE CXML_ITSOL_SET_PRINT_ROUTINE(USER_PRINT_ROUTINE,CONTEXT,IPARAM)

       SUBROUTINE USER_PRINT_ROUTINE(CONTEXT,BUF,SIZE)
```

Fatal error messages are always printed out. The only exception to this is when the value of **iolevel** is negative. In such cases, no output is produced by the solver. Therefore it is important to check the error flag on exit.

10.9 Hints on the Use of the Iterative Solver

The iterative solvers included in CXML provide you with a wide choice of iterative methods and preconditioners. Additional flexibility is provided via the adoption of a matrix-free formulation of the iterative method. This allows you to use any storage scheme for the matrix, but implies that you have to write the routines for the matrix operations. You also have the option of using routines included in CXML for the matrix operations, but this restricts you to the storage schemes and preconditioners provided by CXML. It is also possible to mix the two approaches and use a storage scheme included in CXML, but provide your own routines to create and apply the preconditioner of your choice.

CXML provides further flexibility by allowing you to set various parameters such as the form of preconditioner, the stopping criterion, the maximum number of iterations allowed, the degree of the polynomial for polynomial preconditioning and so on. These enable you to control the iterative procedure and fine tune it to suit the needs of your application.

The steps in using the iterative solver can be summarized as follows:

- Choose the storage scheme for the coefficient matrix A.

  You can either choose one of the schemes provided by CXML (SDIA, UDIA, or GENR) or choose your own storage scheme.

- Select an iterative method (DITSOL_PCG, DITSOL_PLSCG, DITSOL_PBCG, DITSOL_PCGS, DITSOL_PGMRES, or DITSOL_PTFQMR), a form of preconditioner (none, left, right, split, or SPD split), and if necessary, a preconditioner (DIAG, POLY, or ILU).

  The preconditioner and the form of preconditioning should match. For example, DIAG and POLY preconditioners cannot be used in the split form as they do not explicitly generate the matrices Q_L and Q_R. However, they can be used in SPD split preconditioning as it requires only the matrix Q. The form of preconditioning is chosen via the parameter ipcond (IPARAM(7)). You also have the option of providing your own preconditioner.

- Write the routines MATVEC (required) and, if necessary, the routines PCONDL and PCONDR.

The reference descriptions for each iterative method at the end of this chapter describe the functionality that must be provided by these routines. If you have chosen your own storage scheme for the coefficient matrix or chosen your own preconditioner, then you must provide the functionality required by the routines MATVEC, PCONDL, and PCONDR. If, however, you have chosen one of the preconditioners and storage schemes included in CXML, the functionality required by these routines is provided via a call to the appropriate CXML routines. In this case, you should be consistent in the use of storage schemes, that is, the same storage schemes should be used in all operations.

Whether you use the routines for the matrix operations provided by CXML or not, it is your responsibility to provide the routine MATVEC and, if applicable, the routines PCONDL and PCONDR, with the standard interface.

You also have the option of using the driver routine, DITSOL_DRIVER, in which case, you do not have to provide the routines MATVEC, PCONDL and PCONDR; instead you use the versions of these routines provided by CXML.

- Assign values to the variables in array IPARAM and RPARAM.

  This could be done via a call to the routine DITSOL_DEFAULTS. The routine DITSOL_DEFAULTS does not set the values of all parameters in the arrays IPARAM and RPARAM and it is your responsibility to ensure that all appropriate variables have been assigned valid values before a call to the iterative solver. Information such as the size of the work arrays is provided in the routine descriptions at the end of this chapter. In addition to the assignment of values to the variables, any associated setup should also be done at this time such as the opening of files for I/O. If you choose to implement your own stopping criterion, you must provide the routine MSTOP, with the standard interface given in Table 10–3.

- Generate the preconditioner.

  This is done either by a call to one of CXML's routines, if you are using a storage scheme and preconditioner provided by CXML, or by writing your own routine. Unlike the routines for the application of the preconditioner, there is no standard interface for the routine to generate the preconditioner as it is formed before the call to the iterative solver. However, the preconditioner must be generated in a manner that would be consistent with the use of the standard interface for the routines PCONDL and PCONDR.

  If you use a CXML routine to generate the preconditioner, it is your responsibility to ensure that the preconditioner does exist. For example, in the case of diagonal preconditioning, the diagonal elements of the coefficient matrix A must be nonzero. If a CXML routine is called to create a preconditioner and it does not exist, the routine terminates with an appropriate system message such as a division by zero error or a square-root of a negative number error.

  If you are using the driver routine, DITSOL_DRIVER, you must create the appropriate preconditioner using the appropriate storage scheme, prior to the call to the driver routine.

- Call the appropriate iterative solver routine with the standard interface given in Table 10–7.

On exit from the solver, the error flag, ierror, should be checked to ensure that the iterations converged normally. A return value of 0 indicates a normal exit from the routine SOLVER, with the iterations converging under the specified conditions. A negative return value implies a fatal error such as incorrect input or insufficient workspace, while a positive return value indicates a warning such as the solver terminating after the maximum number of iterations.

The best solver and preconditioner for a given problem is very dependent on the problem itself. Often, a choice is made based on prior experience. In the absence of this, the following factors may influence the selection of a particular solver or preconditioner:

- Applicability of a solver

  Each solver is applicable under certain conditions. Some solvers can be applied to symmetric matrices only; others require the evaluation of both Ax and $A^T x$. The reference description for each solver includes the conditions under which it is applicable. These must be considered in the choice of a solver for a problem.

- Effectiveness of a preconditioner

  Based on the properties of the problem, some preconditioners may be more effective than others in improving the convergence of a solver. However, the increase in time per iteration due to the use of the preconditioner must also be taken into account. For example, increasing the degree of the polynomial in polynomial preconditioning will increase the time per iteration, but may not always reduce the number of iterations sufficiently to lead to an overall reduction in the execution time.

- Amount of memory available

  Different solvers and preconditioners require different amounts of memory. For example, the generalized minimum residual method (DITSOL_PGMRES) allows you to use a variable number of previous residual vectors. As this number increases, the work done per iteration, and the memory required, also increase. Often, but not always, there is a corresponding increase in the convergence rate. A limited amount of memory may preclude the choice of a sufficiently large number of previous residual vectors to ensure convergence.

In addition to choosing a solver and a preconditioner, you also have the choice of a stopping criterion. It is important to select carefully the condition that determines when the iterative process will be terminated. CXML includes four stopping criteria. It also allows you the option of writing your own version. In some cases, a stopping criterion may be obtained at a low cost from the iterative process. But, this may not be the most effective criterion for judging the convergence of your particular problem. In the initial stages of experimenting with different stopping criteria, it may help to calculate the residual of the system explicitly at the end of the iterative process in order to determine if the choice of stopping criteria was an appropriate one.

The preceding guidelines should be taken into consideration in your choice of a solver, preconditioner and stopping criterion. As this choice is very dependent on the problem, some experimentation may be necessary to determine the most efficient method. CXML provides you a flexible interface that allows different solvers, preconditioners and stopping criterion to be tested easily. In addition, the input parameters allow you to generate extensive information on the solution process. These can be used to gain a better insight into the behavior of various

solvers and preconditioners for your problem, helping you to choose a combination that will provide a solution efficiently.

10.10 A Look at Some Iterative Solvers

To illustrate the use of the sparse iterative solvers and the concepts of matrix-free formulation and preconditioning, consider the linear system of equations derived from the discretization of the Laplace's equation on the unit square with Dirichlet boundary conditions, using the standard five point central differencing scheme:

$$-u_{xx} - u_{yy} = 0$$

$$0 \leq x \leq 1$$

$$0 \leq y \leq 1$$

Assuming nx grid points in x direction and ny grid points in the y direction, the coefficient matrix A has the following form for $nx = ny = 4$:

```
 4 -1        | -1           |            |
-1  4 -1     |    -1        |            |
   -1  4 -1  |       -1     |            |
      -1  4  |          -1  |            |
 ----------- |------------- |------------|-----------
-1           |  4 -1        |-1          |
   -1        | -1  4 -1     |   -1       |
      -1     |    -1  4 -1  |      -1    |
         -1  |       -1  4  |         -1 |
 ----------- |------------- |------------|-----------
             | -1           | 4 -1       |-1
             |    -1        |-1  4 -1    |   -1
             |       -1     |   -1  4 -1 |      -1
             |          -1  |      -1  4 |         -1
 ----------- |------------- |------------|-----------
             |              |-1          | 4 -1
             |              |   -1       |-1  4 -1
             |              |      -1    |   -1  4 -1
             |              |         -1 |      -1  4
```

The elements not defined in the matrix are zero. The exact solution is assumed to be all 1.0 and the starting guess is the zero vector.

Examples 10–2, 10–3, 10–4, and 10–5 illustrate the use of the CXML iterative solver routines from Fortran, C, and C++ codes. Each example is self-contained, and includes comments indicating the operations being performed. The output created by each example program is also included, to illustrate the information that can be obtained from the iterative solvers by setting the appropriate parameters.

These examples, along with additional examples, are included online in the CXML Examples directory. The following is an example of a print routine that users can supply to iterative solvers. Line breaks are already inserted in the proper places in the message string. If you use an unformatted write statement, Fortran will insert more line breaks. Therefore, it is suggested that you use WRITE(filename, '(A)') in order to print the message.

Example 10–1 USER_PRINT_ROUTINE (Fortran Code)

```
          SUBROUTINE USER_PRINT_ROUTINE( CONTEXT, BUF, SIZE)
C
          INTEGER CONTEXT
          INTEGER SIZE
          INTEGER BUF(*)
C
          INCLUDE 'CXML_ITSOL_PRINT.FOR'
C
          CHARACTER*(CXML_ITSOL_MAX_MESSAGE_LENGTH) NEW_BUF
C
          CALL CXML_FORMAT_STRING(BUF, SIZE, NEW_BUF)
          WRITE(CONTEXT, '(A)') NEW_BUF(1:SIZE)
C
          END
```

Example 10–2 Iterative Solver with User-Defined Routines (Fortran Code) - Example filename: example_itsol_1.f

```
      PROGRAM EXAMPLE_ITSOL_1
C
C ***** TO DEMONSTRATE THE USE OF THE SPARSE ITERATIVE SOLVER.
C
C ***** THIS PROGRAM ILLUSTRATES THE FOLLOWING:
C
C       (1) USE OF THE SOLVER TO SOLVE THE TEST PROBLEM VIA
C           PRECONDITIONED CONJUGATE GRADIENT METHOD, USING A
C           USER-DEFINED STORAGE SCHEME.
C       (2) USE OF A USER-DEFINED ROUTINE MATVEC
C       (3) USE OF A USER-DEFINED ROUTINE MSTOP
C       (4) USE OF USER-DEFINED ROUTINE PCONDL
C       (5) USE OF THE ROUTINE DITSOL_DEFAULTS
C       (6) INFORMATION PRINTED OUT FOR IOLEVEL = 3
C       (7) PRINTING MESSAGES TO A FILE
C
      IMPLICIT NONE
      INTEGER NMAX
C
      PARAMETER (NMAX = 100)
C
      REAL*8 X(NMAX), XO(NMAX), RHS(NMAX), QL(NMAX)
      REAL*8 RPARAM(50), RWORK(4*NMAX), DUM, TEMP
      REAL*8 A(NMAX)
C
      INTEGER IPARAM(50), IA(2), IDUM
      INTEGER I,NX, NY, NXNY, IOUNIT, IERROR
C
      REAL*8 A1(NMAX), A2(NMAX), A3(NMAX), A4(NMAX), A5(NMAX)
      COMMON/ MATRIX/ A1, A2, A3, A4, A5
C
      EXTERNAL MATVEC, PCONDL, USER_MSTOP, USER_PRINT_ROUTINE
C
C ***** SET UP PROBLEM SIZE
C
      NX = 10
      NY = 10
      NXNY = NX*NY
C
C ***** SET THE PARAMETERS (INTEGER AND REAL)
C
      CALL DITSOL_DEFAULTS (IPARAM, RPARAM)
C
C ***** CHANGE ANY VALUES THAT ARE DIFFERENT FROM THE DEFAULT
C       ASSIGN VALUES TO PARAMETERS NOT SET BY ROUTINE DEFAULTS
C           CHANGE IPCOND TO 4 (FOR SPD SPLIT PRECONDITIONING)
C           CHANGE IOLEVEL TO 3
C           CHANGE ISTOP TO 0 (FOR USER-DEFINED MSTOP)
C
      IPARAM(3) = 0
      IPARAM(4) = 4*NXNY
C
      IPARAM(5) = 7
      IPARAM(6) = 3
      IPARAM(7) = 4
      IPARAM(8) = 0
```

(continued on next page)

Example 10–2 (Cont.) Iterative Solver with User-Defined Routines (Fortran Code) - Example filename: example_itsol_1.f

```
C
C ***** SETUP OUTPUT FILE
C
      IOUNIT = IPARAM(5)
      OPEN (UNIT=IOUNIT,FILE='OUTPUT.DATA',STATUS='UNKNOWN')
      REWIND IOUNIT
C
C *****  SETUP PRINT ROUTINE
C
      CALL CXML_ITSOL_SET_PRINT_ROUTINE(USER_PRINT_ROUTINE,
     $         IOUNIT, IPARAM)

      WRITE (IOUNIT,101)

  101 FORMAT (/,2X,'SOLVING EXAMPLE PROBLEM WITH SPD SPLIT
     $ PRECONDITIONED CG',/,2X,'DIAGONAL PRECONDITIONING USED ',/)
C
C ***** GENERATE THE MATRIX (USE IA TO PASS NX AND NY TO SOLVER)
C
      CALL GENMAT(NX, NY, NXNY)
      IA(1) = NX
      IA(2) = NY
C
C ***** GENERATE XO, THE TRUE SOLUTION
C
      DO I = 1, NXNY
          XO(I) = 1.0D0
      END DO
C
C ***** OBTAIN THE RIGHT HAND SIDE
C
      CALL MATVEC (0, IPARAM, RPARAM, A, IA, DUM, XO, RHS, NXNY)
C
C ***** OBTAIN INITIAL GUESS (ALL ZEROS)
C
      DO I = 1, NXNY
         X(I) = 0.0D0
      END DO
C
C ***** GENERATE THE DIAGONAL PRECONDITIONER
C
      CALL GEN_PCOND (NXNY, QL)
C
C ***** CALL THE SOLVER
C
       CALL DITSOL_PCG ( MATVEC, PCONDL, DUM, USER_MSTOP,
     $                   A, IA, X, RHS,
     $                   NXNY, QL, IDUM, DUM, IDUM,
     $                   IPARAM, RPARAM, IDUM, RWORK, IERROR)
C
C ***** PRINT OUT THE SOLUTION
C
      WRITE (IOUNIT,102)
102   FORMAT (/,5X,'TRUE SOLUTION',5X,'SOLUTION FROM SOLVER',
     $5X,'ABS. DIFFERENCE'/)
      WRITE (IOUNIT,103) (XO(I),X(I),ABS(XO(I)-X(I)),I=1,NXNY)
103   FORMAT (/,3(5X,E15.8))
C
```

(continued on next page)

Example 10–2 (Cont.) Iterative Solver with User-Defined Routines (Fortran Code) - Example filename: example_itsol_1.f

```
C
C
C ***** FIND MAX ERROR IN SOLUTION
C
      TEMP = ABS(XO(1) - X(1))
      DO I = 2, NXNY
         TEMP = MAX( TEMP, ABS(XO(I) - X(I)) )
      END DO
      WRITE (IOUNIT,104) TEMP
104   FORMAT (/,2X,'MAX ERROR IN SOLUTION= ', E15.8,/)
C
      STOP
      END
C
      SUBROUTINE USER_PRINT_ROUTINE(CONTEXT, BUF, SIZE)
C
      INTEGER CONTEXT
      INTEGER SIZE
      INTEGER BUF(*)
C
      INCLUDE 'cxml_itsol_print.for'
C
      CHARACTER*(CXML_ITSOL_MAX_MESSAGE_LENGTH) NEW_BUF
C
      CALL CXML_FORMAT_STRING(BUF, SIZE, NEW_BUF)
      WRITE(CONTEXT, '(A)') NEW_BUF(1:SIZE)
C
      END
C
C
C
      SUBROUTINE MATVEC(JOB, IPARAM, RPARAM, A, IA, W, X, Y, N)
C
C ***** MULTIPLY THE VECTOR X BY THE MATRIX TO OBTAIN VECTOR Y
C       ONLY JOB = 0 NEEDED FOR THIS EXAMPLE
C
      IMPLICIT NONE
C
      REAL*8 X(*), Y(*), A(*), RPARAM(*), W
      INTEGER IA(*), IPARAM(*), N, JOB
C
      CALL MULA (IA(1), IA(2), N, X, Y)
C
      RETURN
      END
C
C
C
```

(continued on next page)

Example 10–2 (Cont.) Iterative Solver with User-Defined Routines (Fortran Code) - Example filename: example_itsol_1.f

```
      SUBROUTINE PCONDL(JOB, IPARAM, RPARAM, QL, IQL, A, IA,
     $                  W, X, Y, N)
C
C ***** CALL THE LEFT PRECONDITIONER
C       ONLY JOB = 0 NEEDED FOR THIS EXAMPLE
C
      IMPLICIT NONE
      REAL*8 X(*), Y(*),  QL(*), A(*), RPARAM(*), W
      INTEGER IA(*), IPARAM(*), N, IQL, JOB
C
C ***** DIAGONAL PRECONDITIONING
C
      CALL APPLY_PCOND_DIA (N, X, Y, QL)
C
      RETURN
      END
C
C
C
      SUBROUTINE GEN_PCOND (N, QL)
C
C ***** GENERATE THE LEFT PRECONDITIONER
C
      IMPLICIT NONE
      INTEGER NMAX
      PARAMETER (NMAX = 100)
      INTEGER N,I
      REAL*8 QL(*), A1(NMAX), A2(NMAX), A3(NMAX), A4(NMAX), A5(NMAX)
      COMMON /MATRIX/ A1, A2, A3, A4, A5
C
      DO I = 1, N
          QL(I) = 1.0D0 / A3(I)
      END DO
C
      RETURN
      END
C
C
C
      SUBROUTINE APPLY_PCOND_DIA (N, X, Y, QL)
C
C ***** APPLY THE DIAGONAL PRECONDITIONER
C
      IMPLICIT NONE
      REAL*8 X(*), Y(*), QL(*)
      INTEGER N,I
C
      DO I = 1, N
          Y(I) = X(I) * QL(I)
      END DO
C
      RETURN
      END
C
C
C
```

(continued on next page)

Example 10–2 (Cont.) Iterative Solver with User-Defined Routines (Fortran Code) - Example filename: example_itsol_1.f

```
      SUBROUTINE GENMAT (NX, NY, NXNY)
C
C ***** GENERATE THE MATRIX FOR THE EXAMPLE
C
      IMPLICIT NONE
      INTEGER NMAX
      PARAMETER (NMAX = 100)
      REAL*8 A1(NMAX), A2(NMAX), A3(NMAX), A4(NMAX), A5(NMAX)
      COMMON /MATRIX/ A1, A2, A3, A4, A5
      INTEGER NXNY, I, J, K, NX, NY
C
      DO I = 1, NXNY
          A3(I) = 4.0D0
          A1(I) = 0.0D0
          A2(I) = 0.0D0
          A4(I) = 0.0D0
          A5(I) = 0.0D0
      END DO
C
      DO J = 1, NY
          DO I = 2, NX
              K = (J-1)*NX+I
              A2(K) = -1.0D0
      END DO
          DO I = 1, NX-1
              K = (J-1)*NX+I
              A4(K) = -1.0D0
          END DO
      END DO
C
      DO J = 2, NY
          DO I = 1, NX
              K = (J-1)*NX+I
              A1(K) = -1.0D0
          END DO
      END DO
C
      DO J = 1, NY-1
          DO I = 1, NX
              K = (J-1)*NX+I
              A5(K) = -1.0D0
          END DO
      END DO
C
      RETURN
      END
C
C
C
```

(continued on next page)

Example 10–2 (Cont.) Iterative Solver with User-Defined Routines (Fortran Code) - Example filename: example_itsol_1.f

```
      SUBROUTINE MULA (NX, NY, NXNY, TMP1, TMP2)
C
C ***** TO OBTAIN THE MATRIX VECTOR MULTIPLY
C
      IMPLICIT NONE
      INTEGER NMAX
      PARAMETER (NMAX = 100)
      REAL*8 TMP1(*), TMP2(*)
      INTEGER NX,NY,NXNY, I
      REAL*8 A1(NMAX), A2(NMAX), A3(NMAX), A4(NMAX), A5(NMAX)
      COMMON /MATRIX/ A1, A2, A3, A4, A5
C
      DO I = 1, NXNY
          TMP2(I) = A3(I)*TMP1(I)
      END DO
C
      DO I = 1, NXNY-1
          TMP2(I) = TMP2(I) +
     $              A4(I)*TMP1(I+1)
      END DO
C
      DO I = 2, NXNY
          TMP2(I) = TMP2(I) +
     $              A2(I)*TMP1(I-1)
      END DO
C
      DO I = 1, NXNY-NX
          TMP2(I) = TMP2(I) +
     $              A5(I)*TMP1(I+NX)
      END DO
C
      DO I = NX+1, NXNY
          TMP2(I) = TMP2(I) +
     $              A1(I)*TMP1(I-NX)
      END DO
C
      RETURN
      END
C
C
C
      SUBROUTINE USER_MSTOP (IPARAM, RPARAM, X, R, Z, B, N)
C
C ***** ROUTINE FOR THE USER PROVIDED STOPPING CRITERION
C
      IMPLICIT NONE
      REAL*8 X(*), B(*), R(*), Z(*), RPARAM(*), STPTST
      INTEGER ITERS, I, IOUNIT, IPARAM(*), N
C
      IOUNIT = IPARAM(5)
      ITERS = IPARAM(10)
      IF (ITERS.EQ.0) THEN
          WRITE(IOUNIT, 100)
  100     FORMAT(/,2X,'USING USER-DEFINED STOPPING CRITERION',/)
      END IF
```

(continued on next page)

Example 10–2 (Cont.) Iterative Solver with User-Defined Routines (Fortran Code) - Example filename: example_itsol_1.f

```
C
C ***** USER-DEFINED STOPPING CRITERION USES MAX NORM OF RESIDUAL FOR
C       STPTST
C
      STPTST = ABS (R(1))
      DO I = 2, N
         STPTST = MAX ( STPTST,ABS(R(I)) )
      END DO
C
      RPARAM(2) = STPTST
C
      RETURN
      END
```

Output from example_itsol_1.f

```
SOLVING EXAMPLE PROBLEM WITH SPD SPLIT PRECONDITIONED CG
DIAGONAL PRECONDITIONING USED
 METHOD USED : CG WITH SPD SPLIT PRECONDITIONING
 ORDER OF SYSTEM =    100
 STOPPING CRITERION USED :     0
 MAXIMUM ITERATIONS ALLOWED:   100
 TOLERANCE FOR CONVERGENCE :   0.10000000e-05
USING USER-DEFINED STOPPING CRITERION
    ITERATION =         0    STOPPING TEST = 0.20000000e+01
    ITERATION =         1    STOPPING TEST = 0.92307692e+00
    ITERATION =         2    STOPPING TEST = 0.58793970e+00
    ITERATION =         3    STOPPING TEST = 0.63509006e+00
    ITERATION =         4    STOPPING TEST = 0.42973063e+00
    ITERATION =         5    STOPPING TEST = 0.48724587e+00
    ITERATION =         6    STOPPING TEST = 0.41781094e+00
    ITERATION =         7    STOPPING TEST = 0.50288290e+00
    ITERATION =         8    STOPPING TEST = 0.17070529e+00
    ITERATION =         9    STOPPING TEST = 0.38502953e-01
    ITERATION =        10    STOPPING TEST = 0.16076790e-01
    ITERATION =        11    STOPPING TEST = 0.75548469e-02
    ITERATION =        12    STOPPING TEST = 0.15431168e-02
    ITERATION =        13    STOPPING TEST = 0.14025362e-03
    ITERATION =        14    STOPPING TEST = 0.42745516e-05
    ITERATION =        15    STOPPING TEST = 0.63333204e-15
 SOLUTION OBTAINED AFTER          15  ITERATIONS
 NORMAL EXIT FROM SOLVER
 FINAL VALUE OF STOPPING TEST = 0.63333204e-15
   TRUE SOLUTION     SOLUTION FROM SOLVER     ABS. DIFFERENCE
    0.10000000e+01      0.10000000e+01      0.33306691e-15
    0.10000000e+01      0.10000000e+01      0.44408921e-15
                              :
                              : (EDITED FOR BREVITY)
    0.10000000e+01      0.10000000e+01      0.33306691e-15
    0.10000000e+01      0.10000000e+01      0.33306691e-15
MAX ERROR IN SOLUTION=  0.23314684e-14
```

Example 10–3 Iterative Solver with CXML Routines (Fortran Code) - Example filename: example_itsol_4.f

```
      PROGRAM EXAMPLE_ITSOL_4
C
C ***** TO DEMONSTRATE THE USE OF THE SPARSE ITERATIVE SOLVER.
C
C ***** THIS PROGRAM ILLUSTRATES THE FOLLOWING:
C
C       (1) USE OF THE SOLVER TO SOLVE THE TEST PROBLEM VIA
C           PRECONDITIONED GMRES METHOD METHOD, WITH SPLIT INCOMPLETE
C           CHOLESKY PRECONDITIONING. THE MATRIX IS STORED USING
C           THE UNSYMMETRIC DIAGONAL FORMAT
C       (2) USE OF ROUTINE MATVEC (DMATVEC_UDIA)
C       (3) USE OF ROUTINES PCONDL AND PCONDR TO CALL ROUTINES FOR APPLYING
C           THE PRECONDITIONER (DAPPLY_ILU_UDIA_L AND DAPPLY_ILU_UDIA_U)
C       (4) USE OF THE ROUTINE DITSOL_DEFAULTS
C       (5) PRINT MESSAGES TO FILE.
C
C
      IMPLICIT NONE
C
      INTEGER NMAX
      PARAMETER (NMAX = 100)
      INTEGER NDIM
      PARAMETER (NDIM = 100)
      INTEGER KPREV_MAX
      PARAMETER (KPREV_MAX = 5)
      INTEGER NWK
      PARAMETER (NWK = NMAX*(KPREV_MAX+2) + KPREV_MAX*(KPREV_MAX+5)+1 )
C
      REAL*8 X(NMAX), XO(NMAX), RHS(NMAX)
      REAL*8 RPARAM(50), RWORK(NWK), DUM
      REAL*8 A_UDIA(NDIM,5), P_ILU(NDIM,5), TEMP
      INTEGER IP_ILU(5), INDEX_UDIA(5)
C
      INTEGER IPARAM(50), IDUM
      INTEGER I, NX, NY, NXNY, IOUNIT, IERROR, NZEROS
C
      EXTERNAL MATVEC, PCONDL, PCONDR, USER_PRINT_ROUTINE
C
C ***** SET UP PROBLEM SIZE
C
      NX = 10
      NY = 10
      NXNY = NX*NY
      NZEROS = 5
C
C ***** SET THE PARAMETERS (INTEGER AND REAL)
C
      CALL DITSOL_DEFAULTS (IPARAM, RPARAM)
```

(continued on next page)

Example 10–3 (Cont.) Iterative Solver with CXML Routines (Fortran Code) - Example filename: example_itsol_4.f

```
C
C ***** CHANGE ANY VALUES THAT ARE DIFFERENT FROM THE DEFAULT
C       ASSIGN VALUES TO PARAMETERS NOT SET BY DEFAULTS
C              CHANGE IOUNIT TO 7
C              CHANGE IPCOND TO 3 (FOR SPLIT PRECONDITIONING)
C              CHANGE IOLEVEL TO 3
C              CHANGE ISTOP TO 3 (ONLY ISTOP=3 AND 4 ALLOWED)
C
      IPARAM(3) = 0
      IPARAM(4) = NWK
      IPARAM(5) = 7
      IPARAM(6) = 3
      IPARAM(7) = 3
      IPARAM(8) = 3
C
C ***** ASSIGN VALUE TO KPREV (NUMBER OF PREVIOUS RESIDUALS STORED)
C       NOTE THAT THE SIZE OF RWORK ALLOWS A MAXIMUM VALUE OF KPREV = 5
C
      IPARAM(34) = 3
C
C ***** SETUP OUTPUT FILE
C
      IOUNIT = IPARAM(5)
      OPEN (UNIT=IOUNIT,FILE='OUTPUT.DATA',STATUS='UNKNOWN')
      REWIND IOUNIT
C
C *****  SETUP PRINT ROUTINE
C
      CALL CXML_ITSOL_SET_PRINT_ROUTINE(USER_PRINT_ROUTINE,
     $         IOUNIT, IPARAM)
C
      WRITE (IOUNIT,101)
101   FORMAT (/,2X,'SOLVING EXAMPLE PROBLEM WITH SPLIT
     $ PRECONDITIONED GMRES',/,2X,'ILU PRECONDITIONING USED ',/
     $ 2X,'MATRIX STORED IN UNSYMMETRIC DIAGONAL FORMAT',/)
C
C ***** GENERATE THE MATRIX
C
      CALL GENMAT(NX, NY, NXNY, A_UDIA, INDEX_UDIA, NDIM, NZEROS)
      IPARAM(31) = NZEROS
      IPARAM(32) = NDIM
C
C ***** GENERATE XO, THE TRUE SOLUTION
C
      DO I = 1, NXNY
          XO(I) = 1.0D0
      END DO
C
C ***** OBTAIN THE RIGHT HAND SIDE
C
      CALL MATVEC (0, IPARAM, RPARAM, A_UDIA, INDEX_UDIA, DUM, XO,
     $             RHS, NXNY)
C
C ***** OBTAIN INITIAL GUESS (ALL ZEROS)
C
      DO I = 1, NXNY
        X(I) = 0.0D0
      END DO
```

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Example 10–3 (Cont.) Iterative Solver with CXML Routines (Fortran Code) - Example filename: example_itsol_4.f

```
C ***** GENERATE THE ILU PRECONDITIONER
C
      CALL DCREATE_ILU_UDIA (A_UDIA, INDEX_UDIA, NDIM, NZEROS,
     $                      P_ILU, IP_ILU, NXNY)
C
C ***** CALL THE SOLVER
C
       CALL DITSOL_PGMRES ( MATVEC, PCONDL, PCONDR, DUM,
     $                      A_UDIA, INDEX_UDIA, X, RHS, NXNY,
     $                      P_ILU, IP_ILU, P_ILU, IP_ILU,
     $                      IPARAM, RPARAM, IDUM, RWORK, IERROR)
C
C ***** PRINT OUT THE SOLUTION
C
      WRITE (IOUNIT,102)
102   FORMAT (/,5X,'TRUE SOLUTION',5X,'SOLUTION FROM SOLVER',
     $5X,'ABS. DIFFERENCE'/)
      WRITE (IOUNIT,103) (XO(I),X(I),ABS(XO(I)-X(I)),I=1,NXNY)
103   FORMAT (/,3(5X,E15.8))
C
C ***** FIND MAX ERROR IN SOLUTION
C
      TEMP = ABS(XO(1) - X(1))
      DO I =2,NXNY
         TEMP = MAX( TEMP, ABS(XO(I) - X(I)) )
      END DO
      WRITE(IOUNIT,104) TEMP
104   FORMAT(/,2X,'MAX ERROR IN SOLUTION = ', E15.8,/)
C
      STOP
      END
C
C
      SUBROUTINE USER_PRINT_ROUTINE(CONTEXT, BUF, SIZE)

      INTEGER CONTEXT
      INTEGER SIZE
      INTEGER BUF(*)

      INCLUDE 'cxml_itsol_print.for'

      CHARACTER*(CXML_ITSOL_MAX_MESSAGE_LENGTH) NEW_BUF

      CALL CXML_FORMAT_STRING(BUF, SIZE, NEW_BUF)
      WRITE(CONTEXT, '(A)') NEW_BUF(1:SIZE)
C
      END
C
C
      SUBROUTINE MATVEC(JOB, IPARAM, RPARAM, A, IA, DUM, X, Y, N)
C
C     MULTIPLY N VECTOR X BY MATRIX TO OBTAIN Y
C
      IMPLICIT NONE
C
      REAL*8 X(*), Y(*), A(*), RPARAM(*), DUM
      INTEGER IA(*), JOB, NDIM, N, NZEROS, IPARAM(*)
C
      NZEROS = IPARAM(31)
      NDIM = IPARAM(32)
C
```

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Example 10–3 (Cont.) Iterative Solver with CXML Routines (Fortran Code) - Example filename: example_itsol_4.f

```
      CALL DMATVEC_UDIA (JOB, A, IA, NDIM, NZEROS, DUM, X, Y, N)
C
      RETURN
      END
C
C
      SUBROUTINE PCONDL(JOB, IPARAM, RPARAM, QL, IQL, A, IA,
     $                  W, X, Y, N)
C
C ***** CALL THE LEFT PRECONDITIONER
C
      IMPLICIT NONE
      INTEGER NMAX
      PARAMETER (NMAX = 100)
      REAL*8 X(*), Y(*), RPARAM(*), QL(*), A(*), W, TMP(NMAX)
      INTEGER JOB, IPARAM(*), IQL(*), IA(*), IPCOND, NZEROS, N, NDIM
C
C ***** ILU PRECONDITIONING
C
      IPCOND = IPARAM(7)
      NZEROS = IPARAM(31)
      NDIM = IPARAM(32)
C
      CALL DAPPLY_ILU_UDIA_L (JOB, QL, IQL, NDIM, NZEROS,
     $                           X, Y, N)
C
      RETURN
      END
C
C
      SUBROUTINE PCONDR(JOB, IPARAM, RPARAM, QR, IQR, A, IA,
     $                  W, X, Y, N)
C
C ***** CALL THE RIGHT PRECONDITIONER
C
      IMPLICIT NONE
      REAL*8 X(*), Y(*), RPARAM(*), QR(*), A(*), W
      INTEGER JOB, IPARAM(*), IQR(*), IA(*)
      INTEGER IPCOND, NZEROS, N, NDIM
C
C ***** ILU PRECONDITIONING
C
      IPCOND = IPARAM(7)
      NZEROS = IPARAM(31)
      NDIM = IPARAM(32)
C
      CALL DAPPLY_ILU_UDIA_U (JOB, QR, IQR, NDIM, NZEROS,
     $                           X, Y, N)
C
      RETURN
      END
C
C
      SUBROUTINE GENMAT (NX, NY, NXNY, A, IA, NDIM, NZEROS)
```

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Example 10–3 (Cont.) Iterative Solver with CXML Routines (Fortran Code) - Example filename: example_itsol_4.f

```
C
C ***** GENERATE MATRIX FOR THE EXAMPLE IN THE UNSYMMETRIC DIAGONAL FORM
C
      IMPLICIT NONE
      INTEGER NDIM, NXNY, NX, NY, J, I, K, NZEROS
      REAL*8 A(NDIM,*)
      INTEGER IA(*)
C
      DO J = 2, NZEROS
          DO I = 1, NXNY
              A(I,J) = 0.0D0
          END DO
      END DO
C
      DO I = 1, NXNY
          A(I,1) = 4.0D0
      END DO
C
      DO J = 1, NY-1
          DO I = 1, NX
              K = (J-1)*NX+I
              A(K,2) = -1.0D0
          END DO
      END DO
C
      DO J = 1, NY
          DO I = 2, NX
              K = (J-1)*NX+I
              A(K,3) = -1.0D0
          END DO
      END DO
C
      DO J = 1, NY
          DO I = 1, NX-1
              K = (J-1)*NX+I
              A(K,4) = -1.0D0
          END DO
      END DO
C
      DO J = 2, NY
          DO I = 1, NX
              K = (J-1)*NX+I
              A(K,5) = -1.0D0
          END DO
      END DO
C
      IA(1) = 0
      IA(2) = NX
      IA(3) = -1
      IA(4) = 1
      IA(5) = -NX
C
      RETURN
C
      END
```

Output from example_itsol_4.f

```
SOLVING EXAMPLE PROBLEM WITH SPLIT PRECONDITIONED GMRES
ILU PRECONDITIONING USED
MATRIX STORED IN UNSYMMETRIC DIAGONAL FORMAT
 METHOD USED : GMRES WITH SPLIT PRECONDITIONING
          3  PREVIOUS RESIDUAL VECTORS ARE STORED
 ORDER OF SYSTEM =    100
 STOPPING CRITERION USED :     3
 MAXIMUM ITERATIONS ALLOWED:   100
 TOLERANCE FOR CONVERGENCE :   0.10000000e-05
    ITERATION =         0    STOPPING TEST = 0.27403910e+01
    ITERATION =         1    STOPPING TEST = 0.83454209e+00
    ITERATION =         2    STOPPING TEST = 0.44870733e+00
    ITERATION =         3    STOPPING TEST = 0.17433646e+00
    ITERATION =         4    STOPPING TEST = 0.72856695e-01
    ITERATION =         5    STOPPING TEST = 0.38408003e-01
    ITERATION =         6    STOPPING TEST = 0.14164437e-01
    ITERATION =         7    STOPPING TEST = 0.56991076e-02
    ITERATION =         8    STOPPING TEST = 0.28790502e-02
    ITERATION =         9    STOPPING TEST = 0.13411353e-02
    ITERATION =        10    STOPPING TEST = 0.63725219e-03
    ITERATION =        11    STOPPING TEST = 0.32213502e-03
    ITERATION =        12    STOPPING TEST = 0.13084728e-03
    ITERATION =        13    STOPPING TEST = 0.54223092e-04
    ITERATION =        14    STOPPING TEST = 0.27502204e-04
    ITERATION =        15    STOPPING TEST = 0.13133042e-04
    ITERATION =        16    STOPPING TEST = 0.63404914e-05
    ITERATION =        17    STOPPING TEST = 0.32280646e-05
    ITERATION =        18    STOPPING TEST = 0.13311315e-05
    ITERATION =        19    STOPPING TEST = 0.55695871e-06
 SOLUTION OBTAINED AFTER          19  ITERATIONS
 NORMAL EXIT FROM SOLVER
 FINAL VALUE OF STOPPING TEST = 0.55695871e-06
   TRUE SOLUTION     SOLUTION FROM SOLVER     ABS. DIFFERENCE
    0.10000000e+01      0.99999997e+00      0.32325871e-07
    0.10000000e+01      0.99999987e+00      0.13396025e-06
                              :
                              : (edited for brevity)
                              :
    0.10000000e+01      0.99999983e+00      0.16690401e-06
    0.10000000e+01      0.99999995e+00      0.48797753e-07
MAX ERROR IN SOLUTION =  0.78315035e-06
```

Example 10–4 Iterative Solver with CXML Routines (C Code) - Example filename: example_itsol_1.c

```
/*
   This is an example program to illustrate the use of the iterative
   solver ditsol_pcg from a C application program. The program generates
   the matrix and the preconditioner, calls the solver and prints the
   maximum error in the solution. The right hand side of the problem is
   generated assuming a known solution. The problem used is identical to
   the one in the example section of the chapter on iterative solvers
   in the CXML Reference Guide.

   This program illustrates the following:
        - routine naming conventions
        - differences in array limits between Fortran and C:
              C default: x[n] -> 0 to (n-1)
              FORTRAN default:   x(n) -> 1 to n
        - how to store two dimensional arrays in C for use in a
          Fortran library routine
        - how to use the matrix-free formulation from a C program
        - how to print messages to a file.

   For more detailed explanation of the routines used, please
   check the Reference Manual or manpage or the FORTRAN example
   programs in this directory.

   Note: the code used in this example works on all Compaq platforms.
   Conditional compilation is used to select the statements appropriate
   to each operating system.

   All output from this program is sent to file called output.data.
   A sample output is:

   method used : cg with spd split preconditioning
   order of system =      100
   stopping criterion used =     1
   maximum iterations allowed =        100
   tolerance for convergence =   0.10000000E-05
      iteration =         0    stopping test = 0.69282032E+01
      iteration =         1    stopping test = 0.19194193E+01
      iteration =         2    stopping test = 0.12100937E+01
      iteration =         3    stopping test = 0.52439623E+00
      iteration =         4    stopping test = 0.84029860E-01
      iteration =         5    stopping test = 0.20539881E-01
      iteration =         6    stopping test = 0.34309306E-02
      iteration =         7    stopping test = 0.47063334E-03
      iteration =         8    stopping test = 0.16605002E-03
      iteration =         9    stopping test = 0.45072557E-04
      iteration =        10    stopping test = 0.72087304E-05
      iteration =        11    stopping test = 0.88047573E-06
   solution obtained after         11  iterations
   normal exit from solver
   final value of stopping test = 0.88047573E-06

maximum error in the solution: 5.6260082260e-08

*/
```

(continued on next page)

Example 10–4 (Cont.) Iterative Solver with CXML Routines (C Code) - Example filename: example_itsol_1.c

```
#include <stdio.h>
#include <stdlib.h>

#define ABS(x) (((x) < 0) ? -(x) : (x))
#define MAX(x,y) (((x) < (y)) ? (y) : (x))

/*
    Add trailing underscores to Fortran routines on unix and linux
*/

#if defined(linux)
#  define ditsol_defaults ditsol_defaults__
#  define dcreate_ilu_sdia dcreate_ilu_sdia__
#  define ditsol_pcg ditsol_pcg__
#  define dmatvec_sdia dmatvec_sdia__
#  define dapply_ilu_sdia dapply_ilu_sdia__
#  define cxml_itsol_set_print_routine cxml_itsol_set_print_routine__
#elif defined(__unix__)
#  define ditsol_defaults ditsol_defaults_
#  define dcreate_ilu_sdia dcreate_ilu_sdia_
#  define ditsol_pcg ditsol_pcg_
#  define dmatvec_sdia dmatvec_sdia_
#  define dapply_ilu_sdia dapply_ilu_sdia_
#  define cxml_itsol_set_print_routine cxml_itsol_set_print_routine_
#endif


extern void  pcondl1();
extern void  matvec1();
extern void  genmat1();
extern void ditsol_defaults();
extern void dcreate_ilu_sdia();
extern void ditsol_pcg();
extern void dmatvec_sdia();
extern void dapply_ilu_sdia();
extern void user_print_routine();
extern void cxml_itsol_set_print_routine();

/*
    illustrating the use of the iterative solver:
    preconditioned conjugate gradient method, with incomplete
    cholesky preconditioning. the matrix is stored using the
    symmetric diagonal format
*/

int main()
{
    FILE *fp;
    char *filename;
    double *a_sdia;
    double *a_ilu;
    double *rwork1;
    double *rhs;
    double *x;
    double *xo;

    double rparam[50];

    double dum, max1, tmp1;

    int *index_sdia;
    int *index_ilu;

    int iparam[50];
```

(continued on next page)

Example 10–4 (Cont.) Iterative Solver with CXML Routines (C Code) - Example filename: example_itsol_1.c

```
    int  nx, ny, nxny, length, ndim, nzeros;
    int  i, j, idum, ierror;
    int  job;

    filename = "output.data";

    fp = fopen(filename, "w");

/*
    define the size of the problem
*/

    nx = 10;
    ny = 10;
    nzeros = 3;
    nxny = nx * ny;
    ndim = nxny;

/*
   get the memory for the 2-dimensional arrays a_sdia and a_ilu
*/

    a_sdia = (double *)malloc (nzeros*ndim*sizeof(double));
    if (a_sdia == 0) perror("malloc");

    a_ilu = (double *)malloc (nzeros*ndim*sizeof(double));
    if (a_ilu == 0) perror("malloc");

/*
    get the memory for the 1-dimensional arrays
*/

    rwork1 = (double *)malloc(4*nxny*sizeof(double));
    if (rwork1 == 0) perror("malloc");

    rhs = (double *)malloc(nxny*sizeof(double));
    if (rhs == 0) perror("malloc");

    x = (double *)malloc(nxny*sizeof(double));
    if (x == 0) perror("malloc");

    xo = (double *)malloc(nxny*sizeof(double));
    if (xo == 0) perror("malloc");

    index_sdia = (int *)malloc(nzeros*sizeof(int));
    if (index_sdia == 0) perror("malloc");

    index_ilu = (int *)malloc(nzeros*sizeof(int));
    if (index_ilu == 0) perror("malloc");

/*
    set the parameters (integer and real)
*/

    ditsol_defaults(iparam, rparam);

    iparam[2] = 0;
    iparam[3] = 4 * nxny;

/*
    direct all output to the file
*/

    iparam[5] = 3;
    iparam[6] = 4;
    cxml_itsol_set_print_routine(user_print_routine, fp, iparam);
```

(continued on next page)

Example 10–4 (Cont.) Iterative Solver with CXML Routines (C Code) - Example filename: example_itsol_1.c

```
/*
    generate the matrix
*/

    genmat1(nx, ny, nxny, a_sdia, index_sdia, ndim, nzeros);

    iparam[30] = nzeros;
    iparam[31] = ndim;

/*
    generate xo, the true solution
*/

    for (i=0; i<nxny; i++)
        xo[i] = 1.0;

/*
    obtain the right hand side
*/

    job = 0;
    matvec1(&job, iparam, rparam, a_sdia, index_sdia,
            &dum, xo, rhs, &nxny);

/*
    obtain initial guess (all zeros)
*/

    for (i=0; i<nxny; i++)
        x[i] = 0.0;

/*
    generate the preconditioner
*/

    dcreate_ilu_sdia(a_sdia, index_sdia, &ndim, &nzeros,
                     a_ilu, index_ilu, &nxny);

/*
    call the solver
*/

    ditsol_pcg(matvec1, pcondl1, &dum, &dum,
               a_sdia, index_sdia,
               x, rhs, &nxny,
               a_ilu, index_ilu, &dum, &idum,
               iparam, rparam, &idum, rwork1, &ierror);

    if (ierror != 0)
        fprintf(fp,"ditsol_pcg returned with error flag: %d\n",ierror);

/*
    find the maximum absolute error in the solution
*/

    max1 = ABS((x[0]-xo[0]));

    for (i=1; i<nxny; i++)
        {
            tmp1 = ABS((x[i]-xo[i]));
            max1 = MAX((max1),(tmp1));
        }
```

(continued on next page)

Example 10–4 (Cont.) Iterative Solver with CXML Routines (C Code) - Example filename: example_itsol_1.c

```
/*
    print the maximum absolute error
*/

    fprintf(fp,"maximum error in the solution: %.10e\n",max1);

/*
    release the memory
*/

    free(a_sdia);
    free(a_ilu);
    free(rwork1);
    free(rhs);
    free(x);
    free(xo);
    free(index_sdia);
    free(index_ilu);

}  /* end of main() */

/*
    generate the matrix for the problem described in the chapter on
    iterative solvers in the CXML Reference Guide
*/

void genmat1(int nx, int ny, int nxny, double a[],
             int index[], int ndim, int nzeros)
{
    int  i, j, k;

    for (j=0; j<nxny; j++)
        for (i=1; i<nzeros; i++)
            a[i*ndim+j] = 0.0;

    for (j=0; j<nxny; j++)
        a[0*ndim+j] = 4.0;

    for (j=0; j<ny; j++)
        for (i=1; i<nx; i++)
            {
                k = j * nx + i;
                a[2*ndim+k] = -1.0;
            }

    for (j=1; j<ny; j++)
        for (i=0; i<nx; i++)
            {
                k = j * nx + i;
                a[1*ndim+k] = -1.0;
            }
    index[0] = 0;
    index[2] = -1;
    index[1] = -nx;

}  /* end of genmat1() */
```

(continued on next page)

Example 10–4 (Cont.) Iterative Solver with CXML Routines (C Code) - Example filename: example_itsol_1.c

```
/*
   prints the messages to a file
*/

void user_print_routine(void *context, char *buf, int *size)
{
    fprintf((FILE*)context, buf);
}

/*
    provide the matrix-vector routine using the standard parameter list
    as described in the CXML Reference Guide
*/

void matvec1(int *job, int *iparam, double *rparam, double *a, int *ia,
             double *w, double *x, double *y, int *n)
{
    int  nzeros, ndim;
    double dum;

    nzeros = iparam[30];
    ndim = iparam[31];

    dmatvec_sdia(job, a, ia, &ndim, &nzeros, &dum, x, y, n, iparam);

}  /* end of matvec1() */

/*
    provide the left preconditioning routine using the standard parameter
    list as described in the CXML Reference Guide
*/

void pcondl1(int *job, int *iparam, double *rparam, double *ql, int *iql,
             double *a, int *ia, double *w, double *x, double *y, int *n)
{
    int job1;
    int  nzeros, ndim;
    double *tmp;

/*
    ilu preconditioning
*/

    nzeros = iparam[30];
    ndim = iparam[31];

/*
    get memory for temporary vector
*/

    tmp = (double *)malloc((*n)*sizeof(double));
    job1 = 0;
    dapply_ilu_sdia(&job1, ql, iql, &ndim, &nzeros, x, tmp, n);
    job1 = 1;
    dapply_ilu_sdia(&job1, ql, iql, &ndim, &nzeros, tmp, y, n);

/*
    release memory for temporary vector
*/

    free(tmp);

}  /* end of pcondl1() */
```

Output from example_itsol_1.c

```
   method used : cg with spd split preconditioning
   order of system =       100
   stopping criterion used =     1
   maximum iterations allowed =         100
   tolerance for convergence =   0.10000000E-05
      iteration =         0    stopping test = 0.69282032E+01
      iteration =         1    stopping test = 0.19194193E+01
      iteration =         2    stopping test = 0.12100937E+01
      iteration =         3    stopping test = 0.52439623E+00
      iteration =         4    stopping test = 0.84029860E-01
      iteration =         5    stopping test = 0.20539881E-01
      iteration =         6    stopping test = 0.34309306E-02
      iteration =         7    stopping test = 0.47063334E-03
      iteration =         8    stopping test = 0.16605002E-03
      iteration =         9    stopping test = 0.45072557E-04
      iteration =        10    stopping test = 0.72087304E-05
      iteration =        11    stopping test = 0.88047573E-06
   solution obtained after          11  iterations
   normal exit from solver
   final value of stopping test = 0.88047573E-06

maximum error in the solution: 5.6260082260e-08
```

Example 10–5 Iterative Solver with CXML Routines (C++ Code) - Example filename: example_itsol_1.cxx

```
//   This is an example program to illustrate the use of the iterative
//   solver ditsol_pcg from a C application program. The program generates
//   the matrix and the preconditioner, calls the solver and prints the
//   maximum error in the solution. The right hand side of the problem is
//   generated assuming a known solution.
//
//   This program illustrates the following:
//        - routine naming conventions
//        - Differences in endexing arrays:
//              C default: x[n] -> 0 to (n-1)
//              FORTRAN default: x(n) -> 1 to n
//        - how to use two dimensional arrays in C to interface with a
//          Fortran library routine
//        - how to use the matrix-free formulation from a C program
//
//    For more detailed explanation of the routines used, please
//    check the reference section of the CXML Reference Guide.
//
//    Note: the code used in this example works on all Compaq platforms.
//    Conditional compilation is used to select the statements
//    appropriate to each operating system.
//
//    All output from this program is sent to the screen. A sample
//    output is:
//
//   method used : cg with spd split preconditioning
//   order of system =       100
//   stopping criterion used =     1
//   maximum iterations allowed =         100
//   tolerance for convergence =   0.10000000E-05
//      iteration =          0    stopping test = 0.69282032E+01
//      iteration =          1    stopping test = 0.19194193E+01
//      iteration =          2    stopping test = 0.12100937E+01
//      iteration =          3    stopping test = 0.52439623E+00
//      iteration =          4    stopping test = 0.84029860E-01
//      iteration =          5    stopping test = 0.20539881E-01
//      iteration =          6    stopping test = 0.34309306E-02
//      iteration =          7    stopping test = 0.47063334E-03
//      iteration =          8    stopping test = 0.16605002E-03
//      iteration =          9    stopping test = 0.45072557E-04
//      iteration =         10    stopping test = 0.72087304E-05
//      iteration =         11    stopping test = 0.88047573E-06
//   solution obtained after          11  iterations
//   normal exit from solver
//   final value of stopping test = 0.88047573E-06
//
//maximum error in the solution: 5.6260082260e-08
//

#include <iostream.h>
#include <iomanip.h>
#include <stdlib.h>
#include <new.h>
```

(continued on next page)

Example 10–5 (Cont.) Iterative Solver with CXML Routines (C++ Code) - Example filename: example_itsol_1.cxx

```
//
//   Add trailing underscores to Fortran routines on unix and linux
//

#if defined(linux)
#  define ditsol_defaults ditsol_defaults__
#  define dcreate_ilu_sdia dcreate_ilu_sdia__
#  define ditsol_pcg ditsol_pcg__
#  define dmatvec_sdia dmatvec_sdia__
#  define dapply_ilu_sdia dapply_ilu_sdia__
#elif defined(__unix__)
#  define ditsol_defaults ditsol_defaults_
#  define dcreate_ilu_sdia dcreate_ilu_sdia_
#  define ditsol_pcg ditsol_pcg_
#  define dmatvec_sdia dmatvec_sdia_
#  define dapply_ilu_sdia dapply_ilu_sdia_
#endif

inline double ABS(double x)
{
    return(((x) < 0) ? -(x) : (x));
}

inline double MAX(double x, double y)
{
    return(((x) < (y)) ? (y) : (x));
}

//  extern void (*set_new_handler(void (*memory_err)()))();
void memory_err()
{
    cout << "memory allocation error\n";
    exit(1); // quit program
}

extern void pcondl1(int &, int [], double [],
                    double [], int [],
                    double [], int [],
                    double [], double [], double [], int &);
extern void  matvec1(int &, int [], double [],
                     double [], int [],
                     double [], double [], double [], int &);
extern void  genmat1(int, int, int,
                     double [], int [],
                     int, int);
```

(continued on next page)

Example 10–5 (Cont.) Iterative Solver with CXML Routines (C++ Code) - Example filename: example_itsol_1.cxx

```
//
//   Declare the Fortran routines
//

extern "C"
{
void ditsol_defaults(int [], double []);
void dcreate_ilu_sdia(double [], int [],
                      int &, int &,
                      double [], int [],
                      int &);
void ditsol_pcg(void (*)(int &, int [], double [],
                         double [], int [],
                         double [], double [], double [],
                         int &),
                void (*)(int &, int [], double [],
                          double [], int [],
                          double [], int [],
                          double [], double [], double [], int &),
                double &, double &,
                double [], int [],
                double [], double [], int &,
                double [], int [],
                double &, int &,
                int [], double [],
                int &, double [],
                int &);
void dmatvec_sdia(int &, double [], int [],
                  int &, int &, double [], double [], double [],
                  int &, int []);
void dapply_ilu_sdia(int &,
                     double [], int [],
                     int [], int [],
                     double [], double [], int &);
}

//
//     illustrating the use of the iterative solver:
//     preconditioned conjugate gradient method, with incomplete
//     cholesky preconditioning. the matrix is stored using the
//     symmetric diagonal format
//

void main()
{
    double *a_sdia;
    double *a_ilu;
    double *rwork1;
    double *rhs;
    double *x;
    double *xo;

    double rparam[50];

    double dum, max1, tmp1;

    int *index_sdia;
    int *index_ilu;
```

(continued on next page)

Example 10–5 (Cont.) Iterative Solver with CXML Routines (C++ Code) - Example filename: example_itsol_1.cxx

```
    int iparam[50];

    int nxny, length, ndim, nzeros;
    int i, j, idum, ierror;
    int job;

// set up exception handler

    set_new_handler(memory_err);

// define the problem size

    const int nx = 10;
    const int ny = 10;

    nxny = nx * ny;
    ndim = nxny;
    nzeros = 3;

// allocate memory for the 2-dimensional arrays

    a_sdia = new double [nzeros*ndim];
    a_ilu = new double [nzeros*ndim];

// allocate memory for the 1-dimensional arrays

    rwork1 = new double [4*nxny];
    rhs = new double [nxny];
    x = new double [nxny];
    xo = new double [nxny];

    index_sdia = new int [nzeros];
    index_ilu = new int [nzeros];

// set the parameters (integer and real)

    ditsol_defaults(iparam, rparam);

    iparam[2] = 0;
    iparam[3] = 4 * nxny;

// direct all output to the screen

    iparam[4] = 6;
    iparam[5] = 3;
    iparam[6] = 4;

// generate the matrix

    genmat1(nx, ny, nxny,
            a_sdia, index_sdia,
            ndim, nzeros);

    iparam[30] = nzeros;
    iparam[31] = ndim;
```

(continued on next page)

Example 10–5 (Cont.) Iterative Solver with CXML Routines (C++ Code) - Example filename: example_itsol_1.cxx

```
// generate xo, the true solution

    for (i=0; i<nxny; i++)
        xo[i] = 1.0;

// obtain the right hand side

    job = 0;
    matvec1(job, iparam, rparam,
            a_sdia, index_sdia,
            &dum, xo, rhs, nxny);

// obtain initial guess (all zeros)

    for (i=0; i<nxny; i++)
        x[i] = 0.0;

// generate the preconditioner

    dcreate_ilu_sdia(a_sdia, index_sdia,
                     ndim, nzeros,
                     a_ilu, index_ilu,
                     nxny);

// call the solver

    ditsol_pcg(matvec1, pcondl1, dum, dum,
               a_sdia, index_sdia,
               x, rhs, nxny,
               a_ilu, index_ilu,
               dum, idum,
               iparam, rparam,
               idum, rwork1,
               ierror);

    if (ierror != 0)
        cout << "ditsol_pcg returned with error flag: " << ierror
            << endl;

// find the maximum absolute error in the solution

    max1 = ABS((x[0]-xo[0]));

    for (i=1; i<nxny; i++)
        {
            tmp1 = ABS((x[i]-xo[i]));
            max1 = MAX((max1),(tmp1));
        }
// print the maximum absolute error

    cout << "maximum error in the solution: " << max1 << endl;
```

(continued on next page)

Example 10–5 (Cont.) Iterative Solver with CXML Routines (C++ Code) - Example filename: example_itsol_1.cxx

```
// deallocate the memory

    delete a_sdia;
    delete a_ilu;
    delete rwork1;
    delete xo;
    delete x;
    delete rhs;

    delete index_sdia;
    delete index_ilu;

}  // end of main()


//
//    generate the matrix for the problem described in the chapter on
//    iterative solvers in the CXML Reference Guide
//

void genmat1(int nx, int ny, int nxny,
             double a[], int index[],
             int ndim, int nzeros)
{
    int  i, j, k;

    for (j=0; j<nxny; j++)
        for (i=1; i<nzeros; i++)
            a[i*ndim+j] = 0.0;

    for (j=0; j<nxny; j++)
        a[0*ndim+j] = 4.0;

    for (j=0; j<ny; j++)
        for (i=1; i<nx; i++)
            {
                k = j * nx + i;
                a[2*ndim+k] = -1.0;
            }

    for (j=1; j<ny; j++)
        for (i=0; i<nx; i++)
            {
                k = j * nx + i;
                a[1*ndim+k] = -1.0;
            }

    index[0] = 0;
    index[2] = -1;
    index[1] = -nx;

}  // end of genmat1()
```

(continued on next page)

Example 10–5 (Cont.) Iterative Solver with CXML Routines (C++ Code) - Example filename: example_itsol_1.cxx

```
//
//    provide the matrix-vector routine using the standard parameter list
//    as described in the CXML Reference Guide
//

void matvec1(int &job, int iparam[], double rparam[],
             double a[], int ia[],
             double w[], double x[], double y[], int &n)
{
    int  nzeros, ndim;
    double dum;

    nzeros = iparam[30];
    ndim = iparam[31];

    dmatvec_sdia(job, a, ia, ndim, nzeros, &dum, x, y, n, iparam);

}  // end of matvec1()


//
//    provide the left preconditioning routine using the standard parameter
//    list as described in the CXML Refernce Guide
//

void pcondl1(int &job, int iparam[], double rparam[],
             double ql[], int iql[],
             double a[], int ia[],
             double w[], double x[], double y[], int &n)
{
    int  nzeros, ndim, job1;
    double *tmp;

// ilu preconditioning

    nzeros = iparam[30];
    ndim = iparam[31];

// allocate temporary storage

    tmp = new double [n];

    job1 = 0;
    dapply_ilu_sdia(job1, ql, iql, &ndim, &nzeros, x, tmp, n);
    job1 = 1;
    dapply_ilu_sdia(job1, ql, iql, &ndim, &nzeros, tmp, y, n);

// deallocate temporary storage

    delete tmp;

}  // end of pcondl1()
```

Output from example_itsol_1.cxx

```
   method used : cg with spd split preconditioning
   order of system =       100
   stopping criterion used =     1
   maximum iterations allowed =         100
   tolerance for convergence =   0.10000000E-05
      iteration =         0    stopping test = 0.69282032E+01
      iteration =         1    stopping test = 0.19194193E+01
      iteration =         2    stopping test = 0.12100937E+01
      iteration =         3    stopping test = 0.52439623E+00
      iteration =         4    stopping test = 0.84029860E-01
      iteration =         5    stopping test = 0.20539881E-01
      iteration =         6    stopping test = 0.34309306E-02
      iteration =         7    stopping test = 0.47063334E-03
      iteration =         8    stopping test = 0.16605002E-03
      iteration =         9    stopping test = 0.45072557E-04
      iteration =        10    stopping test = 0.72087304E-05
      iteration =        11    stopping test = 0.88047573E-06

   solution obtained after          11  iterations
   normal exit from solver
   final value of stopping test = 0.88047573E-06

maximum error in the solution: 5.6260082260e-08
```

11 Using Direct Sparse Solvers

CXML provides user-callable direct sparse solver subroutines to solve symmetric and symmetricly-structured matrices with real or complex coefficients. For symmetric matrices, these CXML subroutines can solve both positive definite and indefinite systems.

The *Introduction* (Section 11.1) and the two sections that follow, *Matrix Basics* (Section 11.2) and *The Direct Method* (Section 11.3), discuss all of the terms and concepts required to understand the use of the CXML direct sparse solver routines. If you are familiar with direct sparse solvers, you can omit reading these sections and go directly to the section titled *Sparse Matrix Storage Format* (Section 11.4) for a discussion of how sparse matrices are stored for CXML direct sparse solver routines. The direct sparse solver routines themselves are described in the reference section. Refer to Direct Sparse Solver Subprograms.

11.1 Introduction

Many applications in science and engineering require the solution of a system of linear equations. This problem is usually expressed mathematically by the matrix-vector equation, $Ax = b$, where A is an n by n matrix and x and b are n element column vectors. The matrix A is usually referred as the **coefficient matrix**, and the vectors x and b are referred to as the **solution vector** and the **right-hand side**, respectively.

In many real-life applications, most of the elements in A are zero. Such a matrix is referred to as **sparse**. Conversely, matrices with very few zero elements are called dense. For sparse matrices, computing the solution to the equation $Ax = b$ can be made much more efficient with respect to both storage and computation time, if the sparsity of the matrix can be exploited. The more an algorithm can exploit the sparsity without sacrificing the correctness, the better the algorithm.

Generally speaking, computer software that finds solutions to systems of linear equations is called a solver. A solver designed to work specifically on sparse systems of equations is called a **sparse solver**. Sparse solvers are usually classified into two groups - **direct** and **iterative**.

Iterative Solvers

Iterative solvers start with an initial approximation to a solution and attempt to estimate the difference between the approximation and the true result. Based on the difference, an iterative solver calculates a new approximation that is closer to the true result than the initial approximation. This process is repeated until the difference between the approximation and the true result is sufficiently small. The main drawback to iterative solvers is that the rate of convergence depends greatly on the values in the matrix A. Consequently, it is not possible to predict how long it will take for an iterative solver to produce a solution. In fact, for ill-conditioned matrices, the iterative process will not converge to a solution at all. However, for well-conditioned matrices it is possible for iterative solvers

to converge to a solution very quickly. Consequently for the right applications, iterative solvers can be very efficient.

Direct Solvers

Direct solvers, on the other hand, factor the matrix *A* into the product of two triangular matrices and then perform a forward and backward triangular solve. This approach makes the time required to solve a systems of linear equations relatively predictable, based on the size of the matrix. In fact, for sparse matrices, the solution time can be predicted based on the number of non-zero elements in the array A.

11.2 Matrix Basics

A **matrix** is a rectangular array of either real or complex numbers. A matrix is denoted by a capital letter; its elements are denoted by the same lower case letter with row/column subscripts. For example, the value of the element in row *i* and column *j* in matrix *A* is denoted by a(i,j).

Matrix *A*, a 3 by 4 matrix, is written as follows:

$$A = \begin{bmatrix} a(1,1) & a(1,2) & a(1,3) & a(1,4) \\ a(2,1) & a(2,2) & a(2,3) & a(2,4) \\ a(3,1) & a(3,2) & a(3,3) & a(3,4) \end{bmatrix}$$

Note that with the above notation, we assume the standard Fortran programming language convention of starting array indices at 1 rather than the C programming language convention of starting them at 0.

A matrix in which all of the elements are real numbers is called a **real matrix**. A matrix that contains at least one complex number is called a **complex matrix**. A real or complex matrix, *A*, with the property that $a(i,j) = a(j,i)$, is called a **symmetric matrix**. A complex matrix, *A*, with the property that $a(i,j) = conj(a(j,i))$, is called a **Hermitian matrix**. Note that programs that manipulate symmetric and Hermitian matrices need only store half of the matrix values, since the values of the non-stored elements can be quickly reconstructed from the stored values.

A matrix that has the same number of rows as it has columns is referred to as a **square matrix**. The elements in a square matrix that have same row index and column index are called the diagonal elements of the matrix, or simply the diagonal of the matrix.

The **transpose** of a matrix *A* to is the matrix obtained by "flipping" the elements of the array about its diagonal. That is, we exchange the elements *a(i,j)* and *a(j,i)*.

For a complex matrix, if we both flipped the elements about the diagonal and than take the complex conjugate of the element, the resulting matrix is called the **Hermitian transpose** or **conjugate transpose** of the original matrix. The transpose and Hermitian transpose of a matrix *A* are denoted by A^t and A^h respectively.

A **column vector**, or simply a **vector**, is a *n x 1* matrix, and a **row vector** is a *1 x n* matrix.

A real or complex matrix, *A*, is said to be **positive definite** if the vector-matrix product $x^t Ax$ is greater than zero for all non-zero vectors *x*. A matrix that is not positive definite is referred to as **indefinite**.

An upper (or lower) **triangular matrix**, is a square matrix in which all elements below (or above) the diagonal are zero. A unit triangular matrix is an upper or lower triangular matrix with all 1's along the diagonal.

A matrix P is called a **permutation matrix** if, for any matrix A, the result of the matrix product PA is identical to A except for interchanging the rows of A. For a square matrix, it can be shown that if PA is a permutation of the rows of A, then AP^t is the same permutation of the columns of A. Additionally, it can be shown that the inverse of P is P^t.

In order to save space, a permutation matrix is usually stored as a linear array, called a **permutation vector**, rather than as an array. Specifically, if the permutation matrix maps the i-th row of a matrix to the j-th row, then the i-th element of the permutation vector is j.

A matrix with non-zero elements only on the diagonal is called a **diagonal matrix**. As is the case with a permutation matrix, it is usually stored as a vector of values, rather than as a matrix.

11.3 The Direct Method

For solvers that use the direct method, the basic technique employed in finding the solution of the system $Ax = b$ is to first factor A into triangular matrices. That is, find a lower triangular matrix L and an upper triangular matrix U, such that $A = LU$. Having obtained such a factorization (usually referred to as an *LU decomposition* or *LU factorization*), the solution to the original problem can be rewritten as follows.

$$\begin{aligned} & Ax = b \\ \Longrightarrow \quad & LUx = b \\ \Longrightarrow \quad & L(Ux) = b \end{aligned}$$

This leads to the following two-step process for finding the solution to the original system of equations:

1. Solve the systems of equations $Ly = b$.
2. Solve the system $Ux = y$.

Solving the systems $Ly = b$ and $Ux = y$ is referred to as a **forward solve** and a **backward solve**, respectively.

If a symmetric matrix, A, is also positive definite, it can be shown that A can be factored as LL^t where L is a lower triangular matrix. Similarly, a Hermitian matrix, A, that is positive definite can be factored as $A = LL^h$. For both symmetric and Hermitian matrices, a factorization of this form is called a **Cholesky factorization**.

In a Cholesky factorization, the matrix U in an LU decomposition is either L^t or L^h. Consequently, a sparse solver can increase its efficiency by only storing L, and one-half of A, and not computing U. Therefore, users who can express their application as the solution of a system of positive definite equations will gain a significant performance improvement over using a general sparse representation.

For matrices that are symmetric (or Hermitian) but not positive definite, there are still some significant efficiencies to be had. It can be shown that if A is symmetric but not positive definite, then A can be factored as $A = LDL^t$, where D is a diagonal matrix and L is a lower unit triangular matrix. Similarly, if A is Hermitian, it can be factored as $A = LDL^h$. In either case, we again only need

to store L, D and half of A and we need not compute U. However, the backward solve phases must be amended to solving $L^t x = D^{-1} y$ rather than $L^t x = y$.

Fill-In and Reordering of Matrices

Two important concepts associated with the solution of sparse systems of equations are **fill-in** and **reordering**. The following example illustrates these concepts.

Consider the system of linear equation $Ax = b$, where A is the symmetric positive definite matrix defined by the following:

$$A = \begin{bmatrix} 9 & \frac{3}{2} & 6 & \frac{3}{4} & 3 \\ \frac{3}{2} & \frac{1}{2} & * & * & * \\ 6 & * & 12 & * & * \\ \frac{3}{4} & * & * & \frac{5}{8} & * \\ 3 & * & * & * & 16 \end{bmatrix} \quad b = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$$

A star (*) is used to represent zeros and to emphasize the sparsity of A.
The Cholesky factorization of A is: $A = LL^t$, where L is the following:

$$L = \begin{bmatrix} 3 & * & * & * & * \\ \frac{1}{2} & \frac{1}{2} & * & * & * \\ 2 & -2 & 2 & * & * \\ \frac{1}{4} & \frac{1}{-4} & \frac{1}{-2} & \frac{1}{2} & * \\ 1 & -1 & -2 & -3 & 1 \end{bmatrix}$$

Notice that even though the matrix A is relatively sparse, the lower triangular matrix L has no zeros below the diagonal. If we computed L and then used it for the forward and backward solve phase, we would do as much computation as if A had been dense.

The situation of L having non-zeros in places where A has zeros is referred to as **fill-in**. Computationally, it would be more efficient if a solver could exploit the non-zero structure of A in such a way as to reduce the fill-in when computing L. By doing this, the solver would only need to compute the non-zero entries in L.

Toward this end, consider permuting the rows and columns of A. As described in Section 11.2, the permutations of the rows of A can be represented as a permutation matrix, P. The result of permuting the rows is the product of P and A. Suppose, in the above example, we swap the first and fifth row of A, then swap the first and fifth columns of A, and call the resulting matrix B. From Section 11.2, we see that mathematically, we can express the process of permuting

the rows and columns of A to get B as $B = PAP^t$. After permuting the rows and columns of A, we see that B is given by the following:

$$B = \begin{bmatrix} 16 & * & * & * & 3 \\ * & \frac{1}{2} & * & * & \frac{3}{2} \\ * & * & 12 & * & 6 \\ * & * & * & \frac{5}{8} & \frac{3}{4} \\ 3 & \frac{3}{2} & 6 & \frac{3}{4} & 9 \end{bmatrix}$$

Since B is obtained from A by simply switching rows and columns, the numbers of non-zero entries in A and B are the same. However, when we find the Cholesky factorization, $B = LL^t$, we see the following:

$$L = \begin{bmatrix} 4 & * & * & * & * \\ * & \frac{1}{\sqrt{2}} & * & * & * \\ * & * & 2(\sqrt{3}) & * & * \\ * & * & * & \frac{\sqrt{10}}{4} & * \\ \frac{3}{4} & \frac{3}{\sqrt{2}} & \sqrt{3} & \frac{3}{\sqrt{10}} & \frac{\sqrt{\frac{3}{5}}}{4} \end{bmatrix}$$

The fill-in associated with B is much smaller than the fill-in associated with A. Consequently, the storage and computation time needed to factor B is much smaller than to factor A. Based on this, we see that an efficient solver needs to find permutation P of the matrix A, which minimizes the fill-in for factoring $B = PAP^t$, and then use the factorization of B to solve the original system of equations.

Although the above example is based on a symmetric positive definite matrix and a Cholesky decomposition, the same approach works for a general LU decomposition. Specifically, let P be a permutation matrix, $B = PAP^t$ and suppose that B can be factored as $B = LU$. $\Longrightarrow$

$Ax = b$
$\Longrightarrow PA(P^{-1}P)x = Pb$
$\Longrightarrow PA(P^tP)x = Pb$
$\Longrightarrow (PAP^t)(Px) = Pb$
$\Longrightarrow B(Px) = Pb$
$\Longrightarrow LU(Px) = Pb$

It follows that if we obtain an LU factorization for B, we can solve the original system of equations by a three step process:

1. Solve $Ly = Pb$.
2. Solve $Uz = y$.
3. Set $x = P^tz$.

If we apply this three step process to the current example, we first need to perform the forward solve of the systems of equation $Ly = Pb$:

$$\begin{bmatrix} 4 & * & * & * & * \\ * & \frac{1}{\sqrt{2}} & * & * & * \\ * & * & 2(\sqrt{3}) & * & * \\ * & * & * & \frac{\sqrt{10}}{4} & * \\ \frac{3}{4} & \frac{3}{\sqrt{2}} & \sqrt{3} & \frac{3}{\sqrt{10}} & \frac{\sqrt{\frac{3}{5}}}{4} \end{bmatrix} * \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} = \begin{bmatrix} 5 \\ 2 \\ 3 \\ 4 \\ 1 \end{bmatrix}$$

This gives: $y^t = \frac{5}{4}, 2\sqrt{2}, \frac{\sqrt{3}}{2}, \frac{16}{\sqrt{10}}, \frac{-979\sqrt{\frac{3}{5}}}{12}$.

The second step is to perform the backward solve, $Uz = y$. Or, in this case, since we are using a Cholesky factorization, $L^t z = y$.

$$\begin{bmatrix} 4 & * & * & * & \frac{3}{4} \\ * & \frac{1}{\sqrt{2}} & * & * & \frac{3}{\sqrt{2}} \\ * & * & 2(\sqrt{3}) & * & \sqrt{3} \\ * & * & * & \frac{\sqrt{10}}{4} & \frac{3}{\sqrt{10}} \\ * & * & * & * & \frac{\sqrt{\frac{3}{5}}}{4} \end{bmatrix} * \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \\ z_5 \end{bmatrix} = \begin{bmatrix} \frac{5}{4} \\ 2(\sqrt{2}) \\ \frac{\sqrt{3}}{2} \\ \frac{16}{\sqrt{10}} \\ \frac{-979*\sqrt{\frac{3}{5}}}{12} \end{bmatrix}$$

This gives $z = \frac{123}{2}, 983, \frac{1961}{12}, 398, \frac{-979}{3}$.

The third and final step is to set $x = P^t z$. This gives $x^t = \frac{-979}{3}, 983, \frac{1961}{12}, 398, \frac{123}{2}$.

11.4 Sparse Matrix Storage Format

As discussed in Section 11.3, it is more efficient to store only the non-zeros of a sparse matrix. There are a number of common storage schemes used for sparse matrices, but most of the schemes employ the same basic technique. That is, compress all of the non-zero elements of the matrix into a linear array, and then provide some number of auxiliary arrays to describe the locations of the non-zeros in the original matrix.

The compression of the non-zeros of a sparse matrix A into a linear array is done by walking down each column (column major format) or across each row (row major format) in order, and writing the non-zero elements to a linear array in the order that they appear in the walk.

When storing symmetric matrices, it is necessary to store only the upper triangular half of the matrix (upper triangular format) or the lower triangular half of the matrix (lower triangular format).

The CXML direct sparse solver uses a row major upper triangular storage format. That is, the matrix is compressed row-by-row and for symmetric matrices only non-zeros in the upper triangular half of the matrix are stored.

The CXML storage format for sparse matrices consists of three arrays, which are called the *values*, *column*, and *rowIndex* arrays. The following table describes the arrays in terms of the values, row, and column positions of the non-zero elements in a sparse matrix *A*.

values	A real or complex array that contains the non-zero entries of *A*. The non-zero values of *A* are mapped into the *values* array using the row major, upper triangular storage mapping described above.
columns	Element *i* of the integer array *columns* contains the number of the column in *A* that contained the value in values(i).
rowIndex	Element *j* of the integer array *rowIndex* gives the index into the values array that contains the first non-zero element in a row *j* of *A*.

The length of the *values* and *columns* arrays is equal to the number of non-zeros in *A*.

Since the *rowIndex* array gives the location of the first non-zero within a row, and the non-zeros are stored consecutively, then we would like to be able to compute the number of non-zeros in the *i*-th row as the difference of *rowIndex(i)* and *rowIndex(i+1)*.

In order have this relationship hold for the last row of *A*, we need to add an entry (dummy entry) to the end of *rowIndex* whose value is equal to the number of non-zeros in *A*, plus one. This makes the total length of the *rowIndex* array one larger than the number of rows of *A*.

Note

The CXML sparse storage scheme uses the Fortran programming language convention of starting array indices at 1, rather than the C programming language convention of starting at 0.

With the above in mind, consider storing the symmetric matrix discussed in the example from Section 11.3.

$$A = \begin{bmatrix} 9 & \frac{3}{2} & 6 & \frac{3}{4} & 3 \\ * & \frac{1}{2} & * & * & * \\ * & * & \frac{1}{2} & * & * \\ * & * & * & \frac{5}{8} & * \\ * & * & * & * & 16 \end{bmatrix}$$

In this case, *A* has nine non-zero elements, so the lengths of the *values* and *columns* arrays will be nine. Also, since the matrix *A* has five rows, the *rowIndex* array is of length six. The actual values for each of the arrays for the example matrix are as follows:

```
values   = ( 9  3/2  6  3/4  3 1/2  12  5/8  16 )
columns  = ( 1   2   3   4   5  2    3   4    5 )
rowIndex = ( 1   6   7   8   9  10)
```

For a non-symmetric or non-Hermitian array, all of the non-zeros need to be stored. Consider the non-symmetric matrix B defined by the following:

$$B = \begin{bmatrix} 1 & -1 & * & -3 & * \\ -2 & 5 & * & * & * \\ * & * & 4 & 6 & 4 \\ -4 & * & 2 & 7 & * \\ * & 8 & * & * & -5 \end{bmatrix}$$

We see that B has 13 non-zeros, and we store B as follows:

```
values   = (1 -1 -3 -2 5 4 6 4 -4 2 7 8 -5)
columns  = (1  2  4  1 2 3 4 5  1 3 4 2  5)
rowIndex = (1 4 6 9 12 14)
```

In this version of CXML, direct sparse solvers cannot solve non-symmetric systems of equations. However, it can solve **symmetrically structured** systems of equations. A symmetrically structured system of equations is one where the pattern of non-zeros is symmetric. That is, a matrix has a symmetric structure if $a(i,j)$ is non-zero if and only if $a(j,i)$ is non-zero.

However, from the point of view of the solver software, a non-zero element of a matrix is anything that is stored in the *values* array. In that sense, we can turn any non-symmetric matrix into a symmetrically structured matrix by carefully adding zeros to the *values* array.

For example, suppose we consider the matrix B to have the following set of non-zero entries:

$$B = \begin{bmatrix} 1 & -1 & * & -3 & * \\ -2 & 5 & * & * & 0 \\ * & * & 4 & 6 & 4 \\ -4 & * & 2 & 7 & * \\ * & 8 & 0 & * & -5 \end{bmatrix}$$

Now B can be considered to be symmetrically structured with 15 non-zero entries. We would represent the matrix as:

```
values   = (1 -1 -3 -2 5 0 4 6 4 -4 2 7 8 0 -5)
columns  = (1  2  4  1 2 5 3 4 5  1 3 4 2 3  5)
rowIndex = (1 4 7 10 13 16)
```

11.4.1 Storage Format Restrictions

The storage format for DSS must conform to two important restrictions: First, the non-zero values in a given row must be placed into the *values* array *in the order in which they occur in the row* (from left to right). Second, no diagonal element can be omitted from the *values* array.

The second restriction implies that when dealing with matrices that have zeros on the diagonal, the zero diagonal elements must be *explicitly* represented in the *values* array.

11.5 Direct Sparse Solver (DSS) Routine Overview

The CXML direct sparse solver uses the general scheme described in Section 11.4 for solving sparse systems of linear equations. The solver consists of eight user callable routines that are conceptually divided into six phases. The following table lists the names of the eight routines, grouped by phase, and describes their general use. Full descriptions of these routines are provided in Part XV.

Table 11–1 Direct Sparse Solver Routines

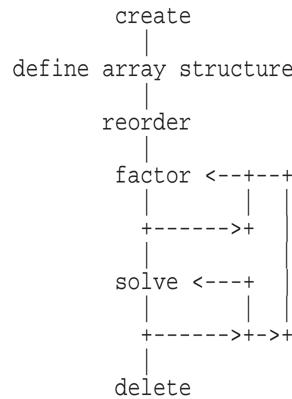
Routine	Description
dss_create	Initializes the solver and creates the basic data structures necessary for the solver. This routine must be called before any other solver routine.
dss_define_structure	This routine is used to inform the solver of the locations of the non-zero elements of the array.
dss_reorder	Based on the non-zero structure of the matrix, this routine computes a permutation vector to reduce fill-in during the factoring process.
dss_factor_real dss_factor_complex	Computes the LU, LDT^t or LL^T factorization of a real or complex matrix.
dss_solve_real dss_solve_complex	Computes the solution vector for a system of equations based on the factorization computed by the previous phase.
dss_delete	Deletes all of the data structures created during the solutions process.

To find a single solution vector for a single system of equations with a single right hand side, the CXML direct sparse routines are invoked in the order in which they are listed in the above table.

However, in certain applications it is necessary to produce solution vectors for multiple right-hand sides for a given factorization and/or factor several matrices with the same non-zero structure.

Consequently, it is necessary to be able to invoke the CXML sparse routines in an order other than listed above. The following diagram indicates the typical order(s) in which the direct sparse routines can be invoked:

Figure 11–1 Typical order for invoking direct sparse solver routines



11.6 Direct Sparse Solver Routine Interfaces

This section describes the direct sparse solver routine interfaces.

11.6.1 Portability Issues

Several aspects of the CXML direct sparse solver are platform-specific and language-specific. In order to promote portability across platforms and ease of use across different languages, users are encouraged to include one of the CXML direct sparse solver language-specific header files. Currently, there are four language specific header files:

- cxml_dss.f77 for F77 programs
- cxml_dss.f90 for F90 programs
- cxml_dss.h for C programs
- cxml_dss.hxx for C++ programs

These language-specific header files define symbolic constants for error returns, function options, certain defined data types, and function prototypes.

Note

It is strongly recommended that you refer to the constants for options, error returns, and message severities **only** by the symbolic names that are defined in the header files. Use of the CXML direct sparse solver without including one of the above header files is not supported.

11.6.1.1 Error Reporting

When a CXML direct sparse solver routine encounters an error, the CXML message dispatcher is invoked. Based on the severity of the error and certain user-specifiable options (see Section 11.6.2.1), the message dispatcher optionally prints an explanatory message to the screen and exits the application. If the message dispatcher does not exit the application, then an error code indicating the type of error that occurred is returned to the user.

CXML recognizes the following error severities (listed in increasing order of severity):

SUCCESS

INFO
WARNING
ERROR
FATAL

All of the CXML direct sparse solver routines return an error code. A error code of CXML_DSS_SUCCESS indicates a successful completion. Any other error code indicates some type of problem.

User code should check the return value from all CXML direct sparse solver routines, and continue only if the result is equal to CXML_DSS_SUCCESS. Note that any error code other than CXML_DSS_SUCCESS from a direct sparse solver routine simply indicates that an error has occur. No effort is made by the routines to clean up data structures or to correct the problem.

The numerical values of the CXML direct sparse solver error codes are platform dependent. Users are strongly encouraged to use only the symbolic error code defined in the language-specific header files supplied with the solver.

The following table lists the symbolic error codes that are currently defined.

Table 11–2 CXML Symbolic Error Codes

Error	Description
CXML_DSS_SUCCESS	No error occurred.
CXML_DSS_ZERO_PIVOT	The matrix defined is singular.
CXML_DSS_OUT_OF_MEMORY	The system cannot allocate enough memory to proceed with the specified operation.
CXML_DSS_STATE_ERR	The CXML direct sparse solver routines were called in an order other than that permitted by the flow chart in Figure 11–1
CXML_DSS_INVALID_OPTION	One or more of the options supplied to a routine is inappropriate for the routine.
CXML_DSS_OPTION_CONFLICT	Two or more of the options requested for a routine cannot be satisfied simultaneously.
CXML_DSS_ROW	The number of rows specified for matrix is less than one.
CXML_DSS_COL	The number of columns specified for matrix is less than one.
CXML_DSS_NOT_SQUARE	The number of rows is not equal to the number of columns.
CXML_DSS_TOO_FEW_VALUES	The specified number of non-zeros is less than the number of rows.
CXML_DSS_TOO_MANY_VALUES	The specified number of non-zeros is greater than the product of the number of rows and columns.
CXML_DSS_MSG_LVL_ERR	The specified message level is invalid
CXML_DSS_TERM_LVL_ERR	The specified termination level is invalid
CXML_DSS_STRUCTURE_ERR	The specified structure option is invalid
CXML_DSS_REORDER_ERR	The specified reorder option is invalid

(continued on next page)

Table 11–2 (Cont.) CXML Symbolic Error Codes

Error	Description
CXML_DSS_FACTOR_ERR	The specified factor option is invalid
CXML_DSS_FAILURE	An unclassified error occurred.

Note: All of the above errors have a severity level of ERROR, except for CXML_DSS_FAILURE and CXML_DSS_SUCCESS.

CXML_DSS_FAILURE has severity FATAL.
CXML_DSS_SUCCESS has a severity of SUCCESS.

11.6.1.2 Memory Allocation and Handles

In order to make the CXML direct sparse solver routines as easy to use as possible, the routines do not require the user to allocate any temporary working storage. Any storage required by the solver (that is not a user input) is allocated by the solver itself. In order to allow multiple users to access the solver simultaneously, the solver keeps track of the storage allocated for a particular application by using an opaque data object called a **handle**.

Each of the CXML direct sparse solver routines either creates, uses or deletes a handle. Consequently, user programs must be able to allocate storage for a handle. The exact syntax for allocating storage for a handle varies from language to language. To help standardize the handle declarations, the language-specific header files declare constants and defined data types that should be used when declaring a handle object in user code.

Fortran 90 programmers should declare a handle as:

```
INCLUDE "cxml_dss.f90"
TYPE(CXML_DSS_HANDLE) handle
```

C and C++ programmers should declare a handle as:

```
#include "cxml_dss.h"
_CXML_DSS_HANDLE_t handle;
```

Fortran 77 programmers using compilers that support eight byte integers, should declare a handle as:

```
INCLUDE "cxml_dss.f77"
INTEGER*8 handle
```

otherwise they should replace INTEGER*8 with DOUBLE PRECISION.

In addition to the necessary definition for the correct declaration of a handle, the include file also defines the following:

- function prototypes for languages that support prototypes
- symbolic constants that are used for the error returns
- user options for the solver routines
- message severity

11.6.1.3 Calling Direct Sparse Solver Routines From C/C++

The calling interface for all of the CXML direct sparse solver routines is designed to be used easily from Fortran 77 or Fortran 90. However, any of the direct sparse solver routines can be invoked directly from C or C++ if users are familiar with the inter-language calling conventions of their platforms. These conventions include, but are not limited to, the argument passing mechanisms for the language, the data type mappings from Fortan to C/C++ and how Fortran external names are decorated on the platform.

In order to promote portability and to avoid having most users deal with these issues, the C and C++ header files, cxml_dss.h and cxml_dss.hxx, provide a set of macros and type definitions that are intended to hide the inter-language calling conventions and provide an interface to the Direct Sparse Solver that appears natural for C/C++.

For example, consider a hypothetical library routine, *foo*, that takes real vector of length n, and returns an integer status. Fortran users would access such a function as:

```
INTEGER n, status, foo
REAL x(*)

status = foo(x, n)
```

As noted above, for C users to invoke *foo*, they would need to know what C data types correspond to Fortran types INTEGER and REAL; what argument passing mechanism the Fortran compiler uses; and what, if any, name decoration the is performed by the Fotran compiler when generating the external symbol *foo*. However, by using the C specific header file cmxl_dss.h, the invocation of *foo*, within a C program would look like:

```
#include "cxml_dss.h"

_INTEGER_t  i, status;
_REAL_t x[];

status = foo( x, i );
```

Note that in the above example, the header file *cxml_dss.h* provides definitions for the types _INTEGER_t and _REAL_t that correspond to the Fortran types INTEGER and REAL.

In order to ease the use of direct sparse solver routines from C and C++, the general approach of providing C definitions of Fortran types is used throughout the library. Specifically, if an argument or result from a direct sparse solver is documented as having the Fortran language specific type XXX, then the C and C++ header files provide an appropriate C language type definitions for the name _XXX_t.

11.6.1.3.1 A Caveat for C Users One of the key differences between C/C++ and Fortran is the argument passing mechanisms for the languages: Fortran programs use pass-by-reference semantics and C/C++ programs use pass-by-value semantics. In the example in the previous section, the header file, cxml_dss.h, attempts to hide this difference, by defining a macro, *foo* that takes the address of the appropriate arguments. For example, on Tru64 UNIX, cxml_dss.h would define the macro as:

```
#define foo(a,b)  foo_((a), &(b))
```

An important point to note when using the macro form of foo is how it deals with constants. If we write *foo(x, 10)*, this is translated into *foo_(x, &10)*. In a strictly ANSI compliant C compiler, it is not permissible to take the address of a constant, so a strictly conforming program would look like:

```
_INTEGER_t iTen = 10;
_REAL_t *  x;
status = foo( x, iTen );
```

However, Compaq C compilers in a non-ANSI standard mode (the default mode), allow taking the address of a constant for ease of use with Fortran programs. Thus for Compaq C compilers, the form shown as foo(x, 10) is acceptable.

If users compile their code in strict ANSI-C mode (i.e. use the compiler switch -std1), then the compiler generates correctly functioning code, but normally issues a warning when trying to take the address of a constant. cxml_dss.h contains a pragma to suppress the warnings when the -std1 switch is used. Users can restore the default warning for the -std1 by including cxml_dss.h as follows:

```
#include "cxml_dss.h"
#pragma message enable argaddr
```

11.6.2 Interface Descriptions

As noted in Section 11.6.1.3, each direct sparse solver routine either reads or writes an opaque data structure called a handle. Because the declaration of a handle varies from language to language, it is declared as being of type CXML_DSS_HANDLE in this documentation. You can refer to Section 11.6.1.3 to determine the correct method for declaring a handle argument.

All other types in this documentation refer to the standard Fortran types, INTEGER, REAL, COMPLEX, DOUBLE PRECISION and DOUBLE COMPLEX. C and C++ programmers should refer to Section 11.6.1.3 for information on mapping Fortran types to C/C++ types.

In the routine descriptions in this document, routine arguments are documented using the format:

```
name : intent : type
```

`type` is one of the standard Fortran data types and intent is one of INPUT, OUTPUT or MODIFY. Arguments with INPUT intent are read and not written. Arguments with OUTPUT intent are written but not read. Arguments with MODIFY intent are both read and written.

As noted in section Section 11.6.1.1, all direct sparse solver routines return an integer value that is equal to one of the error codes defined in that section.

11.6.2.1 Routine Options

All of the direct sparse solver routines have an integer argument for passing various options to the routines referred to in the user documentation as *opt*. The permissible values for *opt* should be specified using only the symbol constants defined in the language-specific header files. All of the routines accept options for setting the message termination level as described below. Additionally, all routines accept the following option:

CXML_DSS_DEFAULTS

Specifying CXML_DSS_DEFAULTS establishes the documented default options for each direct sparse solver routine.

All of the direct sparse solver routines accept options for controlling the message and termination level (see Section 11.6.1.1 The following symbolic names for the options are defined in the language-specific header files.

CXML_DSS_MSG_LVL_SUCCESS
CXML_DSS_MSG_LVL_INFO
CXML_DSS_MSG_LVL_WARNING
CXML_DSS_MSG_LVL_ERROR
CXML_DSS_MSG_LVL_FATAL

CXML_DSS_TERM_LVL_SUCCESS
CXML_DSS_TERM_LVL_INFO
CXML_DSS_TERM_LVL_WARNING
CXML_DSS_TERM_LVL_ERROR
CXML_DSS_TERM_LVL_FATAL

The settings for message and termination level can be set on any call to a direct sparse solver routine. However, once set to a particular level, they remain at that level until they are changed in another call to a direct sparse solver routine.

Users can specify multiple options to a direct sparse solver routine by adding the options together. For example, to set the message level to debug and the termination level to error for all direct sparse solver routines, use the call:

```
      CALL dss_create( handle,
     1 CXML_DSS_MSG_LVL_INFO + CXML_DSS_TERM_LVL_ERROR)
```

11.6.2.2 User Data Arrays

Many of the direct sparse solver routines take arrays of user data as input. For example, user arrays are passed to the routine dss_define_structure to describe the location of the non-zero entries in the matrix. In order to minimize storage requirements and improve overall run-time efficiency, the CXML direct sparse solver routines do not make copies of the user input arrays.

! Important

Users cannot modify the contents of these arrays after they are passed to one of the solver routines.

11.7 Direct Sparse Solver Examples

This section contains example code in F77 and C. The example code solves the equations presented in Section 11.3 - a symmetric positive definite system of equations.

11.7.1 Fortran 77 Example of Direct Sparse Solver

Example 11–1 Fortran 77 Example to solve symmetric positive definite system of equations in Section 11.3

(continued on next page)

Example 11–1 (Cont.) Fortran 77 Example to solve symmetric positive definite system of equations in Section 11.3

```
C--------------------------------------------------------------------------
C
C Example program for solving symmetric positive definite system of
equations.
C
C--------------------------------------------------------------------------

 PROGRAM solver_f77_test
 IMPLICIT NONE
 INCLUDE 'cxml_dss.f77'

C--------------------------------------------------------------------------
C  Define the array and rhs vectors
C--------------------------------------------------------------------------

      INTEGER  nRows, nCols, nNonZeros, i, nRhs
      PARAMETER (nRows     = 5,
     1          nCols     = 5,
     2          nNonZeros = 9,
     3          nRhs      = 1)

      INTEGER rowIndex(nRows + 1), columns(nNonZeros)
      DOUBLE PRECISION values(nNonZeros), rhs(nRows)

      DATA rowIndex / 1, 6, 7, 8, 9, 10 /
      DATA columns  / 1, 2, 3, 4, 5, 2, 3, 4, 5 /
      DATA values   / 9, 1.5, 6, .75, 3, 0.5, 12, .625, 16 /
      DATA rhs      / 1, 2, 3, 4, 5 /

C--------------------------------------------------------------------------
C  Allocate storage for the solver handle and the solution vector
C--------------------------------------------------------------------------

      DOUBLE PRECISION solution(nRows)
      INTEGER*8        handle
      INTEGER          error

C--------------------------------------------------------------------------
C  Initialize the solver
C--------------------------------------------------------------------------

      error = dss_create(handle, CXML_DSS_DEFAULTS)
      IF (error .NE. CXML_DSS_SUCCESS ) GOTO 999

C--------------------------------------------------------------------------
C  Define the non-zero structure of the matrix
C--------------------------------------------------------------------------


      error = dss_define_structure( handle, CXML_DSS_SYMMETRIC,
     &               rowIndex, nRows, nCols, columns, nNonZeros )
      IF (error .NE. CXML_DSS_SUCCESS ) GOTO 999

C--------------------------------------------------------------------------
C  Reorder the matrix
C--------------------------------------------------------------------------

      error = dss_reorder( handle, CXML_DSS_DEFAULTS, 0)
      IF (error .NE. CXML_DSS_SUCCESS ) GOTO 999

C--------------------------------------------------------------------------
C  Factor the matrix
C--------------------------------------------------------------------------
```

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Example 11–1 (Cont.) Fortran 77 Example to solve symmetric positive definite system of equations in Section 11.3

```
      error = dss_factor_real( handle,
     &           CXML_DSS_DEFAULTS, VALUES)
      IF (error .NE. CXML_DSS_SUCCESS ) GOTO 999

C---------------------------------------------------------------------------
C  Get the solution vector
C---------------------------------------------------------------------------
      error = dss_solve_real( handle, CXML_DSS_DEFAULTS,
     &                          rhs, nRhs, solution)
      IF (error .NE. CXML_DSS_SUCCESS ) GOTO 999
C---------------------------------------------------------------------------
C  Deallocate solver storage
C---------------------------------------------------------------------------
      error = dss_delete( handle, CXML_DSS_DEFAULTS )
      IF (error .NE. CXML_DSS_SUCCESS ) GOTO 999
C---------------------------------------------------------------------------
C  Print solution vector
C---------------------------------------------------------------------------
      WRITE(*,900) (solution(i), i = 1, nCols)
  900 FORMAT(' Solution Array: ',5(F10.3))
      GOTO 1000
  999 WRITE(*,*) "Solver returned error code ", error
 1000 END
```

11.7.2 C Example of Direct Sparse Solver

Example 11–2 C Example to solve symmetric positive definite system of equations in Section 11.3

```
/*
**
** Example program to solve symmetric positive definite system of equations.
**
*/
#include<stdio.h>
#include<stdlib.h>
#include "cxml_dss.h"
/*
** Define the array and rhs vectors
*/
#define nRows 5
#define nCols 5
#define nNonZeros 9
#define nRhs  1
```

(continued on next page)

Example 11–2 (Cont.) C Example to solve symmetric positive definite system of equations in Section 11.3

```
static _INTEGER_t          rowIndex[nRows+1]  = { 1, 6, 7, 8, 9, 10 };
static _INTEGER_t          columns[nNonZeros] = { 1, 2, 3, 4, 5, 2, 3, 4, 5
};
static _DOUBLE_PRECISION_t values[nNonZeros]  = { 9, 1.5, 6, .75, 3, 0.5,
                                                  12, .625, 16 };
static _DOUBLE_PRECISION_t rhs[nCols]         = { 1, 2, 3, 4, 5 };

void main() {

    int i;

    /* Allocate storage for the solver handle and the right-hand side.  */

    _DOUBLE_PRECISION_t solValues[nRows];
    _CXML_DSS_HANDLE_t  handle;
    _INTEGER_t          error;

    /* --------------------- */
    /* Initialize the solver */
    /* --------------------- */

    error = dss_create(handle, CXML_DSS_DEFAULTS );
    if ( error != CXML_DSS_SUCCESS ) goto printError;

    /* ------------------------------------------- */
    /* Define the non-zero structure of the matrix */
    /* ------------------------------------------- */

    error = dss_define_structure(
             handle, CXML_DSS_SYMMETRIC, rowIndex, nRows, nCols,
             columns, nNonZeros );
    if ( error != CXML_DSS_SUCCESS ) goto printError;

    /* ------------------ */
    /* Reorder the matrix */
    /* ------------------ */

    error = dss_reorder( handle, CXML_DSS_DEFAULTS, 0);
    if ( error != CXML_DSS_SUCCESS ) goto printError;

    /* ------------------ */
    /*  Factor the matrix */
    /* ------------------ */

    error = dss_factor_real( handle, CXML_DSS_POSITIVE_DEFINITE, values );
    if ( error != CXML_DSS_SUCCESS ) goto printError;

    /* ------------------------ */
    /*  Get the solution vector */
    /* ------------------------ */

    error = dss_solve_real( handle, CXML_DSS_DEFAULTS, rhs, nRhs, solValues );
    if ( error != CXML_DSS_SUCCESS ) goto printError;

    /* -------------------------- */
    /*  Deallocate solver storage */
    /* -------------------------- */

    error = dss_delete( handle, CXML_DSS_DEFAULTS );
    if ( error != CXML_DSS_SUCCESS ) goto printError;

    /* ---------------------- */
    /*  Print solution vector */
    /* ---------------------- */
```

(continued on next page)

Example 11–2 (Cont.) C Example to solve symmetric positive definite system of equations in Section 11.3

```
    printf(" Solution array: ");

    for(i = 0; i< nCols; i++)
        printf(" %g", solValues[i] );
    printf("\n");

    return;

printError:

    printf("Solver returned error code %d\n", error);
}
```

11.7.3 Fortran 90 Example of Direct Sparse Solver

Example 11–3 Fortran 90 Example to solve symmetric positive definite system of equations in Section 11.3

```
!---------------------------------------------------------------------------
!
! Example program for solving a symmetric positive definite system of
!  equations.
!
!---------------------------------------------------------------------------

PROGRAM solver_f90_test

  INCLUDE 'cxml_dss.f90'  !  Include the standard DSS "header file."

  IMPLICIT NONE

  INTEGER, PARAMETER :: dp = KIND(1.0D0)

  INTEGER :: error
  INTEGER :: i

!  Define the data arrays and the solution and rhs vectors.

  INTEGER, ALLOCATABLE :: columns( : )
  INTEGER :: nCols
  INTEGER :: nNonZeros
  INTEGER :: nRhs
  INTEGER :: nRows
  REAL(KIND=DP), ALLOCATABLE :: rhs( : )
  INTEGER, ALLOCATABLE :: rowIndex( : )
  REAL(KIND=DP), ALLOCATABLE :: solution( : )
  REAL(KIND=DP), ALLOCATABLE :: values( : )

  TYPE(CXML_DSS_HANDLE) :: handle  !  Allocate storage for the solver
  handle.

!  Set the problem to be solved.
```

(continued on next page)

Example 11–3 (Cont.) Fortran 90 Example to solve symmetric positive definite system of equations in Section 11.3

```
  nRows = 5
  nCols = 5
  nNonZeros = 9
  nRhs = 1
  ALLOCATE( rowIndex( nRows + 1 ) )
  rowIndex = (/ 1, 6, 7, 8, 9, 10 /)
  ALLOCATE( columns( nNonZeros ) )
  columns = (/ 1, 2, 3, 4, 5, 2, 3, 4, 5 /)
  ALLOCATE( values( nNonZeros ) )
  values = (/ 9.0_DP, 1.5_DP, 6.0_DP, 0.75_DP, 3.0_DP, 0.5_DP, 12.0_DP,  &
  &           0.625_DP, 16.0_DP /)
  ALLOCATE( rhs( nRows ) )
  rhs = (/ 1.0_DP, 2.0_DP, 3.0_DP, 4.0_DP, 5.0_DP /)

  !  Initialize the solver.
  error = dss_create( handle, CXML_DSS_DEFAULTS )
  IF (error /= CXML_DSS_SUCCESS) GOTO 999

  !  Define the non-zero structure of the matrix.
  error = dss_define_structure( handle, CXML_DSS_SYMMETRIC, rowIndex, nRows, &
  &                             nCols, columns, nNonZeros )
  IF (error /= CXML_DSS_SUCCESS) GOTO 999

  !  Reorder the matrix.
  error = dss_reorder( handle, CXML_DSS_DEFAULTS, 0 )
  IF (error /= CXML_DSS_SUCCESS) GOTO 999

  !  Factor the matrix.
  error = dss_factor_real( handle, CXML_DSS_DEFAULTS, values )
  IF (error /= CXML_DSS_SUCCESS) GOTO 999

  !  Allocate the solution vector and solve the problem.
  ALLOCATE( solution( nRows ) )
  error = dss_solve_real(handle, CXML_DSS_DEFAULTS, rhs, nRhs, solution )
  IF (error /= CXML_DSS_SUCCESS) GOTO 999

  !  Deallocate solver storage and various local arrays.
  error = dss_delete( handle, CXML_DSS_DEFAULTS )
  IF (error /= CXML_DSS_SUCCESS ) GOTO 999
  IF ( ALLOCATED( rowIndex) ) DEALLOCATE( rowIndex )
  IF ( ALLOCATED( columns ) ) DEALLOCATE( columns )
  IF ( ALLOCATED( values ) ) DEALLOCATE( values )
  IF ( ALLOCATED( rhs ) ) DEALLOCATE( rhs )

  !  Print the solution vector, deallocate it and exit
  WRITE(*,"('Solution Array: '(5F10.3))") ( solution(i), i = 1, nCols )
  IF ( ALLOCATED( solution ) ) DEALLOCATE( solution )
  GOTO 1000

  !  Print an error message and exit
999 WRITE(*,*) "Solver returned error code ", error

1000 CONTINUE

END PROGRAM solver_f90_test
```

12
Using the VLIB Routines

CXML includes a special set of routines that are similar to industry standard array processor library routines. This special set of run-time library routines operates on vectors—thus the name VLIB. This chapter provides information about the following topics:

- Operations performed by the VLIB subprograms (Section 12.1)
- Vector storage (Section 12.2)
- Subprogram naming conventions (Section 12.3)
- Subprogram summaries (Section 12.4)
- Calling VLIB subprograms (Section 12.5)
- Arguments used in the subprograms (Section 12.6)
- Error handling for VLIB subprograms (Section 12.7)
- A look at a VLIB subprogram and its use (Section 12.8)

12.1 VLIB Operations

VLIB operations work with vectors. The VLIB subprograms operate on only one vector (or possibly scalar), returning one or more vectors (or possibly scalars) as output. These routines make it easier to port existing array processor-oriented code, as well as provide enhanced performance, where possible. Many simple array-oriented routines (such as adding a constant to each element of an array) are more suitably coded by using the corresponding loop and letting compiler optimizations improve performance. More complex routines are suitably encapsulated in highly tuned routines such as those in VLIB.

For example, the VLIB routines include routines for transcendental functions. In this case, the VLIB functions generally deliver performance 1.5 to 2 times faster than the alternative of simply calling the appropriate run-time library function in a loop. Careful code scheduling and algorithm design within the VLIB routines take advantage of the fact that the input is a vector.

The results of these operations do not depend on the order in which the elements of the vector are processed.

12.2 Vector Storage

For the VLIB subprograms, a vector is stored in a one-dimensional array. The calling conventions for negative increment accesses to an array differ from BLAS1 conventions, but follow conventions used in existing array processor libraries. See Section 12.2.2.

12.2.1 Defining a Vector in an Array

A vector is usually stored in a one-dimensional array. The elements of a vector are stored in order, but the elements are not necessarily contiguous.

An array can be much larger than a vector that is stored in the array. The storage of a vector is defined using three arguments in a CXML subprogram argument list:

- Vector length: Number of elements in the vector
- Vector location: Base address of the vector in the array
- Stride: Space, or increment, between consecutive elements of the vector as stored in the array

These three arguments together specify which elements of an array are selected to become the vector.

12.2.1.1 Vector Length

To specify the length n of a vector, you specify an integer value for a length argument, such as the **n** argument. The length of a vector can be less than the length of the array that specifies the vector.

Vector length can also be thought of as the number of elements of the associated array that a subroutine will process. Processing continues until n elements have been processed.

12.2.1.2 Vector Location

The location of a vector is specified by the argument for the vector in the CXML subprogram argument list. Usually, an array such as X is declared, for example, X(1:20) or X(20). In this case, if you want to specify vector x as starting at the first element of an array X, the argument is specified as X(1) or X. If you want to specify vector x as starting at the fifth element of X, the argument is specified as X(5).

However, in an array X that is declared as X(3:20), with a lower bound and an upper bound given for the dimension, specifying vector x as starting at the fifth element of X means that the argument is specified as X(7).

Most of the examples shown in this manual assume that the lower bound in each dimension of an array is 1. Therefore, the lower bound is not specified, and the value of the upper bound is the number of elements in that dimension. So, a declaration of X(50) means X has 50 elements.

12.2.1.3 Stride of a Vector

The spacing parameter, called the increment or stride, indicates how to move from the starting point through the array to select the vector elements from the array. The increment is specified by an argument in the CXML subprogram argument list, such as the **incx** argument.

The vector elements are stored in the array in the order $x_1, x_2, ..., x_n$. An increment of 1 indicates that the vector elements are contiguous in the array.

12.2.1.4 Selecting Vector Elements from an Array

CXML VLIB routines use the stride to select elements from the array to construct the vector composed of these elements. The stride associates consecutive elements of the vector with equally spaced elements of the array.

12.2.2 Storing a Vector in an Array

Suppose X is a real one-dimensional array of $ndim$ elements. Let vector x have length n and let $incx$ be the increment used to access the elements of vector x whose components x_i, $i = 1, \ldots, n$, are stored in X.

If $incx > 0$, and if the first element of the vector is specified at the first element of the array, then x_i is stored in the array location as shown in (12–1):

$$\mathrm{X}(1 + (i - 1) * incx) \qquad (12\text{–}1)$$

Therefore, $ndim$, the number of elements in the array, should satisfy the condition shown in (12–2):

$$ndim \geq 1 + (n - 1) * |incx| \qquad (12\text{–}2)$$

For the general case where the first element of the vector in the array is at the point X(BP) rather than at the first element of the array, (12–3) can be used to find the position of each vector element x_i in a one-dimensional array.

For $incx \neq 0$, the position of x_i is as follows:

$$X(\mathrm{BP} + (i - 1) * incx) \qquad (12\text{–}3)$$

For example, suppose that $\mathrm{BP} = 3$, $ndim = 20$, and $n = 5$. Then a value of $incx = 2$ implies that x_1, x_2, x_3, x_4, and x_5 are stored in array elements X(3), X(5), X(7), X(9), and X(11). Using $\mathrm{BP} = 11$ and $incx = -2$ would mean that x_1, x_2, x_3, x_4, x_5 were stored in X(11), X(9), X(7), X(5), X(3).

12.3 Naming Conventions

Table 12–1 shows the characters used in the names of the VLIB subprograms and what the characters mean.

Table 12–1 Naming Conventions: VLIB Subprograms

Character Group	Mnemonic	Meaning
First group	V	Operates on a vector.
Second group	A combination of letters at the end such as SIN or RECIP	Type of computation such as sine (SIN) of a vector or reciprocal (RECIP) of the elements of a vector.

For example, the name VSQRT is the subprogram for computing the square-root of the elements of a vector. All VLIB routines accept double-precision input arrays and return double-precision output arrays.

12.4 Summary of VLIB Subprograms

Table 12–2 summarizes the VLIB subprograms.

Table 12–2 Summary of VLIB Subprograms

Subprogram Name	Operation
VCOS	Calculates, in double-precision arithmetic, the cosine of the elements of a real vector.
VCOS_SIN	Calculates, in double-precision arithmetic, the sine and cosine of the elements of a real vector.
VEXP	Calculates, in double-precision arithmetic, the exponential of the elements of a real vector.
VLOG	Calculates, in double-precision arithmetic, the natural logarithm of the elements of a real vector.
VRECIP	Calculates, in double-precision arithmetic, the reciprocal of the elements of a real vector.
VSIN	Calculates, in double-precision arithmetic, the sine of the elements of a real vector.
VSQRT	Calculates, in double-precision arithmetic, the square root of the elements of a real vector.

12.5 Calling Subprograms

The VLIB subprograms consist of only subroutines.

12.6 Argument Conventions

The VLIB subprograms use a list of arguments to specify the requirements and control the result of the subprogram. All arguments are required. The argument list is in the same order for each subprogram:

- Arguments that describe the input and output vectors
  The following arguments describe a vector:
  - The arguments **x**, **y**, and **z** define the location of the vectors x, y, and z in the array. In the usual case, the argument **x** specifies the location in the array as X(1), but the location can be specified at any other element of the array. An array can be much larger than the vector that it contains.
  - The arguments **incx**, **incy**, and **incz** provide the increment between the locations of the elements of the vector x, vector y, and vector z, respectively.
- Arguments that define the number of elements to process
  The **n** argument specifies the number of elements to process. If $n \leq 0$, the output vector is unchanged.

12.7 Error Handling

Where applicable, the elements of the input vector (to the VLIB routines) are checked for the possibility that a later arithmetic exception will occur. Nonfinite operands will trap within the routine. Other situations such as finite inputs that are illegal or exception causing inputs to the corresponding RTL routine are typically caught by detecting the offending input argument, and then calling the corresponding RTL routine with the offending argument. Thus, essentially the same "traditional Fortran" exception behavior as with an RTL call is preserved.

12.8 A Look at a VLIB Subprogram

To understand the meaning of the arguments, consider the subroutine VSQRT. VSQRT computes the square root of a real (n-element) vector x, and the result is returned in the vector y. VSQRT has the arguments **x**, **incx**, **y**, **incy** and **n**.

For example, suppose that arrays X and Y are declared as follows:

```
REAL*8 X(-10:10), Y(41)
```

Then, the statements:

```
INCX = 1
INCY = 2
N = 21
CALL VSQRT(X,INCX,Y,INCY,N))
```

yield the following results:

```
Y(1)  = SQRT(X(-10))
Y(3)  = SQRT(X(-9)))
Y(5)  = SQRT(X(-8))
      .
      .
      .
Y(39) = SQRT(X(9))
Y(41) = SQRT(X(10))
```

This call to routine VSQRT obtains the same results as the following Fortran code segment:

```
DO I = 1, 41, 2
   Y(I) = SQRT( X( (I+1)/2 - 11) )
END DO
```

The argument **x** specifies the array X with 21 elements and specifies X(-10) as the location of the vector x whose elements are embedded in X. Since **n** = 21, the vector also has 21 elements. The length of the array X is the same as the length of the vector x. The value of the argument **incx** = 1 specifies that the vector elements are contiguous in the array. Since **incy** is 2, the square root of each element of the array X is stored in array Y, beginning at Y(1), in the locations Y(1), Y(3), Y(5), and so on.

13 Using Random Number Generator Subprograms

CXML provides four random number generator (RNG) subprograms and two auxiliary input subprograms for parallel applications.

This chapter provides information about the following topics:

- Standard Uniform RNG Subprograms (Section 13.2)
- Long Period Uniform RNG Subprogram (Section 13.3)
- Normally Distributed RNG Subprogram (Section 13.4)
- Input Subprograms for Parallel Applications Using RNG Subprograms (Section 13.5)
- Summary of RNG Subprograms (Section 13.6)
- Error Handling (Section 13.7)
- RNG subprogram reference descriptions

13.1 Introduction

RNGs are an important part of many simulation programs and test procedures. CXML provides the following RNG subprograms:

- Three subprograms that generate uniform [0,1] random number distributions using algorithms based on the following:
  - Multiplicative generators — See Section 13.2 for a description of the RAN16807 subprogram.
  - Linear congruential generators — See Section 13.2 for a description of the RAN69069 subprogram.
  - Combined multiplicative generators — See Section 13.3 for a description of the RANL subprogram.
- One subprogram that generates normally distributed (N(0,1)) random numbers using a sum-type algorithm based on the central limit theorem — see Section 13.4 for a description of the RANL_NORMAL subprogram.
- Two subprograms that generate input for two other CXML RNG subprograms when they are used in parallel computing applications. Both input subprograms use a repeated squaring algorithm — see Section 13.5 for descriptions of the RANL_SKIP2 and RANL_SKIP64 subprograms.

13.2 Standard Uniform RNG Subprograms

CXML provides the RAN16807 and the RAN69069 subprograms to generate full period (m or $m-1$), sequences of uniform random numbers. Both subprograms use a single precision, function call interface. CXML provides these RNGs since they are perhaps the two most commonly used 32-bit generators.

The RAN16807 subprogram uses an algorithm that corresponds to the "minimal standard generator" recommended by Park and Miller. For further information see Section G.8. The algorithm is based on a multiplicative generator of the form:

$s = as \quad mod\ m$, with $s \geq 1$, and $m = 2^{31} - 1$.
$x = s/m$

The RAN69069 subprogram uses an algorithm that has been used in Compaq run-time libraries. The algorithm is based on a linear congruential generator of the form:

$s = as + c \quad mod\ m$, with $m = 2^{32}$.
$x = s/m$

For a further discussion of this algorithm, refer to Knuth in Section G.8.

13.3 Long Period Uniform RNG Subprogram

CXML provides the RANL subprogram to generate very long period, uniform random numbers. The RANL subprogram implements the combined multiplicative algorithm introduced by L'Ecuyer. This algorithm uses two 32-bit seeds and combines two separate generators to yield a very long period generator.

Here is a brief summary of the L'Ecuyer algorithm:

- The initial seeds $s1, s2$ are user input, with $1 \leq s1 \leq m1$, $1 \leq s2 \leq m2$. (See $m1, m2$ values in the following paragraphs.)
- In each step, updated values of $s1, s2$ are used to produce the next single precision uniform random number u according to the following:

  $s1 = a1 * s1 \quad (mod\ m1) \quad m1 = 2147483563,\ a1 = 40014$
  $s2 = a2 * s2 \quad (mod\ m2) \quad m2 = 2147483399,\ a2 = 40692$

  The algorithm then calculates $z = s1 - s2\,(mod\ \ (m1-1))$, and if z is 0, puts $z = m1 - 1$.
- Finally, the algorithm returns with $u = z/m1$.

The period can be shown to be $(m1-1)(m2-1)/2$.

CXML provides a subroutine call interface that can return a vector v(1),...,v(n) of outputs. The vector form is very useful when speed is paramount.

For more information about the L'Ecuyer algorithm, see Section G.8.

For parallel applications using the RANL subprogram, CXML provides two auxiliary, input subprograms that generate nonoverlapping streams of independent random numbers. See Section 13.5 for more information.

13.4 Normally Distributed RNG Subprogram

CXML provides the RANL_NORMAL subprogram to generate random normal N(0,1) numbers. The RANL_NORMAL subprogram uses an algorithm based on the central limit, which uses the following sum to approximate a normally distributed variate.

$$s = x1 + x2 + ... + x12 - 6.0$$

The number 12 is used, because the variance of a uniform [0,1] variable is 1/12. Summing 12 uniform variables and subtracting their mean should yield an N(0,1) variate.

The RANL_NORMAL subprogram generalizes this procedure to an arbitrary number of summands and then uses scaling to get back to an N(0,1) result. The RANL_NORMAL subprogram overcomes the common drawback of sum-type algorithms, in that it uses CXML's vector call interface to the RANL subprogram's uniform [0,1] random number generator. Consequently, the RANL_NORMAL subprogram can obtain, for example, 12 uniform random numbers per subroutine call.

For parallel applications using the RANL_NORMAL subprogram, CXML provides two auxiliary, input subprograms that generate nonoverlapping streams of independent random numbers. See Section 13.5 for more information.

13.5 Input Subprograms for Parallel Applications Using RNG Subprograms

For parallel applications using either the RANL or the RANL_NORMAL subprograms, CXML provides two auxiliary, input subprograms - RANL_SKIP2 and RANL_SKIP64[1]. Both subprograms skip over a user specified number of seeds. The RANL_SKIP2 subprogram skips a number 2^d $(d{\geq}0)$ of seeds. The RANL_SKIP64 subprogram skips an arbitrary 64-bit number d $(d{\geq}0)$ of seeds. These subprograms provide a way to generate nonoverlapping streams of independent random numbers. Both subprograms use a well-known, repeated squaring algorithm for computing:

$$a^{2^k} s \quad mod\ m$$

This algorithm for finding the next seed skips over 2^k steps of the multiplicative algorithm:

$$s = as \quad mod\ m$$

The RANL_SKIP64 subprogram makes it convenient to generate nonoverlapping, random sequences. This is useful in parcelling out the same set of random numbers to different numbers of processors in a multiprocessor environment.

The RANL_SKIP64 subprogram is currently available only on Alpha platforms.

13.6 Summary of RNG Subprograms

Table 13–1 gives a description of each RNG subprogram.

Table 13–1 Summary of RNG Subprograms

Subprogram Name	Description
RANL	Generates a vector of uniform [0,1] random numbers.
RANL_SKIP2	Generates starting seeds for parallel, independent streams of random numbers. Auxiliary subprogram for parallel applications using RANL or RANL_NORMAL.
RANL_SKIP64[1]	Generates starting seeds for parallel, independent streams of random numbers by skipping forward a given number d of seeds. Auxiliary subprogram for parallel applications using RANL or RANL_NORMAL.
RANL_NORMAL	Generates a vector of N(0,1) normally distributed random numbers.
RAN69069	Generates single precision uniform [0,1] random numbers using $a = 69069$ in the linear multiplicative algorithm.
RAN16807	Generates single precision uniform [0,1] random numbers using $a = 16807$ in the "minimal standard" multiplicative generator.

[1]The RANL_SKIP64 subprogram is currently available on Alpha platforms only.

13.7 Error Handling

The RNG subprograms assume that input parameters are correct and provide no feedback when errors occur.

14
Using Sort Subprograms

This chapter provides information about CXML quick sort and general purpose sort subprograms.

- Quick Sort Subprograms (Section 14.1)
- General Purpose Sort (Section 14.2)
- Naming Conventions (Section 14.3)
- Summary of Sort Subprograms (Section 14.4)
- Error Handling (Section 14.5)
- Sort subprogram reference descriptions

14.1 Quick Sort Subprograms

The _SORTQ and _SORTQX subprograms use a quick sort algorithm to sort a vector of data. In the case of _SORTQX, the data vector is indexed. Both subprograms implement the quick sort algorithm by recursing until the partition size is less than 16. At that point, _SORTQ uses a simple replacement sort to sort the elements of the partition, while _SORTQX uses a modified insertion sort to sort the elements of the partition. Subprogram _SORTQX permutes only elements of the index vector, leaving the data vector unchanged.

14.2 General Purpose Sort Subprograms

The GEN_SORT subprogram is a general purpose, in memory, sort routine that uses a radix algorithm to sort the data. The GEN_SORTX subprogram is a general purpose, in memory, indexed sort routine that uses an indexed radix algorithm to sort the data.

14.3 Naming Conventions

Table 14–1 shows the characters used in the names of the quick sort subprograms and what the characters mean.

Table 14–1 Naming Conventions: _SORTQ_ Subprograms

Character Group	Mnemonic	Meaning
First group	I	Integer
	S	Single-precision real
	D	Double-precision real
Second group	SORTQ	Quick sort algorithm
Third group	X	Refers to indexed quick sort

For example, the name DSORTQX is the subprogram for performing an indexed quick sort on a vector of double-precision data.

14.4 Summary of Sort Subprograms

Table 14–2 gives a description of each sort subprogram.

Table 14–2 Summary of Sort Subprograms

Subprogram Name	Description
ISORTQ	Quick sorts the elements of a vector of integer data.
SSORTQ	Quick sorts the elements of a vector of single-precision data.
DSORTQ	Quick sorts the elements of a vector of double-precision data.
ISORTQX	Performs an indexed quick sort of a vector of integer data.
SSORTQX	Performs an indexed quick sort of a vector of single-precision data.
DSORTQX	Performs an indexed quick sort of a vector of double-precision data.
GEN_SORT	Performs a general purpose, in memory, sort routine.
GEN_SORTX	Performs a general purpose, in memory, sort of an indexed vector of data.

14.5 Error Handling

The sort subprograms assume that input parameters are correct and provide no feedback when errors occur.

15 Using Sciport

Sciport is a Cray SciLib compatibility interface library on CXML supplied by Compaq Computer Corporation. Sciport implements the functionality and user interface of many of the Cray **SciLib** routines by calling appropriate sequences of CXML routines. The primary function of the Sciport library is to aid in porting Cray applications to platforms supported by CXML. Sciport is not supported on the Windows NT platform. This section describes the SciLib functions that are supported in Sciport.

What Sciport Provides

Compaq Sciport provides the following:

- Cray compatible versions of SciLib *single-precision* BLAS-1, BLAS-2, and BLAS-3 routines
- Cray SciLib LAPACK single-precision routines
- Cray SciLib Special Linear System Solver routines
- Cray SciLib Signal Processing routines
- Cray SciLib Sorting and Searching routines
- CF77 intrinsic functions that are not directly supported by Compaq Fortran Compilers

These Compaq Sciport routines are compatible with their Cray SciLib counterparts and require no source code changes except as described in this documentation.

It is important to note that Sciport *is not* intended to be a complete implementation of Cray SciLib. Instead Sciport implements a very common subset of SciLib that is useful for porting most Cray applications. In particular, it should be noted that Sciport *does not* support any of the SciLib distributed memory routines. However, support for SMP (symmetric multiprocessing) is provided by linking Sciport with the parallel CXML.

15.1 How Data is Handled

The Cray Fortran compiler (CF77) treats `REAL`, `COMPLEX`, and `INTEGER` data as 64, 128, and 64 bit quantities, respectively. The Compaq Fortran compiler treats `REAL`, `COMPLEX`, and `INTEGER` data as 32, 64, and 32 bit quantities. To aid in porting applications, the Compaq Fortran compiler supports switches to override default behavior and automatically treat all `REAL`, `COMPLEX`, and `INTEGER` data as the 64, 128, and 64 bits, respectivvely. The Sciport library is intended to be used in conjunction with these compiler switches to port Cray applications with minimal source changes. Refer to the Compaq Fortran documentation for information about the use of these switches.

15.2 Compatibility and Restrictions

Since the primary objective of Sciport is to enable porting Cray applications to Compaq platforms, great care was taken in the development of Sciport to minimize compatibility issues. In many cases, Sciport routines provide bit-for-bit compatible results. For example, the Sciport version of RANF returns exactly the same sequence of random digits as its Cray SciLib counterpart.

Another important objective of Sciport is to allow ported applications to benefit from the performance enhancement provided by CXML, with minimal source code modification.

When these two objectives come into conflict with one another, the conflict is usually resolved in favor of compatibility. However, in a small number of cases, allowing small incompatibilites enables significant performance gains.

In some cases implementation differences between Cray and Compaq computer hardware and compilers do not allow all details of SciLib routines to be duplicated faithfully. However, the differences between Sciport and SciLib routines are generally minimal. The following sections provide information about any differences that may exist.

15.2.1 The Orders Routine

The `ORDERS` routine performs a radix sort on fixed-length records. In the Sciport version of `ORDER`, the arguments `RECORD` and `KEY` *are not* optional as they are in the SciLib version. Owing to differences in Cray and Compaq system endianness, care must be taken when sorting multi-byte character data. Because of endian considerations, the range of the key argument has been limited to the closed interval [1,8].

15.2.2 CF77 Intrinsic Functions

Many of these CF77 intrinsic functions return a CF77-specific data type of `BOOLEAN`. Since the non-ANSI FORTRAN-77 data type `BOOLEAN` is not supported by Compaq Fortran compilers, it is necessary for users to change the function return types from `BOOLEAN` to `INTEGER`.

15.2.3 BLAS and LAPACK Routines

In order to achieve source code compatibility with SciLib, Sciport single-precision and single-complex BLAS and LAPACK routines support 64-bit integers passed by reference. However, Sciport internally maps these routines onto their corresponding double-precision and double-complex CXML BLAS and LAPACK routines which use 32 bit integers. Consequently, some runtime uses of SciLib are not supported by Sciport. In practice, this does not appear to be a significant restriction.

Note

When necessary, Sciport automatically converts between 64 and 32 bit integers.

Additionally, since the single-precision Sciport BLAS and LAPACK routines have the same names as the single-precision CXML BLAS and LAPACK routines, applications that use Sciport cannot use the shared-library version of CXML. That is, applications that use Sciport must be linked "non-shared" with the Sciport and CXML libraries. In addition, the Sciport library must precede CXML

in the link command. Refer to the *Compiling and Linking Sciport* section for more information about how to link Sciport.

15.2.4 FFT Routines

The interface to the SciLib FFT routines requires that a work array of sufficient size be allocated and passed to the FFT routines. Users are free to write to this work array between calls to the SciLib FFT routines.

Some SciLib FFT routines additionally require that a table array be allocated and passed to the FFT routines. Users cannot write to this table array between FFT calls. It is assumed to be "read-only" after initialization.

For performance reasons, Sciport FFT routines are implemented as calls to CXML FFT routines. CXML FFT routines do not require a user-allocated work space. However they do require a small user-allocated data struture to record information from call-to-call in a thread-safe manner.

In order to preserve the SciLib interface, Sciport FFT routines overlay the table array (if it is present), or the user work array (if the table array is not present), with the CXML FFT data structure. This implementation has the following important side effects:

- Programs that use Sciport FFT routines without table arrays and write to the work array between FFT calls will overwrite the CXML FFT data structures. This can cause incorrect results, memory leaks, memory corruption and/or memory access violations.
- If the length of the FFT data structure is too small, the size of the table array and work array will be insufficient to overlay CXML data sturctures. In this case, users must make sure that the table array (or the work array) is at least 150 (64 bit) words long.
- The CXML FFT routines used to implement the Sciport FFT routines allocate working storage for the user. For a truly correct use of the Sciport FFT routines, users should explicitly free the memory allocated by CXML. Since the SciLib FFT routines require the user to allocate all of the work space, existing Cray applications do not free the allocated memory. In practice, this is generally not a problem because the memory is freed when the application exits.

  However, under certain conditions, it is necessary for users of the Sciport FFT routines to explicitly free the memory allocated by CXML. Specifically, if an application writes to the user-allocated work space between calls to the Sciport FFT routines, it is necessary to explicitly free CXML allocated memory. This is accomplished by calling the Sciport FFT routines with the `INIT` argument set to '80FF0FF0FF0FF0FF'X.

15.3 Compiling and Linking Sciport

As noted in the previous section, Sciport is used in conjuntion with CXML, and must be linked into an application statically. The typical approach is:

- Compile an application using the compiler flags that automatically promote `REAL` and `INTEGER` types to 64 bit quantities. The switches are `real_size 64` (or `-r8`), and `integer_size 64` (or `-i8`).
- Statically link in the Sciport and CXML libraries.

For example, on a UNIX platform this is accomplished with the following command:

```
f77 -o prog -r8 -i8 -double_size 128 prog.f -static -lsciport -lcxml
```

The same command also applies to Linux, except that the name of the Fortran driver is "fort".

On a VMS platform, linking can be accomplished by the following command:

```
LINK PROG, OBJ, SYS$LIBRARY:CXML$FGS_SCIPORT/LIB
```

Note: CXML must be linked in *after* Sciport.

On platforms that support parallel execution, users can link in the parallel CXML rather than the serial CXML.

15.4 Summary of Sciport Routines

The following set of SciLib routines are supported in Sciport. With the exception of BLAS and LAPACK routines, any SciLib routines not listed here are *not* supported in Sciport.

Table 15–1 Summary of CF77 Intrinsics

Routine Name	Operation
snglr	Returns closest real approximation to double precision.
gamma	Computes the natural log of the gamma function.
coss	Computes sine and cosine.
cot, dcot	Computes cotangent.
cbrt, dcbrt	Computes the cube root.
erf, erfc	Returns the value of the error function and the complimentary error function.
j0, j1, jn	Returns the value of the Bessel function of the first kind of orders 0, 1, and n.
y0, y1, yn	Returns the value of the Bessel function of the second kind of orders 0, 1, and n.
ranf, ranget, ranset	Computes pseudo-random numbers.
flmin, flmax	Return the minimum and maximum positive floating-point values, respectively.
ffrac	Returns the fractional accuracy of single precision floating point numbers.
inmax	Returns the maximum positive integer value.
and	Computes logical product.
or	Computes logical sum.
compl	Computes logical complement.
eqv	Computes logical equivalence.
xor, neqv	Computes logical difference.
shift	Performs a left circular shift.

(continued on next page)

Table 15–1 (Cont.) Summary of CF77 Intrinsics

Routine Name	Operation
shiftl	Performs a left shift with zero fill.
shiftr	Performs a right shift with zero fill.
dshiftr	Returns the lowermost 64 bits of a right-shifted 128 bit integer.
dshiftl	Returns the uppermost 64 bits of a left-shifted 128 bit integer.
mask	Returns a bit mask.
leadz	Counts number of leading zero bits.
popcnt	Counts number of bits set to 1.
poppar	Computes bit population parity.
cvmgp, cvmgn, cvmgt, cvmgz	Performs a conditional merge.
csmg	Performs a scalar boolean merge.

Table 15–2 Summary of BLAS Extensions

Routine Name	Operation
spaxpy	Adds a scalar multiple of a real vector to a sparse real vector.
saxpby, caxpby	Adds a scalar multiple of a real or complex vector to a scalar multiple of another real or complex vector.
spdot	Computes a sparse dot product of two real vectors.
scopy2	Copies a real or complex vector into another real or complex vector.
shad	Computes the Hadamard product of two vectors.
cgesum, sgesum	Adds a scalar multiple of a real or complex matrix to a scalar multiple of another real or complex matrix.
sspr12	Performs two simultaneous symmetric rank 1 updates of a real symmetric packed matrix.
sgemms, cgemms	Multiplies a real or complex general matrix by a real or complex general matrix using Strassen's algorithm.

Table 15–3 Summary of Signal Processing Routines

Routine Name	Operation
cfft	Applies a complex Fast Fourier Transform (FFT).
cfft2	Applies a complex Fast Fourier Transform (FFT).
cfft2d	Applies a two-dimensional complex Fast Fourier Transform (FFT).
cfft3d	Applies a three-dimensional complex Fast Fourier Transform (FFT).
cfftmlt	Applies complex-to-complex Fast Fourier Transforms (FFT) on multiple input vectors.
crfft2	Applies complex-to-real Fast Fourier Transforms (FFT).

(continued on next page)

Table 15–3 (Cont.) Summary of Signal Processing Routines

Routine Name	Operation
mcfft	Applies a multiple complex Fast Fourier Transform (FFT).
rcfft2	Applies real-to-complex Fast Fourier Transforms (FFT).
rfftmlt	Applies complex-to-real or real-to-complex Fast Fourier Transforms (FFT) on multiple input vectors.
fftfax	Initializes multi-dimensional real Fast Fourier Transforms (FFT).
cftfax	Initializes multi-dimensional complex Fast Fourier Transforms (FFT).
ccfft	Applies a complex-to-complex Fast Fourier Transform (FFT).
ccfft2d	Applies a two-dimensional complex-to-complex Fast Fourier Transform (FFT).
ccfft3d	Applies a three-dimensional complex-to-complex Fast Fourier Transform (FFT).
ccfftm	Applies multiple complex-to-complex Fast Fourier Transforms (FFTs).
csfft	Computes a real-to-complex or complex-to-real Fast Fourier Transform (FFT).
csfft2d	Applies a two-dimensional real-to-complex or complex-to-real Fast Fourier Transform (FFT).
csfft3d	Applies a three-dimensional real-to- complex Fast Fourier Transform (FFT).
csfftm	Applies multiple real-to-complex or complex-to-real Fast Fourier Transforms (FFTs).
scfft	Computes a real-to-complex or complex-to-real Fast Fourier Transform (FFT).
scfft2d	Applies a two-dimensional real-to-complex or complex-to-real Fast Fourier Transform (FFT).
scfft3d	Applies a three-dimensional real-to-complex Fast Fourier Transform (FFT).
scfftm	Applies multiple real-to-complex or complex-to-real Fast Fourier Transforms (FFTs).
ccnvl, ccnvlf	Computes the complex convolution of a sequence with one or more other sequences.
filterg	Computes a correlation of two vectors.
filters	Computes a correlation of two vectors (symmetric coefficient).
opfilt	Solves Weiner-Levinson linear equations.

Table 15–4 Summary of First and Second Order Recurrence Functions

Routine Name	Operation
folr, folrp	Solves first-order linear recurrences.
folrc	Solves first-order linear recurrences with a scalar coefficient.

(continued on next page)

Table 15–4 (Cont.) Summary of First and Second Order Recurrence Functions

Routine Name	Operation
folr2, folr2p	Solves first-order linear recurrences without overwriting the operand vector.
folrn, folrnp	Solves for the last term of a first-order linear recurrence.
solr	Solves a second-order linear recurrence.
solr3	Solves a second-order linear recurrence for three terms.
solrn	Solves a second-order linear recurrence for the last term only.
recpp, recps	Solves a partial products or partial summation problem.

Table 15–5 Summary of Tri-Diagonal Solvers

Routine Name	Operation
sdtsol	Solves a real valued tri-diagonal linear system with one right-hand side.
sdttrf	Factors a real valued tri-diagonal linear system.
sdttrs	Solves a real valued tri-diagonal linear system with one right-hand side, using the matrix factored by SDTTRF.
cdtsol	Solves a complex valued tri-diagonal linear system with one right-hand side.
cdttrf	Factors a complex valued tri-diagonal linear system.
cdttrs	Solves a complex valued tri-diagonal linear system with one right-hand side, using the matrix factored by CDTTRF.

Table 15–6 Summary of Sorting Routines

Routine Name	Operation
isortd, isortb	Sort an integer vector.
ssortb	Sort a real vector.
orders	Internal, fixed-length record-sorting routine optimized for Cray Research computer systems.

Table 15–7 Summary of Vector Scatter/Gather Routines

Routine Name	Operation
cluseq, clusne	Searches a vector for clusters of values equal or not equal to a target.
clusilt, clusile, clusigt, clusige	Searches an integer vector for clusters of values with a specified logical relationship to an integer target.
clusflt, clusfle, clusfgt, clusfge	Searches a real vector for clusters or values with a specified logical relationship to a real target.
isrcheq, isrchne	Searches a vector for the first element equal or not equal to a target.

(continued on next page)

Table 15–7 (Cont.) Summary of Vector Scatter/Gather Routines

Routine Name	Operation
isrchilt, isrchile, isrchigt, isrchige	Searches an integer vector for the first element with a specified logical relationship to an integer target.
isrchflt, isrchfle, isrchfgt, isrchfge	Searches a real vector for the first element with a specified logical relationship to a real target.
isrchmeq, isrchmne	Searches a vector for the first element whose subfield is equal or not equal to a target.
isrchmlt, isrchmle, isrchmgt, isrchmge	Searches a vector for the first element whose subfield has a specified logical relationship with a target.
wheneq, whenne	Searches a vector for the first element equal or not equal to a target.
whenilt, whenile, whenigt, whenige	Searches an integer vector for all elements with a specified relationship to an integer target.
whenflt, whenfle, whenfgt, whenfge	Searches a real vector for all elements with a specified logical relationship to a real target.
whenmeq, whenmne	Searches a vector for all elements whose subfields are equal or not equal to a target.
whenmlt, whenmle, whenmgt, whenmge	Searches a vector for all elements whose subfields have a specified logical relationship with a target.
inflmin, inflmax	Searches for the minimum or maximum value in subfields of a vector element.
intmin, intmax	Searches an integer vector for the maximum or minimum value.
iilz, illz, ilsum	Returns a number of leading occurrences of an object in a vector.
osrchf, osrchi	Searches an ordered vector for the first location that contains a target.
osrchm	Searches an ordered integer vector for the first element whose subfield is equal to an integer target.

Part 3—CXML Subprogram Reference

This section describes the individual subroutines and functions of CXML.

The following groups of subprograms are discussed:

- Level 1 BLAS Subprograms
- Level 1 BLAS Extensions Subprograms
- Sparse Level 1 BLAS Subprograms
- Level 2 BLAS Subprograms
- Level 3 BLAS Subroutines
- Fast Fourier
- Cosine and Sine
- Convolutions and Correlations
- Filters
- Sparse Iterative Solver Subprograms
- Direct Sparse Solver Subprograms
- VLIB Routines
- Random Number Generator Subprograms
- Sort Subprograms

Level 1 BLAS Subprograms

This section provides descriptions of the Level 1 BLAS subprograms, combining real and complex versions of the subprograms.

ISAMAX IDAMAX ICAMAX IZAMAX
Index of the Element of a Vector with Maximum Absolute Value

Format

I{S,D,C,Z}AMAX (n, x, incx)

Function Value

imax
integer*4
The index of the element of the vector x that is the largest in absolute value of all elements of the vector. If $n \leq 0$, **imax** returns the value 0.

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** ≥ 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
On exit, **incx** is unchanged.

Description

These functions determine the first integer i among the elements of the vector x such that:

$$|x_i| = \max \left\{ |x_j|, j = 1, 2, ..., n \right\}$$

You can use these functions to obtain the pivots in Gaussian elimination.

For complex vectors, each element of the vector is a complex number. In these subprograms, the absolute value of a complex number is defined as the absolute value of the real part plus the absolute value of the imaginary part:

$$|x_j| = |a_j| + |b_j| = |\text{real}| + |\text{imaginary}|$$

If $incx < 0$, the result depends on how the program is processed. See the coding information in this document for a discussion of the possible results. If $incx = 0$, the computation is a time-consuming way of setting $imax = 1$.

Example

```
INTEGER*4 IMAX, N, INCX, ISAMAX
REAL*4 X(40)
INCX = 2
N = 20
IMAX = ISAMAX(N,X,INCX)
```

This Fortran code shows how to compute the index of a real vector element with maximum absolute value.

SASUM DASUM SCASUM DZASUM
Sum of the Absolute Values

Format

{S,D}ASUM (n, x, incx)

SCASUM (n, x, incx)

DZASUM (n, x, incx)

Function Value

sum
real*4 | real*8 | complex*8 | complex*16
The sum of the absolute values of the elements of the vector x.
If $n \leq 0$, **sum** returns the value 0.0.

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** ≥ 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
On exit, **incx** is unchanged.

Description

The SASUM and DASUM functions compute the sum of the absolute values of the elements of a real vector x:

$$\sum_{i=1}^{n} |x_i| = |x_1| + |x_2| + \ldots + |x_n|$$

SCASUM and DZASUM compute the sum of the absolute values of the real and imaginary parts of the elements of a complex vector x:

$$\sum_{i=1}^{n} (|a_i| + |b_i|) = (|a_1| + |b_1|) + (|a_2| + |b_2|) + \ldots + (|a_n| + |b_n|)$$

where $x_i = (a_i, b_i)$ and $|x_i| = |a_i| + |b_i| = |\mathrm{real}| + |\mathrm{imaginary}|$

If $incx < 0$, the result is identical to using $|incx|$. If $incx = 0$, the computation is a time-consuming way of setting $\mathrm{sum} = nx_1$.

Because of the efficient coding of these routines, rounding errors can cause the final result to differ from the result computed by a sequential evaluation of the sum of the elements of the vector.

Example

```
INTEGER*4 N, INCX
REAL*4 X(20), SUM, SASUM
INCX = 1
N = 20
SUM = SASUM(N,X,INCX)
```

This Fortran code shows how to compute the sum of the absolute values of the elements of the vector x.

SAXPY DAXPY CAXPY ZAXPY
Vector Plus the Product of a Scalar and a Vector

Format

{S,D,C,Z}AXPY (n, alpha, x, incx, y, incy)

Arguments

n
integer*4
On entry, the number of elements in the vectors x and y.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar multiplier α for the elements of the vector x.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** ≥ 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
On exit, **incx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$, containing the elements of the vector y.

On exit, if $n \leq 0$ or $\alpha = 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; y_i is replaced by $y_i + \alpha x_i$.

incy
integer*4
On entry, the increment for the array Y.
If **incy** > 0, vector y is stored forward in the array, so that y_i is stored in location $Y(1 + (i - 1) * incy)$.
If **incy** < 0, vector y is stored backward in the array, so that y_i is stored in location $Y(1 + (n - i) * |incy|)$.
On exit, **incy** is unchanged.

Description

The _AXPY functions compute the following scalar-vector product and sum:

$$y \leftarrow \alpha x + y$$

where α is a scalar, and x and y are vectors.

If any element of x or the scalar α share a memory location with an element of y, the results are unpredictable.

If $incx = 0$, the computation is a time-consuming way of adding the constant αx_1 to all the elements of y. The following chart shows the operation that results from the interaction of the values for arguments **incx** and **incy**:

	incx = 0	incx $\neq$ 0
incy = 0	$y_1 = y_1 + n\alpha x_1$	$y_1 = y_1 + \sum_{i=1}^{n} \alpha x_i$
incy $\neq$ 0	$y_i = y_i + \alpha x_1$	$y_i = y_i + \alpha x_i$

Example

```
INTEGER*4 N, INCX, INCY
REAL*4 X(20), Y(20), ALPHA
INCX = 1
INCY = 1
ALPHA = 2.0
N = 20
CALL SAXPY(N,ALPHA,X,INCX,Y,INCY)
```

This Fortran code shows how all elements of the real vector x are multiplied by 2.0, added to the elements of the real vector y, and the vector y is set equal to the result.

SCOPY DCOPY CCOPY ZCOPY
Copy of a Vector

Format

{S,D,C,Z}COPY (n, x, incx, y, incy)

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** ≥ 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
On exit, **incx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$.
On exit, if $n \leq 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; y_i is replaced by x_i.

incy
integer*4
On entry, the increment for the array Y.
If **incy** ≥ 0, vector y is stored forward in the array, so that y_i is stored in location $Y(1 + (i - 1) * incy)$.
If **incy** < 0, vector y is stored backward in the array, so that y_i is stored in location $Y(1 + (n - i) * |incy|)$.

On exit, **incy** is unchanged.

Description

The _COPY subprograms copy the elements of the vector x to the vector y, performing the following operation:

$$y_i \leftarrow x_i$$

If $incx = 0$, each y_i is set to x_1. Therefore, you can use $incx = 0$ to initialize all elements to a constant.

If $incy = 0$, the computation is a time-consuming way of setting $y_1 = x_n$, the last referenced element of the vector x.

If $incy = -incx$, the vector x is stored in reverse order in y. In this case, the call format is as follows:

```
CALL SCOPY (N,X,INCX,Y,-INCX)
```

If any element of x shares a memory location with an element of y, the results are unpredictable, except for the following special case. It is possible to move the contents of a vector up or down within itself and not cause unpredictable results even though the same memory location is shared between input and output. To do this when $i > j$, call the subroutine with $incx = incy > 0$ as follows:

```
CALL SCOPY (N,X(I),INCX,X(J),INCX)
```

The call to SCOPY moves elements of the array X $x(i), x(i + 1 * incx), ..., x(i + (n - 1) * incx)$ to new elements of the array X $x(j), x(j + 1 * incx), ..., x(j + (n - 1) * incx)$. If $i < j$, specify a negative value for $incx$ and $incy$ in the call to the subroutine, as follows. The parts that do not overlap are unchanged.

```
CALL SCOPY (N,X(I),-INCX,X(J),-INCX)
```

Examples

1.
```
INTEGER*4 N, INCX, INCY
REAL*4 X(20), Y(20)
INCX = 1
INCY = 1
N = 20
CALL SCOPY(N,X,INCX,Y,INCY)
```

   The preceding Fortran code copies a vector x to a vector y.

2.
```
CALL SCOPY(N,X,-2,X(3),-2))
```

   The preceding call moves the contents of X(1),X(3),X(5), . . . , X(2N-1) to X(3),X(5), . . . , X(2N+1) and leaves the vector x unchanged.

3.
```
CALL SCOPY(99,X(2),1,X,1))
```

   The preceding call moves the contents of X(2),X(3), . . . , X(100) to X(1),X(2), . . . , X(99) and leaves x_{100} unchanged.

4.
```
CALL SCOPY(N,X,1,Y,-1))
```

   The preceding call moves the contents of X(1),X(2),X(3), . . . , X(N) to Y(N),Y(N-1), . . . , Y.

SDOT DDOT DSDOT CDOTC ZDOTC CDOTU ZDOTU Inner Product of Two Vectors

Format

{S,D}DOT (n, x, incx, y, incy)

DSDOT (n, x, incx, y, incy)

{C,Z}DOT{C,U} (n, x, incx, y, incy)

Function Value

dotpr
real*4 | real*8 | complex*8 | complex*16
The dot product of the two vectors x and y.

For real vectors, if $n \leq 0$, **dotpr** returns the value 0.0.
For complex vectors, if $n \leq 0$, **dotpr** returns (0.0, 0.0).

Arguments

n
integer*4
On entry, the number of elements in the vectors x and y.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** $\geq$ 0, vector x is stored forward in the array, so that x_i is stored in location X$(1 + (i - 1) * incx)$.
If **incx** $<$ 0, vector x is stored backward in the array, so that x_i is stored in location X$(1 + (n - i) * |incx|)$.
On exit, **incx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector y.
On exit, **y** is unchanged.

incy
integer*4
On entry, the increment for the array Y.
If **incy** $\geq$ 0, vector y is stored forward in the array, so that y_i is stored in location Y$(1 + (i - 1) * incy)$.
If **incy** $<$ 0, vector y is stored backward in the array, so that y_i is stored in location Y$(1 + (n - i) * |incy|)$.
On exit, **incy** is unchanged.

Description

SDOT, DDOT, and DSDOT compute the dot product of two real vectors. CDOTC and ZDOTC compute the conjugated dot product of two complex vectors. CDOTU and ZDOTU compute the unconjugated dot product of two complex vectors.

SDOT, DDOT, DSDOT are functions that compute the dot product of two n-element real vectors, x and y:

$$x \cdot y = \sum_{i=1}^{n} x_i y_i = x_1 y_1 + x_2 y_2 + \ldots + x_n y_n$$

The order of operations is different from the order in a sequential evaluation of the dot product. The final result can differ from the result of a sequential evaluation. The DSDOT function accepts single-precision input vectors but uses double-precision operations to compute a double-precision result.

CDOTC and ZDOTC are functions that compute the conjugated dot product of two complex vectors, x and y, that is, the complex conjugate of the first vector is used to compute the dot product.

Each element x_j of the vector x is a complex number and each element y_j of the vector y is a complex number. The conjugated dot product of two complex vectors, x and y, is expressed as follows:

$$\overline{x} \cdot y = \sum_{i=1}^{n} \overline{x}_i y_i = \overline{x}_1 y_1 + \overline{x}_2 y_2 + \ldots + \overline{x}_n y_n$$

For example, x and y each have two complex elements:

$$x = (1 + i, 2 - i), y = (3 + i, 3 + 2i)$$

The conjugate of vector x is $\overline{x} = (1 - i, 2 + i)$, and the dot product is:

$$\overline{x} \cdot y = (1 - i)(3 + i) + (2 + i)(3 + 2i) = (4 - 2i) + (4 + 7i) = (8 + 5i)$$

CDOTU and ZDOTU compute the unconjugated dot product of two complex vectors. The unconjugated dot product of two complex vectors, x and y, is expressed as follows:

$$x \cdot y = \sum_{i=1}^{n} x_i y_i = x_1 y_1 + x_2 y_2 + \ldots + x_n y_n$$

For example, for the same complex vectors x and y:

$$x \cdot y = (1 + i)(2 + i) + (2 - i)(3 + 2i) = (1 + 3i) + (8 + i) = 9 + 4i$$

Example

```
INTEGER*4 INCX, INCY
REAL*4 X(20), Y(20), DOTPR, SDOT
INCX = 1
INCY = 1
N = 20
DOTPR = SDOT(N,X,INCX,Y,INCY)
```

This Fortran code shows how to compute the dot product of two vectors, x and y, and return the result in **dotpr**.

```
INTEGER*4 INCX, INCY
COMPLEX*8 X(20), Y(20), DOTPR, CDOTU
INCX = 1
INCY = 1
N = 20
DOTPR = CDOTU(N,X,INCX,Y,INCY)
```

This Fortran code shows how to compute the unconjugated dot product of two complex vectors, x and y, and return the result in dotpr.

SDSDOT
Product of Scaled Vector and Vector

Format

SDSDOT (n, alpha, x, incx, y, incy)

Function Value

dotpr
real*4
The sum of the scalar **alpha** and the dot product of vectors x and y.

If $n \leq 0$, **dotpr** returns the value in **alpha**.

Arguments

n
integer*4
On entry, the number of elements in the vectors x and y.
On exit, **n** is unchanged.

alpha
real*4 | real*8
On entry, a scalar addend summed with the dot product of vectors x and y.
On exit, **alpha** is unchanged.

x
real*4 | real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** ≥ 0, vector x is stored forward in the array, so that x_i is stored in location X$(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location X$(1 + (n - i) * |incx|)$.
On exit, **incx** is unchanged.

y
real*4 | real*8
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector y.
On exit, **y** is unchanged.

incy
integer*4
On entry, the increment for the array Y.
If **incy** ≥ 0, vector y is stored forward in the array, so that y_i is stored in location Y$(1 + (i - 1) * incy)$.
If **incy** < 0, vector y is stored backward in the array, so that y_i is stored in location Y$(1 + (n - i) * |incy|)$.
On exit, **incy** is unchanged.

Description

SDSDOT computes the dot product of two single-precision real vectors, x and y, using double-precision arithmetic. The resulting dot product is added to the single-precision scalar value **alpha** to produce the single precision return value.

Example

```
INTEGER*4 INCX,INCY
REAL*8 X(20),Y(20),ALPHA
REAL*4 DOTPR,SDSDOT
INCX = 1
INCY = 1
ALPHA = 0.4
N = 20
DOTPR = SDSDOT(N,ALPHA,X,INCX,Y,INCY)
```

SNRM2 DNRM2 SCNRM2 DZNRM2
Square Root of Sum of the Squares of the Elements of a Vector

Format

{S,D}NRM2 (n, x, incx)

SCNRM2 (n, x, incx)

DZNRM2 (n, x, incx)

Function Value

e_norm
real*4 | real*8
The Euclidean norm of the vector x, that is, the square root of the conjugated dot product of x with itself.

If $n \leq 0$, **e_norm** returns the value 0.0.

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** ≥ 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
On exit, **incx** is unchanged.

Description

SNRM2 and DNRM2 compute the Euclidean norm of a real vector; SCNRM2 and DZNRM2 compute the Euclidean norm of a complex vector. The Euclidean norm is the square root of the conjugated dot product of a vector with itself.

For real vectors:

$$\sqrt{\sum_{i=1}^{n} x_i^2} = \sqrt{x_1^2 + x_2^2 + \ldots + x_n^2}$$

For complex vectors:

$$\sqrt{\sum_{i=1}^{n} \overline{x}_i * x_i} = \sqrt{(\overline{x}_1 * x_1) + (\overline{x}_2 * x_2) + \ldots + (\overline{x}_n * x_n)}$$

The order of operations is different from the order in a sequential evaluation of the Euclidean norm. The final result can differ from the result of a sequential evaluation.

If $incx < 0$, the result is identical to using $|incx|$. If $incx = 0$, the computation is a time-consuming way of setting $\mathrm{e_norm} = \sqrt{n x_1^2}$.

Example

```
INTEGER*4 INCX, N
REAL*4 X(20), E_NORM
INCX = 1
N = 20
E_NORM = SNRM2(N,X,INCX)
```

This Fortran code shows how to compute the Euclidean norm of a real vector.

SROT DROT CROT ZROT CSROT ZDROT
Apply Givens Plane Rotation

Format

{S,D,C,Z}ROT (n, x, incx, y, incy, c, s)

CSROT (n, x, incx, y, incy, c, s)

ZDROT (n, x, incx, y, incy, c, s)

Arguments

n
integer*4
On entry, the number of elements in the vectors x and y.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, if $n \leq 0$ or if **c** is 1.0 and **s** is 0.0, **x** is unchanged. Otherwise, **x** is overwritten; X contains the rotated vector x.

incx
integer*4
On entry, the increment for the array X.
If **incx** ≥ 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
On exit, **incx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$. Y contains the n elements of the vector y.

On exit, if $n \leq 0$ or if **c** is 1.0 and **s** is 0.0, **y** is unchanged. Otherwise, **y** is overwritten; Y contains the rotated vector y.

incy
integer*4
On entry, the increment for the array Y.
If **incy** ≥ 0, vector y is stored forward in the array, so that y_i is stored in location $Y(1 + (i - 1) * incy)$.

If **incy** < 0, vector y is stored backward in the array, so that y_i is stored in location $\mathrm{Y}(1 + (n - i) * |incy|)$.
On exit, **incy** is unchanged.

c
real*4 | real*8
On entry, the first rotation element, that is, the cosine of the angle of rotation. The argument **c** is the first rotation element generated by the _ROTG subroutines.
On exit, **c** is unchanged.

s
real*4 | real*8 | complex*8 | complex*16
On entry, the second rotation element, that is, the sine of the angle of rotation. The argument **s** is the second rotation element generated by the _ROTG subroutines.
On exit, **s** is unchanged.

Description

SROT and DROT apply a real Givens plane rotation to each element in the pair of real vectors, x and y. CSROT and ZDROT apply a real Givens plane rotation to elements in the complex vectors, x and y. CROT and ZROT apply a complex Givens plane rotation to each element in the pair of complex vectors x and y.

The cosine and sine of the angle of rotation are c and s, respectively, and are provided by the BLAS Level 1 _ROTG subroutines.

The Givens plane rotation for SROT, DROT, CSROT, and ZDROT follows:

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} \leftarrow \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix}$$

The elements of the rotated vector x are $x_i \leftarrow cx_i + sy_i$.
The elements of the rotated vector y are $y_i \leftarrow -sx_i + cy_i$.

The Givens plane rotation for CROT and ZROT follows:

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} \leftarrow \begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix}$$

The elements of the rotated vector x are $x_i \leftarrow cx_i + sy_i$.
The elements of the rotated vector y are $y_i \leftarrow -\bar{s}x_i + cy_i$.

If $n \le 0$ or if $c = 1.0$ and $s = 0.0$, x and y are unchanged. If any element of x shares a memory location with an element of y, the results are unpredictable.

These subroutines can be used to introduce zeros selectively into a matrix.

Example

```
INTEGER*4 INCX, N
REAL X(20,20), A, B, C, S
INCX = 20
N = 20
A = X(1,1)
B = X(2,1)
CALL SROTG(A,B,C,S)
CALL SROT(N,X,INCX,X(2,1),INCX,C,S)
```

This Fortran code shows how to rotate the first two rows of a matrix and zero out the element in the first column of the second row.

SROTG DROTG CROTG ZROTG
Generate Elements for a Givens Plane Rotation

Format

{S,D,C.Z}ROTG (a, b, c, s)

Arguments

a
real*4 | real*8 | complex*8 | complex*16
On entry, the first element of the input vector.
On exit, **a** is overwritten with the rotated element r.

b
real*4 | real*8 | complex*8 | complex*16
On entry, the second element of the input vector. On exit, for SROTG and DROTG, **b** is overwritten with the reconstruction element z. For CROTG and ZROTG, **b** is unchanged.

c
real*4 | real*8
On entry, an unspecified variable.
On exit, **c** is overwritten with the first rotation element, that is, the cosine of the angle of rotation.

s
real*4 | real*8 | complex*8 | complex*16
On entry, an unspecified variable.
On exit, **s** is overwritten with the second rotation element, that is, the sine of the angle of rotation.

Description

The _ROTG subroutines construct a Givens plane rotation that eliminates the second element of a two-element vector and can be used to introduce zeros selectively into a matrix.

Using a and b to represent elements of an input real vector, the SROTG and DROTG functions calculate the elements c and s of an orthogonal matrix such that:

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix} * \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

Using a and b to represent elements of an input complex vector, the CROTG and ZROTG functions calculate the elements real c and complex s of an orthogonal matrix such that:

$$\begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix} * \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

A real Givens plane rotation is constructed for values a and b by computing values for r, c, s, and z, as follows:

$r = p\sqrt{a^2 + b^2}$

$p = \mathrm{SIGN}(a)$ if $|a| > |b|$
$p = \mathrm{SIGN}(b)$ if $|a| \leq |b|$

$c = \frac{a}{r}$ if r is not equal to 0
$c = 1$ if $r = 0$

$s = \frac{b}{r}$ if r is not equal to 0
$s = 0$ if $r = 0$

$z = s$ if $|a| > |b|$
$z = \frac{1}{c}$ if $|a| \leq |b|$, c is not equal to 0, and r is not equal to 0.
$z = 1$ if $|a| \leq |b|$, $c = 0$, and r is not equal to 0.
$z = 0$ if $r = 0$

SROTG and DROTG can use the reconstruction element z to store the rotation elements for future use. The quantities c and s are reconstructed from z as follows:

For $|z| = 1, c = 0.0 \text{ and } s = 1.0$

For $|z| < 1$, $c = \sqrt{1 - z^2}$ and $s = z$

For $|z| > 1, c = \frac{1}{z}$ and $s = \sqrt{1 - c^2}$

A complex Givens plane rotation is constructed for values a and b by computing values for real c, complex s and complex r, as follows:

$p = \sqrt{|a|^2 + |b|^2}$
$q = \frac{a}{|a|}$

$r = qp$ if $|a|$ is not equal to 0.
$r = b$ if $|a|$ is equal to 0.

$c = \frac{|a|}{p}$ if $|a|$ is not equal to 0.
$c = 0$ if $|a|$ is equal to 0.

$s = \frac{q\bar{b}}{p}$ if $|a|$ is not equal to 0.
$s = (1.0, 0.0)$ if $|a|$ is equal to 0.

The absolute value used in the previous definitions corresponds to the strict definition of the absolute value of a complex number.

The arguments **c** and **s** are passed to the _ROT subroutines.

Example

```
REAL*4 A, B, C, S
CALL SROTG(A,B,C,S)
```

This Fortran code shows how to generate the rotation elements for a vector of elements a and b.

SROTM DROTM
Apply Modified Givens Transformation

Format

{S,D}ROTM (n, x, incx, y, incy, param)

Arguments

n
integer*4
On entry, the number of elements in the vectors x and y.
On exit, **n** is unchanged.

x
real*4 | real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, if $n \leq 0$ or if PARAM(1) = (-2.0), **x** is unchanged. Otherwise, **x** is overwritten; X contains the rotated vector x.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location X$(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location X$(1 + (n - i) * |incx|)$.
On exit, **incx** is unchanged.

y
real*4 | real*8
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$. Y contains the n elements of the vector y.

On exit, if $n \leq 0$ or if PARAM(1) = (-2.0), **y** is unchanged. Otherwise, **y** is overwritten; Y contains the rotated vector y.

incy
integer*4
On entry, the increment for the array Y.
If **incy** > 0, vector y is stored forward in the array, so that y_i is stored in location Y$(1 + (i - 1) * incy)$.
If **incy** < 0, vector y is stored backward in the array, so that y_i is stored in location Y$(1 + (n - i) * |incy|)$.
On exit, **incy** is unchanged.

param
real*4 | real*8
On entry, an array defining the type of transform matrix H used:

PARAM(1) specifies the flag characteristic: -1.0, 0.0, 1.0, -2.0
PARAM(2) specifies H_{11} value
PARAM(3) specifies H_{21} value
PARAM(4) specifies H_{12} value
PARAM(5) specifies H_{22} value

On exit, **param** is unchanged.

Description

SROTM and DROTM apply a modified Givens transform to each element in the pair of real vectors, x and y, using the transformation matrix H as follows:

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} = H * \begin{bmatrix} x_i \\ y_i \end{bmatrix}$$

Depending on the value of PARAM(1), the transformation matrix H is defined as follows:

- PARAM(1)= -1.0

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

- PARAM(1)= 0.0

$$\begin{pmatrix} 1.0 & H_{12} \\ H_{21} & 1.0 \end{pmatrix}$$

- PARAM(1)= 1.0

$$\begin{pmatrix} H_{11} & 1.0 \\ -1.0 & H_{22} \end{pmatrix}$$

- PARAM(1)= -2.0

$$\begin{pmatrix} 1.0 & 0.0 \\ 0.0 & 1.0 \end{pmatrix}$$

The array PARAM is generated by a call to the routine _ROTMG.

Results are unpredictable if either **incx** or **incy** are zero.

Example

```
      INTEGER*4 INCA, N
      REAL A(10,10), D(10), SPARAM(5)
C
      INCA = 10
C
C INITIALIZE D TO 1.0
C
      DO I = 1, 10
         D(I) = 1.0
      END DO
C
C FOR EACH ROW OF THE MATRIX, ELIMINATE TO UPPER TRIANGULAR FORM
C
      DO I = 2, 10
C
C ELIMINATE A(I,J) USING ELEMENT A(J,J)
C
         JEND = I-1
         DO J = 1, JEND
            N = 10-J
            CALL SROTMG(D(J),D(I),A(J,J),A(I,J),SPARAM)
            CALL SROTM(N,A(J,J+1),INCA,A(I,J+1),INCA,SPARAM)
         ENDDO
C
      END DO
C
C APPLY ACCUMULATED SCALE FACTORS TO THE ROWS OF A
C
      DO I = 1, 10
         CALL SSCAL(11-I, SQRT(D(I)), A(I,I), INCA)
      END DO
```

This Fortran code shows how to reduce a 10 by 10 matrix to upper triangular form using the routine SROTMG and SROTM.

SROTMG DROTMG
Generate Elements for a Modified Givens Transform

Format

{S,D}ROTMG (d1, d2, x1, y1, param)

Arguments

d1
real*4 | real*8
On entry, the first scale factor for the modified Givens transform.
On exit, **d1** is updated.

d2
real*4 | real*8
On entry, the second scale factor for the modified Givens transform.
On exit, **d2** is updated.

x1
real*4 | real*8
On entry, the first element x_1 of the input vector.
On exit, **x1** is overwritten with the rotated element.

y1
real*4 | real*8
On entry, the second element y_1 of the input vector.
On exit, **y1** is unchanged.

param
real*4 | real*8
On entry, **param** is unspecified.
On exit, **param** contains an array defining the transform matrix H as follows:

PARAM(1) specifies the flag characteristic: -1.0, 0.0, 1.0, -2.0
PARAM(2) specifies H_{11} value
PARAM(3) specifies H_{21} value
PARAM(4) specifies H_{12} value
PARAM(5) specifies H_{22} value

Description

The _ROTMG subroutines construct a modified Givens transform that eliminates the second element of a two-element vector and can be used to introduce zeros selectively into a matrix. These routines use the modification due to Gentleman of the Givens plane rotations. This modification eliminates the square root from the construction of the plane rotation and reduces the operation count when the modified Givens rotation, rather than the standard Givens rotations are applied. In most applications, the scale factors d_1 and d_2 are initially set to 1 and then modified by _ROTMG as necessary.

Given real a and b in factored form:

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} d_1^{\frac{1}{2}} & 0 \\ 0 & d_2^{\frac{1}{2}} \end{bmatrix} * \begin{bmatrix} x_1 \\ y_1 \end{bmatrix}$$

SROTMG and DROTMG construct the modified Givens plane rotation, $\overline{d_1}$, $\overline{d_2}$ and

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}$$

such that

$$\begin{bmatrix} \overline{d}_1^{\frac{1}{2}} & 0 \\ 0 & \overline{d}_2^{\frac{1}{2}} \end{bmatrix} * H * \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = G * \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

where G is a 2 by 2 Givens plane rotation matrix which annihilates b, and where H is chosen for numerical stability and computational efficiency.

The routine _ROTM applies the matrix H, as constructed by _ROTMG, to a pair of real vectors, x and y, each with n elements, as follows:

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} = H * \begin{bmatrix} x_i \\ y_i \end{bmatrix}$$

These vectors may be either rows or columns of matrices and the indexing of the vectors may be either forwards or backwards.

Depending on the value of IPARAM(1), the matrix H is defined as follows:

- PARAM(1)= -1.0

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

- PARAM(1)= 0.0

$$\begin{pmatrix} 1.0 & H_{12} \\ H_{21} & 1.0 \end{pmatrix}$$

- PARAM(1)= 1.0

$$\begin{pmatrix} H_{11} & 1.0 \\ -1.0 & H_{22} \end{pmatrix}$$

- PARAM(1)= -2.0

$$\begin{pmatrix} 1.0 & 0.0 \\ 0.0 & 1.0 \end{pmatrix}$$

Note

The routines _ROTMG and _ROTM perform similar tasks to the routines _ROTG and _ROT, which construct and apply the standard Givens plane rotations. The modified Givens rotations reduce the operation count of constructing and applying the rotations at the cost of increased storage to represent the rotations.

Example

See the example for SROTM.

SSCAL DSCAL CSCAL ZSCAL, CSSCAL ZDSCAL Product of a Scalar and a Vector

Format

{S,D,C,Z}SCAL (n, alpha, x, incx)

CSSCAL (n, alpha, x, incx)

ZDSCAL (n, alpha, x, incx)

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar value used to multiply the elements of vector x.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, if $n \leq 0$ or $\alpha = 1.0$, then **x** is unchanged. Otherwise, **x** is overwritten; x_i is replaced by αx_i.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element in the array is scaled.
On exit, **incx** is unchanged.

Description

These routines perform the following operation:

$$x \leftarrow \alpha x$$

SSCAL and DSCAL scale the elements of a real vector by computing the product of the vector and a real scalar αx. CSCAL and ZSCAL scale the elements of a complex vector by computing the product of the vector and a complex scalar α. CSSCAL and ZDCAL scale the elements of a complex vector by computing the product of the vector and a real scalar α.

If $n \leq 0$ or α = 1.0, x is unchanged.

If $incx < 0$, the result is identical to using $|incx|$.

If α = 0.0 or (0.0, 0.0), the computation is a time-consuming way of setting all elements of the vector x equal to zero. Use the BLAS Level 1 Extensions subroutines _SET to set all the elements of a vector to a scalar.

The _SCAL routines are similar to the BLAS Level 1 Extensions subroutines _VCAL routines, but the _VCAL routines use an output vector different from the input vector.

Example

```
INTEGER*4 INCX, N
COMPLEX*8 X(20), ALPHA
INCX = 1
ALPHA = (2.0, 1.0)
N = 20
CALL CSCAL(N,ALPHA,X,INCX)
```

This Fortran code shows how to scale a complex vector x by the complex scalar (2.0, 1.0).

SSWAP DSWAP CSWAP ZSWAP
Exchange the Elements of Two Vectors

Format

{S,D,C,Z}SWAP (n, x, incx, y, incy)

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, if $n \leq 0$, **x** is unchanged. If $n > 0$, **x** is overwritten; the elements in the array X that are the vector x are overwritten by the vector y.

incx
integer*4
On entry, the increment for the array X.
If **incx** ≥ 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
On exit, **incx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$.

On exit, if $n \leq 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; the elements in the array Y that are the vector y are overwritten by the vector x.

incy
integer*4
On entry, the increment for the array Y.
If **incy** ≥ 0, vector y is stored forward in the array, so that y_i is stored in location $Y(1 + (i - 1) * incy)$.
If **incy** < 0, vector y is stored backward in the array, so that y_i is stored in location $Y(1 + (n - i) * |incy|)$.
On exit, **incy** is unchanged.

Description

These subroutines swap n elements of the vector x with n elements of vector y:

$$x \leftrightarrow y$$

If any element of x shares a memory location with an element of y, the results are unpredictable.

If $n \leq 0$, x and y are unchanged.

You can use these subroutines to invert the storage of elements of a vector within itself. If $incx > 0$, each element x_i is moved from location $X(1 + (i - 1) * incx)$ to location $X(1 + (n - i) * incx)$. The following code fragment inverts the storage of elements of a vector within itself:

```
NN = N/2
LHALF = 1+(N-NN)*INCX
CALL SSWAP(NN,X,INCX,X(LHALF),-INCX)
```

Example

```
INTEGER*4 INCX, INCY, N
REAL*4 X(20), Y(20)
INCX = 1
INCY = 1
N = 20
CALL SSWAP(N,X,INCX,Y,INCY)
```

The preceding Fortran code swaps the contents of vectors x and y.

```
INCX = 1
INCY = -1
N = 50
CALL SSWAP(N,X,INCX,X(51),INCY)
```

The preceding Fortran code inverts the order of storage of the elements of x within itself; that is, it moves $x_1, \ldots, x_{100}$ to $x_{100}, \ldots, x_1$.

Level 1 BLAS Extensions Subprograms

This section provides descriptions of the Level 1 BLAS Extensions subprograms, combining real and complex versions of the subprograms.

ISAMIN IDAMIN ICAMIN IZAMIN
Index of the Element of a Vector with Minimum Absolute Value

Format

I{S,D,C,Z}AMIN (n, x, incx)

Function Value

imin
integer*4

The index of the first element of the vector x such that $X(1 + (imin - 1) * |incx|)$ is the smallest in absolute value of all elements of the vector. If $n \leq 0$, **imin** returns the value 0.

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

These subprograms compute the index of the element of a vector having the minimum absolute value. They determine the first integer i of the vector x such that:

$$|x_i| = \min \left\{ |x_j|, j = 1, 2, ..., n \right\}$$

For complex vectors, each element x_j is a complex number. In this subprogram, the absolute value of a complex number is defined as the absolute value of the real part of the complex number plus the absolute value of the imaginary part of the complex number:

$$|x_j| = |a_j| + |b_j| = |\mathrm{real}| + |\mathrm{imaginary}|$$

If $incx = 0$, the computation is a time-consuming way of setting $imin = 1$.

Example

```
INTEGER*4 N, INCX, IMIN, ISAMIN
REAL*4 X(40)
INCX = 2
N = 20
IMIN = ISAMIN(N,X,INCX)
```

This Fortran example shows how to compute the index of the vector element with minimum absolute value.

ISMAX IDMAX
Index of the Real Vector Element with Maximum Value

Format

I{S,D}MAX (n, x, incx)

Function Value

imax
integer*4

The index of the first element of the real vector x such that
$X(1 + (imax - 1) * |incx|)$ is the largest of all elements of the vector.
If $n \leq 0$, **imax** returns the value 0.

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the real vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

ISMAX and IDMAX determine the first integer i of vector x such that:

$$x_i = \max \left\{ x_j, j = 1, 2, ..., n \right\}$$

If $incx = 0$, the computation is a time-consuming way of setting $imax$ = 1.

Example

```
INTEGER*4 N, INCX, IMAX, ISMAX
REAL*4 X(40)
INCX = 2
N = 20
IMAX = ISMAX(N,X,INCX)
```

This Fortran example shows how to compute the index of the vector element with maximum value.

ISMIN IDMIN
Index of the Real Vector Element with Minimum Value

Format

I{S,D}MIN (n, x, incx)

Function Value

imin
integer*4

The index of the first element of the real vector x such that $X(1 + (imin - 1) * |incx|)$ is the smallest of all elements in the vector. If $n \leq 0$, **imin** returns the value 0.

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the real vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

ISMIN and IDMIN determine the first integer i such that:

$$x_i = \min\left\{x_j, j = 1, 2, ..., n\right\}$$

If $incx = 0$, the computation is a time-consuming way of setting $imin = 1$.

Example

```
INTEGER*4 N, INCX, IMIN, ISMIN
REAL*4 X(40)
INCX = 2
N = 20
IMIN = ISMIN(N,X,INCX)
```

This Fortran example shows how to compute the index of the vector element with minimum value.

SAMAX DAMAX SCAMAX DZAMAX
Maximum Absolute Value

Format

{S,D}AMAX (n, x, incx)

SCAMAX (n, x, incx)

DZAMAX (n, x, incx)

Function Value

amax
real*4 | real*8
The element of the vector with the largest absolute value. If $n \leq 0$, **amax** returns the value 0.0.

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.

If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

These functions determine the largest absolute value of the elements of a vector:

$$\max\left\{|x_j|, j = 1, 2, ..., n\right\}$$

For complex vectors, each element is a complex number. In this subprogram, the absolute value of a complex number is defined as the absolute value of the real part of the complex number plus the absolute value of the imaginary part of the complex number:

$$|x_j| = |a_j| + |b_j| = |\text{real}| + |\text{imaginary}|$$

If $incx < 0$, the result is identical to using $|incx|$. If $incx = 0$, the computation is a time-consuming way of setting $amax = |x_1|$.

Example

```
REAL*4 SCAMAX, AMAX
INTEGER*4 N, INCX
COMPLEX*8 X(40)
INCX = 2
N = 20
AMAX = SCAMAX(N,X,INCX)
```

This Fortran example shows how to compute the element with the largest absolute value.

SAMIN DAMIN SCAMIN DZAMIN
Minimum Absolute Value

Format

{S,D}AMIN   (n, x, incx)

SCAMIN   (n, x, incx)

DZAMIN   (n, x, incx)

Function Value

amin
real*4 | real*8
The element of the vector x with the smallest absolute value.
If $n \leq 0$, **amin** = 0.

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

These functions determine the smallest absolute value of the elements of a vector x:

$$\max \left\{ |x_j|, j = 1, 2, ..., n \right\}$$

For complex vectors, each element x_j is a complex number. In this subprogram, the absolute value of a complex number is defined as the absolute value of the real part of the complex number plus the absolute value of the imaginary part of the complex number:

$$|x_j| = |a_j| + |b_j| = |\text{real}| + |\text{imaginary}|$$

If $incx < 0$, the result is identical to using $|incx|$. If $incx = 0$, the computation is a time-consuming way of setting $amin = |x_1|$.

Example

```
INTEGER*4 N, INCX
REAL*4 X(400), AMIN, SAMIN
INCX = 3
N = 100
AMIN = SAMIN(N,X,INCX)
```

These Fortran examples show how to compute the element with the smallest absolute value.

SMAX DMAX
Largest Element in a Real Vector

Format

{S,D}MAX (n, x, incx)

Function Value

wmax
real*4 | real*8
The largest value among the elements of the real vector x.

If $n \leq 0$, **wmax** = 0.

Arguments

n
integer*4
On entry, the number of elements in real vector x.
On exit, **n** is unchanged.

x
real*4 | real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of real vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location X$(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location X$(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

SMAX and DMAX are functions that determine the largest value among the real elements of a vector x:

$$\max \left\{ x_j, j = 1, 2, ..., n \right\}$$

If $incx < 0$, the result is identical to using $|incx|$. If $incx = 0$, the computation is a time-consuming way of setting $wmax = x_1$.

Example

```
INTEGER*4 N, INCX
REAL*4 X(40), WMAX, SMAX
INCX = 2
N = 20
WMAX = SMAX(N,X,INCX)
```

This Fortran example shows how to compute the largest value of the elements of a vector x.

SMIN DMIN
Minimum Value of the Elements of a Real Vector

Format

{S,D}MIN (n, x, incx)

Function Value

wmin
real*4 | real*8
The smallest value of the elements of the real vector x.
If $n \leq 0$, **wmin** = 0.

Arguments

n
integer*4
On entry, the number of elements n in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$. X contains the n elements of the real vector x.

On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

SMIN and DMIN are functions that determine the smallest value of the elements of a vector x:

$$\min \{x_j, j = 1, 2, ..., n\}$$

If $incx < 0$, the result is identical to using $|incx|$. If $incx = 0$, the computation is a time-consuming way of setting $wmin = x_1$.

Example

```
INTEGER*4 N, INCX
REAL*4 X(40), WMIN, SMIN
INCX = 1
N = 30
WMIN = SMIN(N,X,INCX)
```

This Fortran example shows how to compute the smallest value of the elements of a vector x.

SNORM2 DNORM2 SCNORM2 DZNORM2
Square Root of Sum of the Squares of the Elements of a Vector

Format

{S,D}NORM2 (n, x, incx)

SCNORM2 (n, x, incx)

DZNORM2 (n, x, incx)

Function Value

sum
real*4 | real*8 | complex*8 | complex*16
The Euclidean norm of the vector x, that is, the square root of the sum of the squares of the elements of a real vector or the square root of the sum of the squares of the absolute value of the elements of the complex vector. If $n \leq 0$, **sum** = 0.0.

Arguments

n
integer*4
On entry, the number of elements of the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

SNORM2 and DNORM2 compute the Euclidean norm of a real vector x. The Euclidean norm is the square root of the sum of the squares of the elements of the vector:

$$\sqrt{\sum_{i=1}^{n} x_i^2}$$

SCNORM2 and DZNORM2 compute the square root of the sum of the squares of the absolute value of the elements of a complex vector x:

$$\sqrt{\sum_{i=1}^{n} |x_i|^2}$$

For complex vectors, each element x_j is a complex number. In this subprogram, the absolute value of a complex number is defined as the square root of the sum of the squares of the real part and the imaginary part:

$$|x_j| = \sqrt{a_j^2 + b_j^2} = \sqrt{\text{real}^2 + \text{imaginary}^2}$$

If $incx < 0$, the result is identical to using $|incx|$. If $incx = 0$, the computation is a time-consuming way of setting $\text{sum} = \sqrt{nx_1^2}$ for real operations, and $\text{sum} = |x_i|\sqrt{n}$ for complex operations.

Because of efficient coding, rounding errors can cause the final result to differ from the result computed by a sequential evaluation of the Euclidean norm.

Unlike the _NRM2 and _ _NRM2 subprograms in BLAS Level 1, the _NORM2 and _ _NORM2 subprograms do not perform any special scaling to ensure that intermediate results do not overflow or underflow. Therefore, these routines must use an input vector x so that:

$$|\sqrt{min}| \leq |x_i| \leq |\sqrt{max}|$$

The largest value of x must not overflow when it is squared; the smallest value must not underflow when it is squared.

Example

```
INTEGER*4 N, INCX
REAL*4 X(20), SUM, SNORM2
INCX = 1
N = 20
SUM = SNORM2(N,X,INCX)
```

This Fortran example shows how to compute the Euclidean norm of the vector x.

SNRSQ DNRSQ SCNRSQ DZNRSQ
Sum of the Squares of the Elements of a Vector

Format

{S,D}NRSQ (n, x, incx)

SCNRSQ (n, x, incx)

DZNRSQ (n, x, incx)

Function Value

sum
real*4 | real*8
The sum of the squares of the elements of the real vector x.
The sum of the squares of the absolute value of the elements of the complex vector x.

If $n \leq 0$, **sum** returns the value 0.0.

Arguments

n
integer*4
On entry, the number of elements of the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

SNRSQ and DNRSQ compute the sum of squares of the elements of a real vector. SCNRSQ and DZNRSQ compute the sum of squares of the absolute value of the elements of a complex vector.

SNRSQ and DNRSQ compute the total value of the square roots of each element in the real vector x:

$$\sum_{j=1}^{n} x_j^2$$

SCNRSQ and DZNRSQ compute the total value of the square roots of each element in the complex vector x, using the absolute value of each element:

$$\sum_{j=1}^{n} |x_j|^2$$

For complex vectors, each element x_j is a complex number. In this subprogram, the absolute value of a complex number is defined as the square root of the sum of the square of the real part and the square of the imaginary part:

$$|x_j| = \sqrt{a_j^2 + b_j^2} = \sqrt{\text{real}^2 + \text{imaginary}^2}$$

If $incx < 0$, the result is identical to using $|incx|$. If $incx = 0$, the computation is a time-consuming way of setting $\text{sum} = nx_1^2$.

Because of efficient coding, rounding errors can cause the final result to differ from the result computed by a sequential evaluation of the sum of the squares of the elements of the vector. Use these functions to obtain the square of the Euclidean norm instead of squaring the result obtained from the Level 1 routines SNRM2 and DNRM2. The computation is more accurate.

Example

```
INTEGER*4 N, INCX
REAL*4 X(20), SUM, SNRSQ
INCX = 1
N = 20
SUM = SNRSQ(N,X,INCX)
```

This Fortran example shows how to compute the sum of the squares of the elements of the vector x.

SSET DSET CSET ZSET
Set All Elements of a Vector to a Scalar

Format

{S,D,C,Z}SET (n, alpha, x, incx)

Arguments

n
integer*4
On entry, the number of elements in the vector.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α value.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.

On exit, if $n \leq 0$, **x** is unchanged. If $n > 0$, **x** is overwritten by the updated x.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

The _SET subroutines change all elements of a vector to the same scalar value; each element x_i is replaced with α.

$$x_i \leftarrow \alpha$$

If $incx < 0$, the result is identical to using $|incx|$. If $incx = 0$, the computation is a time-consuming way of setting $x_1 = \alpha$.

Example

```
INTEGER*4 N, INCX
REAL*4 X(200), ALPHA
INCX = 2
ALPHA = 2.0
N = 50
CALL SSET(N,ALPHA,X,INCX)
```

This Fortran example shows how to set all elements of the vector x equal to 2.0.

SSUM DSUM CSUM ZSUM
Sum of the Values of the Elements of a Vector

Format

{S,D,C,Z}SUM (n, x, incx)

Function Value

sum
real*4 | real*8 | complex*8 | complex*16
The total of the values of the elements in the vector x. If $n \leq 0$, **sum** returns the value 0.0.

Arguments

n
integer*4
On entry, the number of elements in the vector x.
On exit, **n** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the n elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

Description

The _SUM subprograms compute the total value of the elements of a vector, performing the following operation:

$$\sum_{i=1}^{n} x_i$$

Because of efficient coding, rounding errors can cause the final result to differ from the result computed by a sequential evaluation of the sum of the elements of the vector.

If $incx < 0$, the result is identical to using $|incx|$. If $incx = 0$, the computation is a time-consuming way of setting $\mathrm{sum} = nx_1$.

Example

```
INTEGER*4 N, INCX
REAL*4 X(200), SUM, SSUM
INCX = 2
N = 50
SUM = SSUM(N,X,INCX)
```

This Fortran example shows how to compute the sum of the values of the elements of the vector x.

SVCAL DVCAL CVCAL ZVCAL CSVCAL, ZDVCAL Product of a Scalar and a Vector

Format

{S,D,C,Z}VCAL (n, alpha, x, incx, y, incy)

CSVCAL (n, alpha, x, incx, y, incy)

ZDVCAL (n, alpha, x, incx, y, incy)

Arguments

n
integer*4
On entry, the number of elements of the vector x.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar multiplier α.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$.
On exit, if $n \leq 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; each element y_i is replaced by αx_i.

incy
integer*4
On entry, the increment for the array Y.
If **incy** ≥ 0, vector y is stored forward in the array, so that y_i is stored in location $Y(1 + (i - 1) * incy)$
If **incy** < 0, vector y is stored backward in the array, so that y_i is stored in location $Y(1 + (n - i) * |incy|)$.
On exit, **incy** is unchanged.

Description

SVCAL and DVCAL compute the product of a real scalar and a real vector, in single or double precision. CVCAL and ZVCAL compute the product of a complex scalar and a complex vector, in single or double precision. CSVCAL and ZDVCAL compute the product of a real scalar and a complex vector in single or double precision.

These subprograms multiply each element of a vector by a scalar value, returning the result in vector y:

$$y \leftarrow \alpha x$$

If $incy = 0$, the result is unpredictable. If $incx = 0$, each element in y is equal to $\alpha X(1)$.

If α = 0, the computation is a time-consuming way of setting all elements of the vector y equal to zero. Use the _SET routines to perform that operation.

EXAMPLES

1.
```
INTEGER*4 N, INCX, INCY
REAL*4 X(20), Y(40), ALPHA
INCX = 1
INCY = 2
ALPHA = 2.0
N = 20
CALL SVCAL(N,ALPHA,X,INCX,Y,INCY)
```

This Fortran example shows how to scale a vector x by 2.0. Vector y is set equal to the result.

2.
```
INTEGER*4 N, INCX, INCY
COMPLEX*8 X(20), Y(40), ALPHA
INCX = 1
INCY = 2
ALPHA = (5.0, 1.0)
N = 20
CALL CVCAL(N,ALPHA,X,INCX,Y,INCY)
```

This Fortran example shows how to scale a vector x by the complex number (5.0,1.0). Vector y is set equal to the result.

SZAXPY DZAXPY CZAXPY ZZAXPY
Vector Plus the Product of a Scalar and a Vector

Format

{S,D,C,Z}ZAXPY (n, alpha, x, incx, y, incy, z, incz)

Arguments

n
integer*4
On entry, the number of elements of the vectors x and y.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar value to be multiplied with the elements of vector x.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the n elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
If **incx** > 0, vector x is stored forward in the array, so that x_i is stored in location $X(1 + (i - 1) * incx)$.
If **incx** < 0, vector x is stored backward in the array, so that x_i is stored in location $X(1 + (n - i) * |incx|)$.
If **incx** = 0, only the first element is accessed.
On exit, **incx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$, containing the n elements of the vector y.
On exit, **y** is unchanged.

incy
integer*4
On entry, the increment for the array Y.

If **incy** ≥ 0, vector y is stored forward in the array, so that y_i is stored in location $Y(1 + (i - 1) * incy)$.
If **incy** < 0, vector y is stored backward in the array, so that y_i is stored in location $Y(1 + (n - i) * |incy|)$.
On exit, **incy** is unchanged.

z
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Z of length at least $(1 + (n - 1) * |incz|)$.
On exit, if $n \leq 0$, then **z** is unchanged. If $n > 0$, **z** is overwritten with the products; each z_i is replaced by $y_i + \alpha x_i$.

incz
integer*4
On entry, the increment for the array Z.
If **incz** ≥ 0, vector z is stored forward in the array, so that z_i is stored in location $Z(1 + (i - 1) * incz)$.
If **incz** < 0, vector z is stored backward in the array, so that z_i is stored in location $Z(1 + (n - i) * |incz|)$.
On exit, **incz** is unchanged.

Description

The _ZAXPY subprograms compute the product of a scalar and a vector, add the result to the elements of another vector, and then store the result in vector z:

$$z \leftarrow \alpha x + y$$

where α is a scalar, and x, y, and z are vectors with n elements.

The scalar α must not share a memory location with any element of the vector z. If $incz = 0$ or if any element of z shares a memory location with an element of x or y, the results are unpredictable.

If $incx = 0$, the computation is a time-consuming way of adding the constant αx_1 to all the elements of y. The following chart shows the resulting operation from the interaction of the **incx** and **incy** arguments:

	incx = 0	incx $\neq$ 0
incy = 0	$z_i = y_1 + \alpha x_1$	$z_i = y_1 + \alpha x_i$
incy $\neq$ 0	$z_i = y_i + \alpha x_1$	$z_i = y_i + \alpha x_i$

Example

```
INTEGER*4 N, INCX, INCY, INCZ
REAL*4 X(20), Y(20), Z(40), ALPHA
INCX = 1
INCY = 1
INCZ = 2
ALPHA = 2.0
N = 20
CALL SZAXPY(N,ALPHA,X,INCX,Y,INCY,Z,INCZ)
```

This Fortran example shows how all elements of the vector x are multiplied by 2.0 and added to the elements of vector y. Vector z contains the result.

Sparse Level 1 BLAS Subprograms

This section provides descriptions of the Sparse Level 1 BLAS subprograms.

SAXPYI DAXPYI CAXPYI ZAXPYI
Vector Plus the Product of a Scalar and a Sparse Vector

Format

{S,D,C,Z}AXPYI (nz, alpha, x, indx, y)

Arguments

nz
integer*4
On entry, the number of elements in the vector in the compressed form.
On exit, **nz** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar multiplier for the elements of vector x.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector x in compressed form.
On exit, **x** is unchanged.

indx
integer*4
On entry, an array containing the indices of the compressed form. The values in the INDX array must be distinct for consistent vector or parallel execution.
On exit, **indx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector y stored in full form.
On exit, if $nz \leq 0$ or if α = 0, **y** is unchanged. If $nz > 0$, the elements in the vector y corresponding to the indices in the INDX array are overwritten.

Description

The _AXPYI subprograms compute the product of a scalar α and a sparse vector x stored in compressed form. The product is then added to a vector y, and the result is stored as vector y in full form. Only the elements of vector y whose indices are listed in INDX are updated. For $i = 1, ..., nz$:

$$y(indx(i)) \longleftarrow y(indx(i)) + \alpha * x(i)$$

If $nz \leq 0$ or $\alpha = 0.0$, y is unchanged. SAXPYI and DAXPYI compute the product of a real scalar and a real sparse vector stored in compressed form, and add the product to a real vector in full form. CAXPYI and ZAXPYI compute the product of a complex scalar and a complex sparse vector stored in compressed form, and add the product to a complex vector stored in full form.

Example

```
INTEGER NZ, INDX(10)
REAL*4 Y(40), X(10), ALPHA
NZ = 10
ALPHA = 2.0
CALL SAXPYI(NZ, ALPHA, X, INDX, Y)
```

This Fortran code shows how the nz elements in y, corresponding to the indices in the INDX array, are updated by the addition of a scalar multiple of the corresponding element of the compressed vector, x.

SDOTI DDOTI CDOTUI ZDOTUI CDOTCI ZDOTCI
Inner Product of a Vector and a Sparse Vector

Format

{S,D}DOTI (nz, x, indx, y)

{C,Z}DOT{U,C}I (nz, x, indx, y)

Function Value

dotpr
real*4 | real*8 | complex*8 | complex*16
The inner product of the sparse vector x and the full vector y.

Arguments

nz
integer*4
On entry, the number of elements in the vector in the compressed form.
On exit, **nz** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector x in compressed form.
On exit, **x** is unchanged.

indx
integer*4
On entry, an array containing the indices of the compressed form.
On exit, **indx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector y stored in full form.
On exit, **y** is unchanged. Only the elements in the vector y corresponding to the indices in the INDX array are accessed.

Description

These routines compute the vector inner product of a sparse vector x stored in compressed form with a vector y stored in full form. If $nz \leq 0$, **dotpr** is set equal to zero.

SDOTI and DDOTI multiply a real vector by a sparse vector of real values stored in compressed form. CDOTUI and ZDOTUI multiply a complex vector by an unconjugated sparse vector of complex values stored in compressed form. CDOTCI and ZDOTCI multiply a complex vector by a conjugated sparse vector of complex values stored in compressed form.

As shown in (Reference–1) and (Reference–2), CDOTUI and ZDOTUI operate on the vector x in the unconjugated form; CDOTCI and ZDOTCI operate on the vector x in conjugated form.

Unconjugated form:

$$dotpr = \sum_{i=1}^{nz} x(i) * y(indx(i)) \qquad \text{(Reference–1)}$$

Conjugated form:

$$dotpr = \sum_{i=1}^{nz} \overline{x}(i) * y(indx(i)) \qquad \text{(Reference–2)}$$

The order of operations for the evaluation of $dotpr$ may be different fom the sequential order of operations. The results obtained from these two evaluations may not be identical.

Example

```
INTEGER NZ, INDX(15)
COMPLEX*8 Y(50), X(15)
NZ = 10
CINNER = CDOTUI(NZ, X, INDX, Y)
```

This Fortran code produces the inner product of two vectors, x and y. Vector y is stored in full form and vector x is stored in compressed form. The elements of vector x are used in unconjugated form.

SGTHR DGTHR CGTHR ZGTHR
Gathers the Specified Elements of a Vector

Format

{S,D,C,Z}GTHR (nz, y, x, indx)

Arguments

nz
integer*4
On entry, the number of elements to be gathered into the compressed form.
On exit, **nz** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector y stored in full form.
On exit, **y** is unchanged. Only the elements in the vector y corresponding to the indices in the INDX array are accessed.

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array that receives the specified elements of the vector y.
On exit, if $nz \leq 0$, **x** is unchanged. If $nz > 0$, array X contains the values gathered into compressed form.

indx
integer*4
On entry, an array containing the indices of the values to be gathered into compressed form.
On exit, **indx** is unchanged.

Description

The _GTHR subprograms gather specified elements from a vector in full form, y, and store them as a vector x in compressed form. For $i = 1, ..., nz$:

$$x(i) \longleftarrow y(indx(i))$$

If $nz \leq 0$, x is unchanged.

SGTHR and DGTHR gather the specified elements from a real vector in full form and store them as a real sparse vector in compressed form. CGTHR and ZGTHR gather the specified elements from a complex vector in full form and store them as a complex sparse vector in compressed form.

Example

```
INTEGER NZ, INDX(10)
REAL*4 Y(40), X(10)
NZ = 10
CALL SGTHR(NZ, Y, X, INDX)
```

This Fortran code shows how the nz elements of the vector y, corresponding to the indices in the INDX array, are gathered in a compressed form into the vector x.

SGTHRS DGTHRS CGTHRS ZGTHRS
Gathers and Scales the Specified Elements of a Vector

Format

{S,D,C,Z}GTHRS (nz, alpha, y, x, indx)

Arguments

nz
integer*4
On entry, the number of elements to be gathered into the compressed form.
On exit, **nz** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar multiplier for the elements of vector y.
On exit, **alpha** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector y stored in full form.
On exit, **y** is unchanged. Only the elements in the vector y corresponding to the indices in the INDX array are accessed.

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array that receives the specified elements of vector y after scaling.
On exit, if $nz \leq 0$, **x** is unchanged. If $nz > 0$, the array X contains the specified elements of vector y after scaling by the scalar, α.

indx
integer*4
On entry, an array containing the indices of the values to be gathered into compressed form.
On exit, **indx** is unchanged.

Description

The _GTHRS subprograms gather specified elements of vector y in full form, multiply the elements by α, and store the result as elements of a sparse vector x in compressed form. For $i = 1, ..., nz$:

$$x(i) \longleftarrow \alpha * y(indx(i))$$

If $nz \leq 0$, x is unchanged.

SGTHRS and DGTHRS gather the elements from a real vector in full storage and scale them into a real vector in compressed storage. CGTHRS and ZGTHRS gather the specified elements from a complex vector in full storage and scale them into a complex vector in compressed storage.

The _GTHRS subprograms are not part of the original set of Sparse BLAS Level 1 subprograms.

Example

```
INTEGER NZ, INDX(10)
REAL*8 Y(40), X(10), ALPHA
NZ = 10
ALPHA = 1.5D0
CALL DGTHRS(NZ, ALPHA, Y, X, INDX)
```

This Fortran code shows how the nz elements of the vector y, corresponding to the indices in the INDX array, are scaled by the scalar **alpha** and gathered in a compressed form into the vector x.

SGTHRZ DGTHRZ CGTHRZ ZGTHRZ
Gathers and Zeros Specified Elements of a Vector

Format

{S,D,C,Z}GTHRZ (nz, y, x, indx)

Arguments

nz
integer*4
On entry, the number of elements to be gathered into the compressed form.
On exit, **nz** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector y stored in full form.
On exit, if $nz \leq 0$, **y** is unchanged. If $nz > 0$, the gathered elements in Y are set to zero. Only the elements in the vector y corresponding to the indices in the INDX array are overwritten.

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array that receives the specified elements of vector y.
On exit, if $nz \leq 0$ **x** is unchanged. If $nz > 0$, the array X contains the values gathered into compressed form.

indx
integer*4
On entry, an array containing the indices of the values to be gathered into compressed form. The values in INDX must be distinct for consistent vector or parallel execution.
On exit, **indx** is unchanged.

Description

The _GTHRZ subprograms gather the specified elements from a vector y stored in full form into a sparse vector x in compressed form. Those elements in y are then set to zero. For $i = 1, ..., nz$:

$$x(i) \longleftarrow y(indx(i))$$

$$y(indx(i)) \longleftarrow 0.0$$

If $nz \leq 0$, both x and y are unchanged. SGTHRZ and DGTHRZ gather the specified elements of a real vector in full form into a real sparse vector in compressed form. CGTHRZ and ZGTHRZ gather the specified elements of a complex vector in full form into a complex sparse vector in compressed form. In each case, the specified elements of the full vector are set equal to zero.

Example

```
INTEGER NZ, INDX(10)
REAL*4 Y(40), X(10)
NZ = 10
CALL SGTHRZ(NZ, Y, X, INDX)
```

This Fortran code shows how the nz elements of the vector y, corresponding to the indices in the INDX array, are gathered in a compressed form into the vector x. The gathered elements in y are set equal to zero.

SROTI DROTI
Real Givens Plane Rotation Applied to Sparse Vector

Format

{S,D}ROTI (nz, x, indx, y, c, s)

Arguments

nz
integer*4
On entry, the number of elements in the vector in the compressed form.
On exit, **nz** is unchanged.

x
real*4 | real*8
On entry, an array of the elements of vector x in compressed form.
On exit, if $nz \leq 0$, **x** is unchanged. If $nz > 0$, the array X is updated.

indx
integer*4
On entry, an array containing the indices of the compressed form. The values in INDX must be distinct for consistent vector or parallel execution.
On exit, **indx** is unchanged.

y
real*4 | real*8
On entry, an array of the elements of vector y stored in full form.
On exit, if $nz \leq 0$, **y** is unchanged. If $nz > 0$, the elements in the vector y corresponding to the indices in the INDX array are overwritten.

c
real*4 | real*8
On entry, **c** is the first rotation element, which can be interpreted as the cosine of the angle of rotation.
On exit, **c** is unchanged.

s
real*4 | real*8
On entry, **s** is the second rotation element, which can be interpreted as the sine of the angle of rotation.
On exit, **s** is unchanged.

Description

The _ROTI routines apply a real Givens rotation to a sparse vector x stored in compressed form and another vector y stored in full form. For $i = 1, ..., nz$:

$$temp \longleftarrow -s * x(i) + c * y(indx(i))$$

$$x(i) \longleftarrow c * x(i) + s * y(indx(i))$$

$$y(indx(i)) \longleftarrow temp$$

If $nz \leq 0$, x and y are unchanged. Only the elements of y whose indices are listed in INDX are referenced or modified.

The output vectors x and y have nonzero elements in the locations where either input vector x or y had nonzero elements. Because the _ROTI subprograms do not handle this fill-in, the arrays X and INDX must take this into account on input. This means that all nonzero elements of y must be listed in the array INDX, resulting in an INDX array containing the indices of all nonzero elements of both vectors x and y.

Example

```
INTEGER NZ, INDX(10)
REAL*8 Y(40), X(10), C, S
NZ = 10
CALL DROTI(NZ, X, INDX, Y, C, S)
```

This Fortran code shows how to apply a Givens rotation to a sparse vector x, stored in compressed form, and another vector y, stored in full form.

SSCTR DSCTR CSCTR ZSCTR
Scatters the Elements of a Sparse Vector

Format

{S,D,C,Z}SCTR (nz, x, indx, y)

Arguments

nz
integer*4
On entry, the number of elements to be scattered from the compressed form.
On exit, **nz** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector x to be scattered from compressed form into full form.
On exit, **x** is unchanged.

indx
integer*4
On entry, an array containing the indices of the values to be scattered from the compressed form. The values in the INDX array must be distinct for consistent vector or parallel execution.
On exit, **indx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array that receives the elements of vector x.
On exit, if $nz \leq 0$, **y** is unchanged. If $nz > 0$, the elements in the vector y corresponding to the indices in the INDX array are set to the corresponding elements in vector x.

Description

The _SCTR routines scatter the elements stored in the sparse vector x in compressed form into the specified elements of the vector y in full form. For $i = 1, ..., nz$:

$$y(indx(i)) \longleftarrow x(i)$$

If $nz \leq 0$, y is unchanged. SSCTR and DSCTR scatter the elements of a real sparse vector stored in compressed form into the specified elements of a real vector in full form. CSCTR and ZSCTR scatter the elements of a complex sparse vector stored in compressed form into the specified elements of a complex vector in full form.

Example

```
INTEGER NZ, INDX(10)
REAL*4 Y(40), X(10)
NZ = 10
CALL SSCTR(NZ, X, INDX, Y)
```

This Fortran code scatters the elements of a sparse vector x, stored in compressed form, into the specified elements of the vector y, stored in full form.

SSCTRS DSCTRS CSCTRS ZSCTRS
Scales and Scatters the Elements of a Sparse Vector

Format

{S,D,C,Z}SCTRS (nz, alpha, x, indx, y)

Arguments

nz
integer*4
On entry, the number of elements to be scattered from the compressed form.
On exit, **nz** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar multiplier for the elements of vector x.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector x to be scattered from compressed form into full form.
On exit, **x** is unchanged.

indx
integer*4
On entry, an array containing the indices of the values to be scattered from the compressed form. The values in INDX must be distinct for consistent vector or parallel execution.
On exit, **indx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array that receives the scaled elements of the vector x.
On exit, if $nz \leq 0$, **y** is unchanged. If $nz > 0$, the elements in the vector y corresponding to the indices in the INDX array are set to the corresponding scaled entries of x.

Description

The _SCTRS subprograms multiply the elements of a sparse vector x stored in compressed form by a scalar α and then scatter them into the specified elements of the vector y stored in full form. For $i = 1, ..., nz$:

$$y(indx(i)) \longleftarrow \alpha * x(i)$$

If $nz \leq 0$, y is unchanged.

SSCTRS and DSCTRS scatter the elements of a real sparse vector stored in compressed form, after scaling, into the specified elements of a real vector stored in full form. CSCTRS and ZSCTRS scatter the elements of a complex sparse vector stored in compressed form, after scaling, into the specified elements of a complex vector stored in full form.

The _SCTRS subprograms are not part of the original set of Sparse BLAS Level 1 subprograms.

Example

```
INTEGER NZ, INDX(10)
REAL*8 Y(40), X(10), ALPHA
NZ = 10
ALPHA = 2.5D0
CALL DSCTRS(NZ, ALPHA, X, INDX, Y)
```

This Fortran code scales the elements of a sparse vector x, stored in compressed form, by the scalar **alpha**, and then scatters them into the specified elements of the vector y, stored in full form.

SSUMI DSUMI CSUMI ZSUMI
Sum of a Vector and a Sparse Vector

Format

{S,D,C,Z}SUMI (nz, x, indx, y)

Arguments

nz
integer*4
On entry, the number of elements in the vector in the compressed form.
On exit, **nz** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector x in compressed form.
On exit, **x** is unchanged.

indx
integer*4
On entry, an array containing the indices of the compressed form. The values in the INDX array must be distinct for consistent vector or parallel execution.
On exit, **indx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array of the elements of vector y stored in full form.
On exit, if $nz \leq 0$, **y** is unchanged. If $nz > 0$, the elements in the vector y corresponding to the indices in the INDX array are overwritten.

Description

SSUMI and DSUMI add a sparse vector of real values stored in compressed form to a real vector stored in full form. CSUMI and ZSUMI add a sparse vector of complex values stored in compressed form to a complex vector stored in full form.

Only the elements of vector y whose indices are listed in array INDX are overwritten. For $i = 1, ..., nz$:

$$y(indx(i)) \longleftarrow y(indx(i)) + x(i)$$

If $nz \leq 0$, y is unchanged. The _SUMI subprograms are an efficient implementation of the _AXPYI subprograms when α = 1.0.

The _SUMI subprograms are not part of the original set of Sparse BLAS Level 1 subprograms.

Example

```
INTEGER NZ, INDX(20)
REAL*8 Y(100), X(20)
NZ = 20
CALL DSUMI(NZ, X, INDX, Y)
```

This Fortran code shows how the nz elements in y, corresponding to the indices in the array INDX, are updated by the addition of the corresponding element of the compressed vector, x.

Level 2 BLAS Subprograms

This section provides descriptions of the Level 2 BLAS subroutines for real and complex operations.

SGBMV DGBMV CGBMV ZGBMV
Matrix-Vector Product for a General Band Matrix

Format

{S,D,C,Z}GBMV (trans, m, n, kl, ku, alpha, a, lda, x, incx, beta, y, incy)

Arguments

trans
character*1
On entry, specifies the operation to be performed:

If **trans** = 'N' or 'n', the operation is $y \leftarrow \alpha Ax + \beta y$.
If **trans** = 'T' or 't', the operation is $y \leftarrow \alpha A^T x + \beta y$.
If **trans** = 'C' or 'c', the operation is $y \leftarrow \alpha A^H x + \beta y$.

On exit, **trans** is unchanged.

m
integer*4
On entry, the number of rows of the matrix A; $m \geq 0$.
On exit, **m** is unchanged.

n
integer*4
On entry, the number of columns of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

kl
integer*4
On entry, the number of sub-diagonals of the matrix A; $kl \geq 0$.
On exit, **kl** is unchanged.

ku
integer*4
On entry, the number of super-diagonals of the matrix A; $ku \geq 0$.
On exit, **ku** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n. The leading m by n part of the array contains the elements of the matrix A, supplied column by column. The leading diagonal of the matrix is stored in row $(ku + 1)$ of the array, the first super-diagonal is stored in row ku starting at position 2, the first sub-diagonal is stored in row $(ku + 2)$ starting at position 1, and so on. Elements in the array A that do not correspond to elements in the matrix (such as the top left ku by ku triangle) are not referenced.
On exit, **a** is unchanged.

lda

integer*4
On entry, the first dimension of array A; $lda \geq (kl + ku + 1)$.
On exit, **lda** is unchanged.

x

real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array containing the vector x. When **trans** is equal to 'N' or 'n', the length of the array is at least $(1 + (n - 1) * |incx|)$. Otherwise, the length is at least $(1 + (m - 1) * |incx|)$.
On exit, **x** is unchanged.

incx

integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

beta

real*4 | real*8 | complex*8 | complex*16
On entry, the scalar β.
On exit, **beta** is unchanged.

y

real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array containing the vector y. When **trans** is equal to 'N' or 'n', the length of the array is at least $(1 + (m - 1) * |incy|)$. Otherwise, the length is at least $(1 + (n - 1) * |incy|)$.

If $\beta = 0$, **y** need not be set. If β is not equal to zero, the incremented array Y must contain the vector y.
On exit, **y** is overwritten by the updated vector y.

incy

integer*4
On entry, the increment for the elements of Y; $incy$ must not equal zero.
On exit, **incy** is unchanged.

Description

The _GBMV subprograms compute a matrix-vector product for either a general band matrix or its transpose:

$$y \leftarrow \alpha Ax + \beta y$$

$$y \leftarrow \alpha A^T x + \beta y$$

In addition to these operations, the CGBMV and ZGBMV subprograms compute a matrix-vector product for the conjugate transpose:

$$y \leftarrow \alpha A^H x + \beta y$$

α and β are scalars, x and y are vectors, and A is an m by n band matrix.

Example

```
COMPLEX*16 A(5,20), X(20), Y(20), ALPHA, BETA
M = 5
N = 20
KL = 2
KU = 2
ALPHA = (1.0D0, 2.0D0)
LDA = 5
INCX = 1
BETA = (0.0D0, 0.0D0)
INCY = 1
CALL ZGBMV('N',M,N,KL,KU,ALPHA,A,LDA,X,INCX,BETA,Y,INCY)
```

This Fortran code multiplies a pentadiagonal matrix A by the vector x to get the vector y. The operation is $y \leftarrow Ax$ where A is stored in banded storage form.

SGEMV DGEMV CGEMV ZGEMV
Matrix-Vector Product for a General Matrix
(Serial and Parallel Versions)

Format

{S,D,C,Z}GEMV (trans, m, n, alpha, a, lda, x, incx, beta, y, incy)

Arguments

trans
character*1
On entry, specifies the operation to be performed:

If **trans** = 'N' or 'n', the operation is $y \leftarrow \alpha Ax + \beta y$.
If **trans** = 'T' or 't', the operation is $y \leftarrow \alpha A^T x + \beta y$.
If **trans** = 'C' or 'c', the operation is $y \leftarrow \alpha A^H x + \beta y$.

On exit, **trans** is unchanged.

m
integer*4
On entry, the number of rows of the matrix A; $m \geq 0$.
On exit, **m** is unchanged.

n
integer*4
On entry, the number of columns of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n. The leading m by n part of the array contains the elements of the matrix A.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A; $lda \geq \max(1, m)$.
On exit, **lda** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array containing the vector x. When **trans** is equal to 'N' or 'n', the length of the array is at least $(1 + (n - 1) * |incx|)$. Otherwise, the length is at least $(1 + (m - 1) * |incx|)$.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

beta
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar β.
On exit, **beta** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array containing the vector y. When **trans** is equal to 'N' or 'n', the length of the array is at least $(1 + (m - 1) * |incy|)$. Otherwise, the length is at least $(1 + (n - 1) * |incy|)$.

If $\beta = 0$, **y** need not be set. If β is not equal to zero, the incremented array Y must contain the vector y.
On exit, **y** is overwritten by the updated vector y.

incy
integer*4
On entry, the increment for the elements of Y; $incy$ must not equal zero.
On exit, **incy** is unchanged.

Description

The _GEMV subprograms compute a matrix-vector product for either a general matrix or its transpose:

$$y \leftarrow \alpha Ax + \beta y$$

$$y \leftarrow \alpha A^T x + \beta y$$

In addition to these operations, the CGEMV and ZGEMV subprograms compute the matrix-vector product for the conjugate transpose:

$$y \leftarrow \alpha A^H x + \beta y$$

α and β are scalars, x and y are vectors, and A is an m by n matrix.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Examples

1.
```
REAL*8 A(20,20), X(20), Y(20), ALPHA, BETA
INCX = 1
INCY = 1
LDA = 20
M = 20
N = 20
ALPHA = 1.0D0
BETA = 0.0D0
CALL DGEMV('T',M,N,ALPHA,A,LDA,X,INCX,BETA,Y,INCY)
```

This Fortran code computes the product $y \leftarrow A^T x$.

2.
```
COMPLEX A(20,20), X(20), Y(20), ALPHA, BETA
INCX = 1
INCY = 1
LDA = 20
M = 20
N = 20
ALPHA = (1.0, 1.0)
BETA = (0.0, 0.0)
CALL CGEMV('T',M,N,ALPHA,A,LDA,X,INCX,BETA,Y,INCY)
```

This Fortran code computes the product $y \leftarrow A^T x$.

SGER DGER CGERC ZGERC CGERU ZGERU Rank-One Update of a General Matrix

Format

{S,D}GER (m, n, alpha, x, incx, y, incy, a, lda)

{C,Z}GER{C,U} (m, n, alpha, x, incx, y, incy, a, lda)

Arguments

m
integer*4
On entry, the number of rows of the matrix A; $m \geq 0$.
On exit, **m** is unchanged.

n
integer*4
On entry, the number of columns of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (m - 1) * |incx|)$. Array X contains the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array of length at least $(1 + (n - 1) * |incy|)$. The incremented array Y must contain the vector y.
On exit, **y** is unchanged.

incy
integer*4
On entry, the increment for the elements of Y; $incy$ must not equal zero.
On exit, **incy** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n. The leading m by n part of the array contains the elements of the matrix A.
On exit, **a** is overwritten by the updated matrix.

lda
integer*4
On entry, the first dimension of A; $lda \geq \max(1, m)$.
On exit, **lda** is unchanged.

Description

SGER and DGER perform a rank-one update of a real general matrix:

$$A \leftarrow \alpha x y^T + A$$

CGERU and ZGERU perform a rank-one update of an unconjugated complex general matrix:

$$A \leftarrow \alpha x y^T + A$$

CGERC and ZGERC perform a rank-one update of a conjugated complex general matrix:

$$A \leftarrow \alpha x y^H + A$$

α is a scalar, x is an m-element vector, y is an n-element vector, and A is an m by n matrix.

Examples

1.
```
REAL*4 A(10,10), X(10), Y(5), ALPHA
INCX = 1
INCY = 1
LDA = 10
M = 3
N = 4
ALPHA = 2.3
CALL SGER(M,N,ALPHA,X,INCX,Y,INCY,A,LDA)
```

This Fortran code computes the rank-1 update $A \leftarrow \alpha x y^T + A$. Only the upper left submatrix of A, of dimension (3,4) and starting at location A(1,1), is updated.

2.
```
COMPLEX A(10,10), X(10), Y(5), ALPHA
INCX = 1
INCY = 1
LDA = 10
M = 3
N = 4
ALPHA = (2.3, 1.2)
CALL CGERC(M,N,ALPHA,X,INCX,Y,INCY,A,LDA)
```

This Fortran code computes the rank-1 update $A \leftarrow \alpha xy^H + A$. Only the upper left submatrix of A, of dimension (3,4) and starting at location A(1,1), is updated.

SSBMV DSBMV CHBMV ZHBMV
Matrix-Vector Product for a Symmetric or Hermitian Band Matrix

Format

{S,D}SBMV (uplo, n, k, alpha, a, lda, x, incx, beta, y, incy)

{C,Z}HBMV (uplo, n, k, alpha, a, lda, x, incx, beta, y, incy)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the array A is referenced:

If **uplo** = 'U' or 'u', the upper-triangular part of A is referenced.
If **uplo** = 'L' or 'l', the lower-triangular part of A is referenced.

On exit, **uplo** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

k
integer*4
On entry, if **uplo** specifies the upper portion of matrix A, **k** represents the number of super-diagonals of the matrix. If **uplo** specifies the lower portion, **k** is the number of subdiagonals; $k \geq 0$.
On exit, **k** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n.

When **uplo** specifies the upper portion of the matrix, the leading $(k+1)$ by n part of the array must contain the upper-triangular band part of the matrix, supplied column by column. The main diagonal of the matrix is stored in row $(k+1)$ of the array, the first super-diagonal is stored in row k starting at position 2, and so on. The top left k by k triangle of the array A is not referenced.

When **uplo** specifies the lower portion of the matrix, the leading $(k+1)$ by n part of the array must contain the lower-triangular band part of the matrix, supplied column by column. The main diagonal of the matrix is stored in row 1 of the array, the first sub-diagonal is stored in row 2, starting at position 1, and so on. The bottom right k by k triangle of the array A is not referenced.

For CHBMV and ZHBMV routines, the imaginary parts of the diagonal elements are not accessed, need not be set, and are assumed to be zero.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A; $lda \geq (k+1)$.
On exit, **lda** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1+(n-1)*|incx|)$. Array X contains the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

beta
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar β.
On exit, **beta** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1+(n-1)*|incy|)$.

If $\beta = 0$, **y** need not be set. If β is not equal to zero, the incremented array Y must contain the vector y.
On exit, **y** is overwritten by the updated vector y.

incy
integer*4
On entry, the increment for the elements of Y; $incy$ must not equal zero.
On exit, **incy** is unchanged.

Description

SSBMV and DSBMV compute a matrix-vector product for a real symmetric band matrix. CHBMV and ZHBMV compute a matrix-vector product for a complex Hermitian band matrix. Both products are described by the following operation:

$$y \leftarrow \alpha Ax + \beta y$$

α and β are scalars, and x and y are vectors with n elements. In the case of SSBMV and DSBMV, A is a symmetric matrix and in the case of CHBMV and ZHBMV, A is a Hermitian matrix.

Example

```
REAL*8 A(2,10), X(10), Y(10), ALPHA, BETA
N = 10
K = 1
ALPHA = 2.0D0
LDA = 2
INCX = 1
BETA = 1.0D0
INCY = 1
CALL DSBMV('U',N,K,ALPHA,A,LDA,X,INCX,BETA,Y,INCY)
```

This Fortran code computes the product $y \leftarrow \alpha Ax + y$ where A is a symmetric tridiagonal matrix, with A stored in upper-triangular form.

```
COMPLEX*8 A(2,10), X(10), Y(10), ALPHA, BETA
N = 10
K = 1
ALPHA = (2.0D0, 2.2D0)
LDA = 2
INCX = 1
BETA = (1.0D0, 0.0D0)
INCY = 1
CALL ZHBMV('U',N,K,ALPHA,A,LDA,X,INCX,BETA,Y,INCY)
```

This Fortran code computes the product $y \leftarrow \alpha Ax + y$ where A is a Hermitian tridiagonal matrix, with the upper diagonal of A stored.

SSPMV DSPMV CHPMV ZHPMV
Matrix-Vector Product for a Symmetric or Hermitian Matrix Stored in Packed Form

Format

{S,D}SPMV (uplo, n, alpha, ap, x, incx, beta, y, incy)

{C,Z}HPMV (uplo, n, alpha, ap, x, incx, beta, y, incy)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the matrix A is supplied in the packed array AP:

If **uplo** = 'U' or 'u', the upper-triangular part of A is supplied.

If **uplo** = 'L' or 'l', the lower-triangular part of A is supplied.

On exit, **uplo** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α.
On exit, **alpha** is unchanged.

ap
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array AP of length at least $n(n+1)/2$.

If **uplo** specifies the upper triangular part of the matrix A, the array contains those elements of the matrix, packed sequentially, column by column, so that AP(1) contains a_{11}, AP(2) and AP(3) contain a_{12} and a_{22} respectively, and so on.

If **uplo** specifies the lower triangular part to the matrix A, the array contains those elements of the matrix, also packed sequentially, so that AP(1) contains a_{11}, AP(2) and AP(3) contain a_{21} and a_{31} respectively, and so on.

For CHPMV and ZHPMV routines, the imaginary parts of the diagonal elements are not accessed, need not be set, and are assumed to be zero.
On exit, **ap** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n-1) * |incx|)$. Array X contains the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

beta
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar β.
On exit, **beta** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n-1) * |incy|)$.

If $\beta = 0$, **y** need not be set. If β is not equal to zero, the incremented array Y must contain the vector y.
On exit, **y** is overwritten by the updated vector y.

incy
integer*4
On entry, the increment for the elements of Y; $incy$ must not equal zero.
On exit, **incy** is unchanged.

Description

SSPMV and DSPMV compute a matrix-vector product for a real symmetric matrix stored in packed form. CHPMV and ZHPMV compute a matrix-vector product for a complex Hermitian matrix stored in packed form. Both products are described by the following operation:

$$y \leftarrow \alpha Ax + \beta y$$

α and β are scalars, and x and y are vectors with n elements. A is an n by n matrix. In the case of SSPMV and DSPMV, matrix A is a symmetric matrix and in the case of CHPMV and ZHPMV, matrix A is a Hermitian matrix.

Example

```
COMPLEX*16 AP(250), X(20), Y(20), ALPHA, BETA
N = 20
ALPHA = (2.3D0, 8.4D0)
INCX = 1
BETA = (4.0D0, 3.3D0)
INCY = 1
CALL ZHPMV('L',N,ALPHA,AP,X,INCX,BETA,Y,INCY)
```

This Fortran code computes the product $y \leftarrow \alpha Ax + \beta y$ where A is a Hermitian matrix with its lower-triangular part stored in packed form in AP.

SSPR DSPR CHPR ZHPR
Rank-One Update of a Symmetric or Hermitian Matrix Stored in Packed Form

Format

{S,D}SPR (uplo, n, alpha, x, incx, ap)

{C,Z}HPR (uplo, n, alpha, x, incx, ap)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the matrix A is supplied in the packed array AP:

If **uplo** = 'U' or 'u', the upper-triangular part of A is supplied.
If **uplo** = 'L' or 'l', the lower-triangular part of A is supplied.

On exit, **uplo** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$. Array X contains the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

ap
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array AP of length at least $n(n + 1)/2$.

If **uplo** specifies the upper triangular part of the matrix A, the array contains those elements of the matrix, packed sequentially, column by column, so that AP(1) contains a_{11}, AP(2) and AP(3) contain a_{12} and a_{22} respectively, and so on.

If **uplo** specifies the lower triangular part to the matrix A, the array contains those elements of the matrix, also packed sequentially, so that AP(1) contains a_{11}, AP(2) and AP(3) contain a_{21} and a_{31} respectively, and so on.

For CHPR and ZHPR routines, the imaginary parts of the diagonal elements are not accessed, need not be set, and are assumed to be zero.

On exit, **ap** is overwritten by the specified part of the updated matrix.

Description

SSPR and DSPR perform the rank-one update of a real symmetric matrix stored in packed form:

$$A \leftarrow \alpha x x^T + A$$

CHPR and ZHPR perform the rank-one update of a complex Hermitian matrix stored in packed form:

$$A \leftarrow \alpha x x^H + A$$

α is a scalar, x is vector with n elements, and A is an n by n matrix in packed form. In the case of SSPR and DSPR, matrix A is a symmetric matrix and in the case of CHPR and ZHPR, matrix A is a Hermitian matrix.

Example

```
REAL*8 AP(500), X(30), Y(30), ALPHA
INCX = 1
ALPHA = 1.0D0
N = 30
CALL DSPR('U',N,ALPHA,X,INCX,AP)
```

This Fortran code computes the rank-1 update $A \leftarrow xx^T + A$ where A is a real symmetric matrix, of order 30, with its upper-triangular part stored in packed form in AP.

SSPR2 DSPR2 CHPR2 ZHPR2
Rank-Two Update of a Symmetric or Hermitian Matrix Stored in Packed Form

Format

{S,D}SPR2 (uplo, n, alpha, x, incx, y, incy, ap)

{C,Z}HPR2 (uplo, n, alpha, x, incx, y, incy, ap)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the matrix A is supplied in the packed array AP:

If **uplo** = 'U' or 'u', the upper-triangular part of matrix A is supplied.
If **uplo** = 'L' or 'l', the lower-triangular part of matrix A is supplied.

On exit, **uplo** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$. Array X contains the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$. The incremented array Y must contain the vector y.
On exit, **y** is unchanged.

incy
integer*4
On entry, the increment for the elements of Y; $incy$ must not equal zero.
On exit, **incy** is unchanged.

ap
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array AP of length at least $n(n+1)/2$.

If **uplo** specifies the upper triangular part of the matrix A, the array contains those elements of the matrix, packed sequentially, column by column, so that AP(1) contains a_{11}, AP(2) and AP(3) contain a_{12} and a_{22} respectively, and so on.

If **uplo** specifies the lower triangular part to the matrix A, the array contains those elements of the matrix, also packed sequentially, so that AP(1) contains a_{11}, AP(2) and AP(3) contain a_{21} and a_{31} respectively, and so on.

For CHPR2 and ZHPR2 routines, the imaginary parts of the diagonal elements are not accessed, need not be set, and are assumed to be zero.

On exit, **ap** is overwritten by the specified part of the updated matrix.

Description

SSPR2 and DSPR2 perform the rank-two update of a real symmetric matrix stored in packed form:

$$A \leftarrow \alpha x y^T + \alpha y x^T + A$$

CHPR2 and ZHPR2 perform the rank-two update of a complex Hermitian matrix stored in packed form:

$$A \leftarrow \alpha x y^H + \overline{\alpha} y x^H + A$$

α is a scalar, x is vector with n elements, and A is an n by n matrix in packed form. In the case of SSPR2 and DSPR2, matrix A is a symmetric matrix and in the case of CHPR2 and ZHPR2, matrix A is a Hermitian matrix.

Example

```
REAL*4 AP(250), X(20), Y(20), ALPHA
INCX = 1
INCY = 1
ALPHA = 2.0
N = 20
CALL SSPR2('L',N,ALPHA,X,INCX,Y,INCY,AP)
```

This Fortran code computes the rank-2 update of a real symmetric matrix A, given by $A \leftarrow \alpha x y^T + \alpha y x^T + A$. A is a real symmetric matrix, of order 20, with its lower-triangular part stored in packed form in AP.

SSYMV DSYMV CHEMV ZHEMV
Matrix-Vector Product for a Symmetric or Hermitian Matrix

Format

{S,D}SYMV (uplo, n, alpha, a, lda, x, incx, beta, y, incy)

{C,Z}HEMV (uplo, n, alpha, a, lda, x, incx, beta, y, incy)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the array A is referenced:

If **uplo** = 'U' or 'u', the upper-triangular part of A is referenced.
If **uplo** = 'L' or 'l', the lower-triangular part of A is referenced.

On exit, **uplo** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n.

When **uplo** specifies the upper portion of the matrix, the leading n by n part of the array contains the upper-triangular part of the matrix, and the lower-triangular part of array A is not referenced.

When **uplo** specifies the lower portion of the matrix, the leading n by n part of the array contains the lower-triangular part of the matrix, and the upper-triangular part of array A is not referenced.

For CHEMV and ZHEMV routines, the imaginary parts of the diagonal elements are not accessed, need not be set, and are assumed to be zero.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A; $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n-1) * |incx|)$. Array X contains the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

beta
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar β.
On exit, **beta** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$.

If $\beta = 0$, **y** need not be set. If β is not equal to zero, the incremented array Y must contain the vector y.
On exit, **y** is overwritten by the updated vector y.

incy
integer*4
On entry, the increment for the elements of Y; $incy$ must not equal zero.
On exit, **incy** is unchanged.

Description

SSYMV and DSYMV compute a matrix-vector product for a real symmetric matrix. CHEMV and ZHEMV compute a matrix-vector product for a complex Hermitian matrix. Both products are described by the following operation:

$$y \leftarrow \alpha A x + \beta y$$

α and β are scalars, x and y are vectors with n elements, and A is an n by n matrix. In the case of SSYMV and DSYMV, matrix A is a symmetric matrix and in the case of CHEMV and ZHEMV, matrix A is a Hermitian matrix.

Examples

1.
```
REAL*8 A(100,40), X(40), Y(40), ALPHA, BETA
N = 40
INCX = 1
INCY = 1
ALPHA = 1.0D0
BETA = 0.0D0
LDA = 100
CALL DSYMV('U',N,ALPHA,A,LDA,X,INCX,BETA,Y,INCY)
```

   This Fortran code computes the product $y \leftarrow Ax$ where A is a symmetric matrix, of order 40, with its upper-triangular part stored.

2.
```
COMPLEX A(100,40), X(40), Y(40), ALPHA, BETA
N = 40
INCX = 1
INCY = 1
ALPHA = (1.0, 0.5)
BETA = (0.0, 0.0)
LDA = 100
CALL CHEMV('U',N,ALPHA,A,LDA,X,INCX,BETA,Y,INCY)
```

   This Fortran code computes the product $y \leftarrow Ax$ where A is a Hermitian matrix, of order 40, with its upper-triangular part stored.

SSYR DSYR CHER ZHER
Rank-One Update of a Symmetric or Hermitian Matrix

Format

{S,D}SYR (uplo, n, alpha, x, incx, a, lda)

{C,Z}HER (uplo, n, alpha, x, incx, a, lda)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the array A is referenced:

If **uplo** = 'U' or 'u', the upper-triangular part of A is referenced.
If **uplo** = 'L' or 'l', the lower-triangular part of A is referenced.

On exit, **uplo** is unchanged.

n
integer*4
On entry, the order of the matrix A and the number of elements in vector x; $n \geq 0$.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$. Array X contains the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n.

When **uplo** specifies the upper portion of the matrix, the leading n by n part of the array contains the upper-triangular part of the matrix, and the lower-triangular part of array A is not referenced.

When **uplo** specifies the lower portion of the matrix, the leading n by n part of the array contains the lower-triangular part of the matrix, and the upper-triangular part of array A is not referenced.

For CHER and ZHER routines, the imaginary parts of the diagonal elements are not accessed, need not be set, and are assumed to be zero.

On exit, **a** is overwritten; the specified part of the array A is overwritten by the part of the updated matrix.

lda
integer*4
On entry, the first dimension of array A; $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

Description

SSYR and DSYR perform the rank-one update of a real symmetric matrix:

$$A \leftarrow \alpha x x^T + A$$

CHER and ZHER perform the rank-one update of a complex Hermitian matrix:

$$A \leftarrow \alpha x x^H + A$$

α is a scalar, x is vector with n elements, and A is an n by n matrix in packed form. In the case of SSYR and DSYR, matrix A is a symmetric matrix and in the case of CHER and ZHER, matrix A is a Hermitian matrix.

Examples

1.
```
REAL*4 A(50,20), X(20), ALPHA
INCX = 1
LDA = 50
N = 20
ALPHA = 2.0
CALL SSYR('L',N,ALPHA,X,INCX,A,LDA)
```

   This Fortran code computes the rank-1 update of the matrix A, given by $A \leftarrow \alpha x x^T + A$. A is a real symmetric matrix with its lower-triangular part stored.

2.
```
COMPLEX*16 A(50,20), X(20), ALPHA
INCX = 1
LDA = 50
N = 20
ALPHA = (2.0D0, 1.0D0)
CALL ZHER('L',N,ALPHA,X,INCX,A,LDA)
```

   This Fortran code computes the rank-1 update of the matrix A, given by $A \leftarrow \alpha x x^H + A$. A is a complex Hermitian matrix with its lower-triangular part stored.

SSYR2 DSYR2 CHER2 ZHER2
Rank-Two Update of a Symmetric or Hermitian Matrix

Format

{S,D}SYR2 (uplo, n, alpha, x, incx, y, incy, a, lda)

{C,Z}HER2 (uplo, n, alpha, x, incx, y, incy, a, lda)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the array A is referenced:

If **uplo** = 'U' or 'u', the upper-triangular part of A is referenced.
If **uplo** = 'L' or 'l', the lower-triangular part of A is referenced.

On exit, **uplo** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, the scalar α.
On exit, **alpha** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$. Array X contains the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$. The incremented array Y must contain the vector y.
On exit, **y** is unchanged.

incy
integer*4
On entry, the increment for the elements of Y; $incy$ must not equal zero.
On exit, **incy** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n.

When **uplo** specifies the upper portion of the matrix, the leading n by n part of the array contains the upper-triangular part of the matrix, and the lower-triangular part of array A is not referenced.

When **uplo** specifies the lower portion of the matrix, the leading n by n part of the array contains the lower-triangular part of the matrix, and the upper-triangular part of array A is not referenced.

For complex routines, the imaginary parts of the diagonal elements need not be set. They are assumed to be 0, and on exit they are set to 0.

On exit, **a** is overwritten; the specified part of the array A is overwritten by the specified part of the updated matrix.

lda
integer*4
On entry, the first dimension of array A; $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

Description

SSYR2 and DSYR2 perform the rank-two update of a real symmetric matrix:

$$A \leftarrow \alpha x y^T + \alpha y x^T + A$$

CHER2 and ZHER2 perform the rank-two update of a complex Hermitian matrix:

$$A \leftarrow \alpha x y^H + \overline{\alpha} y x^H + A$$

α is a scalar, x and y are vectors with n elements, and A is an n by n matrix. In the case of SSYR2 and DSYR2, matrix A is a symmetric matrix and in the case of CHER2 and ZHER2, matrix A is a Hermitian matrix.

Example

```
REAL*8 A(50,20), X(20), Y(20), ALPHA
INCX = 1
LDA = 50
N = 20
INCY = 1
ALPHA = 1.0D0
CALL DSYR2('U',N,ALPHA,X,INCX,Y,INCY,A,LDA)
```

This Fortran code computes the rank-2 update of a real symmetric matrix A, given by $A \leftarrow xy^T + yx^T + A$. Only the upper-triangular part of A is stored.

STBMV DTBMV CTBMV ZTBMV
Matrix-Vector Product for a Triangular Band Matrix

Format

{S,D,C,Z}TBMV (uplo, trans, diag, n, k, a, lda, x, incx)

Arguments

uplo
character*1
On entry, specifies whether the matrix A is an upper- or lower-triangular matrix:

If **uplo** = 'U' or 'u', A is an upper-triangular matrix.
If **uplo** = 'L' or 'l', A is a lower-triangular matrix.

On exit, **uplo** is unchanged.

trans
character*1
On entry, specifies the operation to be performed:

If **trans** = 'N' or 'n', the operation is $y \leftarrow \alpha Ax + \beta y$.

If **trans** = 'T' or 't', the operation is $y \leftarrow \alpha A^T x + \beta y$.
If **trans** = 'C' or 'c', the operation is $y \leftarrow \alpha A^H x + \beta y$.

On exit, **trans** is unchanged.

diag

character*1
On entry, specifies whether the matrix A is unit-triangular:

If **diag** = 'U' or 'u', A is a unit-triangular matrix.
If **diag** = 'N' or 'n', A is not a unit-triangular matrix.

On exit, **diag** is unchanged.

n

integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

k

integer*4
On entry, if **uplo** is equal to 'U' or 'u', the number of super-diagonals k of the matrix A. If **uplo** is equal to 'L' or 'l', the number of sub-diagonals k of the matrix A; $k \geq 0$.
On exit, **k** is unchanged.

a

real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n.

When **uplo** specifies the upper portion of the matrix, the leading $(k+1)$ by n part of the array must contain the upper-triangular band part of the matrix, supplied column by column. The main diagonal of the matrix is stored in row $(k+1)$ of the array, the first super-diagonal is stored in row k starting at position 2, and so on. The bottom left k by k triangle of the array A is not referenced.

When **uplo** specifies the lower portion of the matrix, the leading $(k+1)$ by n part of the array must contain the lower-triangular band part of the matrix, supplied column by column. The main diagonal of the matrix is stored in row 1 of the array, the first sub-diagonal is stored in row 2, starting at position 1, and so on. The top right k by k triangle of the array A is not referenced.

If **diag** is equal to 'U' or 'u', the elements of the array A corresponding to the diagonal elements of the matrix are not referenced, but are assumed to be unity.
On exit, **a** is unchanged.

lda

integer*4
On entry, the first dimension of array A; $lda \geq (k+1)$.
On exit, **lda** is unchanged.

x

real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n-1) * |incx|)$. Array X contains the vector x.
On exit, **x** is overwritten with the transformed vector x.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

Description

The _TBMV subprograms compute a matrix-vector product for a triangular band matrix or its transpose: $x \leftarrow Ax$ or $x \leftarrow A^T x$.

In addition to these operations, the CTBMV and ZTBMV subprograms compute the matrix-vector product for the conjugate transpose: $x \leftarrow A^H x$.

x is a vector with n elements and A is an n by n band matrix, with $(k + 1)$ diagonals. The band matrix is a unit or nonunit, upper- or lower-triangular matrix.

Example

```
REAL*4 A(5,100), X(100)
INCX = 1
LDA = 5
K = 4
N = 100
CALL STBMV('U','N','N',N,K,A,LDA,X,INCX)
```

This Fortran code computes the product $x \leftarrow Ax$ where A is an upper-triangular, nonunit diagonal matrix, with 4 superdiagonals.

STBSV DTBSV CTBSV ZTBSV
Solver of a System of Linear Equations with a Triangular Band Matrix

Format

{S,D,C,Z}TBSV (uplo, trans, diag, n, k, a, lda, x, incx)

Arguments

uplo
character*1
On entry, specifies whether the matrix A is an upper- or lower-triangular matrix:

If **uplo** = 'U' or 'u', A is an upper-triangular matrix.
If **uplo** = 'L' or 'l', A is a lower-triangular matrix.

On exit, **uplo** is unchanged.

trans
character*1
On entry, specifies the system to be solved:

If **trans** = 'N' or 'n', the system is $Ax = b$.
If **trans** = 'T' or 't', the system is $A^T x = b$.
If **trans** = 'C' or 'c', the system is $A^H x = b$.

On exit, **trans** is unchanged.

diag
character*1
On entry, specifies whether the matrix A is unit-triangular:

If **diag** = 'U' or 'u', A is a unit-triangular matrix.
If **diag** = 'N' or 'n', A is not a unit-triangular matrix.

On exit, **diag** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

k
integer*4
On entry, if **uplo** is equal to 'U' or 'u', the number of super-diagonals k of the matrix A. If **uplo** is equal to 'L' or 'l', the number of sub-diagonals k of the matrix A; $k \geq 0$.
On exit, **k** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n.

When **uplo** specifies the upper portion of the matrix, the leading $(k + 1)$ by n part of the array contains the upper-triangular band part of the matrix, supplied column by column. The main diagonal of the matrix is stored in row $(k+1)$ of the array, the first super-diagonal is stored in row k starting at position 2, and so on. The top left k by k triangle of the array A is not referenced.

When **uplo** specifies the lower portion, the leading $(k + 1)$ by n part of the array contains the lower-triangular band part of the matrix, supplied column by column. The main diagonal of the matrix is stored in row 1 of the array, the first sub-diagonal is stored in row 2 starting at position 1, and so on. The top right k by k triangle of the array A is not referenced.

If **diag** is equal to 'U' or 'u', the elements of the array A corresponding to the diagonal elements of the matrix are not referenced, but are assumed to be unity.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A; $lda \geq (k + 1)$.
On exit, **lda** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$. Array X contains the vector b.
On exit, **x** is overwritten with the solution vector x.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

Description

The _TBSV subprograms solve one of the following systems of linear equations for x: $Ax = b$ or $A^T x = b$. In addition to these operations, the CTBSV and ZTBSV subprograms solve the following system of linear equations for x: $A^H x = b$.

b and x are vectors with n elements and A is an n by n band matrix with $(k + 1)$ diagonals. The matrix is a unit or nonunit, upper- or lower-triangular band matrix.

The _TBSV routines do not perform checks for singularity or near singularity of the triangular matrix. The requirements for such a test depend on the application. If necessary, perform the test in your application program before calling the routine.

Example

```
REAL*8 A(10,100), X(100)
INCX = 1
K = 9
LDA = 10
N = 100
CALL DTBSV('L','T','U',N,K,A,LDA,X,INCX)
```

This Fortran code solves the system $A^T x = b$ where A is a lower-triangular matrix, with a unit diagonal and 9 subdiagonals. The right hand side b is originally contained in the vector x.

STPMV DTPMV CTPMV ZTPMV
Matrix-Vector Product for a Triangular Matrix in Packed Form

Format

{S,D,C,Z}TPMV (uplo, trans, diag, n, ap, x, incx)

Arguments

uplo
character*1
On entry, specifies whether the matrix A is an upper- or lower-triangular matrix:

If **uplo** = 'U' or 'u', A is an upper-triangular matrix.
If **uplo** = 'L' or 'l', A is a lower-triangular matrix.

On exit, **uplo** is unchanged.

trans
character*1
On entry, specifies the operation to be performed:

If **trans** = 'N' or 'n', the operation is $x \leftarrow Ax$.
If **trans** = 'T' or 't', the operation is $x \leftarrow A^T x$.
If **trans** = 'C' or 'c', the operation is $x \leftarrow A^H x$.

On exit, **trans** is unchanged.

diag
character*1
On entry, specifies whether the matrix A is unit-triangular:

If **diag** = 'U' or 'u', A is a unit-triangular matrix.
If **diag** = 'N' or 'n', A is not a unit-triangular matrix.

On exit, **diag** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

ap
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array AP of length at least $\frac{n(n+1)}{2}$.

If **uplo** specifies the upper triangular part of the matrix A, the array contains those elements of the matrix, packed sequentially, column by column, so that AP(1) contains a_{11}, AP(2) and AP(3) contain a_{12} and a_{22} respectively, and so on.

If **uplo** specifies the lower triangular part to the matrix A, so that AP(1) contains a_{11}, AP(2) and AP(3) contain a_{21} and a_{31} respectively, and so on.

If **diag** is equal to 'U' or 'u', the diagonal elements of A are not referenced, but are assumed to be unity.

On exit, **ap** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$. Array X contains the vector x.
On exit, **x** is overwritten with the transformed vector x.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

Description

The _TPMV subprograms compute a matrix-vector product for a triangular matrix stored in packed form or its transpose: $x \leftarrow Ax$ or $x \leftarrow A^T x$. In addition to these operations, the CTPMV and ZTPMV subprograms compute a matrix-vector product for the conjugate transpose: $x \leftarrow A^H x$.

x is a vector with n elements and A is an n by n, unit or nonunit, upper- or lower-triangular matrix, supplied in packed form.

Example

```
REAL*4 AP(250), X(20)
INCX = 1
N = 20
CALL STPMV('U','N','N',N,AP,X,INCX)
```

This Fortran code computes the product $x \leftarrow Ax$ where A is an upper-triangular matrix of order 20, with nonunit diagonal, stored in packed form.

STPSV DTPSV CTPSV ZTPSV
Solve a System of Linear Equations with a Triangular Matrix in Packed Form

Format

{S,D,C,Z}TPSV (uplo, trans, diag, n, ap, x, incx)

Arguments

uplo
character*1
On entry, specifies whether the matrix A is an upper- or lower-triangular matrix:

If **uplo** = 'U' or 'u', A is an upper-triangular matrix.
If **uplo** = 'L' or 'l', A is a lower-triangular matrix.

On exit, **uplo** is unchanged.

trans
character*1
On entry, specifies the system to be solved:

If **trans** = 'N' or 'n', the system is $Ax = b$.
If **trans** = 'T' or 't', the system is $A^T x = b$.
If **trans** = 'C' or 'c', the system is $A^H x = b$.

On exit, **trans** is unchanged.

diag
character*1
On entry, specifies whether the matrix A is unit-triangular:

If **diag** = 'U' or 'u', A is a unit-triangular matrix.
If **diag** = 'N' or 'n', A is not a unit-triangular matrix.

On exit, **diag** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

ap
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array AP of length at least $n(n + 1)/2$.

If **uplo** specifies the upper triangular part of the matrix A, the array contains those elements of the matrix, packed sequentially, column by column, so that AP(1) contains a_{11}, AP(2) and AP(3) contain a_{12} and a_{22} respectively, and so on.

If **uplo** specifies the lower triangular part to the matrix A, so that AP(1) contains a_{11}, AP(2) and AP(3) contain a_{21} and a_{31} respectively, and so on.

If **diag** is equal to 'U' or 'u', the diagonal elements of A are not referenced, but are assumed to be unity.
On exit, **ap** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$. Array X contains the vector b.
On exit, **x** is overwritten with the solution vector x.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

Description

The _TPSV subprograms solve one of the following systems of linear equations for x: $Ax = b$ or $A^T x = b$. In addition to these operations, the CTPSV and ZTPSV subprograms solve the following system of equations: $A^H x = b$.

b and x are vectors with n elements and A is an n by n, unit or nonunit, upper- or lower-triangular matrix, supplied in packed form.

The _TPSV routines do not perform checks for singularity or near singularity of the triangular matrix. The requirements for such a test depend on the application. If necessary, perform the test in your application program before calling this routine.

Example

```
REAL*8 A(500), X(30)
INCX = 1
N = 30
CALL DTPSV('L','T','N',N,AP,X,INCX)
```

This Fortran code solves the system $A^T x = b$ where A is a lower-triangular matrix of order 30, with nonunit diagonal, stored in packed form. The right hand side b is originally contained in the vector x.

STRMV DTRMV CTRMV ZTRMV
Matrix-Vector Product for a Triangular Matrix

Format

{S,D,C,Z}TRMV (uplo, trans, diag, n, a, lda, x, incx)

Arguments

uplo
character*1
On entry, specifies whether the matrix A is an upper- or lower-triangular matrix:

If **uplo** = 'U' or 'u', A is an upper-triangular matrix.
If **uplo** = 'L' or 'l', A is a lower-triangular matrix.

On exit, **uplo** is unchanged.

trans
character*1
On entry, specifies the operation to be performed:

If **trans** = 'N' or 'n', the operation is $x \leftarrow Ax$.
If **trans** = 'T' or 't', the operation is $x \leftarrow A^T x$.
If **trans** = 'C' or 'c', the operation is $x \leftarrow A^H x$.

On exit, **trans** is unchanged.

diag
character*1
On entry, specifies whether the matrix A is unit-triangular:

If **diag** = 'U' or 'u', A is a unit-triangular matrix.
If **diag** = 'N' or 'n', A is not a unit-triangular matrix.

On exit, **diag** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n.

When **uplo** specifies the upper portion of the matrix, the leading n by n part of the array contains the upper-triangular part of the matrix, and the lower-triangular part of array A is not referenced.

When **uplo** specifies the lower portion of the matrix, the leading n by n part of the array contains the lower-triangular part of the matrix, and the upper-triangular part of array A is not referenced.

If **diag** is equal to 'U' or 'u', the diagonal elements of A are also not referenced, but are assumed to be unity.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A; $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n-1) * |incx|)$. Array X contains the vector x.
On exit, **x** is overwritten with the transformed vector x.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

Description

The _TRMV subprograms compute a matrix-vector product for a triangular matrix or its transpose: $x \leftarrow Ax$ or $x \leftarrow A^T x$. In addition to these operations, the CTRMV and ZTRMV subprograms compute a matrix-vector product for conjugate transpose: $x \leftarrow A^H x$.

x is a vector with n elements, and A is an n by n, unit or nonunit, upper- or lower-triangular matrix.

Example

```
REAL*4 A(50,20), X(20)
INCX = 1
N = 20
LDA = 50
CALL STRMV('U','N','N',N,A,LDA,X,INCX)
```

This Fortran code computes the product $x \leftarrow Ax$ where A is an upper-triangular matrix, of order 20, with a nonunit diagonal.

STRSV DTRSV CTRSV ZTRSV
Solver of a System of Linear Equations with a Triangular Matrix

Format

{S,D,C,Z}TRSV (uplo, trans, diag, n, a, lda, x, incx)

Arguments

uplo
character*1
On entry, specifies whether the matrix A is an upper- or lower-triangular matrix:

If **uplo** = 'U' or 'u', A is an upper-triangular matrix.
If **uplo** = 'L' or 'l', A is a lower-triangular matrix.

On exit, **uplo** is unchanged.

trans
character*1
On entry, specifies the system to be solved:

If **trans** = 'N' or 'n', the system is $Ax = b$.
If **trans** = 'T' or 't', the system is $A^T x = b$.
If **trans** = 'C' or 'c', the system is $A^H x = b$.

On exit, **trans** is unchanged.

diag
character*1
On entry, specifies whether the matrix A is unit-triangular:

If **diag** = 'U' or 'u', A is a unit-triangular matrix.
If **diag** = 'N' or 'n', A is not a unit-triangular matrix.

On exit, **diag** is unchanged.

n
integer*4
On entry, the order of the matrix A; $n \geq 0$.
On exit, **n** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions lda by n.

When **uplo** specifies the upper portion of the matrix, the leading n by n part of the array contains the upper-triangular part of the matrix, and the lower-triangular part of array A is not referenced.

When **uplo** specifies the lower portion of the matrix, the leading n by n part of the array contains the lower-triangular part of the matrix, and the upper-triangular part of array A is not referenced.

If **diag** is equal to 'U' or 'u', the diagonal elements of A are also not referenced, but are assumed to be unity.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A; $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

x
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array X of length at least $(1 + (n-1) * |incx|)$. Array X contains the vector b.
On exit, **x** is overwritten with the solution vector x.

incx
integer*4
On entry, the increment for the elements of X; $incx$ must not equal zero.
On exit, **incx** is unchanged.

Description

The _TRSV subprograms solve one of the following systems of linear equations for x: $Ax = b$ or $A^T x = b$. In addition to these operations, the CTRSV and ZTRSV subprograms solve the following systems of linear equation: $A^H x = b$.

b and x are vectors with n elements and A is an n by n, unit or nonunit, upper- or lower-triangular matrix.

The _TRSV routines do not perform checks for singularity or near singularity of the triangular matrix. The requirements for such a test depend on the application. If necessary, perform the test in your application program before calling this routine.

Example

```
REAL*8 A(100,40), X(40)
INCX = 1
N = 40
LDA = 100
CALL DTRSV('L','N','U',N,A,LDA,X,INCX)
```

This Fortran code solves the system $Ax = b$ where A is a lower-triangular matrix of order 40, with a unit diagonal. The right hand side b is originally stored in the vector x.

Level 3 BLAS Subroutines

This section provides descriptions of the Level 3 BLAS subroutines for real and complex operations.

For real operations, $\overline{A} = A$ and $A^H = A^T$.

SGEMA DGEMA CGEMA ZGEMA
Matrix-Matrix Addition

Format

{S,D,C,Z}GEMA (transa, transb, m, n, alpha, a, lda, beta, b, ldb, c, ldc)

Arguments

transa
character*1
On entry, specifies the form of $\mathrm{op}(A)$ as follows:

If **transa** = 'N' or 'n', $\mathrm{op}(A) = A$
If **transa** = 'T' or 't', $\mathrm{op}(A) = A^T$
If **transa** = 'R' or 'r', $\mathrm{op}(A) = \overline{A}$
If **transa** = 'C' or 'c', $\mathrm{op}(A) = A^H$

On exit, **transa** is unchanged.

transb
character*1
On entry, specifies the form of $\mathrm{op}(B)$ as follows:

If **transb** = 'N' or 'n', $\mathrm{op}(B) = B$
If **transb** = 'T' or 't', $\mathrm{op}(B) = B^T$
If **transb** = 'R' or 'r', $\mathrm{op}(B) = \overline{B}$
If **transb** = 'C' or 'c', $\mathrm{op}(B) = B^H$

On exit, **transb** is unchanged.

m
integer*4
On entry, the number of rows in the matrices $\mathrm{op}(A)$, $\mathrm{op}(B)$, and C; $m \geq 0$.
On exit, **m** is unchanged.

n
integer*4
On entry, the number of columns in the matrices $\mathrm{op}(A)$, $\mathrm{op}(B)$, and C; $n \geq 0$.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by k.
For $\mathrm{op}(A) = A$ or $\overline{A}$, $k = n$ and the leading m by n part of array A contains the matrix A.
For $\mathrm{op}(A) = A^T$ or A^H, $k = m$ and the leading n by m part of array A contains the matrix A.
On exit, **a** is unchanged.

lda
integer*4
On entry, specifies the first dimension of array A.
For $\mathrm{op}(A) = A$ or $\overline{A}$, $lda \geq \max(1, m)$.
For $\mathrm{op}(A) = A^T$ or A^H, $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

beta
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar β.
On exit, **beta** is unchanged.

b
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with dimensions ldb by k.
For $\mathrm{op}(B) = B$ or $\overline{B}$, $k = n$ and the leading m by n part of array B contains the matrix B.
For $\mathrm{op}(B) = B^T$ or B^H, $k = m$ and the leading n by m part of array B contains the matrix B.

ldb
integer*4
On entry, specifies the first dimension of array B.
For $\mathrm{op}(B) = B$ or $\overline{B}$, $ldb \geq \max(1, m)$.
For $\mathrm{op}(B) = B^T$ or B^H, $ldb \geq \max(1, n)$.
On exit, **ldb** is unchanged.

c
real*4 | real*8 | complex*8 | complex*16
On entry, an array with the dimension ldc by n.
On exit, the leading m by n part of array C is overwritten by the matrix $\alpha\mathrm{op}(A) + \beta\mathrm{op}(B)$.

ldc
integer*4
On entry, specifies the first dimension of array C; $ldc \geq \max(1, m)$.
On exit, **ldc** is unchanged.

Description

The _GEMA routines perform the following operations:

$$C \leftarrow \alpha\mathrm{op}(A) + \beta\mathrm{op}(B)$$

where $\mathrm{op}(X) = X, X^T, \overline{X},$ or X^H, α and β are scalars, and A, B, and C are matrices. $\mathrm{op}(A)$, $\mathrm{op}(B)$, and C are m by n matrices.

These subroutines can also perform the following operation when $lda = ldc$, and **transa** = 'N' or 'n', that is, when $\mathrm{op}(A) = A$:

$$A \leftarrow \alpha A + \beta\mathrm{op}(B)$$

where $\mathrm{op}(X) = X, X^T, \overline{X},$ or X^H, α and β are scalars, and A and B are m by n matrices.

SGEMM DGEMM CGEMM ZGEMM
Matrix-Matrix Product and Addition (Serial and Parallel Versions)

Format

{S,D,C,Z}GEMM (transa, transb, m, n, k, alpha, a, lda, b, ldb, beta, c, ldc)

Arguments

transa
character*1
On entry, specifies the form of $\mathrm{op}(A)$ used in the matrix multiplication:

If **transa** = 'N' or 'n', $\mathrm{op}(A) = A$
If **transa** = 'T' or 't', $\mathrm{op}(A) = A^T$
If **transa** = 'R' or 'r', $\mathrm{op}(A) = \overline{A}$
If **transa** = 'C' or 'c', $\mathrm{op}(A) = A^H$

On exit, **transa** is unchanged.

transb
character*1
On entry, specifies the form of $\mathrm{op}(B)$ used in the matrix multiplication:

If **transb** = 'N' or 'n', $\mathrm{op}(B) = B$
If **transb** = 'T' or 't', $\mathrm{op}(B) = B^T$
If **transb** = 'R' or 'r', $\mathrm{op}(B) = \overline{B}$
If **transb** = 'C' or 'c', $\mathrm{op}(B) = B^H$

m
integer*4
On entry, the number of rows of the matrix $\mathrm{op}(A)$ and of the matrix C; $m \geq 0$
On exit, **m** is unchanged.

n
integer*4
On entry, the number of columns of the matrix $\mathrm{op}(B)$ and of the matrix C; $n \geq 0$
On exit, **n** is unchanged.

k
integer*4
On entry, the number of columns of the matrix $\mathrm{op}(A)$ and the number of rows of the matrix $\mathrm{op}(B)$; $k \geq 0$
On exit, **k** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by ka.
For $\mathrm{op}(A) = A$ or $\overline{A}$, $ka \geq k$ and the leading m by k portion of the array A contains the matrix A.

For $\mathrm{op}(A) = A^T$ or A^H, $ka \geq m$ and the leading k by m part of the array A contains the matrix A.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A.
For $\mathrm{op}(A) = A$ or $\overline{A}$, $lda \geq \max(1, m)$.
For $\mathrm{op}(A) = A^T$ or A^H, $lda \geq \max(1, k)$.
On exit, **lda** is unchanged.

b
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array B with dimensions ldb by kb.
For $\mathrm{op}(B) = B$ or $\overline{B}$, $kb \geq n$ and the leading k by n portion of the array contains the matrix B.
For $\mathrm{op}(B) = (B)^T$ or B^H, $kb \geq k$ and the leading n by k part of the array contains the matrix B.
On exit, **b** is unchanged.

ldb
integer*4
On entry, the first dimension of array B.
For $\mathrm{op}(B) = B$ or $\overline{B}$, $ldb \geq \max(1, k)$.
For $\mathrm{op}(B) = B^T$ or B^H, $ldb \geq \max(1, n)$.
On exit, **ldb** is unchanged.

beta
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar β.
On exit, **beta** is unchanged.

c
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with the dimension ldc by at least n.
On exit, the leading m by n part of array C is overwritten by the matrix $\alpha \mathrm{op}(A)\mathrm{op}(B) + \beta C$.

ldc
integer*4
On entry, the first dimension of array C; $ldc \geq \max(1, m)$
On exit, **ldc** is unchanged.

Description

The _GEMM routines perform the following operations:

$$C \leftarrow \alpha \mathrm{op}(A)\mathrm{op}(B) + \beta C$$

where $\mathrm{op}(X) = X, X^T, \overline{X},$ or X^H, α and β are scalars, and A, B, and C are matrices. $\mathrm{op}(A)$ is an m by k matrix, $\mathrm{op}(B)$ is a k by n matrix, and C is an m by n matrix.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Example

```
REAL*4 A(20,40), B(20,30), C(40,30), ALPHA, BETA
M = 10
N = 20
K = 15
LDA = 20
LDB = 20
LDC = 40
ALPHA = 2.0
BETA = 2.0
CALL SGEMM ('T','N',M,N,K,ALPHA,A,LDA,B,LDB,BETA,C,LDC)
```

This Fortran code computes the product $C \leftarrow \alpha A^T B + \beta C$ where A is a real general matrix. A is a 15 by 10 real general matrix embedded in array A. B is a 15 by 20 real general matrix embedded in array B. C is a 10 by 20 real general matrix embedded in array C.

SGEMS DGEMS CGEMS ZGEMS
Matrix-Matrix Subtraction

Format

{S,D,C,Z}GEMS (transa, transb, m, n, alpha, a, lda, beta, b, ldb, c, ldc)

Arguments

transa
character*1
On entry, specifies the form of $\text{op}(A)$ as follows:

If **transa** = 'N' or 'n', $\text{op}(A) = A$
If **transa** = 'T' or 't', $\text{op}(A) = A^T$
If **transa** = 'R' or 'r', $\text{op}(A) = \overline{A}$
If **transa** = 'C' or 'c', $\text{op}(A) = A^H$

On exit, **transa** is unchanged.

transb
character*1
On entry, specifies the form of $\text{op}(B)$ as follows:

If **transb** = 'N' or 'n', $\text{op}(B) = B$
If **transb** = 'T' or 't', $\text{op}(B) = B^T$
If **transb** = 'R' or 'r', $\text{op}(B) = \overline{B}$
If **transb** = 'C' or 'c', $\text{op}(B) = B^H$

On exit, **transb** is unchanged.

m
integer*4
On entry, the number of rows in the matrices $\text{op}(A)$, $\text{op}(B)$, and C; $m \geq 0$.
On exit, **m** is unchanged.

n
integer*4
On entry, the number of columns in the matrices $\text{op}(A)$, $\text{op}(B)$, and C; $m \geq 0$.
On exit, **n** is unchanged.

alpha
Input real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by k.
For $\text{op}(A) = A$ or $\overline{A}$, $k = n$ and the leading m by n part of array A contains the matrix A.
For $\text{op}(A) = A^T$ or A^H, $k = m$ and the leading n by m part of array A contains the matrix A.
On exit, **a** is unchanged.

lda
integer*4
On entry, specifies the first dimension of array A.
For $\text{op}(A) = A$ or $\overline{A}$, $lda \geq \max(1, m)$.
For $\text{op}(A) = A^T$ or A^H, $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

beta
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar β.
On exit, **beta** is unchanged.

b
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array A with dimensions ldb by k.
For $\text{op}(B) = B$ or $\overline{B}$, $k = n$ and the leading m by n part of array B contains the matrix B.
For $\text{op}(B) = B^T$ or B^H, $k = m$ and the leading n by m part of array B contains the matrix B.

ldb
integer*4
On entry, specifies the first dimension of array B.
For $\text{op}(B) = B$ or $\overline{B}$, $ldb \geq \max(1, m)$.
For $\text{op}(B) = B^T$ or B^H, $ldb \geq \max(1, n)$.
On exit, **ldb** is unchanged.

c
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with the dimension ldc by at least n.
On exit, the leading m by n part of array C is overwritten by the matrix $\alpha\text{op}(A) - \beta\text{op}(B)$.

ldc
integer*4
On entry, specifies the first dimension of array C; $ldc \geq \max(1, m)$.
On exit, **ldc** is unchanged.

Description

The _GEMS routines perform one of the following matrix-matrix operations:

$$C \leftarrow \alpha \mathrm{op}(A) - \beta \mathrm{op}(B)$$

where $\mathrm{op}(X) = X, X^T, \overline{X},$ or $\overline{X}^T$, α and β are scalars, and A, B, and C are matrices. $\mathrm{op}(A)$, $\mathrm{op}(B)$, and C are m by n matrices.

These subroutines can also perform the following operation when $lda = ldc$, and **transa** = 'N' or 'n', that is, when $\mathrm{op}(A) = A$:

$$A \leftarrow \alpha A - \beta \mathrm{op} B$$

where $\mathrm{op}(X) = X, X^T, \overline{X},$ or X^H, α and β are scalars, and A and B are m by n matrices.

SGEMT DGEMT CGEMT ZGEMT
Matrix-Matrix Copy

Format

{S,D,C,Z}GEMT (trans, m, n, alpha, a, lda, b, ldb)

Arguments

trans
character*1
On entry, specifies the form of op(A) as follows:

When **trans** = 'N' or 'n', $\mathrm{op}(A) = A$
When **trans** = 'T' or 't', $\mathrm{op}(A) = A^T$
When **trans** = 'R' or 'r', $\mathrm{op}(A) = \overline{A}$
When **trans** = 'C' or 'c', $\mathrm{op}(A) = A^H$

On exit, **trans** is unchanged.

m
integer*4
On entry, the number of rows in the matrices $\mathrm{op}(A)$ and B; $m \geq 0$.
On exit, **m** is unchanged.

n
integer*4
On entry, the number of columns in the matrices $\mathrm{op}(A)$, and B; $n \geq 0$.
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by k.
For $\mathrm{op}(A) = A$ or $\overline{A}$, $k = n$ and the leading m by n part of array A contains the matrix A.
For $\mathrm{op}(A) = A^T$ or A^H, $k = m$ and the leading n by m part of array A contains the matrix A.
On exit, **a** is unchanged.

lda
integer*4
On entry, specifies the first dimension of array A.
For $\mathrm{op}(A) = A$ or $\overline{A}$, $lda \geq \max(1, m)$.
For $\mathrm{op}(A) = A^T$ or A^H, $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

b
real*4 | real*8 | complex*8 | complex*16
On entry, an array with dimensions ldb by n.
On exit, the leading m by n part of the array B is overwritten by the matrix $\alpha\mathrm{op}(A)$.

ldb
integer*4
On entry, specifies the first dimension of array B; $ldb \geq \max(1, m)$.
On exit, **ldb** is unchanged.

Description

The _GEMT routines perform the following operation:

$$B \leftarrow \alpha\mathrm{op}(A)$$

$\mathrm{op}(X) = X, X^T, \overline{X},$ or $\overline{X}^T$, α is a scalar, and A and B are matrices. $\mathrm{op}(A)$ and B are m by n matrices.

These subroutines can also perform matrix scaling when $lda = ldb$, and **trans** = 'N', 'n', 'R', or 'r':

$$A \leftarrow \alpha\mathrm{op}(A)$$

where $\mathrm{op}(X) = X$ or $\overline{X}$, α is a scalar, and A and $\mathrm{op}(A)$ are m by n matrices.

An in place matrix transpose or conjugate transpose may be performed when $lda = ldb$, **trans** = 'T', 't', 'C', or 'c', and $m = n$:

$$A \leftarrow \alpha\mathrm{op}(A)$$

where $\mathrm{op}(X) = X^T$ or X^H, α is a scalar, and A and $\mathrm{op}(A)$ are m by n matrices.

SSYMM DSYMM CSYMM ZSYMM CHEMM ZHEMM Matrix-Matrix Product and Addition for a Symmetric or Hermitian Matrix

Format

{S,D,C,Z}SYMM (side, uplo, m, n, alpha, a, lda, b, ldb, beta, c, ldc)

{C,Z}HEMM (side, uplo, m, n, alpha, a, lda, b, ldb, beta, c, ldc)

Arguments

side
character*1
On entry, specifies whether the symmetric matrix A multiplies B on the left side or the right side:

> If **side** = 'L' or 'l', the operation is $C \leftarrow \alpha AB + \beta C$.
> If **side** = 'R' or 'r', the operation is $C \leftarrow \alpha BA + \beta C$.

On exit, **side** is unchanged.

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the symmetric matrix A is referenced:

> If **uplo** = 'U' or 'u', the upper-triangular part of A is referenced.
> If **uplo** = 'L' or 'l', the lower-triangular part of A is referenced.

On exit, **uplo** is unchanged.

m
integer*4
On entry, the number of rows of the matrix C; $m \geq 0$
On exit, **m** is unchanged.

n
integer*4
On entry, the number of columns of the matrix C; $n \geq 0$
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by ka.
If the multiplication is on the left side, $ka \geq m$ and the leading m by m part of the array contains the matrix A.
If the multiplication is on the right side, $ka \geq n$ and the leading n by n part of the array A must contain the matrix A.
In either case, when the leading part of the array is specified as the upper part, the upper triangular part of array A contains the upper-triangular part of the matrix A, and the lower-triangular part of matrix A is not referenced. When

the lower part is specified, the lower triangular part of the array A contains the lower triangular part of the matrix A, and the upper-triangular part of A is not referenced.

In complex Hermitian matrices, the imaginary parts of the diagonal elements need not be initialized. They are assumed to be zero.

On exit, **a** is unchanged.

lda

integer*4
On entry, the first dimension of array A. When multiplication is on the left, $lda \geq \max(1, m)$. When multiplication is on the right, $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

b

real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array B of dimensions ldb by at least n. The leading m by n part of the array B must contain the matrix B.
On exit, **b** is unchanged.

ldb

integer*4
On entry, the first dimension of B; $ldb \geq \max(1, m)$
On exit, **ldb** is unchanged.

beta

real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar β.
On exit, **beta** is unchanged.

c

real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array with the dimension ldc by at least n.
On exit, **c** is overwritten; the array C is overwritten by the m by n updated matrix.

ldc

integer*4
On entry, the first dimension of array C; $ldc \geq \max(1, n)$
On exit, **ldc** is unchanged.

Description

These routines compute a matrix-matrix product and addition for a real or complex symmetric matrix or a complex Hermitian matrix:

$$C \leftarrow \alpha AB + \beta C$$

$$C \leftarrow \alpha BA + \beta C$$

α and β are scalars, A is the symmetric or Hermitian matrix, and B and C are m by n matrices.

Example

```
REAL*4 A(20,20), B(30,40), C(30,50), ALPHA, BETA
M = 10
N = 20
LDA = 20
LDB = 30
LDC = 30
ALPHA = 2.0
BETA = 3.0
CALL SSYMM ('L','U',M,N,ALPHA,A,LDA,B,LDB,BETA,C,LDC)
```

This Fortran code computes the product of a symmetric matrix and a rectangular matrix. The operation is $C \leftarrow \alpha AB + \beta C$ where A is a 10 by 10 real symmetric matrix embedded in array A, B is a 10 by 20 real matrix embedded in array B, and C is a 10 by 20 real matrix embedded in array C. The leading 10 by 10 upper-triangular part of the array A contains the upper-triangular part of the matrix A. The lower-triangular part of A is not referenced.

```
COMPLEX*16 A(30,40), B(15,20), C(19,13), ALPHA, BETA
M = 12
N = 7
LDA = 30
LDB = 15
LDC = 19
ALPHA = (2.0D0, 0.0D0)
BETA = (0.0D0, -2.0D0)
CALL ZHEMM ('R','L',M,N,ALPHA,A,LDA,B,LDB,BETA,C,LDC)
```

This Fortran code computes the product of a Hermitian matrix and a rectangular matrix. The operation is $C \leftarrow \alpha BA + \beta C$ where A is a 7 by 7 complex Hermitian matrix embedded in array A, B is a 12 by 7 complex matrix embedded in array B, and C is a 12 by 7 complex matrix embedded in array C. The leading 7 by 7 lower-triangular part of the array A contains the lower-triangular part of the matrix A. The upper-triangular part of A is not referenced.

SSYRK DSYRK CSYRK ZSYRK
Rank-k Update of a Symmetric Matrix

Format

{S,D,C,Z}SYRK (uplo, trans, n, k, alpha, a, lda, beta, c, ldc)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the symmetric matrix C is to be referenced:

If **uplo** = 'U' or 'u', the upper-triangular part of C is to be referenced.
If **uplo** = 'L' or 'l', the lower-triangular part of C is to be referenced.

On exit, **uplo** is unchanged.

trans
character*1
On entry, specifies the operation to be performed:

If **trans** = 'N' or 'n', $C \leftarrow \alpha AA^T + \beta C$
If **trans** = 'T' or 't', $C \leftarrow \alpha A^T A + \beta C$

On exit, **trans** is unchanged.

n
integer*4
On entry, specifies the order of the matrix C; $n \geq 0$
On exit, **n** is unchanged.

k
integer*4
On entry, the number of columns of the matrix A when **trans** = 'N' or 'n', or the number of rows of the matrix A when **trans** = 'T' or 't'; $k \geq 0$.
On exit, **k** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by ka.
For **trans** = 'N' or 'n', $ka \geq k$ and the leading n by k portion of the array A contains the matrix A.
For **trans** = 'T' or 't', $ka \geq n$ and the leading k by n part of the array A contains the matrix A.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A.
For **trans** = 'N' or 'n', $lda \geq \max(1, n)$.
For **trans** = 'T', 't', 'C' or 'c', $lda \geq \max(1, k)$.
On exit, **lda** is unchanged.

beta
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar β.
On exit, **beta** is unchanged.

c
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array C of dimensions ldc by at least n. If **uplo** specifies the upper part, the leading n by n upper-triangular part of the array C must contain the upper-triangular part of the symmetric matrix C, and the strictly lower-triangular part of C is not referenced.

If **uplo** specifies the lower part, the leading n by n lower-triangular part of the array C must contain the lower-triangular part of the symmetric matrix C, and the strictly upper-triangular part of C is not referenced.

On exit, **c** is overwritten; the triangular part of the array C is overwritten by the triangular part of the updated matrix.

ldc
integer*4
On entry, the first dimension of array C; $ldc \geq \max(1, n)$
On exit, **ldc** is unchanged.

Description

The _SYRK routines perform the rank-k update of a symmetric matrix:

$$C \leftarrow \alpha AA^T + \beta C$$

$$C \leftarrow \alpha A^T A + \beta C$$

α and β are scalars, C is an n by n symmetric matrix. In the first case, A is an n by k matrix, and in the second case, A is a k by n matrix.

Example

```
REAL*4 A(40,20), C(20,20), ALPHA, BETA
LDA = 40
LDC = 20
N = 10
K = 15
ALPHA = 1.0
BETA = 2.0
CALL SSYRK ('U','N',N,K,ALPHA,A,LDA,BETA,C,LDC)
```

This Fortran code computes the rank-k update of the real symmetric matrix C: $C \leftarrow \alpha AA^T + \beta C$. C is a 10 by 10 matrix, and A is a 10 by 15 matrix. Only the upper-triangular part of C is referenced. The leading 10 by 15 part of array A contains the matrix A. The leading 10 by 10 upper-triangular part of array C contains the upper-triangular matrix C.

CHERK ZHERK
Rank-k Update of a Complex Hermitian Matrix

Format

{C,Z}HERK (uplo, trans, n, k, alpha, a, lda, beta, c, ldc)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the Hermitian matrix C is to be referenced:

If **uplo** = 'U' or 'u', the upper-triangular part of C is to be referenced.
If **uplo** = 'L' or 'l', the lower-triangular part of C is to be referenced.

On exit, **uplo** is unchanged.

trans
character*1
On entry, specifies the operation to be performed:

If **trans** = 'N' or 'n', $C \leftarrow \alpha AA^H + \beta C$
If **trans** = 'C' or 'c', $C \leftarrow \alpha A^H A + \beta C$

On exit, **trans** is unchanged.

n
integer*4
On entry, the order of the matrix C; $n \geq 0$
On exit, **n** is unchanged.

k
integer*4
On entry, the number of columns of the matrix A when **trans** = 'N' or 'n', or the number of rows of the matrix A when **trans** = 'C' or 'c'; $k \geq 0$.
On exit, **k** is unchanged.

alpha
real*4 | real*8
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by ka.
For **trans** = 'N' or 'n', $ka \geq k$ and the leading n by k portion of the array A contains the matrix A.
For **trans** = 'T', 't', 'C', or 'c', $ka \geq n$ and the leading k by n part of the array A contains the matrix A.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A.
For **trans** = 'N' or 'n' $lda \geq \max(1, n)$.
For **trans** = 'C' or 'c', $lda \geq \max(1, k)$.
On exit, **lda** is unchanged.

beta
real*4 | real*8
On entry, the scalar β.
On exit, **beta** is unchanged.

c
complex*8 | complex*16
On entry, a two-dimensional array C of dimensions ldc by at least n.

If **uplo** specifies the upper part, the leading n by n upper-triangular part of the array C must contain the upper-triangular part of the Hermitian matrix C, and the strictly lower-triangular part of C is not referenced.

If **uplo** specifies the lower part, the leading n by n lower-triangular part of the array C must contain the lower-triangular part of the Hermitian matrix C, and the strictly upper-triangular part of C is not referenced.

The imaginary parts of the diagonal elements need not be initialized. They are assumed to be 0, and on exit, they are set to 0.
On exit, **c** is overwritten; the triangular part of the array C is overwritten by the triangular part of the updated matrix.

ldc
integer*4
On entry, the first dimension of array C; $ldc \geq \max(1, n)$
On exit, **ldc** is unchanged.

Description

CHERK and ZHERK perform the rank-k update of a complex Hermitian matrix:

$$C \leftarrow \alpha AA^H + \beta C$$

$$C \leftarrow \alpha A^H A + \beta C$$

α and β are real scalars, C is an n by n Hermitian matrix, and A is an n by k matrix in the first case and a k by n matrix in the second case.

Example

```
COMPLEX*8 A(40,20), C(20,20)
REAL*4 ALPHA, BETA
LDA = 40
LDC = 20
N = 10
K = 15
ALPHA = 1.0
BETA = 2.0
CALL CHERK ('U','N',N,K,ALPHA,A,LDA,BETA,C,LDC)
```

This Fortran code computes the rank-k update of the complex Hermitian matrix C: $C \leftarrow \alpha AA^H + \beta C$. C is a 10 by 10 matrix, and A is a 10 by 15 matrix. Only the upper-triangular part of C is referenced. The leading 10 by 15 part of array A contains the matrix A. The leading 10 by 10 upper-triangular part of array C contains the upper-triangular matrix C.

SSYR2K DSYR2K CSYR2K ZSYR2K
Rank-2k Update of a Symmetric Matrix

Format

{S,D,C,Z}SYR2K (uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the symmetric matrix C is to be referenced:

If **uplo** = 'U' or 'u', the upper-triangular part of C is to be referenced.
If **uplo** = 'L' or 'l', the lower-triangular part of C is to be referenced.

On exit, **uplo** is unchanged.

trans
character*1
On entry, specifies the operation to be performed:

If **trans** = 'N' or 'n', $C \leftarrow \alpha AB^T + \alpha BA^T + \beta C$
If **trans** = 'T' or 't', $C \leftarrow \alpha A^T B + \alpha B^T A + \beta C$

On exit, **trans** is unchanged.

n
integer*4
On entry, the order n of the matrix C; $n \geq 0$
On exit, **n** is unchanged.

k
integer*4
On entry, the number of columns of the matrices A and B when **trans** = 'N' or 'n', or the number of rows of the matrix A and B when **trans** = 'T' or 't': $k \geq 0$.
On exit, **k** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by ka.
For **trans** = 'N' or 'n', $ka \geq k$ and the leading n by k portion of the array A contains the matrix A.
For **trans** = 'T' or 't', $ka \geq n$ and the leading k by n part of the array A contains the matrix A.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A.
For **trans** = 'N' or 'n' $lda \geq \max(1, n)$.
For **trans** = 'T' or 't', $lda \geq \max(1, k)$.
On exit, **lda** is unchanged.

b
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array B with dimensions ldb by kb.
For **trans** = 'N' or 'n', $kb \geq k$ and the leading n by k portion of the array B contains the matrix B.
For **trans** = 'T' or 't', $kb \geq n$ and the leading k by n part of the array B contains the matrix B.
On exit, **b** is unchanged.

ldb
integer*4
On entry, the first dimension of array B.
For **trans** = 'N' or 'n', $ldb \geq \max(1, n)$.
For **trans** = 'T' or 't', $ldb \geq \max(1, k)$.
On exit, **ldb** is unchanged.

beta
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar β.
On exit, **beta** is unchanged.

c
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array C of dimensions ldc by at least n.

If **uplo** specifies the upper part, the leading n by n upper-triangular part of the array C must contain the upper-triangular part of the symmetric matrix C, and the strictly lower-triangular part of C is not referenced.

If **uplo** specifies the lower part, the leading n by n lower-triangular part of the array C must contain the lower-triangular part of the symmetric matrix C, and the strictly upper-triangular part of C is not referenced.
On exit, **c** is overwritten; the triangular part of the array C is overwritten by the triangular part of the updated matrix.

ldc
integer*4
On entry, the first dimension of array C; $ldc \geq \max(1, n)$
On exit, **ldc** is unchanged.

Description

The _SYR2K routines perform the rank-2k update of a symmetric matrix:

$$C \leftarrow \alpha AB^T + \alpha BA^T + \beta C$$

$$C \leftarrow \alpha A^T B + \alpha B^T A + \beta C$$

α and β are scalars, C is an n by n symmetric matrix, and A and B are n by k matrices in the first case and k by n matrices in the second case.

Example

```
REAL*4 A(40,10), B(40,10), C(20,20), ALPHA, BETA
LDA = 40
LDB = 30
LDC = 20
N = 18
K = 10
ALPHA = 1.0
BETA = 2.0
CALL SSYR2K ('U','N',N,K,ALPHA,A,LDA,B,LDB,BETA,C,LDC)
```

This Fortran code computes the rank-2k update of the real symmetric matrix C: $C \leftarrow \alpha AB^T + \alpha BA^T + \beta C$. Only the upper-triangular part of C is referenced. The leading 18 by 10 part of array A contains the matrix A. The leading 18 by 10 part of array B contains the matrix B. The leading 18 by 18 upper-triangular part of array C contains the upper-triangular matrix C.

CHER2K ZHER2K
Rank-2k Update of a Complex Hermitian Matrix

Format

{C,Z}HER2K (uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc)

Arguments

uplo
character*1
On entry, specifies whether the upper- or lower-triangular part of the Hermitian matrix C is to be referenced:

If **uplo** = 'U' or 'u', the upper-triangular part of C is to be referenced.
If **uplo** = 'L' or 'l', the lower-triangular part of C is to be referenced.

On exit, **uplo** is unchanged.

trans
character*1
On entry, specifies the operation to be performed:

If **trans** = 'N' or 'n', $C \leftarrow \alpha AB^H + \overline{\alpha}BA^H + \beta C$
If **trans** = 'C' or 'c', $C \leftarrow \alpha A^H B + \overline{\alpha}B^H A + \beta C$

On exit, **trans** is unchanged.

n
integer*4
On entry, the order of the matrix C; $n \geq 0$
On exit, **n** is unchanged.

k
integer*4
On entry, the number of columns of the matrices A and B when **trans** = 'N' or 'n', or the number of rows of the matrices A and B when **trans** = 'C' or 'c'; $k \geq 0$.
On exit, **k** is unchanged.

alpha
complex*8 | complex*16
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by ka.
For **trans** = 'N' or 'n', $ka \geq k$ and the leading n by k portion of the array A contains the matrix A.
For **trans** = 'C' or 'c', $ka \geq n$ and the leading k by n part of the array A contains the matrix A.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of array A.
For **trans** = 'N' or 'n', $lda \geq \max(1, n)$.
For **trans** = 'C' or 'c', $lda \geq \max(1, k)$.
On exit, **lda** is unchanged.

b
complex*8 | complex*16
On entry, a two-dimensional array B with dimensions ldb by kb.
For **trans** = 'N' or 'n', $kb \geq k$ and the leading n by k portion of the array B contains the matrix B.
For **trans** = 'C' or 'c', $kb \geq n$ and the leading k by n part of the array B contains the matrix B.
On exit, **b** is unchanged.

ldb
integer*4
For **trans** = 'N' or 'n' $ldb \geq \max(1, n)$.
For **trans** = 'C' or 'c', $ldb \geq \max(1, k)$.
On exit, **ldb** is unchanged.

beta
real*4 | real*8
On entry, specifies the scalar β.
On exit, **beta** is unchanged.

c
complex*8 | complex*16
On entry, a two-dimensional array C of dimensions ldc by at least n.

If **uplo** specifies the upper part, the leading n by n upper-triangular part of the array C must contain the upper-triangular part of the Hermitian matrix C, and the strictly lower-triangular part of C is not referenced.

If **uplo** specifies the lower part, the leading n by n lower-triangular part of the array C must contain the lower-triangular part of the Hermitian matrix C, and the strictly upper-triangular part of C is not referenced.

The imaginary parts of the diagonal elements need not be initialized. They are assumed to be 0, and on exit, they are set to 0.

On exit, **c** is overwritten; the triangular part of the array C is overwritten by the triangular part of the updated matrix.

ldc
integer*4
On entry, the first dimension of array C; $ldc \geq \max(1, n)$
On exit, **ldc** is unchanged.

Description

CHER2K and ZHER2K perform the rank-2k update of a complex Hermitian matrix:

$$C \leftarrow \alpha AB^H + \overline{\alpha} BA^H + \beta C$$

$$C \leftarrow \alpha A^H B + \overline{\alpha} B^H A + \beta C$$

where α is a complex scalar, β is a real scalar, and C is an n by n Hermitian matrix. In the first case, A and B are n by k matrices, and in the second case, they are k by n matrices.

Example

```
COMPLEX*8 A(40,10), B(40,10), C(20,20), ALPHA
REAL*4 BETA
LDA = 40
LDB = 30
LDC = 20
N = 18
K = 10
ALPHA = (1.0, 1.0)
BETA = 2.0
CALL CHER2K ('U','N',N,K,ALPHA,A,LDA,B,LDB,BETA,C,LDC)
```

This Fortran code computes the rank-2k update of the complex Hermitian matrix C: $C \leftarrow \alpha AB^H + \overline{\alpha} BA^H + \beta C$. Only the upper-triangular part of C is referenced. The leading 18 by 10 part of array A contains the matrix A. The leading 18 by 10 part of array B contains the matrix B. The leading 18 by 18 upper-triangular part of array C contains the upper-triangular matrix C.

STRMM DTRMM CTRMM ZTRMM
Matrix-Matrix Product for Triangular Matrix

Format

{S,D,C,Z}TRMM (side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb)

Arguments

side
character*1
On entry, specifies whether $\mathrm{op}(A)$ multiplies B on the left or right in the operation:

If **side** = 'L' or 'l', the operation is $B \leftarrow \alpha \mathrm{op}(A)B$.
If **side** = 'R' or 'r', the operation is $B \leftarrow \alpha B\mathrm{op}(A)$.

On exit, **side** is unchanged.

uplo
character*1
On entry, specifies whether the matrix A is an upper- or lower-triangular matrix:

If **uplo** = 'U' or 'u', the matrix A is an upper-triangular matrix.
If **uplo** = 'L' or 'l', the matrix A is a lower-triangular matrix.

On exit, **uplo** is unchanged.

transa
character*1
On entry, specifies the form of $\mathrm{op}(A)$ used in the matrix multiplication:

If **transa** = 'N' or 'n', $\mathrm{op}(A) = A$.
If **transa** = 'T' or 't', $\mathrm{op}(A) = A^T$.

If **transa** = 'C' or 'c', $\mathrm{op}(A) = A^H$.

On exit, **transa** is unchanged.

diag
character*1
On entry, specifies whether the matrix A is unit-triangular:

If **diag** = 'U' or 'u', A is a unit-triangular matrix.
If **diag** = 'N' or 'n', A is not a unit-triangular matrix.

On exit, **diag** is unchanged.

m
integer*4
On entry, the number of rows of the matrix B; $m \geq 0$
On exit, **m** is unchanged.

n
integer*4
On entry, the number of columns of the matrix B; $n \geq 0$
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by k.
If the multiplication is on the left side, $k \geq m$ and the leading m by m part of the array contains the matrix A.
If the multiplication is on the right side, $k \geq n$ and the leading n by n part of the array A must contain the matrix A.
In either case, when the leading part of the array is specified as the upper part, the upper triangular part of array A contains the upper-triangular part of the matrix A, and the lower-triangular part of matrix A is not referenced. When the lower part is specified, the lower triangular part of the array A contains the lower triangular part of the matrix A, and the upper-triangular part of A is not referenced.

If matrix A is unit-triangular, its diagonal elements are assumed to be unity and are not referenced.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of A. When multiplication is on the left, $lda \geq \max(1, m)$. When multiplication is on the right, $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

b
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array B of dimensions ldb by at least n. The leading m by n part of the array B must contain the matrix B.
On exit, **b** is overwritten by the m by n updated matrix.

ldb
integer*4
On entry, the first dimension of B; $ldb \geq \max(1, m)$
On exit, **ldb** is unchanged.

Description

STRMM and DTRMM compute a matrix-matrix product for a real triangular matrix or its transpose. CTRMM and ZTRMM compute a matrix-matrix product for a complex triangular matrix, its transpose, or its conjugate transpose.

$$B \leftarrow \alpha \mathrm{op}(A) B$$

$$B \leftarrow \alpha B(\mathrm{op}(A))$$

where $\mathrm{op}(A) = A, A^T, \text{ or } A^H$

α is a scalar, B is an m by n matrix, and A is a unit or non-unit, upper- or lower-triangular matrix.

Example

```
REAL*8 A(25,40), B(30,35), ALPHA
M = 15
N = 18
LDA = 25
LDB = 30
ALPHA = -1.0D0
CALL DTRMM ('R','L','T','U',M,N,ALPHA,A,LDA,B,LDB)
```

This Fortran code solves the system $B \leftarrow \alpha B A^T$ where A is a lower-triangular real matrix with a unit diagonal. A is an 18 by 18 real triangular matrix embedded in array A, and B is a 15 by 18 real rectangular matrix embedded in array B. The leading 18 by 18 lower-triangular part of the array A must contain the lower-triangular matrix A. The upper-triangular part of A and the diagonal are not referenced.

```
COMPLEX*16 A(25,40), B(30,35), ALPHA
M = 15
N = 18
LDA = 25
LDB = 30
ALPHA = (-1.0D0, 2.0D0)
CALL ZTRMM ('R','L','T','U',M,N,ALPHA,A,LDA,B,LDB)
```

This Fortran code solves the system $B \leftarrow \alpha B A^T$ where A is a lower-triangular complex matrix with a unit diagonal. A is an 18 by 18 complex triangular matrix embedded in array A, and B is a 15 by 18 complex rectangular matrix embedded in array B. The leading 18 by 18 lower-triangular part of the array A must contain the lower-triangular matrix A. The upper-triangular part of A and the diagonal are not referenced.

STRSM DTRSM CTRSM ZTRSM
Solve a Triangular System of Equations with a Triangular Coefficient Matrix

Format

{S,D,C,Z}TRSM (side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb)

Arguments

side
character*1
On entry, specifies whether $\mathrm{op}(A)$ is on the left side or the right side of X in the system of equations:

If **side** = 'L' or 'l', the system is $\mathrm{op}(A)X = \alpha B$.
If **side** = 'R' or 'r', the system is $X\mathrm{op}(A) = \alpha B$.

On exit, **side** is unchanged.

uplo
character*1
On entry, specifies whether the matrix A is an upper- or lower-triangular matrix:

If **uplo** = 'U' or 'u', the matrix A is an upper-triangular matrix.
If **uplo** = 'L' or 'l', the matrix A is a lower-triangular matrix.

On exit, **uplo** is unchanged.

transa
character*1
On entry, specifies the form of $\mathrm{op}(A)$ used in the system of equations:

If **transa** = 'N' or 'n', $\mathrm{op}(A) = A$.
If **transa** = 'T' or 't', $\mathrm{op}(A) = A^T$.
If **transa** = 'C' or 'c', $\mathrm{op}(A) = A^H$.

On exit, **transa** is unchanged.

diag
character*1
On entry, specifies whether the matrix A is unit-triangular:

If **diag** = 'U' or 'u', A is a unit-triangular matrix.
If **diag** = 'N' or 'n', A is not a unit-triangular matrix.

On exit, **diag** is unchanged.

m
integer*4
On entry, the number of rows m of the matrix B; $m \geq 0$
On exit, **m** is unchanged.

n
integer*4
On entry, the number of columns n of the matrix B; $n \geq 0$
On exit, **n** is unchanged.

alpha
real*4 | real*8 | complex*8 | complex*16
On entry, specifies the scalar α.
On exit, **alpha** is unchanged.

a
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array A with dimensions lda by k.
If the multiplication is on the left side, $k \geq m$ and the leading m by m part of the array contains the matrix A.
If the multiplication is on the right side, $k \geq n$ and the leading n by n part of the array A must contain the matrix A.
In either case, when the leading part of the array is specified as the upper part, the upper triangular part of array A contains the upper-triangular part of the matrix A, and the lower-triangular part of matrix A is not referenced. When the lower part is specified, the lower triangular part of the array A contains the lower triangular part of the matrix A, and the upper-triangular part of A is not referenced.

If matrix A is unit-triangular, its diagonal elements are assumed to be unity and are not referenced.
On exit, **a** is unchanged.

lda
integer*4
On entry, the first dimension of A. When multiplication is on the left, $lda \geq \max(1, m)$. When multiplication is on the right, $lda \geq \max(1, n)$.
On exit, **lda** is unchanged.

b
real*4 | real*8 | complex*8 | complex*16
On entry, a two-dimensional array B of dimensions ldb by at least n. The leading m by n part of the array B must contain the right-hand-side matrix B.
On exit, **b** is overwritten by the m by n solution matrix X.

ldb
integer*4
On entry, the first dimension of B; $ldb \geq \max(1, m)$
On exit, **ldb** is unchanged.

Description

The _TRSM routines solve a triangular system of equations where the coefficient matrix A is a triangular matrix:

$$\mathrm{op}(A)X = \alpha B$$

$$X\mathrm{op}(A) = \alpha B$$

$\mathrm{op}(A) = A, A^T,$ or A^H, α is a scalar, X and B are m by n matrices, and A is a unit or non-unit, upper- or lower-triangular matrix.

Example

```
REAL*8 A(100,40), B(40,20), ALPHA
M = 16
N = 18
LDA = 100
LDB = 40
ALPHA = 2.0D0
CALL DTRSM ('L','U','N','U',M,N,ALPHA,A,LDA,B,LDB)
```

This Fortran code solves the system $AX = \alpha B$ where A is an upper-triangular real matrix with a unit diagonal. X and B are 16 by 18 matrices. The leading 16 by 16 upper-triangular part of the array A must contain the upper-triangular matrix A. The leading 16 by 18 part of the array B must contain the matrix B. The lower-triangular part of A and the diagonal are not referenced. The leading 16 by 18 part of B is overwritten by the solution matrix X.

Fast Fourier

This section provides descriptions of the routines for fast transforms. The four versions of each routine are titled by the name using a leading underscore character. The section is ordered in the following way:

- By the type of FFT:

  one-dimensional
  two-dimensional
  three-dimensional
  group

- By function within each type of FFT:

  one-step procedure
  initialization
  application
  exit

SFFT DFFT CFFT ZFFT
Fast Fourier Transform in One Dimension (Serial and Parallel Versions)

Format

Real transform:

status = {S,D}FFT (input_format, output_format, direction, in, out, n, stride)

Complex transform in complex data format:

status = {C,Z}FFT (input_format, output_format, direction, in, out, n, stride)

Complex transform in real data format:

status = {C,Z}FFT (input_format, output_format, direction, in_real, in_imag, out_real, out_imag, n, stride)

Arguments

input_format, output_format
character*(*)
Identifies the data type of the input and the format to be used to store the data, regardless of the data type. For example, a complex sequence can be stored in real format.

The character 'R' specifies the format as real; the character 'C' specifies the format as complex. As convenient, use either uppercase or lowercase characters, and either spell out or abbreviate the word.

The following table shows the valid values:

Subprogram	Input Format	Output Format	Direction
{S,D}	'R'	'C'	'F'
	'C'	'R'	'B'
	'R'	'R'	'F' or 'B'
{C,Z}	'R'	'R'	'F' or 'B'
	'C'	'C'	'F' or 'B'

For complex transforms, the type of data determines what other arguments are needed. When both the input and output data are real, the complex functions store the data as separate arrays for imaginary and real data so additional arguments are needed.

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8 | complex*8 | complex*16
Both the arguments are one-dimensional arrays. The input and output arrays can be the same array. The IN array contains the data to be transformed. The OUT array contains the transformed data.

in_real, out_real, in_imag, out_imag
real*4 | real*8
Use these arguments when performing a complex transform on real data format and storing the result in a real data format.

n
integer*4
Specifies the number of values to be transformed, that is, the length of the array to be transformed, and therefore the required size of the resulting array; $n > 0$.

Subprogram	Input Format	Output Format	Minimum Size
{S,D}	'R'	'C'	n+2 (n must be even)
	'C'	'R'	n+2 (n must be even)
	'R'	'R'	n (n must be even)
{C,Z}	'R'	'R'	n
	'C'	'C'	n

stride
integer*4
Specifies the distance between consecutive elements in the input and output arrays. The distance must be at least 1.

Description

The _FFT functions compute the fast Fourier transform of one-dimensional data in one step. The SFFT and DFFT functions perform the forward Fourier transform of a real sequence and store the result in either real or complex data format. These functions also perform the inverse Fourier transform of a complex sequence into a real sequence.

The CFFT and ZFFT functions perform Fourier transforms on a complex sequence. However, the argument list is different, depending on the data format in which the output data is stored. See Section 9.1.3.2 for an explanation of real and complex data format.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
4 (real transforms only)	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()
16	DXML_BAD_FORMAT_STRING()
18 (real transforms only)	DXML_BAD_FORMAT_FOR_DIRECTION()

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N, STATUS
COMPLEX*16 A(1024), B(1024)
REAL*8 C_REAL(1024),C_IMAG(1024),D_REAL(1024),D_IMAG(1024)
REAL*8 E(1026),F(1026)
REAL*8 G(1024),H(1024)
N = 1024
STATUS = ZFFT('C','C','F',A,B,N,1)
STATUS = ZFFT('R','R','F',C_REAL,C_IMAG,D_REAL,D_IMAG,N,1)
STATUS = DFFT('R','C','F',E,F,N,1)
STATUS = DFFT('C','R','B',F,E,N,1)
STATUS = DFFT('R','R','F',G,H,N,1)
```

This Fortran code computes the following:

- Forward Fourier transform of the complex sequence A to the complex sequence B.
- Forward Fourier transform of the complex sequence C to the complex sequence D. The data C and D are each stored as two real arrays.
- Forward Fourier transform of the real sequence E to the complex sequence F. The data F is stored in complex format.
- Backward Fourier transform of the complex sequence F to the real sequence E.
- Backward Fourier transform of the real sequence G to the complex sequence H stored in real format.

SFFT_INIT DFFT_INIT CFFT_INIT ZFFT_INIT Initialization Step for Fast Fourier Transform in One Dimension (Serial and Parallel Versions)

Format

status = {S,D,C,Z}FFT_INIT (n, fft_struct, stride_1_flag)

Arguments

n
integer*4
Specifies the number of values to be transformed, that is, the length of the array to be transformed; $n > 0$. For real operations, **n** must be even.

fft_struct
record /dxml_s_fft_structure/ for single-precision real operations
record /dxml_d_fft_structure/ for double-precision real operations
record /dxml_c_fft_structure/ for single-precision complex operations
record /dxml_z_fft_structure/ for double-precision complex operations
You must include this argument but it needs no additional definitions. The argument is declared in the program before this function. See Section 9.1.3.3 for more information.

stride_1_flag
logical
Specifies the allowed distance between consecutive elements in the input and output arrays:

TRUE: Stride must be 1.
FALSE: Stride is at least 1.

Description

The _FFT_INIT functions build internal data structures needed to compute fast Fourier transforms of one-dimensional data. These functions are the first step in a three-step procedure. They create the internal data structures, using attributes defined in the file `DXMLDEF.FOR`.

Use the initialization function that is appropriate for the data format. Then use the corresponding application and exit functions to complete the transform. For example, use SFFT_INIT for the internal data structures used by SFFT_APPLY and end with the SFFT_EXIT function.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
4(real transforms only)	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
12	DXML_INS_RES()

SFFT_APPLY DFFT_APPLY CFFT_APPLY ZFFT_APPLY Application Step for Fast Fourier Transform in One Dimension (Serial and Parallel Versions)

Format

Real transform:

status = {S,D}FFT_APPLY (input_format, output_format, direction, in, out, fft_struct, stride)

Complex transform in complex data format:

status = {C,Z}FFT_APPLY (input_format, output_format, direction, in, out, fft_struct, stride)

Complex transform in real data format:

status = {C,Z}FFT_APPLY (input_format, output_format, direction, in_real, in_imag, out_real, out_imag, fft_struct, stride)

Arguments

input_format, output_format
character*(*)
Identifies the data type of the input and the format to be used to store the data, regardless of the data type. For example, a complex sequence can be stored in real format.

The character 'R' specifies the format as real; the character 'C' specifies the format as complex. As convenient, use either uppercase or lowercase characters, and either spell out or abbreviate the word.

The following table shows the valid values:

Subprogram	Input Format	Output Format	Direction
{S,D}	'R'	'C'	'F'
	'C'	'R'	'B'
	'R'	'R'	'F' or 'B'
{C,Z}	'R'	'R'	'F' or 'B'
	'C'	'C'	'F' or 'B'

For complex transforms, the type of data determines what other arguments are needed. When both the input and output data are real, the complex functions store the data as separate arrays for imaginary and real data so additional arguments are needed. See Section 9.1.3.2 for an explanation of real and complex data format.

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8 | complex*8 | complex*16
Both the arguments are one-dimensional arrays. The input and output arrays can be the same array. The IN array contains the data to be transformed. The OUT array contains the transformed data. The size of the output array is determined by the value of **n** provided to the _INIT function.

Subprogram	Input Format	Output Format	Minimum Size
{S,D}	'R'	'C'	n+2 (n must be even)
	'C'	'R'	n+2 (n must be even)
	'R'	'R'	n (n must be even)
{C,Z}	'R'	'R'	n
	'C'	'C'	n

in_real, out_real, in_imag, out_imag
real*4 | real*8
Use these arguments to perform a complex transform on real data format and storing the result in a real data format.

fft_struct
record /dxml_s_fft_structure/ for single-precision real operations
record /dxml_d_fft_structure/ for double-precision real operations
record /dxml_c_fft_structure/ for single-precision complex operations
record /dxml_z_fft_structure/ for double-precision complex operations
The argument refers to the structure created by the _INIT function.

stride
integer*4
Specifies the distance between consecutive elements in the input and output arrays, depending on the value of **stride_1_flag** provided in the _INIT function.

Description

The _FFT_APPLY routine performs the fast Fourier transform of one-dimensional data, in either the forward or backward direction. These routines are the second step of a three-step procedure. The _FFT_APPLY routine computes the fast forward or inverse Fourier transform, using the internal data structures created by the _FFT_INIT subroutine.

Use the _APPLY routines with their corresponding _INIT and _EXIT routines. For example, use SFFT_APPLY after the SFFT_INIT and end with the SFFT_EXIT routine.

The SFFT_APPLY and DFFT_APPLY functions perform the Fourier transform of a real sequence (forward) or a complex sequence (inverse) into real sequence.

The CFFT_APPLY and ZFFT_APPLY functions perform Fourier transforms of a complex sequence into a complex sequence, storing the output in either real or complex data format. However, the argument list depends on the data format of the output. See Section 9.1.3.2 for an explanation of real and complex data format.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()
16	DXML_BAD_FORMAT_STRING()
18 (real transform only)	DXML_BAD_FORMAT_FOR_DIRECTION()

Examples

1.
```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N, STATUS
REAL*8 A(1026), B(1026)
RECORD /DXML_D_FFT_STRUCTURE/ FFT_STRUCT
N = 1024
STATUS = DFFT_INIT(N,FFT_STRUCT,.TRUE.)
STATUS = DFFT_APPLY('R','C','F',A,B,FFT_STRUCT,1)
STATUS = DFFT_EXIT(FFT_STRUCT)
```

This Fortran code computes the forward, real FFT of a vector, a, with length of 1024. The result of the transform is stored in b in complex form. The length of b is 1026 to hold 513 complex values.

2.
```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N, STATUS
COMPLEX*8 A(1024), B(1024)
RECORD /DXML_C_FFT_STRUCTURE/ FFT_STRUCT
N = 1024
STATUS = CFFT_INIT(N,FFT_STRUCT,.TRUE.)
STATUS = CFFT_APPLY('C','C','F',A,B,FFT_STRUCT,1)
STATUS = CFFT_EXIT(FFT_STRUCT)
```

This Fortran code computes the forward, complex FFT of a vector a, with length of 1024. The result of the transform is stored in b in complex form.

SFFT_EXIT DFFT_EXIT CFFT_EXIT ZFFT_EXIT
Final Step for Fast Fourier Transform in One Dimension (Serial and Parallel Versions)

Format

status = {S,D,C,Z}FFT_EXIT (fft_struct)

Arguments

fft_struct
record /dxml_s_fft_structure/ for single-precision real operations
record /dxml_d_fft_structure/ for double-precision real operations
record /dxml_c_fft_structure/ for single-precision complex operations
record /dxml_z_fft_structure/ for double-precision complex operations
This argument must be included but it is not necessary to modify it in any way. It refers to the data structure that was specified by the initialization step. See Section 9.1.3.3 for more information on the data structure.

Description

The _FFT_EXIT functions remove the internal data structures created in the _FFT_INIT functions. These functions are the final step in a three-step procedure. They release the virtual memory that was allocated by the _FFT_INIT functions.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
12	DXML_INS_RES()

SFFT_2D DFFT_2D CFFT_2D ZFFT_2D Fast Fourier Transform in Two Dimensions (Serial and Parallel Versions)

Format

Real transform:

status = {S,D}FFT_2D (input_format, output_format, direction, in, out, ni, nj, lda, ni_stride, nj_stride)

Complex transforms in complex format:

status = {C,Z}FFT_2D (input_format, output_format, direction, in, out, ni, nj, lda, ni_stride, nj_stride)

Complex transform in real data format:

status = {C,Z}FFT_2D (input_format, output_format, direction, in_real, in_imag, out_real, out_imag, ni, nj, lda, ni_stride, nj_stride)

Arguments

input_format, output_format
character*(*)
Identifies the data type of the input and the format to be used to store the data, regardless of the data type. For example, a complex sequence can be stored in real format.

The character 'R' specifies the format as real; the character 'C' specifies the format as complex. As convenient, use either uppercase or lowercase characters, and either spell out or abbreviate the word.

The following table shows the valid values:

Subprogram	Input Format	Output Format	Direction
{S,D}	'R'	'C'	'F'
	'C'	'R'	'B'
	'R'	'R'	'F' or 'B'
{C,Z}	'R'	'R'	'F' or 'B'
	'C'	'C'	'F' or 'B'

For complex data, the type of data determines what other arguments are needed. When both the input and output data are real, the complex routines store the

data as separate arrays for imaginary and real data so additional arguments are needed.

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8 | complex*8 | complex*16
Both the arguments are two-dimensional arrays. The input and output arrays can be the same array. The IN array contains the data to be transformed. The OUT array contains the transformed data.

in_real, out_real, in_imag, out_imag
real*4 | real*8
Use these arguments when performing a complex transform on real data format and storing the result in a real data format.

ni, nj
integer*4
Specifies the size of the first and second dimension of data in the input array; $ni > 0$, $nj > 0$. For SFFT_2D and DFFT_2D, **ni** must be even.

lda
integer*4
Specifies the number of rows in the IN and OUT arrays; $lda \geq ni$. For {S,D} routines, $lda \geq ni + 2$ when the input format is 'R' and the output format is 'C' or the input format is 'C' and the output format is 'R'.

ni_stride, nj_stride
integer*4
Specifies the distance between consecutive elements in a column and row in the IN and OUT arrays; $ni_stride \geq 1$, $nj_stride \geq 1$.

Description

The _FFT_2D routines compute the fast forward or inverse Fourier transform of two-dimensional data in one step. The SFFT_2D and DFFT_2D functions perform the forward Fourier transform of a real sequence and store the result in either real or complex data format. These functions also perform the inverse Fourier transform of a complex sequence into a real sequence.

The CFFT_2D and ZFFT_2D functions perform Fourier transforms on a complex sequence. However, the argument list is different, depending on the data format in which the output data is stored. See Section 9.1.3.2 for an explanation of real and complex data format.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
4 (with real transforms only)	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
11	DXML_ILL_LDA()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()
16	DXML_BAD_FORMAT_STRING()
18	DXML_BAD_FORMAT_FOR_DIRECTION()

Examples

1.
```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N_I, N_J, STATUS, LDA
REAL*8 A(1026,512), B(1026,513)
N_I = 1024
N_J = 512
LDA = 1026
STATUS = DFFT_2D('R','C','F',A,B,N_I,N_J,LDA,1,1)
```

This Fortran code computes the forward, two-dimensional, real FFT of a 1024x512 matrix A. The result of the transform is stored in B in complex form. The leading dimension of B is 1026 in order to hold the extra complex values (see section on data storage). The input matrix A also requires a leading dimension of at least 1026.

2.
```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N_I, N_J, STATUS, LDA
COMPLEX*8 A(1024,512), B(1024,512)
N_I = 1024
N_J = 512
LDA = 1024
STATUS = CFFT_2D('C','C','F',A,B,N_I,N_J,LDA,1,1)
```

This Fortran code computes the forward, two-dimensional, complex FFT of a matrix A, of dimension 1024 by 512. The result of the transform is stored in B in complex form.

SFFT_INIT_2D DFFT_INIT_2D CFFT_INIT_2D ZFFT_INIT_2D Initialization Step for Fast Fourier Transform in Two Dimensions (Serial and Parallel Versions)

Format

status = {S,D,C,Z}FFT_INIT_2D (ni, nj, fft_struct, ni_stride_1_flag)

Arguments

ni, nj
integer*4
Specifies the size of the first and second dimension of data in the input array; $ni > 0$, $nj > 0$. For SFFT_INIT_2D and DFFT_INIT_2D, **ni** must be even.

fft_struct
record /dxml_s_fft_structure_2d/ for single-precision real operations
record /dxml_d_fft_structure_2d/ for double-precision real operations
record /dxml_c_fft_structure_2d/ for single-precision complex operations
record /dxml_z_fft_structure_2d/ for double-precision complex operations
This argument must be included but needs no additional definitions. The argument is declared in the program before this routine. See Section 9.1.3.3 for more information.

ni_stride_1_flag
logical
Specifies whether to allow a stride of more than 1 between elements in the row:

TRUE: Stride must be 1.
FALSE: Stride is at least 1.

Description

The _FFT_INIT_2D functions build internal data structures needed to compute fast Fourier transforms of two-dimensional data. These routines are the first step in a three-step procedure. They create the internal data structures, using attributes defined in the file `DXMLDEF.FOR`.

Use the initialization routine that is appropriate for the data format. Then, use the corresponding application and exit steps to complete the procedure. For example, use the SFFT_2D_INIT routine with the SFFT_2D_APPLY and SFFT_2D_EXIT routine.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
4 (real transform only)	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
12	DXML_INS_RES()

SFFT_APPLY_2D DFFT_APPLY_2D CFFT_APPLY_2D ZFFT_APPLY_2D Application Step for Fast Fourier Transform in Two Dimensions (Serial and Parallel Versions)

Format

Real transform:

```
status = {S,D}FFT_APPLY_2D    (input_format, output_format, direction, in, out, lda,
                              fft_struct, ni_stride, nj_stride)
```

Complex transform in complex data format:

```
status = {C,Z}FFT_APPLY_2D    (input_format, output_format, direction, in, out, lda,
                              fft_struct, ni_stride, nj_stride)
```

Complex transform in real data format:

status = {C,Z}FFT_APPLY_2D (input_format, output_format, direction, in_real, in_imag, out_real, out_imag, lda, fft_struct, ni_stride, nj_stride)

Arguments

input_format, output_format
character*(*)
Identifies the data type of the input and the format to be used to store the data, regardless of the data type. For example, a complex sequence can be stored in real format.

The character 'R' specifies the format as real; the character 'C' specifies the format as complex. As convenient, use either uppercase or lowercase characters, and either spell out or abbreviate the word.

The following table shows the valid values:

Subprogram	Input Format	Output Format	Direction
{S,D}	'R'	'C'	'F'
	'C'	'R'	'B'
	'R'	'R'	'F' or 'B'
{C,Z}	'R'	'R'	'F' or 'B'
	'C'	'C'	'F' or 'B'

For complex data, the type of data determines what other arguments are needed. When both the input and output data are real, the complex routines store the data as separate arrays for imaginary and real data so additional arguments are needed.

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8 | complex*8 | complex*16
Both the arguments are two-dimensional arrays. The input and output arrays can be the same array. The IN array contains the data to be transformed. The OUT array contains the transformed data.

in_real, out_real, in_imag, out_imag
real*4 | real*8
Use these arguments when performing a complex transform on real data format and storing the result in a real data format.

lda
integer*4
Specifies the number of rows in the IN and OUT arrays; $lda \geq ni$. For {S,D} routines, $lda \geq ni + 2$ when the input format is 'R' and the output format is 'C' or the input format is 'C' and the output format is 'R'.

fft_struct
record /dxml_s_fft_structure_2d/ for single-precision real operations
record /dxml_d_fft_structure_2d/ for double-precision real operations
record /dxml_c_fft_structure_2d/ for single-precision complex operations
record /dxml_z_fft_structure_2d/ for double-precision complex operations
The argument refers to the structure created by the _2D_INIT routine.

ni_stride, nj_stride
integer*4
Specifies the distance between consecutive elements in a column and row in the IN and OUT arrays; the valid stride depends on the _INIT routine; *ni_stride* $\geq$ 1, *nj_stride* $\geq$ 1.

Description

The _FFT_APPLY_2D routines compute the fast Fourier transform of two-dimensional data in either the forward or backward direction. These routines are the second step of the three-step procedure. They compute the fast forward or inverse Fourier transform, using the internal data structures created by the _FFT_2D_INIT subroutine.

Use the _APPLY_2D routines with their corresponding _INIT_2D and _EXIT_2D routines. For example, use SFFT_APPLY after the SFFT_INIT and end with the SFFT_EXIT routine. See Section 9.1.3.2 for an explanation of real and complex data format.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
11	DXML_ILL_LDA()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()
16	DXML_BAD_FORMAT_STRING()
18 (for real transform only)	DXML_BAD_FORMAT_FOR_DIRECTION()

Examples

1.
```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N_I, N_J, STATUS, LDA
REAL*8 A(1026,512), B(1026,513)
RECORD /DXML_D_FFT_STRUCTURE_2D/ FFT_STRUCT
N_I = 1024
N_J = 512
LDA = 1026
STATUS = DFFT_INIT_2D(N_I,N_J,FFT_STRUCT,.TRUE.)
STATUS = DFFT_APPLY_2D('R','C','F',A,B,LDA,FFT_STRUCT,1,1)
STATUS = DFFT_EXIT_2D(FFT_STRUCT)
```

This Fortran code computes the forward, two-dimensional, real FFT of a 1024x512 matrix A. The result of the transform is stored in B in complex

form. The leading dimension of B is 1026 in order to hold the extra complex values (see section on data storage). Also the input matrix A also requires a leading dimension of at least 1026.

2.
```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N_I, N_J, STATUS, LDA
COMPLEX*16 A(1024,512), B(1024,512)
RECORD /DXML_Z_FFT_STRUCTURE_2D/ FFT_STRUCT
N_I = 1024
N_J = 512
LDA = 1024
STATUS = ZFFT_INIT_2D(N_I,N_J,FFT_STRUCT,.TRUE.)

STATUS = ZFFT_APPLY_2D('C','C','F',A,B,LDA,FFT_STRUCT,1,1)
STATUS = ZFFT_EXIT_2D(FFT_STRUCT)
```

This Fortran code computes the forward, two-dimensional, complex FFT of a matrix A, of dimension 1024 by 512. The result of the transform is stored in B in complex form.

SFFT_EXIT_2D DFFT_EXIT_2D CFFT_EXIT_2D ZFFT_EXIT_2D Final Step for Fast Fourier Transform in Two Dimensions (Serial and Parallel Versions)

Format

status = {S,D,C,Z}FFT_EXIT_2D (fft_struct)

Arguments

fft_struct
record /dxml_s_fft_structure/ for single-precision real operations
record /dxml_d_fft_structure/ for double-precision real operations
record /dxml_c_fft_structure/ for single-precision complex operations
record /dxml_z_fft_structure/ for double-precision complex operations
This argument must be included but it is not necessary to modify it in any way. It refers to the data structure that was created in the initialization step.

Description

The _FFT_EXIT_2D functions remove the internal data structures created in the _FFT_INIT_2D functions. These functions are the final step in a three-step procedure. They release the virtual memory that was allocated by the _FFT_INIT_2D functions.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
12	DXML_INS_RES()

SFFT_3D DFFT_3D CFFT_3D ZFFT_3D Fast Fourier Transform in Three Dimensions (Serial and Parallel Versions)

Format

Real transform:

status = {S,D}FFT_3D (input_format, output_format, direction, in, out, ni, nj, nk, lda_i, lda_j, ni_stride, nj_stride, nk_stride)

Complex transforms in complex format:

status = {C,Z}FFT_3D (input_format, output_format, direction, in, out, ni, nj, nk, lda_i, lda_j, ni_stride, nj_stride, nk_stride)

Complex transform in real data format:

status = {C,Z}FFT_3D (input_format, output_format, direction, in_real, in_imag, out_real, out_imag, ni, nj, nk, lda_i, lda_j, ni_stride, nj_stride, nk_stride)

Arguments

input_format, output_format
character*(*)
Identifies the data type of the input and the format to be used to store the data, regardless of the data type. For example, a complex sequence can be stored in real format.

The character 'R' specifies the format as real; the character 'C' specifies the format as complex. As convenient, use either uppercase or lowercase characters, and either spell out or abbreviate the word.

The following table shows the valid values:

Subprogram	Input Format	Output Format	Direction
{S,D}	'R'	'C'	'F'
	'C'	'R'	'B'
	'R'	'R'	'F' or 'B'
{C,Z}	'R'	'R'	'F' or 'B'
	'C'	'C'	'F' or 'B'

For complex data, the type of data determines what other arguments are needed. When both the input and output data are real, the complex routines store the data as separate arrays for imaginary and real data so additional arguments are needed.

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8 | complex*8 | complex*16
Both the arguments are three-dimensional arrays. The input and output arrays can be the same array. The IN array contains the data to be transformed. The OUT array contains the transformed data.

in_real, out_real, in_imag, out_imag
REAL*4 | REAL*8
Use these arguments when performing a complex transform on real data format and storing the result in a real data format.

ni, nj, nk
integer*4
Specifies the size of the first, second, and third dimension of data in the input array; $ni > 0$, $nj > 0$, $nk > 0$. For SFFT_3D and DFFT_3D, **ni** must be even.

lda_i, lda_j
integer*4
Specifies the number of rows and columns in the IN and OUT arrays; $lda_i \geq ni$, $lda_j \geq nj$. For {S,D} routines, $lda_i \geq ni + 2$ when the input format is 'R' and the output format is 'C' or the input format is 'C' and the output format 'R'.

ni_stride, nj_stride, nk_stride
integer*4
Specifies the distance between consecutive elements in the IN and OUT arrays; $ni_stride \geq 1$, $nj_stride \geq 1$, $nk_stride \geq 1$.

Description

The _FFT_3D routines compute the fast forward or inverse Fourier transform of three-dimensional data in one step.

The SFFT_3D and DFFT_3D functions perform the forward Fourier transform of a real sequence and store the result in either real or complex data format. These functions also perform the inverse Fourier transform of a complex sequence into a real sequence.

The CFFT_3D and ZFFT_3D functions perform Fourier transforms on a complex sequence. However, the argument list is different, depending on the data format in which the output data is stored. See Section 9.1.3.2 for an explanation of real and complex data format.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
4 (with real transforms only)	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
11	DXML_ILL_LDA()
12	DXML_INS_RES()

13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()
16	DXML_BAD_FORMAT_STRING()
18	DXML_BAD_FORMAT_FOR_DIRECTION()

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N_I, N_J, N_K, STATUS, LDA_I, LDA_J
REAL*8 A(130,128,128), B(130,128,128)
N_I = 128
N_J = 128
N_K = 128
LDA_I = 130
LDA_J = 128
STATUS = DFFT_3D('R','C','F',A,B,N_I,N_J,N_K,LDA_I,LDA_J,1,1,1)
```

This Fortran code computes the forward, three-dimensional, real FFT of a 128x128x128 matrix A. The result of the transform is stored in B in complex form. The leading dimension of B is 130 to hold the extra complex values (see section on data storage). Also the input matrix A requires a leading dimension of at least 130.

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N_I, N_J, N_K, STATUS, LDA_I, LDA_J
COMPLEX*8 A(130,128,128), B(130,128,128)
N_I = 128
N_J = 128
N_K = 128
LDA_I = 128
LDA_J = 128
STATUS = CFFT_3D('C','C','F',A,B,N_I,N_J,N_K,LDA_I,LDA_J,1,1,1)
```

This Fortran code computes the forward, three-dimensional, complex FFT of a matrix A, of dimension 128x128x128. The result of the transform is stored in B in complex form.

SFFT_INIT_3D DFFT_INIT_3D CFFT_INIT_3D ZFFT_INIT_3D Initialization Step for Fast Fourier Transform in Three Dimensions (Serial and Parallel Versions)

Format

status = {S,D,C,Z}FFT_INIT_3D   (ni, nj, nk, fft_struct, ni_stride_1_flag)

Arguments

ni, nj, nk
integer*4
Specifies the size of the first, second, and third dimension of data in the input array; $ni > 0$, $nj > 0$, $nk > 0$. For SFFT_INIT_3D and DFFT_INIT_3D, **ni** must be even.

fft_struct
record /dxml_s_fft_structure_3d/ for single-precision real operations
record /dxml_d_fft_structure_3d/ for double-precision real operations
record /dxml_c_fft_structure_3d/ for single-precision complex operations
record /dxml_z_fft_structure_3d/ for double-precision complex operations
This argument must be included but needs no additional definitions. The argument is declared in the program before this routine. See Section 9.1.3.3 for more information.

ni_stride_1_flag
logical
Specifies whether to allow a stride of more than 1 between elements in the row:

TRUE: Stride must be 1.
FALSE: Stride is at least 1.

Description

The _FFT_INIT_3D functions build internal data structures needed to compute fast Fourier transforms of three-dimensional data. These routines are the first step in a three-step procedure. They create the internal data structures, using attributes defined in the file `DXMLDEF.FOR`.

Use the initialization routine that is appropriate for the data format. Then, use the corresponding application and exit steps to complete the procedure. For example, use the SFFT_3D_INIT routine with the SFFT_3D_APPLY and SFFT_3D_EXIT routine.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
4 (real transform only)	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
12	DXML_INS_RES()

SFFT_APPLY_3D DFFT_APPLY_3D CFFT_APPLY_3D ZFFT_APPLY_3D Application Step for Fast Fourier Transform in Three Dimensions (Serial and Parallel Versions)

Format

Real transform:

status = {S,D}FFT_APPLY_3D (input_format, output_format, direction, in, out, lda_i, lda_j, fft_struct, ni_stride, nj_stride, nk_stride)

Complex transforms in complex format:

status = {C,Z}FFT_APPLY_3D (input_format, output_format, direction, in, out, lda_i, lda_j, fft_struct, ni_stride, nj_stride, nk_stride)

Complex transform in real data format:

status = {C,Z}FFT_APPLY_3D (input_format, output_format, direction, in_real, in_imag, out_real, out_imag, lda_i, lda_j, fft_struct, ni_stride, nj_stride, nk_stride)

Arguments

input_format, output_format
character*(*)
Identifies the data type of the input and the format to be used to store the data, regardless of the data type. For example, a complex sequence can be stored in real format.

The character 'R' specifies the format as real; the character 'C' specifies the format as complex. As convenient, use either uppercase or lowercase characters, and either spell out or abbreviate the word.

The following table shows the valid values:

Subprogram	Input Format	Output Format	Direction
{S,D}	'R'	'C'	'F'
	'C'	'R'	'B'
	'R'	'R'	'F' or 'B'
{C,Z}	'R'	'R'	'F' or 'B'
	'C'	'C'	'F' or 'B'

For complex data, the type of data determines what other arguments are needed. When both the input and output data are real, the complex routines store the data as separate arrays for imaginary and real data so additional arguments are needed.

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8 | complex*8 | complex*16
Both the arguments are three-dimensional arrays. The input and output arrays can be the same array. The IN array contains the data to be transformed. The OUT array contains the transformed data.

in_real, out_real, in_imag, out_imag
REAL*4 | REAL*8
Use these arguments when performing a complex transform on real data format and storing the result in a real data format.

lda_i, lda_j
integer*4
Specifies the number of rows and columns in the IN and OUT arrays; $lda_i \geq ni$, $lda_j \geq nj$. For {S,D} routines, $lda_i \geq ni + 2$ when the input format is 'R' and the output format is 'C' or the input format is 'C' and the output format is 'R'.

fft_struct
record /dxml_s_fft_structure_3d/ for single-precision real operations
record /dxml_d_fft_structure_3d/ for double-precision real operations
record /dxml_c_fft_structure_3d/ for single-precision complex operations
record /dxml_z_fft_structure_3d/ for double-precision complex operations
The argument refers to the structure created by the _INIT routine.

ni_stride, nj_stride, nk_stride
integer*4
Specifies the distance between consecutive elements in the IN and OUT arrays; the valid stride depends on the _INIT routine. *ni_stride* ≥ 1, *nj_stride* ≥ 1, *nk_stride* ≥ 1.

Description

The _FFT_APPLY_3D routines compute the fast Fourier transform of three-dimensional data in either the forward or backward direction. These routines are the second step of the three-step procedure for the fast Fourier transform of three-dimensional data. They compute the fast forward or inverse Fourier transform, using the internal data structures created by the _FFT_3D_INIT subroutine.

Use the _APPLY_3D routines with their corresponding _INIT_3D and _EXIT_3D routines. For example, use SFFT_APPLY after the SFFT_INIT and end with the SFFT_EXIT routine. See Section 9.1.3.2 for an explanation of real and complex data format.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
11	DXML_ILL_LDA()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
18 (for real transform only)	DXML_BAD_FORMAT_FOR_DIRECTION()
15	DXML_BAD_DIRECTION_STRING()
16	DXML_BAD_FORMAT_STRING()

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N_I, N_J, N_K, STATUS, LDA_I, LDA_J
REAL*8 A(130,128,128), B(130,128,128)
RECORD /DXML_D_FFT_STRUCTURE_3D/ FFT_STRUCT
N_I = 128
N_J = 128
N_K = 128
LDA_I = 130
LDA_J = 128
STATUS = DFFT_INIT_3D(N_I,N_J,N_K,FFT_STRUCT,.TRUE.)
STATUS = DFFT_APPLY_3D('R','C','F',A,B,LDA_I,LDA_J,FFT_STRUCT,1,1,1)
STATUS = DFFT_EXIT_3D(FFT_STRUCT)
```

This Fortran code computes the forward, three-dimensional, real FFT of a 128x128x128 matrix A. The result of the transform is stored in B in complex form. The leading dimension of B is 130 to hold the extra complex values (see section on data storage). Also the input matrix A requires a leading dimension of at least 130.

SFFT_EXIT_3D DFFT_EXIT_3D CFFT_EXIT_3D ZFFT_EXIT_3D Final Step for Fast Fourier Transform in Three Dimensions (Serial and Parallel Versions)

Format

status = {S,D,C,Z}FFT_EXIT_3D (fft_struct)

Arguments

fft_struct
record /dxml_s_fft_structure/ for single-precision real operations
record /dxml_d_fft_structure/ for double-precision real operations
record /dxml_c_fft_structure/ for single-precision complex operations
record /dxml_z_fft_structure/ for double-precision complex operations
This argument must be included but it is not necessary to modify it in any way. It refers to the data structure that was created in the initialization step.

Description

The _FFT_EXIT_3D functions remove the internal data structures created in the _FFT_INIT_3D functions. These functions are the final step in a three-step procedure. They release the virtual memory that was allocated by the _FFT_INIT_3D functions.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

Return Values

0	DXML_SUCCESS()
12	DXML_INS_RES()

SFFT_GRP DFFT_GRP CFFT_GRP ZFFT_GRP
Group Fast Fourier Transform in One Dimension

Format

Real transform:

status = {S,D}FFT_GRP (input_format, output_format, direction, in, out, n, grp_size, lda, stride, grp_stride)

Complex transform in complex data format:

status = {C,Z}FFT_GRP (input_format, output_format, direction, in, out, n, grp_size, lda, stride, grp_stride)

Complex transform real data format:

status = {C,Z}FFT_GRP (input_format, output_format, direction, in_real, in_imag, out_real, out_imag, n, grp_size, lda, stride, grp_stride)

Arguments

input_format, output_format
character*(*)
Identifies the data type of the input and the format to be used to store the data, regardless of the data type. For example, a complex sequence can be stored in real format.

The character 'R' specifies the format as real; the character 'C' specifies the format as complex. As convenient, use either uppercase or lowercase characters, and either spell out or abbreviate the word.

The following table shows the valid values:

Subprogram	Input Format	Output Format	Direction
{S,D}	'R'	'C'	'F'
	'C'	'R'	'B'
	'R'	'R'	'F' or 'B'
{C,Z}	'R'	'R'	'F' or 'B'
	'C'	'C'	'F' or 'B'

For complex transforms, the type of data determines what other arguments are needed. When both the input and output data are real, the complex functions store the data as separate arrays for imaginary and real data so additional arguments are needed.

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8 | complex*8 | complex*16
Both arguments are two-dimensional arrays. The IN array contains the data to be transformed. The OUT array contains the transformed data. The IN and OUT arrays can be the same array. The IN and OUT arrays must be the same size.

in_real, in_imag, out_real, out_imag
real*4 | real*8
Use these arguments when performing a complex transform on real data format and storing the result in a real data format.

n
integer*4
Specifies the number of elements in the column within each one-dimensional data array; $n > 0$. For SFFT_GRP and DFFT_GRP, **n** must be even.

grp_size
integer*4
Specifies the number of one-dimensional data arrays; *grp_size*> 0.

lda
integer*4
Specifies the the number of rows in two-dimensional data arrays; *lda* ≥ *grp_size*. Using *lda* = *grp_size* $+ \{ 3 \; or \; 5\}$ can sometimes achieve better performance by avoiding cache thrashing.

stride
integer*4
Specifies the distance between columns of active data arrays; $stride \geq 1$. **stride** permits columns of IN and OUT arrays to be skipped when they are not part of the group.

grp_stride
integer*4
Specifies the distance between consecutive elements in a row in the IN and OUT arrays; *grp_stride* ≥ 1. **grp_stride** permits rows of IN and OUT arrays to be skipped when they are not part of the group.

Description

_FFT_GRP computes the fast forward or inverse Fourier transform on a group of one-dimensional data arrays. The transform is performed on the first row of elements of one-dimensional data arrays within the group. Data arrays can be skipped by setting the **stride** parameter. The transform then goes to the next row of elements. Similarly, rows of elements can be skipped by setting the **grp_stride** parameter. _FFT_GRP contrasts with _FFT in that _FFT performs a transform on each element of a data array before going to the next data array. Although _FFT_GRP gives the same result as _FFT, _FFT_GRP is more efficient at completing the transform.

Return Values

0	DXML_SUCCESS()
4 (real transforms only)	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()

16	DXML_BAD_FORMAT_STRING()
18 (real transforms only)	DXML_BAD_FORMAT_FOR_DIRECTION()

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N,GRP_SIZE
REAL*8 A(100,514),B(100,514)
N=512
LDA=100
GRP_SIZE=100
STATUS=DFFT_GRP('R','C','F',A,B,N,GRP_SIZE,LDA,1,1)
```

This Fortran code computes a set of 100 FFT of size 512. The results of the transforms are stored in B in complex format. The second dimension of A and B is 514 to hold the extra complex values.

SFFT_INIT_GRP DFFT_INIT_GRP CFFT_INIT_GRP ZFFT_INIT_GRP Initialization Step for Group Fast Fourier Transform in One Dimension

Format

status = {S,D,C,Z}FFT_INIT_GRP (n, fft_struct, grp_stride_1_flag, max_grp_size)

Arguments

n
integer*4
Specifies the number of elements in the column within each one-dimensional data array; $n > 0$. For SFFT_INIT_GRP and DFFT_INIT_GRP, **n** must be even.

fft_struct
record /dxml_s_grp_fft_structure/ for single-precision real operations
record /dxml_d_grp_fft_structure/ for double-precision real operations
record /dxml_c_grp_fft_structure/ for single-precision complex operations
record /dxml_z_grp_fft_structure/ for double-precision complex operations
You must include this argument but it needs no additional definitions. The argument is declared in the program before this routine. See Section 9.1.3.3 for more information.

grp_stride_1_flag
logical
Specifies whether to allow a distance greater than 1 between elements:

TRUE: Group stride must be 1.
FALSE: Group stride is at least 1.

max_grp_size
integer*4
Specifies the expected number of sets of data. If unknown, set *max_grp_size* = 0.

Description

The _FFT_INIT_GRP functions build internal data structures needed to compute fast Fourier transforms of one-dimensional data. These routines are the first step in a three-step procedure. They create the internal data structures, using attributes defined in the file `DXMLDEF.FOR`.

Return Values

0	DXML_SUCCESS()
4 (real transforms only)	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
12	DXML_INS_RES()

SFFT_APPLY_GRP DFFT_APPLY_GRP CFFT_APPLY_GRP ZFFT_APPLY_GRP Application Step for Group Fast Fourier Transform in One Dimension

Format

Real transform:

status = {S,D}FFT_APPLY_GRP (input_format, output_format, direction, in, out, grp_size, lda, fft_struct, stride, grp_stride)

Complex transform of real data format:

status = {C,Z}FFT_APPLY_GRP (input_format, output_format, direction, in, out, grp_size, lda, fft_struct, stride, grp_stride)

Complex transform of real data to real data:

status = {C,Z}FFT_APPLY_GRP (input_format, output_format, direction, in_real, in_imag, out_real, out_imag, grp_size, lda, fft_struct, stride, grp_stride)

Arguments

input_format, output_format
character*(*)
Identifies the data type of the input and the format to be used to store the data, regardless of the data type. For example, a complex sequence can be stored in real format.

The character 'R' specifies the format as real; the character 'C' specifies the format as complex. As convenient, use either uppercase or lowercase characters, and either spell out or abbreviate the word.

The following table shows the valid values:

Subprogram	Input Format	Output Format	Direction
{S,D}	'R'	'C'	'F'
	'C'	'R'	'B'
	'R'	'R'	'F' or 'B'
{C,Z}	'R'	'R'	'F' or 'B'
	'C'	'C'	'F' or 'B'

For complex transforms, the type of data determines what other arguments are needed. When both the input and output data are real, the complex functions store the data as separate arrays for imaginary and real data so additional arguments are needed.

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8 | complex*8 | complex*16
Both arguments are two-dimensional arrays. The IN array contains the data to be transformed. The OUT array contains the transformed data. The IN and OUT arrays can be the same array.

in_real, in_imag, out_real, out_imag
real*4 | real*8
Use these arguments when performing a complex transform on real data format and storing the result in a real data format.

grp_size
integer*4
Specifies the number of one-dimensional data arrays; $grp_size > 0$.

lda
integer*4
Specifies the the number of rows in two-dimensional data arrays; $lda \geq grp_size$. Using $lda = grp_size + \{3 \; or \; 5\}$ can sometimes achieve better performance by avoiding cache thrashing.

fft_struct
record /dxml_s_grp_fft_structure/ for single-precision real operations
record /dxml_d_grp_fft_structure/ for double-precision real operations
record /dxml_c_grp_fft_structure/ for single-precision complex operations
record /dxml_z_grp_fft_structure/ for double-precision complex operations
The argument refers to the structure created by the _INIT routine.

stride
integer*4
Specifies the distance between columns of active data arrays; $stride \geq 1$. **stride** permits columns of IN and OUT arrays to be skipped when they are not part of the group.

grp_stride
integer*4
Specifies the distance between consecutive elements in a row in the IN and OUT arrays; *grp_stride* $\geq$ 1. **grp_stride** permits rows of IN and OUT arrays to be skipped when they are not part of the group.

Description

The _FFT_APPLY_GRP computes the fast forward or inverse Fourier transform on a group of one-dimensional data arrays. The transform is performed on the first row of elements of one-dimensional data arrays within the group. Data arrays can be skipped by setting the **stride** parameter. The transform then goes to the next row of elements. Similarly, rows of elements can be skipped by setting the **grp_stride** parameter. _FFT_APPLY_GRP contrasts with _FFT_APPLY in that _FFT_APPLY performs a transform on each element of a data array before going to the next data array. Although _FFT_APPLY_GRP gives the same result as _FFT_APPLY, _FFT_APPLY_GRP is more efficient at completing the transform.

Return Values

0	DXML_SUCCESS()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()
16	DXML_BAD_FORMAT_STRING()
18 (real transform only)	DXML_BAD_FORMAT_FOR_DIRECTION()

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 GRP_SIZE,N,STATUS
REAL*8 A(100,514),B(100,514)
RECORD /DXML_D_GRP_FFT_STRUCTURE/FFT_STRUCT
GRP_SIZE=100
N=512
LDA=100
STATUS = DFFT_INIT_GRP(N,FFT_STRUCT,.TRUE.,100)
STATUS = DFFT_APPLY_GRP('R','C','F',A,B,GRP_SIZE,LDA,FFT_STRUCT,1,1)
STATUS = DFFT_EXIT_GRP(FFT_STRUCT)
```

This Fortran code computes a set of 100 FFT of size 512. The results of the transforms are stored in B in complex format. The second dimension is 514 to hold the extra complex values.

SFFT_EXIT_GRP DFFT_EXIT_GRP CFFT_EXIT_GRP ZFFT_EXIT_GRP Exit Step for Group Fast Fourier Transform in One Dimension

Format

status = {S,D,C,Z}FFT_EXIT_GRP (fft_struct)

Arguments

fft_struct
record /dxml_s_grp_fft_structure/ for single-precision real operations
record /dxml_d_grp_fft_structure/ for double-precision real operations
record /dxml_c_grp_fft_structure/ for single-precision complex operations
record /dxml_z_grp_fft_structure/ for double-precision complex operations
This argument must be included but it is not necessary to modify it in any way. It refers to the data structure that was created in the initialization step.

Description

The _FFT_EXIT_GRP functions remove the internal data structures created in the _FFT_INIT_GRP functions. These functions are the final step in a three-step procedure. They release the virtual memory that was allocated by the _FFT_INIT_GRP functions.

Return Values

0	DXML_SUCCESS()
12	DXML_INS_RES()

Cosine and Sine

This section provides descriptions of the routines for the Cosine and Sine transforms.

SFCT DFCT
Fast Cosine Transform in One Dimension

Format

status = {S,D}FCT (direction, in, out, n, type, stride)

Arguments

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8
Both the arguments are one-dimensional arrays. The input and output arrays can be the same array. The IN array contains the data to be transformed. The OUT array contains the transformed data. For type-I FCT, the length of the IN,OUT array must $\geq N + 1$. For type-II FCT, the length of the IN,OUT array must be $\geq N$.

n
integer*4
Specifies the size of the transform. The minimum size of the IN, OUT array is **n**; where **n**> 0 and even.

type
integer*4
Specifies the type of the Cosine transform desired. Currently only type-1 and type-2 transforms are supported.

stride
integer*4
Specifies the distance between consecutive elements in the IN and OUT arrays. The distance must be at least 1.

Description

The _FCT functions compute the fast Cosine transform of one-dimensional data in one step.

Return Values

0	DXML_SUCCESS()
4	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()
17	DXML_OPTION_NOT_SUPPORTED()

Example

```
INTEGER*4 N
PARAMETER (N=1024)

INCLUDE 'DXMLDEF.FOR'
INTEGER*4 STATUS
REAL*8 C(0:N),D(0:N)
REAL*4 E(1:N-1),F(1:N-1)

STATUS = DFCT('F',C,D,N,1,1)
STATUS = DFCT('B',D,C,N,1,1)
STATUS = SFCT('F',E,F,N,2,1)
STATUS = SFCT('B',F,E,N,2,1)
```

This Fortran code computes the following:

- Forward Type-1 Cosine transform of the real sequence C to real sequence D.
- Backward Type-1 Cosine transform of the real sequence D to real sequence C.
- Forward Type-2 Cosine transform of the real sequence E to real sequence F.
- Backward Type-2 Cosine transform of the real sequence F to real sequence E.

SFCT_INIT DFCT_INIT
Initialization Step for Fast Cosine Transform in One Dimension

Format

status = {S,D}FCT_INIT (n, fct_struct, type, stride_1_flag)

Arguments

n
integer*4
Specifies the size of the transform. **n** must be even and > 0.

fct_struct
record /dxml_s_fct_structure/ for single-precision operations
record /dxml_d_fct_structure/ for double-precision operations

type
integer*4
Specifies the type of Cosine transform desired. Currently only type-1 and type-2 transforms are supported.

stride_1_flag
logical
Specifies the allowed distance between consecutive elements in the input and output arrays:

TRUE: Stride must be 1.
FALSE: Stride is at least 1.

Description

The _FCT_INIT functions build internal data structures needed to compute fast Cosine transforms of one-dimensional data. These functions are the first step in a three-step procedure. They create the internal data structures, using attributes defined in the file DXMLDEF.FOR.

Use the initialization function that is appropriate for the data format. Then use the corresponding application and exit functions to complete the transform. For example, use SFCT_INIT for the internal data structures used by SFCT_APPLY and end with the SFCT_EXIT function.

Return Values

0	DXML_SUCCESS()
4	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
12	DXML_INS_RES()
17	DXML_OPTION_NOT_SUPPORTED()

SFCT_APPLY SFCT_APPLY
Application Step for Fast Cosine Transform in One Dimension

Format

status = {S,D}FCT_APPLY   (direction, in, out, fct_struct, stride)

Arguments

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8
Both the arguments are one-dimensional arrays. The input and output arrays can be the same array. The IN array contains the data to be transformed. The OUT array contains the transformed data.

fct_struct
record /dxml_s_fct_structure/ for single-precision operations
record /dxml_d_fct_structure/ for double-precision operations

stride
integer*4
Specifies the distance between consecutive elements in the input and output arrays, depending on the value of **stride_1_flag** provided in the _INIT function.

Description

The _FCT_APPLY functions compute the fast Cosine transform of one-dimensional data in three steps.

Return Values

0	DXML_SUCCESS()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()
17	DXML_OPTION_NOT_SUPPORTED()

Example

```
INTEGER*4 N
PARAMETER (N=1024)

INCLUDE 'DXMLDEF.FOR'
INTEGER*4 STATUS
RECORD /DXML_S_FCT_STRUCTURE/ D_FCT_STRUCT
RECORD /DXML_D_FCT_STRUCTURE/ D_FCT_STRUCT
REAL*8 C(0:N),D(0:N)
REAL*4 E(0:N-1),F(0:N-1)

STATUS = DFCT_INIT(N,D_FCT_STRUCT,1,.TRUE.)
STATUS = DFCT_APPLY('F',C,D,D_FCT_STRUCT,1)
STATUS = DFCT_APPLY('B',D,C,D_FCT_STRUCT,1)
STATUS = DFCT_EXIT(D_FCT_STRUCT)

STATUS = SFCT_INIT(N,S_FCT_STRUCT,2,.TRUE.)
STATUS = SFCT_APPLY('F',E,F,S_FCT_STRUCT,1)
STATUS = SFCT_APPLY('B',F,E,S_FCT_STRUCT,1)
STATUS = SFCT_EXIT(D_FCT_STRUCT)
```

This Fortran code computes the following:

- Forward Type-1 Cosine transform of the real sequence C to real sequence D.
- Backward Type-1 Cosine transform of the real sequence D to real sequence C.
- Forward Type-2 Cosine transform of the real sequence E to real sequence F.
- Backward Type-2 Cosine transform of the real sequence F to real sequence E.

SFCT_EXIT DFCT_EXIT
Final Step for Fast Cosine Transform in One Dimension

Format

status = {S,D}FCT_EXIT (fct_struct)

Arguments

fct_struct
record /dxml_s_fct_structure/ for single-precision operations
record /dxml_d_fct_structure/ for double-precision operations

Description

The _FCT_EXIT functions remove the internal data structures created in the _FCT_INIT functions. These functions are the final step in a three-step procedure. They release the virtual memory that was allocated by the _FCT_INIT functions.

Return Values

0	DXML_SUCCESS()
12	DXML_INS_RES()

SFST DFST
Fast Sine Transform in One Dimension

Format

status = {S,D}FST (direction, in, out, n, type, stride)

Arguments

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8
Both the arguments are one-dimensional arrays. The input and output arrays can be the same array. The IN array contains the data to be transformed. The OUT array contains the transformed data.

n
integer*4
Specifies the size of the transform. The minimum size of the IN, OUT array is **n**; where **n**> 0 and even.

type
integer*4
Specifies the type of Sine transform desired. Currently only type-1 and type-2 transforms are supported.

stride
integer*4
Specifies the distance between consecutive elements in the input and output arrays. The distance must be at least 1.

Description

The _FST functions compute the fast type-1 and type-2 Sine transform of one-dimensional data in one step.

Return Values

0	DXML_SUCCESS()
4	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()
17	DXML_OPTION_NOT_SUPPORTED()

Example

```
INTEGER*4 N
PARAMETER (N=1024)

INCLUDE 'DXMLDEF.FOR'
INTEGER*4 STATUS
REAL*8 C(1:N),D(1:N)
REAL*4 E(1:N),F(1:N)

STATUS = DFST('F',C,D,N,1,1)
STATUS = DFST('B',D,C,N,1,1)
STATUS = SFST('F',E,F,N,2,1)
STATUS = SFST('B',F,E,N,2,1)
```

This Fortran code computes the following:

- Forward Type-1 Sine transform of the real sequence C to real sequence D.
- Backward Type-1 Sine transform of the real sequence D to real sequence C.
- Forward Type-2 Sine transform of the real sequence E to real sequence F.
- Backward Type-2 Sine transform of the real sequence F to real sequence E.

SFST_INIT DFST_INIT
Initialization Step for Fast Sine Transform in One Dimension

Format

status = {S,D}FST_INIT (n, fst_struct, type, stride_1_flag)

Arguments

n
integer*4
Specifies the size of the transform. **n** must be even and > 0.

fst_struct
record /dxml_s_fst_structure/ for single-precision operations
record /dxml_d_fst_structure/ for double-precision operations

type
integer*4
Specifies the type of Sine transform desired. Currently only type-1 and type-2 transforms are supported.

stride_1_flag
logical
Specifies the allowed distance between consecutive elements in the input and output arrays:

TRUE: Stride must be 1.
FALSE: Stride is at least 1.

Description

The _FST_INIT functions build internal data structures needed to compute fast Sine transforms of one-dimensional data. These functions are the first step in a three-step procedure. They create the internal data structures, using attributes defined in the file `DXMLDEF.FOR`.

Use the initialization function that is appropriate for the data format. Then use the corresponding application and exit functions to complete the transform. For example, use SFST_INIT for the internal data structures used by SFST_APPLY and end with the SFST_EXIT function.

Return Values

0	DXML_SUCCESS()
4	DXML_ILL_N_IS_ODD()
8	DXML_ILL_N_RANGE()
12	DXML_INS_RES()
17	DXML_OPTION_NOT_SUPPORTED()

SFST_APPLY DFST_APPLY
Application Step for Fast Sine Transform in One Dimension

Format

status = {S,D}FST_APPLY (direction, in, out, fst_struct, stride)

Arguments

direction
character*(*)
Specifies the operation as either the forward or inverse transform. Use 'F' or 'f' to specify the forward transform. Use 'B' or 'b' to specify the inverse transform.

in, out
real*4 | real*8
Both the arguments are one-dimensional arrays. The input and output arrays can be the same array. The IN array contains the data to be transformed. The OUT array contains the transformed data.

fst_struct
record /dxml_s_fst_structure/ for single-precision operations
record /dxml_d_fst_structure/ for double-precision operations

stride
integer*4
Specifies the distance between consecutive elements in the input and output arrays, depending on the value of **stride_1_flag** provided in the _INIT function.

Description

The _FST_APPLY functions compute the fast Sine transform of one-dimensional data in three steps.

Return Values

0	DXML_SUCCESS()
12	DXML_INS_RES()
13	DXML_BAD_STRIDE()
15	DXML_BAD_DIRECTION_STRING()
17	DXML_OPTION_NOT_SUPPORTED()

Example

```
INTEGER*4 N
PARAMETER (N=1024)

INCLUDE 'DXMLDEF.FOR'
INTEGER*4 STATUS
RECORD /DXML_S_FST_STRUCTURE/ D_FST_STRUCT
RECORD /DXML_D_FST_STRUCTURE/ D_FST_STRUCT
REAL*8 C(1:N),D(1:N)
REAL*4 E(1:N),F(1:N)

STATUS = DFST_INIT(N,D_FST_STRUCT,1,.TRUE.)
STATUS = DFST_APPLY('F',C,D,D_FST_STRUCT,1)
STATUS = DFST_APPLY('B',D,C,D_FST_STRUCT,1)
STATUS = DFST_EXIT(D_FST_STRUCT)

STATUS = SFST_INIT(N,S_FST_STRUCT,2,.TRUE.)
STATUS = SFST_APPLY('F',E,F,S_FST_STRUCT,1)
STATUS = SFST_APPLY('B',F,E,S_FST_STRUCT,1)
STATUS = SFST_EXIT(D_FST_STRUCT)
```

This Fortran code computes the following:

- Forward Type-1 Sine transform of the real sequence C to real sequence D.
- Backward Type-1 Sine transform of the real sequence D to real sequence C.
- Forward Type-2 Sine transform of the real sequence E to real sequence F.
- Backward Type-2 Sine transform of the real sequence F to real sequence E.

SFST_EXIT DFST_EXIT
Final Step for Fast Sine Transform in One Dimension

Format

status = {S,D}FST_EXIT (fst_struct)

Arguments

fst_struct
record /dxml_s_fst_structure/ for single-precision operations
record /dxml_d_fst_structure/ for double-precision operations

Description

The _FST_EXIT functions remove the internal data structures created in the _FST_INIT functions. These functions are the final step in a three-step procedure. They release the virtual memory that was allocated by the _FST_INIT functions.

Return Values

0	DXML_SUCCESS()
12	DXML_INS_RES()

Convolutions and Correlations

This section provides descriptions of the convolution and correlation subroutines. The four versions of each routine are titled by name using a leading underscore character. The section is ordered in the following way:

- By type of subprogram:

  Convolution
  Correlation

- By function within each type:

  Nonperiodic
  Periodic

- Extensions to each subprogram

  The extended versions of each subprogram perform the same operation as the corresponding short subprogram but the argument list controls the operation, in the following way:

  – Specify a stride for both the input and output arrays
  – Scale the output by either a scalar or a vector
  – Add an output array to prior output, instead of overwriting
  – Operate on portions of the output array, instead of the entire array

SCONV_NONPERIODIC DCONV_NONPERIODIC CCONV_NONPERIODIC ZCONV Nonperiodic Convolution

Format

{S,D,C,Z}CONV_NONPERIODIC (x, y, out, nx, ny, status)

Arguments

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the data to be convolved.
On exit, **x** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the convolution or “filter” function that is to be convolved with the data from the X array.
On exit, **y** is unchanged.

out
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array OUT of length $nx + ny - 1$.
On exit, **out** contains the convolved data.

nx
integer*4
On entry, the number of values to be convolved, that is, the length of the X array; $nx > 0$.
On exit, **nx** is unchanged.

ny
integer*4
On entry, the length of the array containing the convolution function; $ny > 0$.
On exit, **ny** is unchanged.

status
integer*4

0 DXML_SUCCESS()
8 DXML_ILL_N_RANGE()

Description

The _CONV_NONPERIODIC routines compute the nonperiodic convolution of two arrays using a discrete summing technique.

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N_F, N_M, STATUS
REAL*4 A(500), B(15000), C(15499)
N_A = 500
N_B = 15000
CALL SCONV_NONPERIODIC(A,B,C,N_A,N_B,STATUS)
```

This Fortran code computes the nonperiodic convolution of two vectors of real

numbers, a and b, with lengths of 500 and 15000, respectively. The result is stored in c with length of 15499.

SCONV_PERIODIC DCONV_PERIODIC CCONV_PERIODIC ZCONV_PERIODIC Periodic Convolution

Format

{S,D,C,Z}CONV_PERIODIC (x, y, out, n, status)

Arguments

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the data to be convolved.
On exit, **x** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the convolution or “filter” function that is to be convolved with the data from the X array.
On exit, **y** is unchanged.

out
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array OUT of length n.
On exit, **out** is overwritten and contains the convolved data.

n
integer*4
On entry, the length of the input arrays X and Y and the length of the output array OUT; $n > 0$.
On exit, **n** is unchanged.

status
integer*4

0 DXML_SUCCESS()
8 DXML_ILL_N_RANGE()

Description

The _CONV_PERIODIC functions compute the periodic convolution of two arrays using a discrete summing technique.

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N, STATUS
REAL*8 A(15000), B(15000), C(15000)
N = 15000
CALL DCONV_PERIODIC(A,B,C,N,STATUS)
```

This Fortran code computes the periodic convolution of two vectors of double-precision real numbers, a and b, with lengths of 15000. The result is stored in c with length of 15000.

SCORR_NONPERIODIC DCORR_NONPERIODIC CCORR_NONPERIODIC ZCOR Nonperiodic Correlation

Format

{S,D,C,Z}CORR_NONPERIODIC (x, y, out, nx, ny, status)

Arguments

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the data to be correlated.
On exit, **x** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the function to be correlated with the data from the X array.
On exit, **y** is unchanged.

out
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array OUT with the length nx.
On exit, **out** contains the positive correlation coefficients.

nx
integer*4
On entry, the number of values to be correlated, that is, the length of the X array; $nx > 0$.
On exit, **nx** is unchanged.

ny
integer*4
On entry, the length of the Y array containing the correlation function; $ny > 0$.
On exit, **ny** is unchanged.

status
integer*4

0 DXML_SUCCESS()
8 DXML_ILL_N_RANGE()

Description

The _CORR_NONPERIODIC functions compute the nonperiodic correlation of two arrays using a discrete summing technique.

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N_F, N_M, STATUS
REAL*8 A(500), B(15000), C(500)
N_A = 500
N_B = 15000
CALL DCORR_NONPERIODIC(A,B,C,N_A,N_B,STATUS)
```

This Fortran code computes the nonperiodic correlation of two vectors of double-precision real numbers, a and b, with lengths of 500 and 15000, respectively. The result is stored in c with length of 15499.

SCORR_PERIODIC DCORR_PERIODIC CCORR_PERIODIC ZCORR_PERIODIC Periodic Correlation

Format

{S,D,C,Z}CORR_PERIODIC (x, y, out, n, status)

Arguments

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the data to be correlated.
On exit, **x** is unchanged.

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the correlation function to be correlated with the data from the X array.
On exit, **y** is unchanged.

out
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array OUT of length n.
On exit, **out** contains the positive correlation coefficients.

n
integer*4
On entry, the length of the input arrays X and Y and the length of the output array OUT; $n > 0$.
On exit, **n** is unchanged.

status
integer*4

0 DXML_SUCCESS()
8 DXML_ILL_N_RANGE()

Description

The _CORR_PERIODIC computes the periodic correlation of two arrays using a discrete summing technique.

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N, STATUS
REAL*8 A(15000), B(15000), C(15000)
N = 15000
CALL DCORR_PERIODIC(A,B,C,N,STATUS)
```

This Fortran code computes the periodic correlation of two vectors of double-precision real numbers, a and b, with lengths of 15000. The result is stored in c with length of 15000.

SCONV_NONPERIODIC_EXT DCONV_NONPERIODIC_EXT CCONV_NONPERIO Extended Nonperiodic Convolution

Format

status = {S,D,C,Z}CONV_NONPERIODIC_EXT (x, nx_stride, y, ny_stride, out, out_stride, nx, ny, n_out_start, n_out_end, add_flag, scale_flag, scale, scale_stride)

Arguments

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the data to be convolved.
On exit, **x** is unchanged.

nx_stride
integer*4
Distance between elements in the X array; *nx_stride* > 0

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the convolution or "filter" function that is to be convolved with the data from the X array.
On exit, **y** is unchanged.

ny_stride
integer*4
Distance between elements in the Y array; *ny_stride* > 0

out
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array OUT of length $nx + ny - 1$.
On exit, **out** contains the convolution coefficients.

out_stride
integer*4
Specifies the distance between elements in the OUT array; *out_stride* > 0

nx, ny
integer*4
Specifies the number of values to be operated on; $nx, ny > 0$

n_out_start, n_out_end
integer*4
Specifies the range of coefficients computed; *n_out_end* $>$ *n_out_start*. The OUT array has zero values for indices less than 0 or greater than $nx + ny - 2$.

For example, in the case of nx = 50 and ny = 100, the range of locations is 0 through 148. If you specify *n_out_start* = 5 and *n_out_end* = 10, the convolution function generates numbers for OUT(5) through OUT(10) and puts the results in location 0 through 5 of the OUT array.

You can also specify a range that is larger than the array, creating null elements in the output array. For example, using the same input array, you can specify *n_out_start* = -10 and *n_out_end* = 200. The convolution function can generate values for 0 through 148, putting them in location 10 through 158 of the output array. It puts null elements in the locations between 0 and 9 and between 159 and 200.

add_flag
logical*4
Defines the operation of the convolution to add output to an existing OUT array, without overwriting it:

TRUE: Add the result of the operation to OUT array.
FALSE: Overwrite the existing OUT array.

scale_flag
logical*4
Defines the operation of the convolution to scale the output:

TRUE: Scale the output.
FALSE: Do not scale.

scale
real*4 | real*8 | complex*8 | complex*16
The value used to scale the output. The type of value depends on **scale_stride**.

scale_stride
integer*4
Defines how the scale operation is performed. *scale_stride* $\geq$ 0:

= 0 : Scale by a scalar value
$>$ 0: Scale by a vector, used as the stride of **scale**

Description

The _CONV_NONPERIODIC_EXT functions compute the nonperiodic convolution with options to control the result.

Return Values

0	DXML_SUCCESS()
8	DXML_ILL_N_RANGE()
13	DXML_BAD_STRIDE()

Example

```
  INCLUDE 'DXMLDEF.FOR'
  INTEGER*4 N,STATUS
  REAL*8 A(50),B(100),C(6),SCALE_VALUE

  SCALE_VALUE = 2.0
  STATUS = DCONV_NONPERIODIC_EXT(A,1,B,1,C,1,50,100,5,10,.FALSE.,.TRUE.,
* SCALE_VALUE,0)
```

This Fortran code computes six values of a nonperiodic convolution of two vectors, C(5) to C(10), of double-precision real numbers, a and b, with lengths of 50 and 100, respectively. The result is scaled by 2.0 and stored in c with length of 6.

SCONV_PERIODIC_EXT DCONV_PERIODIC_EXT CCONV_PERIODIC_EXT ZCO Extended Periodic Convolution

Format

status = {S,D,C,Z}CONV_PERIODIC_EXT (x, nx_stride, y, ny_stride, out, out_stride, n, n_out_start, n_out_end, add_flag, scale_flag, scale, scale_stride)

Arguments

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the data to be convolved.
On exit, **x** is unchanged.

nx_stride
integer*4
Distance between elements in the X array; *nx_stride* > 0

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the convolution or "filter" function that is to be convolved with the data from the X array.
On exit, **y** is unchanged.

ny_stride
integer*4
Distance between elements in the Y array; *ny_stride* > 0

out
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array OUT of length n.
On exit, **out** contains the convoluted data.

out_stride
integer*4
Specifies the distance between elements in the OUT array; *out_stride* > 0

n
integer*4
Specifies the number of values to be operated on; $n > 0$

n_out_start, n_out_end
integer*4
Specifies the range of coefficients computed; *n_out_end* > *n_out_start*. The OUT array has zero values for indices less than 0 or greater than $n - 1$.

For example, in the case of n = 100, the locations range from 0 through 99. If you specify *n_out_start* = 5 and *n_out_end* = 10, the convolution function generates numbers for OUT(5) through OUT(10) and puts the results in location 0 through 5 of the OUT array.

You can also specify a range that is larger than the array. For example, using the same input array, you can specify *n_out_start* = -10 and *n_out_end* = 200. The convolution function can generate values OUT(0) through OUT(99), putting them in location 10 through 109 of the output array. The locations outside of the range do not get null values; they are not affected.

add_flag
logical*4
Defines the operation of the convolution to add output to an existing OUT array, without overwriting it:

TRUE: Add the result of the operation to OUT array.
FALSE: Overwrite the existing OUT array.

scale_flag
logical*4
Defines the operation of the convolution to scale the output:

TRUE: Scale the output.
FALSE: Do not scale.

scale
real*4 | real*8 | complex*8 | complex*16
The value by which to scale the output.

scale_stride
integer*4
Defines how the scale operation is performed. *scale_stride* ≥ 0:

= 0 : Scale by a scalar value
> 0: Scale by a vector, used as the stride of **scale**

Description

The _CONV_PERIODIC_EXT functions compute the periodic convolution with options to control the result.

Return Values

0	DXML_SUCCESS()
8	DXML_ILL_N_RANGE()
13	DXML_BAD_STRIDE()

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N,STATUS
REAL*8 A(100),B(100),C(6),SCALE_VALUE

SCALE_VALUE = 2.0
STATUS = DCONV_PERIODIC_EXT(A,1,B,1,C,1,100,5,10,.FALSE.,.TRUE.,SCALE_VALUE,0)
```

This Fortran code computes six values of a periodic convolution of two vector, C(5) to C(10), of double-precision real numbers, a and b, with length of 100. The result is scaled by 2.0 and stored in c with length of 6.

SCORR_NONPERIODIC_EXT DCORR_NONPERIODIC_EXT CCORR_NONPERIOC Extended Nonperiodic Correlation

Format

status = {S,D,C,Z}CORR_NONPERIODIC_EXT (x, nx_stride, y, ny_stride, out, out_stride, nx, ny, n_out_start, n_out_end, add_flag, scale_flag, scale, scale_stride)

Arguments

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the data to be correlated.
On exit, **x** is unchanged.

nx_stride
integer*4
Distance between elements in the X array; $nx_stride > 0$

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the function that is to be correlated with the data from the X array.
On exit, **y** is unchanged.

ny_stride
integer*4
Distance between elements in the Y array; $ny_stride > 0$

out
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array OUT of length $nx + ny - 1$.
On exit, **out** contains the correlated data.

out_stride
integer*4
Specifies the distance between elements in the OUT array; $out_stride > 0$

nx, ny
integer*4
Specifies the number of values to be operated on; $nx, ny > 0$

n_out_start, n_out_end
integer*4
Specifies the range of coefficients computed; *n_out_end* > *n_out_start*. The OUT array has zero values for indices less than $1 - ny$ or greater than $nx - 1$.

For example, in the case of nx = 50 and ny = 100, the range of locations is -99 through 49. If you specify *n_out_start* = 5 and *n_out_end* = 10, the correlation function generates numbers for OUT(5) through OUT(10) and puts the results in location 0 through 5 of the OUT array.

You can also specify a range that is larger than the array, creating null elements in the output array. For example, using the same input array, you can specify *n_out_start* = -110 and *n_out_end* = 60. The correlation function can generate values for OUT(-99) through OUT(49), putting the results in locations 11 through 159. The locations 0 through 10 and 160 through 170 have no values, because OUT(-110) through OUT(-100) and OUT(50) through OUT(60) are out of range.

add_flag
logical*4
Defines the operation of the correlation to add output to an existing OUT array, without overwriting it:

TRUE: Add the result of the operation to OUT array.
FALSE: Overwrite the existing OUT array.

scale_flag
logical*4
Defines the operation of the correlation to scale the output:

TRUE: Scale the output.
FALSE: Do not scale.

scale
real*4 | real*8 | complex*8 | complex*16
The value by which to scale the output.

scale_stride
integer*4
Defines how the scale operation is performed. *scale_stride* $\geq$ 0:

= 0 : Scale by a scalar value
$>$ 0: Scale by a vector, used as the stride of **scale**

Description

The _CORR_NONPERIODIC_EXT functions compute the nonperiodic correlation with options to control the result.

Return Values

0	DXML_SUCCESS()
8	DXML_ILL_N_RANGE()
13	DXML_BAD_STRIDE()

Example

```
  INCLUDE 'DXMLDEF.FOR'
  INTEGER*4 N,STATUS
  REAL*8 A(50),B(100),C(6),SCALE_VALUE

  SCALE_VALUE = 2.0
  STATUS = DCORR_NONPERIODIC_EXT(A,1,B,1,C,1,50,100,-99,-94,
* .FALSE.,.TRUE.,SCALE_VALUE,0)
```

This Fortran code computes six values of a nonperiodic correlation of two vectors, C(-99) to C(-94), of double-precision real numbers, *a* and *b*, with lengths of 50 and 100, respectively. The result is scaled by 2.0 and stored in *c* with a length of 6.

SCORR_PERIODIC_EXT DCORR_PERIODIC_EXT CCORR_PERIODIC_EXT ZCO Extended Periodic Correlation

Format

status = {S,D,C,Z}CORR_PERIODIC_EXT (x, nx_stride, y, ny_stride, out, out_stride, n, n_out_start, n_out_end, add_flag, scale_flag, scale, scale_stride)

Arguments

x
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the data to be correlated.
On exit, **x** is unchanged.

nx_stride
integer*4
Distance between elements in the X array; $nx_stride > 0$

y
real*4 | real*8 | complex*8 | complex*16
On entry, an array containing the function that is to be correlated with the data from the X array.
On exit, **y** is unchanged.

ny_stride
integer*4
Distance between elements in the Y array; $ny_stride > 0$

out
real*4 | real*8 | complex*8 | complex*16
On entry, a one-dimensional array OUT of length n.
On exit, **out** contains the correlated data.

out_stride
integer*4
Specifies the distance between elements in the OUT array; *out_stride* > 0

n
integer*4
Specifies the number of values to be operated on; $n > 0$

n_out_start, n_out_end
integer*4
Specifies the range of coefficients computed; *n_out_end* > *n_out_start*. The OUT array has zero values for indices less than 0 or greater than $n - 1$.

For example, in the case of n = 100, the locations range from 0 through 99. If you specify *n_out_start* = 5 and *n_out_end* = 10, the correlation function generates numbers for OUT(5) through OUT(10) and puts the results in location 0 through 5 of the OUT array.

You can also specify a range that is larger than the array. For example, using the same input array, you can specify *n_out_start* = -10 and *n_out_end* = 200. The convolution function can generate values OUT(0) through OUT(99), putting them in location 10 through 109 of the output array. The locations outside of the range do not get null values; they are not affected.

add_flag
logical*4
Defines the operation of the function to add the output to an existing OUT array, without overwriting it:

TRUE: Add the result of the operation to OUT array.
FALSE: Overwrite the existing OUT array.

scale_flag
logical*4
Defines the operation of the function to multiply the output by a factor:

TRUE: Scale the output.
FALSE: Do not scale.

scale
real*4 | real*8 | complex*8 | complex*16
The value by which to scale the output.

scale_stride
integer*4
Defines how the scale operation is performed. *scale_stride* ≥ 0:

= 0 : Scale by a scalar value
> 0: Scale by a vector, used as the stride of **scale**

Description

The _CORR_PERIODIC_EXT functions compute the periodic correlation with options to control the result.

Return Values

0	DXML_SUCCESS()
8	DXML_ILL_N_RANGE()
13	DXML_BAD_STRIDE()

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N,STATUS
REAL*8 A(100),B(100),C(6),SCALE_VALUE

SCALE_VALUE = 2.0
STATUS = DCORR_PERIODIC_EXT(A,1,B,1,C,1,100,5,10,.FALSE.,.TRUE.,SCALE_VALUE,0)
```

This Fortran code computes six values of a periodic convolution of two vectors, C(5) to C(10), of double-precision real numbers, *a* and *b*, with length of 100. The result is scaled by 2.0 and stored in *c* with a length of 6.

Filters

This section provides descriptions of the filter subroutines. The filter subroutines are ordered by the type of filter: the one-step filter subprogram, then the two-step filter subprograms.

SFILTER_NONREC
Nonrecursive Filter

The SFILTER_NONREC subroutine performs filtering in lowpass, highpass, bandpass, or bandstop (notch) mode.

Format

SFILTER_NONREC (in, out, n, flow, fhigh, wiggles, nterms, status)

Arguments

in

REAL*4
On entry, a one-dimensional array IN containing the data to be filtered.
On exit, **in** is unchanged.

out

REAL*4
On entry, a one-dimensional array OUT containing the filtered data. The IN and OUT arrays can be the same array.
On exit, **out** is overwritten and contains the filtered data.

n

INTEGER*4
On entry, the number of values to be filtered; $n > 2$ and $n \geq 2(nterms) + 1$.
On exit, **n** is unchanged.

flow

REAL*4
On entry, the lower frequency of the filter, given as a fraction of the Nyquist sampling frequency $1/(2\Delta t)$; $0.0 \leq flow \leq 1.0$.
On exit, **flow** is unchanged.

fhigh

REAL*4
On entry, the upper frequency of the filter, given as a fraction of the Nyquist sampling frequency $1/(2\Delta t)$; $0.0 \leq fhigh \leq 1.0$.
On exit, **fhigh** is unchanged.

wiggles

REAL*4
On entry, a number in -dB units which is proportional to the oscillation from the Gibbs phenomenon; $0.0 \leq wiggles \leq 500.0$.
On exit, **wiggles** is unchanged.

nterms

INTEGER*4
On entry, the order of the filter, that is, the number of filter coefficients in the filter equation; $2 \leq nterms \leq 500$ and $n \geq 2(nterms) + 1$.
On exit, **nterms** is unchanged.

status
INTEGER*4
On entry, **status** is a variable with an unspecified value.
On exit, **status** is an integer value that describes the status of the operation. The following table shows the status function names, their associated integer values, and the status description associated with each integer:

Status Function	Value Returned	Description
DXML_SUCCESS()	0	Successful execution
DXML_MAND_ARG()	1	Mandatory argument is missing
DXML_ILL_WIGGLES()	5	wiggles is out of range
DXML_ILL_FLOW()	6	flow is equal to fhigh
DXML_ILL_F_RANGE()	7	flow or fhigh is out of range
DXML_ILL_N_RANGE()	8	n is out of range
DXML_ILL_N_NONREC()	9	n is less than (2*nterms+1)
DXML_ILL_NTERMS()	10	nterms is out of range

Description

The SFILTER_NONREC subroutine performs nonrecursive filtering in either lowpass, highpass, bandpass, or bandstop (notch) mode. See Table 9–16 for information on controlling the filter type with the **flow** and **fhigh** arguments.

Example

```
INCLUDE 'DXMLDEF.FOR'
INTEGER*4 N, NTERMS, STATUS
REAL*4    SA(510), SB(510), FLOW, FHIGH, WIGGLES
FLOW =    0.0
FHIGH =   0.75
WIGGLES = 200.0
N =       200
NTERMS =  20
CALL SFILTER_NONREC(SA, SB, N, FLOW, FHIGH, WIGGLES, NTERMS, STATUS)
```

This Fortran code filters the 200 values in array SA in lowpass mode.

SFILTER_INIT_NONREC
Initialization Step for Nonrecursive Filter

The SFILTER_INIT_NONREC subroutine computes a working array that is used by DXML_FILTER_APPLY_NONREC.

Format

SFILTER_INIT_NONREC (n, flow, fhigh, wiggles, nterms, temp_array, status)

Arguments

n
INTEGER*4
On entry, the number of values to be filtered; $n > 2$ and $n \geq 2(nterms) + 1$.
On exit, **n** is unchanged.

flow
REAL*4

On entry, the lower frequency of the filter, given as a fraction of the Nyquist sampling frequency $1/(2\Delta t)$; $0.0 \leq flow \leq 1.0$.
On exit, **flow** is unchanged.

fhigh
REAL*4
On entry, the upper frequency of the filter, given as a fraction of the Nyquist sampling frequency $1/(2\Delta t)$; $0.0 \leq fhigh \leq 1.0$.
On exit, **fhigh** is unchanged.

wiggles
REAL*4
On entry, a number in -dB units that is proportional to the oscillation from the Gibbs phenomenon; $0.0 \leq wiggles \leq 500.0$.
On exit, **wiggles** is unchanged.

nterms
INTEGER*4
On entry, the order of the filter, that is, the number of filter coefficients in the filter equation; $2 \leq nterms \leq 500$ and $n \geq 2(nterms) + 1$.
On exit, **nterms** is unchanged.

temp_array
REAL*4
On entry, a temporary array of length 510 used for temporary storage.
On exit, **temp_array** is overwritten and contains the internally-generated filter coefficients.

status
INTEGER*4
On entry, **status** is a variable with an unspecified value.
On exit, **status** is an integer value that describes the status of the operation. The following table shows the status function names, their associated integer values, and the status description associated with each integer:

Status Function	Value Returned	Description
DXML_SUCCESS()	0	Successful execution
DXML_MAND_ARG()	1	Mandatory argument is missing
DXML_ILL_WIGGLES()	5	wiggles is out of range
DXML_ILL_FLOW()	6	flow is equal to fhigh
DXML_ILL_F_RANGE()	7	flow or fhigh is out of range

Status Function	Value Returned	Description
DXML_ILL_N_RANGE()	8	n is out of range
DXML_ILL_N_NONREC()	9	n is less than (2*nterms+1)
DXML_ILL_NTERMS()	10	nterms is out of range

Description

The SFILTER_INIT_NONREC subroutine computes a working array that is used by the SFILTER_APPLY_NONREC subroutine. See Table 9–16 for information on controlling the filter type with the **flow** and **fhigh** arguments.

SFILTER_APPLY_NONREC
Application Step for Nonrecursive Filter

The SFILTER_APPLY_NONREC subroutine performs filtering in lowpass, highpass, bandpass, or bandstop (notch) mode by using the working array that was computed by SFILTER_INIT_NONREC.

Format

SFILTER_APPLY_NONREC (in, out, temp_array, status)

Arguments

in
REAL*4
On entry, an array IN containing the data to be filtered.
On exit, **in** is unchanged.

out
REAL*4
On entry, a one-dimensional array OUT to contain the filtered data. The IN and OUT arrays can be the same array.
On exit, **out** is overwritten and contains the filtered data.

temp_array
REAL*4
On entry, the temporary array of length 510 used for temporary storage of the filter coefficients generated by the DXML_FILTER_INIT_NONREC subroutine.
On exit, **temp_array** is unchanged.

status
INTEGER*4
On entry, **status** is a variable with an unspecified value.
On exit, **status** is an integer value that describes the status of the operation. The following table shows the status function names, their associated integer values, and the status description associated with each integer:

Status Function	Value Returned	Description
DXML_SUCCESS()	0	Successful execution
DXML_MAND_ARG()	1	Mandatory argument is missing
DXML_ILL_TEMP_ARRAY()	2	temp_array is corrupted or incorrect

Description

The SFILTER_APPLY_NONREC subroutine uses the working array that was computed by SFILTER_INIT_NONREC for repeated filtering operations.

Sparse Iterative Solver Subprograms

This section provides descriptions of the iterative solver subprograms for real double-precision operations. The subprograms are grouped by functionality starting with the iterative solvers, followed by the routines for matrix-vector product, the routines for the creation of the preconditioners, and finally the routines for the application of the preconditioners.

DITSOL_DEFAULTS
Set Default Values

Format

DITSOL_DEFAULTS (iparam, rparam)

Arguments

iparam
integer*4
On entry, a one-dimensional array of length at least 50.
On exit, the variables in the IPARAM array are assigned the default values, listed in Table 10–4. Of the first 50 elements, the variables that are not assigned a default value, are set equal to zero.

rparam
real*8
On entry, a one-dimensional array of length at least 50.
On exit, the variables in the RPARAM array are assigned the default values, listed in Table 10–5. Of the first 50 elements, the variables that are not assigned a default value, are set equal to zero.

Description

DITSOL_DEFAULTS sets the default values for the variables in the arrays IPARAM and RPARAM. Of the first 50 elements, the variables that are not assigned a default value, are set equal to zero. It is your responsibility to ensure that any variables in IPARAM and RPARAM that are required by the iterative solver are set to an appropriate value before the call to the solver routine.

CXML_ITSOL_SET_PRINT_ROUTINE
Pass address of user-supplied print routine

Format

CXML_ITSOL_SET_PRINT_ROUTINE (user_print_routine, context, iparam)

Arguments

user_print_routine
procedure
User-supplied print routine that iterative solvers call to print messages.

context
integer*4
Integer array of length determined by the user. This argument is passed by the user to retain information for later use in USER_PRINT_ROUTINE.

iparam
integer*4
On entry, a one-dimensional array of length at least 50. The variables in the IPARAM array are assigned the values listed in Table 10–4. Of the first 50 values, the 30th - 50th elements in IPARAM are reserved for the use of CXML.

Description

CXML_ITSOL_SET_PRINT_ROUTINE passes the address of the user-supplied USER_PRINT_ROUTINE to the iterative solvers, along with context and IPARAM array.

For further information and examples about how to use this routine, refer to Chapter 10.

USER_PRINT_ROUTINE
User-supplied print routine

Format

USER_PRINT_ROUTINE (context, buf, size)

Arguments

context
integer*4
Integer array of length determined by the user. This argument is passed by the user in CXML_ITSOL_SET_PRINT_ROUTINE to retain information for use by this routine.

buf
integer*4
Null-terminated string passed by iterative solver.

size
integer*4
Size of null-terminated string passed by iterative solver.

Description

USER_PRINT_ROUTINE is a user-supplied print routine that can be called by the iterative solvers to print messages. Iterative solvers send a null-terminated string to this routine.

Note: CXML provides a routine that can be called by USER_PRINT_ROUTINE to format the null-terminated strings returned to it by the iterative solvers. This routine, CXML_FORMAT_STRING, avoids the problems associated with passing character strings from C to Fortran on various platforms. It is highly recommended that you call CXML_FORMAT_STRING in your USER_PRINT_ROUTINE.

CXML_FORMAT_STRING
General routine to format null-terminated strings

Format

cxml_format_string (buf, size, new_buf)

Arguments

buf
integer*4
Null-terminated string passed by iterative solver.

size
integer*4
Size of null-terminated string passed by iterative solver.

new_buf
character*cxml_itsol_max_message_length
Formatted character string consisting of message from iterative solver.

Description

CXML_FORMAT_STRING formats null-terminated strings returned by the iterative solvers. This routine is specifically designed for Fortran users who wish to write a USER_PRINT_ROUTINE. CXML_FORMAT_STRING can be called by USER_PRINT_ROUTINE to avoid problems that may occur when character strings are passed from C to Fortran on various platforms. The use of this routine is highly recommended.

Note: 'cxml_itsol_print.for' must be included in USER_PRINT_ROUTINE.

DITSOL_DRIVER
Driver for Sparse Iterative Solvers (Serial and Parallel Versions)

Format

DITSOL_DRIVER (dmatvec_driver, dpcondl_driver, dpcondr_driver, mstop, a, ia, x, b, n, ql, iql , qr, iqr, iparam, rparam, iwork, rwork, ierror)

Arguments

DITSOL_DRIVER has the standard parameter list for an iterative solver, with the exception of the first three arguments which must be DMATVEC_DRIVER, DPCONDL_DRIVER, and DPCONDR_DRIVER. These must be declared external in your calling (sub)program.

Description

DITSOL_DRIVER solves the system of linear equations:

$$Ax = b$$

using one of the five iterative methods provided in CXML. By a suitable choice of the variables $isolve$, $istore$ and $iprec$ in the array IPARAM, an appropriate solver, storage scheme and preconditioner are selected. The preconditioner must be created in the appropriate storage scheme, prior to the call to the driver routine.

The following table shows the preconditioning options and the preconditioners that are permitted:

Preconditioner	Left	Right	Split	SPD Split
Diagonal	X	X		X
Polynomial	X	X		X
ILU	X	X	X	X

The preconditioning options applicable to the various iterative solvers are summarized in Table 10–8.

The following table shows the real workspace requirements ($nrwk$) for each method and the corresponding preconditioning option:

Method	None	Left	Right	Split
DITSOL_PCG	$3n$			$4n$ (SPD split)
DITSOL_PLSCG	$4n$	$5n$	$5n$	$6n$
DITSOL_PBCG	$5n$	$7n$	$6n$	$7n$
DITSOL_PCGS	$6n$	$7n$	$6n$	$7n$
DITSOL_PGMRES	$nrwk1$	$nrwk1 + n$	$nrwk1 + n$	$nrwk1 + n$
DITSOL_PTFQMR	$7n$	$8n$	$8n$	$9n$

In DITSOL_PGMRES, $nrwk1 = n(kprev + 1) + kprev(kprev + 5) + 1$ where $kprev$ is the number of previous vectors stored. If ILU preconditioning is used, then an additional real workspace of length n is required.

If you use the option of defining your own MSTOP routine, see the reference description of each solver for the definition of the vector z. format.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, refer to Section A.1. For information about linking to the serial or to the parallel library, refer to Chapter 3.

DITSOL_PCG
Preconditioned Conjugate Gradient Method
(Serial and Parallel Versions)

Format

DITSOL_PCG (matvec, pcondl, pcondr, mstop, a, ia, x, b, n, ql, iql , qr, iqr, iparam, rparam, iwork, rwork, ierror)

Arguments

DITSOL_PCG has the standard parameter list for an iterative solver.

Description

DITSOL_PCG implements the conjugate gradient method [Hestenes and Stiefel 1952, Reid 1971] for the solution of a linear system of equations where the coefficient matrix A is symmetric positive definite or mildly nonsymmetric. This method requires the routine MATVEC to provide operations for **job** = 0. The routines MATVEC, PCONDL (if used) and MSTOP (if used) should be declared external in your calling (sub)program. PCONDR is not used by DITSOL_PCG and is therefore a dummy input parameter.

CXML provides the following two forms of the method:

- Unpreconditioned conjugate gradient method:
  This is the conjugate gradient method applied to:

  $$Ax = b$$

  where A is a symmetric positive definite or a mildly nonsymmetric matrix. As no preconditioning is used, both PCONDL and PCONDR are dummy input parameters.
  For the unpreconditioned conjugate gradient method, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $3n$, where n is the order of the matrix A.

  The vector z, passed as an input argument to the routine MSTOP, is not defined.

- Conjugate gradient method with symmetric positive definite split preconditioning:
  This is the conjugate gradient method applied to:

  $$(Q_L^{-1} A Q_L^{-T})(Q_L^T x) = (Q_L^{-1} b)$$

  where:

  $$Q = Q_L Q_L^T$$

  is the symmetric positive definite preconditioning matrix. The routine PCONDL, with **job**= 0 should evaluate:

  $$v = Q^{-1} u$$

  The routine PCONDR is not used and an explicit split of the preconditioner Q into Q_L and Q_R is not required.

For the conjugate gradient method, with symmetric positive definite split preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $4n$, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

The vector z, passed as an input argument to the routine MSTOP, is defined as:

$$z = Q^{-1}r$$

where r is the residual at the i-th iteration.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DITSOL_PLSCG
Preconditioned Least Square Conjugate Gradient Method
(Serial and Parallel Versions)

Format

DITSOL_PLSCG (matvec, pcondl, pcondr, mstop, a, ia, x, b, n, ql, iql , qr, iqr, iparam, rparam, iwork, rwork, ierror)

Arguments

DITSOL_PLSCG has the standard parameter list for an iterative solver.

Description

The least squares conjugate gradient is a robust method for the solution of general linear systems. It is equivalent to applying the conjugate gradient method to the normal equations:

$$A^T Ax = A^T b$$

This method requires the evaluation of two matrix products, involving matrix A and A^T. It suffers from the drawback that the condition number of $A^T A$ is the square of the condition number of A, and therefore the convergence of the method is slow. To alleviate the numerical instability resulting from a straightforward application of the conjugate gradient method to the normal equations, CXML adopts the implementation proposed in [Björck and Elfving 1979].

The implementation of the least squares conjugate gradient method requires the routine MATVEC to provide operations for both **job**= 0 and **job**= 1. The routines MATVEC, PCONDL (if used), PCONDR (if used) and MSTOP (if used) should be declared external in your calling (sub)program.

CXML provides the following four forms of the method:

- Unpreconditioned least squares conjugate gradient method:
  This is the conjugate gradient method applied to:

  $$A^T Ax = A^T b$$

  where A is a general matrix. As no preconditioning is used, both PCONDL and PCONDR are dummy input parameters.

For the unpreconditioned least squares conjugate gradient method, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $4n$, where n is the order of the matrix A.

The vector z, passed as an input argument to the routine MSTOP, is not defined.

- Least squares conjugate gradient method with left preconditioning:
  This is the conjugate gradient method applied to:

  $$(A^T Q_L^{-T} Q_L^{-1} A)x = (A^T Q_L^{-T} Q_L^{-1} b)$$

  The routine PCONDL, with **job**= 0 should evaluate:

  $$v = Q_L^{-1} u$$

  and with **job**= 1 should evaluate:

  $$v = Q_L^{-T} u$$

  The routine PCONDR is not used and is therefore a dummy input parameter.

  For the least squares conjugate gradient method, with left preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least 5n, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

  The vector z, passed as an input argument to the routine MSTOP, is defined as:

  $$z = Q_L^{-1} r$$

  where r is the residual at the i-th iteration.
- Least squares conjugate gradient method with right preconditioning:
  This is the conjugate gradient method applied to:

  $$(Q_R^{-T} A^T A Q_R^{-1})y = (Q_R^{-T} A^T b)$$

  where:

  $$y = Q_R x$$

  The routine PCONDR, with **job**= 0 should evaluate:

  $$v = Q_R^{-1} u$$

  and with **job**= 1 should evaluate:

  $$v = Q_R^{-T} u$$

  The routine PCONDL is not used and is therefore a dummy input parameter.

  For the least squares conjugate gradient method, with right preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least 5n, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

  The vector z, passed as an input argument to the routine MSTOP, is not defined.

- Least squares conjugate gradient method with split preconditioning: This is the conjugate gradient method applied to:

  $$(Q_R^{-T} A^T Q_L^{-T} Q_L^{-1} A Q_R^{-1}) y = (Q_R^{-T} A^T Q_L^{-T} Q_L^{-1} b)$$

  where:

  $$y = Q_R x$$

  The routine PCONDL, with **job**= 0 should evaluate:

  $$v = Q_L^{-1} u$$

  and with **job**= 1 should evaluate:

  $$v = Q_L^{-T} u$$

  The routine PCONDR, with **job**= 0 should evaluate:

  $$v = Q_R^{-1} u$$

  and with **job**= 1 should evaluate:

  $$v = Q_R^{-T} u$$

  For the least squares conjugate gradient method, with split preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $6n$, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

  The vector z, passed as an input argument to the routine MSTOP, is defined as:

  $$z = Q_L^{-1} r$$

  where r is the residual at the i-th iteration.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DITSOL_PBCG
Preconditioned Biconjugate Gradient Method
(Serial and Parallel Versions)

Format

DITSOL_PBCG (matvec, pcondl, pcondr, mstop, a, ia, x, b, n, ql, iql , qr, iqr, iparam, rparam, iwork, rwork, ierror)

Arguments

DITSOL_PBCG has the standard parameter list for an iterative solver.

Description

The biconjugate gradient method is a method for the solution of nonsymmetric linear systems of equations. It is similar to the conjugate gradient method but generates two sequences of mutually orthogonal residuals [Fletcher 1976]. While there is no solid theoretical basis for the convergence behavior of the biconjugate gradient method, it can be efficient for some classes of problems. This method requires two matrix products involving the matrix A and A^T, but there is no squaring of the condition number.

The implementation of the biconjugate gradient method requires the routine MATVEC to provide operations for both **job**= 0 and **job**= 1. The routines MATVEC, PCONDL (if used), PCONDR (if used), and MSTOP (if used) should be declared external in your calling (sub)program.

CXML provides the following four forms of the method:

- Unpreconditioned biconjugate gradient method:
  This is the biconjugate gradient method applied to:

  $$Ax = b$$

  where A is a general matrix. As no preconditioning is used, both PCONDL and PCONDR are dummy input parameters.

  For the unpreconditioned bi-conjugate gradient method, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $5n$, where n is the order of the matrix A.

  The vector z, passed as an input argument to the routine MSTOP, is not defined.

- Bi-conjugate gradient method with left preconditioning:
  This is the bi-conjugate gradient method applied to:

  $$(Q_L^{-1}A)x = (Q_L^{-1}b)$$

  The routine PCONDL, with **job**= 0 should evaluate:

  $$v = Q_L^{-1}u$$

  and with **job**= 1 should evaluate:

  $$v = Q_L^{-T}u$$

  The routine PCONDR is not used and is therefore a dummy input parameter.

  For the biconjugate gradient method, with left preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $7n$, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

  The vector z, passed as an input argument to the routine MSTOP, is defined as:

  $$z = Q_L^{-1}r$$

  where r is the residual at the i-th iteration.

- Biconjugate gradient method with right preconditioning:
  This is the bi-conjugate gradient method applied to:

  $$(AQ_R^{-1})y = b$$

  where:

  $$y = Q_R x$$

  The routine PCONDR, with **job**= 0 should evaluate:

  $$v = Q_R^{-1} u$$

  and with **job**= 1 should evaluate:

  $$v = Q_R^{-T} u$$

  The routine PCONDL is not used and is therefore a dummy input parameter.

  For the biconjugate gradient method, with right preconditioning, the length of the real work space array, defined by the variable nrwk (IPARAM(4)), should be at least 6n, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

  The vector z, passed as an input argument to the routine MSTOP, is not defined.

- Biconjugate gradient method with split preconditioning:
  This is the biconjugate gradient method applied to:

  $$(Q_L^{-1} AQ_R^{-1})y = (Q_L^{-1} b)$$

  where:

  $$y = Q_R x$$

  The routine PCONDL, with **job**= 0 should evaluate:

  $$v = Q_L^{-1} u$$

  and with **job**= 1 should evaluate:

  $$v = Q_L^{-T} u$$

  The routine PCONDR, with **job**= 0 should evaluate:

  $$v = Q_R^{-1} u$$

  and with **job**= 1 should evaluate:

  $$v = Q_R^{-T} u$$

  For the biconjugate gradient method, with split preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $7n$, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

  The vector z, passed as an input argument to the routine MSTOP, is defined as:

  $$z = Q_L^{-1} r$$

  where r is the residual at the i-th iteration.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DITSOL_PCGS
Preconditioned Conjugate Gradient Squared Method
(Serial and Parallel Versions)

Format

DITSOL_PCGS (matvec, pcondl, pcondr, mstop, a, ia, x, b, n, ql, iql , qr, iqr, iparam, rparam, iwork, rwork, ierror)

Arguments

DITSOL_PCGS has the standard parameter list for an iterative solver.

Description

The conjugate gradient squared method [Sonneveld 1989] accelerates the convergence of the biconjugate gradient method by generating residuals which are related to the original residual by the square of a polynomial in A, instead of a polynomial in A, as in the case of the conjugate gradient and the bi-conjugate gradient methods. In practice, this results in the conjugate gradient squared method converging roughly twice as fast as the biconjugate gradient method. The additional advantage is that only the matrix A is involved and not A^T. The computational cost for both the biconjugate gradient method and the conjugate gradient squared method are about the same per iteration.

The implementation of the conjugate gradient squared method requires the routine MATVEC to provide operations for **job**= 0. The routines MATVEC, PCONDL (if used), PCONDR (if used), and MSTOP (if used) should be declared external in your calling (sub)program.

CXML provides the following four forms of the method:

- Unpreconditioned conjugate gradient squared method:
  This is the conjugate gradient squared method applied to:

  $$Ax = b$$

  where A is a general matrix. As no preconditioning is used, both PCONDL and PCONDR are dummy input parameters.
  For the unpreconditioned conjugate gradient squared method, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $6n$, where n is the order of the matrix A.

  The vector z, passed as an input argument to the routine MSTOP, is not defined.

- Conjugate gradient squared method with left preconditioning:
  This is the conjugate gradient squared method applied to:

  $$(Q_L^{-1}A)x = (Q_L^{-1}b)$$

  The routine PCONDL, with **job**= 0 should evaluate:

  $$v = Q_L^{-1}u$$

  The routine PCONDR is not used and is therefore a dummy input parameter.

For the conjugate gradient squared method, with left preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $7n$, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

The vector z, passed as an input argument to the routine MSTOP, is defined as:

$$z = Q_L^{-1} r$$

where r is the residual at the i-th iteration.

- Conjugate gradient squared method with right preconditioning:
  This is the conjugate gradient squared method applied to:

  $$(AQ_R^{-1})y = b$$

  where:

  $$y = Q_R x$$

  The routine PCONDR, with **job**= 0 should evaluate:

  $$v = Q_R^{-1} u$$

  The routine PCONDL is not used and is therefore a dummy input parameter.

  For the conjugate gradient squared method, with right preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $6n$, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

  The vector z, passed as an input argument to the routine MSTOP, is not defined.

- Conjugate gradient squared method with split preconditioning:
  This is the conjugate gradient squared method applied to:

  $$(Q_L^{-1} A Q_R^{-1})y = (Q_L^{-1} b)$$

  where:

  $$y = Q_R x$$

  The routine PCONDL, with **job**= 0 should evaluate:

  $$v = Q_L^{-1} u$$

  and the routine PCONDR, with **job**= 0 should evaluate:

  $$v = Q_R^{-1} u$$

  For the conjugate gradient squared method, with split preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $7n$, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

  For split preconditioning, the vector z, passed as an input argument to the routine MSTOP, is defined as:

  $$z = Q_L^{-1} r$$

  where r is the residual at the i-th iteration.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DITSOL_PGMRES
Preconditioned Generalized Minimum Residual Method
(Serial and Parallel Versions)

Format

DITSOL_PGMRES (matvec, pcondl, pcondr, mstop, a, ia, x, b, n, ql, iql , qr, iqr, iparam, rparam, iwork, rwork, ierror)

Arguments

DITSOL_PGMRES has the standard parameter list for an iterative solver.

Description

The generalized minimum residual method [Saad and Schultz 1986] obtains a solution x of the form:

$$x = x_0 + z$$

where x_0 is the initial guess and z is a vector that minimizes the two norm of the residual:

$$r = b - A(x_0 + z)$$

over the Krylov space:

$$K = \text{span}\left\{r_0, Ar_0, A^2r_0, \ldots, A^{k-1}r_0\right\}$$

of dimension k, with the initial residual r_0 defined as:

$$r_0 = b - Ax_0$$

CXML implements the restarted generalized minimum residual method, where the method is restarted every $kprev$ steps. This implies that only the $kprev$ residuals need to be stored, instead of all the previous residuals as in the generalized minimum residual method, resulting in a substantial savings in memory.

The choice of $kprev$ is crucial and requires some skill and experience — too small a value could result in poor convergence or no convergence at all, while too large a value could result in excessive memory requirements. $kprev$ should be assigned a value prior to a call to DITSOL_PGMRES with the parameter IPARAM(34) in the array IPARAM. A suggested starting value for $kprev$ is in the range of 3 to 6. If convergence is not obtained, the value should be increased.

While the generalized minimum residual method is applicable to a general problem and the residuals guaranteed not to increase, it is possible for the residuals to stagnate and for the convergence criterion never to be satisfied. Therefore, the convergence of the method should be monitored closely.

The two norm of the residual generated by the generalized minimum residual method is obtained during its implementation at no extra cost. However, this is the residual of the system to which the method is applied, which, in the left and split preconditioned case is the preconditioned residual $Q_L^{-1}r$. To obtain the true residual, a non-negligible amount of extra computation would be required. Hence, for this method, only stopping criteria (10–5) and (10–6) are allowed. Additionally, a user-defined MSTOP is not allowed. In the unpreconditioned case, the stopping criteria default to (10–3) and (10–4), respectively. Thus only $istop$ = 3 and $istop$ = 4 are permitted for the preconditioned case.

The implementation of the generalized minimum residual method requires the routine MATVEC to provide operations for **job**= 0. The routines MATVEC, PCONDL (if used), PCONDR (if used) should be declared external in your calling (sub)program. A user-defined MSTOP is not allowed.

CXML provides the following four forms of the method:

- Unpreconditioned generalized minimum residual method:
  This is the generalized minimum residual method applied to:

  $$Ax = b$$

  where A is a general matrix. As no preconditioning is used, both PCONDL and PCONDR are dummy input parameters.

  For the unpreconditioned generalized minimum residual method, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least:

  $$nrwk = n(kprev + 1) + kprev(kprev + 5) + 1$$

  where n is the order of the matrix A and $kprev$ is the number of previous residuals stored.
- Generalized minimum residual method with left preconditioning:
  This is the generalized minimum residual method applied to:

  $$(Q_L^{-1}A)x = (Q_L^{-1}b)$$

  The routine PCONDL, with **job** = 0 should evaluate:

  $$v = Q_L^{-1}u$$

  The routine PCONDR is not used and is therefore a dummy input parameter.

  For the generalized minimum residual method, with left preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least:

  $$nrwk = n(kprev + 2) + kprev(kprev + 5) + 1$$

  where n is the order of the matrix A and $kprev$ is the number of previous residuals stored. This does not include the memory requirements of the preconditioner.
- Generalized minimum residual method with right preconditioning:
  This is the generalized minimum residual method applied to:

  $$(AQ_R^{-1})y = b$$

  where:

  $$y = Q_R x$$

  The routine PCONDR, with **job** = 0 should evaluate:

  $$v = Q_R^{-1}u$$

  The routine PCONDL is not used.

For the generalized minimum residual method, with right preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least:

$$nrwk = n(kprev + 2) + kprev(kprev + 5) + 1$$

where n is the order of the matrix A and $kprev$ is the number of previous residuals stored. This does not include the memory requirements of the preconditioner.

- GMRES with split preconditioning: This is the generalized minimum residual method applied to:

  $$(Q_L^{-1} A Q_R^{-1}) y = (Q_L^{-1} b)$$

  where:

  $$y = Q_R x$$

  The routine PCONDL, with **job**= 0 should evaluate:

  $$v = Q_L^{-1} u$$

  and the routine PCONDR, with **job**= 0 should evaluate:

  $$v = Q_R^{-1} u$$

  For the generalized minimum residual method, with split preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least:

  $$nrwk = n(kprev + 2) + kprev(kprev + 5) + 1$$

  where n is the order of the matrix A and $kprev$ is the number of previous residuals stored. This does not include the memory requirements of the preconditioner.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DITSOL_PTFQMR
Preconditioned Transpose_free Quasiminimal Residual Method (Serial and Parallel Versions)

Format

DITSOL_PTFQMR (matvec, pcondl, pcondr, mstop, a, ia, x, b, n, ql, iql , qr, iqr, iparam, rparam, iwork, rwork, ierror)

Arguments

DITSOL_PTFQMR has the standard parameter list for an iterative solver.

Description

The quasiminimal residual (QMR) method [Freund and Nachtigal 1991] is one of the algorithms proposed as a remedy for the irregular convergence behavior of the bi-conjugate gradient and the conjugate gradient squared algorithms. Since these algorithms are not characterized by a minimization property, the residual norm often oscillates wildly. The QMR algorithm, by generating iterates that are defined by a quasiminimization of the residual norm, results in smooth convergence curves.

CXML includes TFQMR, the transpose-free variant of the QMR method, implemented without look-ahead [Freund 1993]. The implementation of the transpose-free quasiminimal residual method requires the routine MATVEC to provide operations for **job** = 0. The routines MATVEC, PCONDL (if used), PCONDR (if used) and MSTOP (if used) should be declared external in your calling (sub)program.

An upper bound for the two norm of the residual of the system being solved, is obtained during the implementation of the TFQMR method at no extra cost. This is the residual of the system to which the method is applied, which in the left and split preconditioned case is the preconditioned residual, $Q_L^{-1}r$. To obtain the true residual, a non-negligible amount of extra computation would be required. Hence, for this method, only stopping criteria (10–5) and (10–6) are allowed. In the unpreconditioned case, the stopping criteria default to (10–3) and (10–4), respectively. Thus only $istop$ = 3 and $istop$ = 4 are permitted for both the preconditioned and unpreconditioned case. Additionally, a user-defined MSTOP is allowed, but the vectors r and z, corresponding to the real and preconditioned residuals, respectively, and passed as input parameters to the routine MSTOP, are undefined.

CXML provides the following four forms of the method:

- Unpreconditioned transpose-free, quasiminimal residual method:
  This is the transpose-free, quasiminimal residual method applied to:

  $$Ax = b$$

  where A is a general matrix. As no preconditioning is used, both PCONDL and PCONDR are dummy input parameters.
  For the unpreconditioned transpose-free, quasiminimal residual method, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $7n$, where n is the order of the matrix A.

  The vectors r and z, passed as input arguments to the routine MSTOP, are not defined.

- Transpose-free, quasiminimal residual method with left preconditioning:
  This is the transpose-free, quasiminimal residual method applied to:

  $$(Q_L^{-1}A)x = (Q_L^{-1}b)$$

  The routine PCONDL, with **job** = 0 should evaluate:

  $$v = Q_L^{-1}u$$

  The routine PCONDR is not used and is therefore a dummy input parameter.

For the transpose-free, quasiminimal residual method, with left preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $8n$, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

The vectors r and z, passed as input arguments to the routine MSTOP, are undefined.

- Transpose-free, quasiminimal residual method with right preconditioning: This is the transpose-free, quasiminimal residual method applied to:

  $$(AQ_R^{-1})y = b$$

  where:

  $$y = Q_R x$$

  The routine PCONDR, with **job** = 0 should evaluate:

  $$v = Q_R^{-1} u$$

  The routine PCONDL is not used and is therefore a dummy input parameter.

  For the transpose-free, quasiminimal residual method, with right preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $8n$, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner.

  The vectors r and z, passed as input arguments to the routine MSTOP, are undefined.

- Transpose-free, quasiminimal residual method with split preconditioning: This is the transpose-free, quasiminimal residual method applied to:

  $$(Q_L^{-1} A Q_R^{-1})y = (Q_L^{-1} b)$$

  where:

  $$y = Q_R x$$

  The routine PCONDL, with **job** = 0 should evaluate:

  $$v = Q_L^{-1} u$$

  and the routine PCONDR, with **job** = 0 should evaluate:

  $$v = Q_R^{-1} u$$

  For the transpose-free, quasiminimal residual method, with split preconditioning, the length of the real work space array, defined by the variable $nrwk$ (IPARAM(4)), should be at least $9n$, where n is the order of the matrix A. This does not include the memory requirements of the preconditioner. The vectors r and z, passed as input arguments to the routine MSTOP, are undefined.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DMATVEC_SDIA
Matrix-Vector Product for Symmetric Diagonal Storage
(Serial and Parallel Versions)

Format

DMATVEC_SDIA (job, a, ia, ndim, nz, w, x, y, n, iparam)

Arguments

job
integer*4
On entry, defines the operation to be performed:

job = 0 : $y = Ax$
job = 1 : $y = A^T x$
job = 2 : $y = w - Ax$
job = 3 : $y = w - A^T x$

On exit, **job** is unchanged.

a
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals from the main diagonal.
On exit, **ia** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array A.
On exit, **nz** is unchanged.

w
real*8
On entry, a one-dimensional array of length at least n containing the vector w when **job** = 2 or 3. The elements are accessed with unit increment. When **job** = 0 or 1, array W is not needed so **w** can be a dummy parameter.
On exit, **w** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

iparam
integer*4
On entry, a one-dimensional array of length at least 50. The variables in the IPARAM array are assigned the values listed in Table 10–4. Of the first 50, the 30th - 50th elements in IPARAM are reserved for the use of CXML.

Description

DMATVEC_SDIA obtains the matrix-vector product for a sparse matrix stored using the symmetric diagonal storage scheme. Depending on the value of the input parameter **job**, either the matrix or its transpose is used in the operation.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DMATVEC_UDIA
Matrix-Vector Product for Unsymmetric Diagonal Storage (Serial and Parallel Versions)

Format

DMATVEC_UDIA (job, a, ia, ndim, nz, w, x, y, n)

Arguments

job
integer*4
On entry, defines the operation to be performed:

job = 0 : $y = Ax$
job = 1 : $y = A^T x$
job = 2 : $y = w - Ax$
job = 3 : $y = w - A^T x$

On exit, **job** is unchanged.

a
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals from the main diagonal.
On exit, **ia** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array A.
On exit, **nz** is unchanged.

w
real*8
On entry, a one-dimensional array of length at least n containing the vector w when **job** = 2 or 3. The elements are accessed with unit increment. When **job** = 0 or 1, array W is not needed so **w** can be a dummy parameter.
On exit, **w** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DMATVEC_UDIA obtains the matrix-vector product for a sparse matrix stored using the unsymmetric diagonal storage scheme. Depending on the value of the input parameter **job**, either the matrix or its transpose is used in the operation.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DMATVEC_GENR
Matrix-Vector Product for General Storage by Rows (Serial and Parallel Versions)

Format

DMATVEC_GENR (job, a, ia, ja, nz, w, x, y, n, iparam)

Arguments

job
integer*4
On entry, defines the operation to be performed:

job = 0 : $y = Ax$
job = 1 : $y = A^T x$
job = 2 : $y = w - Ax$
job = 3 : $y = w - A^T x$

On exit, **job** is unchanged.

a
real*8
On entry, a one-dimensional array of length at least nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least $n + 1$, containing the starting indices of each row in arrays JA and A.
On exit, **ia** is unchanged.

ja
integer*4
On entry, a one-dimensional array of length at least nz, containing the column values of each nonzero element of the matrix A, stored using the general storage by rows scheme.
On exit, **ja** is unchanged.

nz
integer*4
On entry, the number of nonzero elements stored in array A.
On exit, **nz** is unchanged.

w
real*8
On entry, a one-dimensional array of length at least n containing the vector w when **job** = 2 or 3. The elements are accessed with unit increment. When **job** = 0 or 1, array W is not needed so **w** can be a dummy parameter.
On exit, **w** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

iparam
integer*4
On entry, a one-dimensional array of length at least 50. The variables in the IPARAM array are assigned the values listed in Table 10–4. Of the first 50, the 30th - 50th elements in IPARAM are reserved for the use of CXML.

Description

DMATVEC_GENR obtains the matrix-vector product for a sparse matrix stored using the general storage by rows scheme. Depending on the value of the input parameter **job**, either the matrix or its transpose is used in the operation.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DCREATE_DIAG_SDIA
Generate Diagonal Preconditioner for Symmetric Diagonal Storage (Serial and Parallel Versions)

Format

DCREATE_DIAG_SDIA (a, ia, ndim, nz, p, n)

Arguments

a
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals from the main diagonal.
On exit, **ia** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array A.
On exit, **nz** is unchanged.

p
real*8
On entry, a one-dimensional array of length at least n.
On exit, array P contains information for use by the diagonal preconditioner.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DCREATE_DIAG_SDIA computes the information required by the diagonal preconditioner for a sparse matrix stored using the symmetric diagonal storage scheme. The real part of this information is returned in the array P. There is no integer information returned for this preconditioner.

The routine DCREATE_DIAG_SDIA is called prior to a call to one of the iterative solver routines with diagonal preconditioning.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DCREATE_DIAG_UDIA
Generate Diagonal Preconditioner for Unsymmetric Diagonal Storage (Serial and Parallel Versions)

Format

DCREATE_DIAG_UDIA (a, ia, ndim, nz, p, n)

Arguments

a
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals from the main diagonal.
On exit, **ia** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array A.
On exit, **nz** is unchanged.

p
real*8
On entry, a one-dimensional array of length at least n.
On exit, array P contains information for use by the diagonal preconditioner.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DCREATE_DIAG_UDIA computes the information required by the diagonal preconditioner for a sparse matrix stored using the unsymmetric diagonal storage scheme. The real part of this information is returned in the array P. There is no integer information returned for this preconditioner.

The routine DCREATE_DIAG_UDIA is called prior to a call to one of the iterative solver routines with diagonal preconditioning.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DCREATE_DIAG_GENR
Generate Diagonal Preconditioner for General Storage by Rows (Serial and Parallel Versions)

Format

DCREATE_DIAG_GENR (a, ia, ja, nz, p, n)

Arguments

a
real*8
On entry, a one-dimensional array of length at least nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least $n + 1$, containing the starting indices of each row in arrays JA and A.
On exit, **ia** is unchanged.

ja
integer*4
On entry, a one-dimensional array of length at least nz, containing the column values of each nonzero element of the matrix A.
On exit, **ja** is unchanged.

nz
integer*4
On entry, the number of nonzero elements stored in array A.
On exit, **nz** is unchanged.

p
real*8
On entry, a one-dimensional array of length at least n.
On exit, array P contains information for use by the diagonal preconditioner.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DCREATE_DIAG_GENR computes the information required by the diagonal preconditioner for a sparse matrix stored using the general storage by rows scheme. The real part of this information is returned in the array P. There is no integer information returned for this preconditioner.

The routine DCREATE_DIAG_GENR is called prior to a call to one of the iterative solver routines with diagonal preconditioning.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DCREATE_POLY_SDIA
Generate Polynomial Preconditioner for Symmetric Diagonal Storage (Serial and Parallel Versions)

Format

DCREATE_POLY_SDIA (a, ia, ndim, nz, p, n)

Arguments

a
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals from the main diagonal.
On exit, **ia** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array A.
On exit, **nz** is unchanged.

p
real*8
On entry, a one-dimensional array of length at least $3n$.
On exit, array P contains information for use by the polynomial preconditioner.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DCREATE_POLY_SDIA computes the information required by the polynomial preconditioner for a sparse matrix stored using the symmetric diagonal storage scheme. The real part of this information is returned in the array P. There is no integer information returned for this preconditioner. Part of the array P is used as workspace during the application of the preconditioner.

The routine DCREATE_POLY_SDIA is called prior to a call to one of the iterative solver routines with polynomial preconditioning.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DCREATE_POLY_UDIA
Generate Polynomial Preconditioner for Unsymmetric Diagonal Storage (Serial and Parallel Versions)

Format

DCREATE_POLY_UDIA (a, ia, ndim, nz, p, n)

Arguments

a
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals from the main diagonal.
On exit, **ia** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array A.
On exit, **nz** is unchanged.

p
real*8
On entry, a one-dimensional array of length at least $3n$.
On exit, array P contains information for use by the polynomial preconditioner.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DCREATE_POLY_UDIA computes the information required by the polynomial preconditioner for a sparse matrix stored using the unsymmetric diagonal storage scheme. The real part of this information is returned in the array P. There is no integer information returned for this preconditioner. Part of the array P is used as workspace during the application of the preconditioner.

The routine DCREATE_POLY_UDIA is called prior to a call to one of the iterative solver routines with polynomial preconditioning.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DCREATE_POLY_GENR
Generate Polynomial Preconditioner for General Storage by Rows (Serial and Parallel Versions)

Format

DCREATE_POLY_GENR (a, ia, ja, nz, p, n)

Arguments

a
real*8
On entry, a one-dimensional array of length at least nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least $n+1$, containing the starting indices of each row in arrays JA and A.
On exit, **ia** is unchanged.

ja
integer*4
On entry, a one-dimensional array of length at least nz, containing the column values of each nonzero element of the matrix A.
On exit, **ja** is unchanged.

nz
integer*4
On entry, the number of nonzero elements stored in array A.
On exit, **nz** is unchanged.

p
real*8
On entry, a one-dimensional array of length at least $3n$.
On exit, array P contains information for use by the diagonal preconditioner.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DCREATE_POLY_GENR computes the information required by the polynomial preconditioner for a sparse matrix stored using the general storage by rows scheme. The real part of this information is returned in the array P. There is no integer information returned for this preconditioner. Part of the array P is used as workspace during the application of the preconditioner.

The routine DCREATE_POLY_GENR is called prior to a call to one of the iterative solver routines with polynomial preconditioning.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DCREATE_ILU_SDIA
Generate Incomplete Cholesky Preconditioner for Symmetric Diagonal Storage

Format

DCREATE_ILU_SDIA (a, ia, ndim, nz, p, ip, n)

Arguments

a
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals from the main diagonal.
On exit, **ia** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array A.
On exit, **nz** is unchanged.

p
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz.
On exit, array P contains information used by the Incomplete Cholesky preconditioner.

ip
integer*4
On entry, a one-dimensional array of length at least nz.
On exit, IP contains information for the Incomplete Cholesky preconditioner.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DCREATE_ILU_SDIA computes the information required by the Incomplete Cholesky preconditioner for a sparse matrix stored using the symmetric diagonal storage scheme. The arrays P and IP contain the real and integer information, respectively, for use by the preconditioner.

If the lower triangular part of the matrix A is stored, the decomposition is LL^T, where L is a lower triangular matrix. If the upper triangular part is stored, the decomposition is U^TU, where U is an upper triangular matrix.

The routine DCREATE_ILU_SDIA is called prior to a call to one of the iterative solver routines with Incomplete Cholesky preconditioning.

DCREATE_ILU_UDIA
Generate Incomplete LU Preconditioner for Unsymmetric Diagonal Storage

Format

DCREATE_ILU_UDIA (a, ia, ndim, nz, plu, iplu, n)

Arguments

a
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals from the main diagonal.
On exit, **ia** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array A.
On exit, **nz** is unchanged.

plu
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz.
On exit, array PLU contains information used by the Incomplete LU preconditioner.

iplu
integer*4
On entry, a one-dimensional array of length at least nz.
On exit, array IPLU contains information used by the Incomplete LU preconditioner.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DCREATE_ILU_UDIA computes the information required by the Incomplete LU preconditioner for a sparse matrix stored using the unsymmetric diagonal storage scheme. The arrays PLU and IPLU contain the real and integer information, respectively, for use by the preconditioner.

The routine DCREATE_ILU_UDIA is called prior to a call to one of the iterative solver routines with Incomplete LU preconditioning.

DCREATE_ILU_GENR
Generate Incomplete LU Preconditioner for General Storage by Rows

Format

DCREATE_ILU_GENR (a, ia, ja, nz, plu, n)

Arguments

a
real*8
On entry, a one-dimensional array of length at least nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least $n + 1$, containing the starting indices of each row in arrays JA and A.
On exit, **ia** is unchanged.

ja
integer*4
On entry, a one-dimensional array of length at least nz, containing the column values of each nonzero element of the matrix A.
On exit, **ja** is unchanged.

nz
integer*4
On entry, the number of nonzero elements in array A.
On exit, **nz** is unchanged.

plu
real*8
On entry, a one-dimensional array of length at least nz.
On exit, array PLU contains information used by the Incomplete LU preconditioner.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DCREATE_ILU_GENR computes the information required by the Incomplete LU preconditioner for a sparse matrix stored using the general storage by rows scheme. The array PLU contains the real information for use by the preconditioner. The integer information is identical to the information in arrays IA and JA and is therefore not generated.

The routine DCREATE_ILU_GENR is called prior to a call to one of the iterative solver routines with Incomplete LU preconditioning.

DAPPLY_DIAG_ALL
Apply Diagonal Preconditioner for Any Storage Scheme (Serial and Parallel Versions)

Format

DAPPLY_DIAG_ALL (p, x, y, n)

Arguments

p
real*8
On entry, a one-dimensional array of length at least n containing information for use by the polynomial preconditioner.
On exit, **p** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by $Q^{-1}x$, where Q is the diagonal preconditioner. The elements of Y are accessed with unit increment.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DAPPLY_DIAG_ALL applies the diagonal preconditioner for a sparse matrix stored using any one of the three storage schemes — symmetric diagonal, unsymmetric diagonal, or general storage by rows. The input vector, p, contains information for use by the routine. This vector is generated by a call to one of the routines DCREATE_DIAG_SDIA, DCREATE_DIAG_UDIA or DCREATE_DIAG_GENR prior to a call to one of the iterative solvers with diagonal preconditioning.

DAPPLY_DIAG_ALL applies the diagonal preconditioner, Q, using information stored in the vector p, to the vector x and returns the result in vector y:

$$y \leftarrow Q^{-1}x$$

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DAPPLY_POLY_SDIA
Apply Polynomial Preconditioner for Symmetric Diagonal Storage (Serial and Parallel Versions)

Format

DAPPLY_POLY_SDIA (job, p, a, ia, ndim, nz, x, y, ndeg, n, iparam)

Arguments

job
integer*4
On entry, defines the operation to be performed:

job = 0 : $y = Q^{-1}x$
job = 1 : $y = Q^{-T}x$

where Q is the polynomial preconditioner.
On exit, **job** is unchanged.

p
real*8
On entry, a one-dimensional array of length at least $3n$ that contains information for use by the polynomial preconditioner and workspace.
On exit, the part of array P that contains the information related to the polynomial preconditioner is unchanged. The part used as workspace is overwritten.

a
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals from the main diagonal.
On exit, **ia** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array A.
On exit, **nz** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

ndeg
integer*4
On entry, the degree of the polynomial in the polynomial preconditioner.
On exit, **ndeg** is unchanged.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

iparam
integer*4
On entry, a one-dimensional array of length at least 50. The variables in the IPARAM array are assigned the values listed in Table 10–4. Of the first 50, the 30th - 50th elements in IPARAM are reserved for the use of CXML.

Description

DAPPLY_POLY_SDIA applies the polynomial preconditioner for a sparse matrix stored using the symmetric diagonal storage scheme. The input vector, p, contains information for use by the routine. This vector is generated by a call to the routine DCREATE_POLY_SDIA prior to a call to one of the iterative solvers with polynomial preconditioning. Depending on the value of the input parameter **job**, DAPPLY_POLY_SDIA operates on either the preconditioning matrix or its transpose.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DAPPLY_POLY_UDIA
Apply Polynomial Preconditioner for Unsymmetric Diagonal Storage (Serial and Parallel Versions)

Format

DAPPLY_POLY_UDIA (job, p, a, ia, ndim, nz, x, y, ndeg, n)

Arguments

job
integer*4
On entry, defines the operation to be performed:

job = 0 : $y = Q^{-1}x$
job = 1 : $y = Q^{-T}x$

where Q is the polynomial preconditioner.
On exit, **job** is unchanged.

p
real*8
On entry, a one-dimensional array of length at least $3n$ that contains information for use by the polynomial preconditioner and workspace.
On exit, the part of array P that contains the information related to the polynomial preconditioner is unchanged. The part used as workspace is overwritten.

a
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals from the main diagonal.
On exit, **ia** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array A.
On exit, **nz** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

ndeg
integer*4
On entry, the degree of the polynomial in the polynomial preconditioner.
On exit, **ndeg** is unchanged.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DAPPLY_POLY_UDIA applies the polynomial preconditioner for a sparse matrix stored using the unsymmetric diagonal storage scheme. The input vector, p, contains information for use by the routine. This vector is generated by a call to the routine DCREATE_POLY_UDIA prior to a call to one of the iterative solvers with polynomial preconditioning. Depending on the value of the input parameter **job**, DAPPLY_POLY_UDIA operates on either the preconditioning matrix or its transpose.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DAPPLY_POLY_GENR
Apply Polynomial Preconditioner for General Storage by Rows (Serial and Parallel Versions)

Format

DAPPLY_POLY_GENR (job, p, a, ia, ja, nz, x, y, ndeg, n, iparam)

Arguments

job
integer*4
On entry, defines the operation to be performed:

job = 0 : $y = Q^{-1}x$
job = 1 : $y = Q^{-T}x$

where Q is the polynomial preconditioner.
On exit, **job** is unchanged.

p
real*8
On entry, a one-dimensional array of length at least $3n$ that contains information for use by the polynomial preconditioner and workspace.
On exit, the part of array P that contains the information related to the polynomial preconditioner is unchanged. The part used as workspace is overwritten.

a
real*8
On entry, a one-dimensional array of length at least nz containing the nonzero elements of the matrix A.
On exit, **a** is unchanged.

ia
integer*4
On entry, a one-dimensional array of length at least $n + 1$, containing the starting indices of each row in arrays JA and A.
On exit, **ia** is unchanged.

ja
integer*4
On entry, a one-dimensional array of length at least nz, containing the column values of each nonzero element of the matrix A.
On exit, **ja** is unchanged.

nz
integer*4
On entry, the number of nonzero elements stored in array A.
On exit, **nz** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

ndeg
integer*4
On entry, the degree of the polynomial in the polynomial preconditioner.
On exit, **ndeg** is unchanged.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

iparam
integer*4
On entry, a one-dimensional array of length at least 50. The variables in the IPARAM array are assigned the values listed in Table 10–4. Of the first 50, the 30th - 50th elements in IPARAM are reserved for the use of CXML.

Description

DAPPLY_POLY_GENR applies the polynomial preconditioner for a sparse matrix stored using the general storage by rows scheme. The input vector, p, contains information for use by the routine. This vector is generated by a call to the routine DCREATE_POLY_GENR prior to a call to one of the iterative solvers with polynomial preconditioning. Depending on the value of the input parameter **job**, DAPPLY_POLY_GENR operates on either the preconditioning matrix or its transpose.

This routine is available in both serial and parallel versions. The routine names and parameter list are identical for both versions. For information about using the parallel library, see Section A.1. For information about linking to the serial or to the parallel library, see Chapter 3.

DAPPLY_ILU_SDIA
Apply ILU Preconditioner for Symmetric Diagonal Storage

Format

DAPPLY_ILU_SDIA (job, p, ip, ndim, nz, x, y, n)

Arguments

job
integer*4
On entry, defines the operation to be performed. If the lower triangular part of the matrix A is stored, the preconditioner is of the form LL^T, where L is a lower triangular matrix. In this case:

job = 0 : $y = L^{-1}x$

job = 1 : $y = L^{-T}x$

If the upper triangular part of the matrix A is stored, the preconditioner is of the form U^TU, where U is an upper triangular matrix. In this case:

job = 0 : $y = U^{-1}x$
job = 1 : $y = U^{-T}x$

On exit, **job** is unchanged.

p
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing information for use by the Incomplete Cholesky preconditioner.
On exit, **p** is unchanged.

ip
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals in array P from the main diagonal.
On exit, **ip** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array P.
On exit, **nz** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DAPPLY_ILU_SDIA applies the Incomplete Cholesky preconditioner for a sparse matrix stored using the symmetric diagonal storage scheme. The input arrays, P and IP, contain information for use by the routine. These arrays are generated by a call to the routine DCREATE_ILU_SDIA prior to a call to one of the iterative solvers with Incomplete Cholesky preconditioning.

Depending on the value of the input parameter **job**, DAPPLY_ILU_SDIA operates on either the matrix or its transpose. The symmetric diagonal storage scheme, SDIA, allows either the lower or upper triangular part of the matrix to be stored. If the lower triangular part is stored, the routine DCREATE_ILU_SDIA creates the incomplete Cholesky preconditioner in the form LL^T, where L is a lower triangular matrix. In this case, **job** = 0 implies:

$$y = L^{-1}x$$

and **job** = 1 implies:

$$y = L^{-T}x$$

If the upper triangular part of the matrix A is stored, the routine DCREATE_ILU_SDIA creates the incomplete Cholesky preconditioner in the form U^TU, where U is an upper triangular matrix. In this case, **job** = 0 implies:

$$y = U^{-1}x$$

and **job** = 1 implies:

$$y = U^{-T}x$$

DAPPLY_ILU_UDIA_L
Apply ILU Preconditioner for Unsymmetric Diagonal Storage

Format

DAPPLY_ILU_UDIA_L (job, plu, iplu, ndim, nz, x, y, n)

Arguments

job
integer*4
On entry, defines the operation to be performed:

job = 0 : $y = L^{-1}x$
job = 1 : $y = L^{-T}x$

where the incomplete factorization is calculated as LU. L and U are lower and upper triangular matrices, respectively.
On exit, **job** is unchanged.

plu
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz, containing information for use by the ILU preconditioner.
On exit, **plu** is unchanged.

iplu
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals of PLU from the main diagonal.
On exit, **iplu** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in array PLU.
On exit, **nz** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DAPPLY_ILU_UDIA_L applies the Incomplete LU preconditioner (lower triangular part) for a sparse matrix stored using the unsymmetric diagonal storage scheme. The input arrays, PLU and IPLU, contain information for use by the routine. These arrays are generated by a call to the routine DCREATE_ILU_UDIA prior to a call to one of the solvers with Incomplete LU preconditioning. Depending on the value of the input parameter **job**, DAPPLY_ILU_UDIA_L operates on either the matrix or its transpose.

DAPPLY_ILU_UDIA_U
Apply ILU Preconditioner for Unsymmetric Diagonal Storage

Format

DAPPLY_ILU_UDIA_U (job, plu, iplu, ndim, nz, x, y, n)

Arguments

job
integer*4
On entry, defines the operation to be performed:

job = 0 : $y = U^{-1}x$
job = 1 : $y = U^{-T}x$

where the incomplete factorization is calculated as LU. L and U are lower and upper triangular matrices respectively.
On exit, **job** is unchanged.

plu
real*8
On entry, a two-dimensional array with dimensions $ndim$ by nz containing information used by the Incomplete LU preconditioner.
On exit, **plu** is unchanged.

iplu
integer*4
On entry, a one-dimensional array of length at least nz, containing the distances of the diagonals of PLU from the main diagonal.
On exit, **iplu** is unchanged.

ndim
integer*4
On entry, the leading dimension of array A, as declared in the calling subprogram; $ndim \geq n$.
On exit, **ndim** is unchanged.

nz
integer*4
On entry, the number of diagonals stored in arrays PLU and A.
On exit, **nz** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DAPPLY_ILU_UDIA_U applies the Incomplete LU preconditioner (upper triangular part) for a sparse matrix stored using the unsymmetric diagonal storage scheme. The input arrays, PLU and IPLU, contain information for use by the routine. These arrays are generated by a call to the routine DCREATE_ILU_UDIA prior to a call to one of the solvers with Incomplete LU preconditioning. Depending on the value of the input parameter **job**, DAPPLY_ILU_UDIA_U operates on either the matrix or its transpose.

DAPPLY_ILU_GENR_L
Apply Incomplete LU Preconditioner for General Storage by Rows

Format

DAPPLY_ILU_GENR_L (job, plu, iplu, jplu, nz, x, y, n)

Arguments

job
integer*4
On entry, defines the operation to be performed:

job = 0 : $y = L^{-1}x$
job = 1 : $y = L^{-T}x$

where the incomplete factorization is calculated as LU. L and U are lower and upper triangular matrices, respectively.
On exit, **job** is unchanged.

plu
real*8
On entry, a one-dimensional array of length at least nz containing information used by the Incomplete LU preconditioner.
On exit, **plu** is unchanged.

iplu
integer*4
On entry, a one-dimensional array of length at least $n + 1$, containing the starting indices of each row in array PLU and JPLU. IPLU is identical to the array IA used in the storage of the matrix A.
On exit, **iplu** is unchanged.

jplu
integer*4
On entry, a one-dimensional array of length at least nz, containing the column values of each nonzero element of the matrix PLU, stored using the general storage by rows scheme. JPLU is identical to the array JA used in the storage of the matrix A.
On exit, **jplu** is unchanged.

nz
integer*4
On entry, the number of nonzero elements stored in array PLU.
On exit, **nz** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DAPPLY_ILU_GENR_L applies the Incomplete LU preconditioner (lower triangular part) for a sparse matrix stored using the general storage by rows scheme. The input arrays, PLU, IPLU and JPLU, contain information for use by the routine. These arrays are generated by a call to the routine DCREATE_ILU_GENR prior to a call to one of the iterative solvers with Incomplete LU preconditioning. The information in the arrays IPLU and JPLU is identical to the information in the arrays IA and JA. Therefore, routine DCREATE_ILU_GENR does not generate these arrays.

Depending on the value of the input parameter **job**, DAPPLY_ILU_GENR_L operates on either the matrix or its transpose.

DAPPLY_ILU_GENR_U
Apply Incomplete LU Preconditioner for General Storage by Rows

Format

DAPPLY_ILU_GENR_U (job, plu, iplu, jplu, nz, x, y, n)

Arguments

job
integer*4
On entry, defines the operation to be performed:

job = 0 : $y = U^{-1}x$
job = 1 : $y = U^{-T}x$

where the incomplete factorization is calculated as LU. L and U are lower and upper triangular matrices, respectively.
On exit, **job** is unchanged.

plu
real*8
On entry, a one-dimensional array of length at least nz containing information used by the Incomplete LU preconditioner.
On exit, **plu** is unchanged.

iplu
integer*4
On entry, a one-dimensional array of length at least $n + 1$, containing the starting indices of each row in array PLU and JPLU. IPLU is identical to the array IA used in the storage of the matrix A.
On exit, **iplu** is unchanged.

jplu
integer*4
On entry, a one-dimensional array of length at least nz, containing the column values of each nonzero element of the matrix PLU, stored using the general storage by rows scheme. JPLU is identical to the array JA used in the storage of the matrix A in the general storage by rows scheme.
On exit, **jplu** is unchanged.

nz
integer*4
On entry, the number of nonzero elements stored in array PLU.
On exit, **nz** is unchanged.

x
real*8
On entry, a one-dimensional array of length at least n, containing the elements of vector x, accessed with unit increment.
On exit, **x** is unchanged.

y
real*8
On entry, a one-dimensional array of length at least n.
On exit, array Y is overwritten by the output vector y. The elements of array Y are accessed with unit increment.

n
integer*4
On entry, the order of the matrix A.
On exit, **n** is unchanged.

Description

DAPPLY_ILU_GENR_U applies the Incomplete LU preconditioner (upper triangular part) for a sparse matrix stored using the general storage by rows scheme. The input arrays, PLU, IPLU and JPLU, contain information for use by the routine. These arrays are generated by a call to the routine DCREATE_ ILU_GENR prior to a call to one of the iterative solvers with Incomplete LU preconditioning. The information in the arrays IPLU and JPLU is identical to the information in the arrays IA and JA. Therefore, the routine DCREATE_ILU_ GENR does not generate these arrays.

Depending on the value of the input parameter **job**, DAPPLY_ILU_GENR_U operates on either the matrix or its transpose.

Direct Sparse Solver Subprograms

This section describes the user-callable CXML direct sparse solver subroutines.

For each routine, a description is provided along with information about the routine's format, arguments, default options, and errors.

Examples showing the use of these routines are provided in the "Using Direct Sparse Solvers" section of the *CXML Reference Manual* and the *Direct Sparse Solvers Reference* booklet.

Note: The Direct Sparse Solver routines described in this section are new, and replace the set of Direct Solvers for Sparse Linear Systems routines (also known as *Skyline Solvers*), which have been retired.

While the former Direct Sparse Solver routines will be supported for an undetermined amount of time, it is highly recommended that you begin using these new Direct Sparse Solver routines immediately.

Refer to "Direct Solvers for Sparse Linear Systems", in the Appendix of the *CXML Reference Manual* for information about the retired direct sparse solver routines.

dss_create

Format

dss_create (handle, opt)

Arguments

handle : OUTPUT : CXML_DSS_HANDLE
opt : INPUT : INTEGER

Description

dss_create is called to initialize the solver. After the call to dss_create, all subsequent invocations of CXML direct sparse solver routines should use the value of handle returned by dss_create.

Warning: Do not write the value of handle directly.

Default Options

CXML_DSS_MSG_LVL_WARNING
CXML_DSS_TERM_LVL_ERROR

Return Values

CXML_DSS_SUCCESS
CXML_DSS_INVALID_OPTION
CXML_DSS_OUT_OF_MEMORY

dss_delete

Format

dss_delete (handle, opt)

Arguments

handle : OUTPUT : CXML_DSS_HANDLE
opt : INPUT : INTEGER

Description

dss_delete is called to delete all of the data structures created during the solutions process.

Default Options

CXML_DSS_MSG_LVL_WARNING
CXML_DSS_TERM_LVL_ERROR

Return Values

CXML_DSS_SUCCESS
CXML_DSS_INVALID_OPTION
CXML_DSS_OUT_OF_MEMORY

---

dss_define_structure

Format

dss_define_structure (handle, opt, rowIndex, nRows, nCols, columns, nNonZeros)

Arguments

handle : OUTPUT : CXML_DSS_HANDLE
opt : INPUT : INTEGER
rowIndex : INPUT : INTEGER (see 1)
nRows : INPUT : INTEGER
nCols : INPUT : INTEGER
columns : INPUT : INTEGER (see 2)
nNonZeros : INPUT : INTEGER

1. Array of size *min(nRows, nCols)+1*.
2. Array of size *nNonZeros*.

Description

dss_define_structure communicates to the solver the locations of the *nNonZero* number of non-zero elements in a matrix of size *nRows* by *nCols*. Currently, the CXML direct sparse solver only operate on square matrices, so *nRows* must be equal to *nCols*.

Communicating the locations of the non-zeros takes place in two steps:

1. Define the general non-zero structure of the matrix by specifying one of the following option arguments:

   CXML_DSS_SYMMETRIC_STRUCTURE
   CXML_DSS_SYMMETRIC
   CXML_DSS_NON_SYMMETRIC

2. Provide the actual locations of the non-zeros by means of the arrays *rowIndex* and *columns*. Refer to the "Using Direct Sparse Solvers" section of the *CXML Reference Manual* and the *Direct Sparse Solvers Reference* booklet for a detailed description of *rowIndex* and *columns* index.

Note: Currently, DSS does not directly support non-symmetric matrices. Instead, when the CXML_DSS_NON_SYMMETRIC option is specified, DSS will convert non-symmetric matrices into symmetrically structured matrices by adding zeros in the appropiate place.

Default Options

CXML_DSS_SYMMETRIC

Return Values

CXML_DSS_SUCCESS
CXML_DSS_STATE_ERR
CXML_DSS_INVALID_OPTION
CXML_DSS_COL_ERR
CXML_DSS_NOT_SQUARE
CXML_DSS_TOO_FEW_VALUES
CXML_DSS_TOO_MANY_VALUES

---

dss_reorder

Format

dss_reorder (handle, opt, perm)

Arguments

handle : OUTPUT : CXML_DSS_HANDLE
opt : INPUT : INTEGER
perm : (See Description) : INTEGER (See 1)

1. Array of length *nRows*.

Description

If *opt* contains the options CXML_DSS_AUTO_ORDER, then dss_reorder computes a permutation vector that minimizes the fill-in during the factorization phase. For this option, the perm array is never accessed.

If *opt* contains the option CXML_DSS_MY_ORDER, then the array perm is considered to be a permutation vector supplied by the user. In this case, the array perm is of length *nRows*, where *nRows* is the number of rows in the matrix as defined by the previous call to dss_define_structure.

Default Options

CXML_DSS_AUTO_ORDER

Return Values

CXML_DSS_SUCCESS
CXML_DSS_STATE_ERR
CXML_DSS_INVALID_OPTION
CXML_DSS_OUT_OF_MEMORY

dss_factor_real dss_factor_complex

Format

dss_factor_real (handle, opt, rValues)

dss_factor_complex (handle, opt, cValues)

Arguments

handle : INPUT : CXML_DSS_HANDLE
opt : INPUT : INTEGER
rValues : INPUT : DOUBLE PRECISION (see 1)
cValues : INPUT : DOUBLE COMPLEX (see 2)

1. Array of size *nNonZeros*.
2. Array of size *nNonZeros*.

Description

These routines compute the factorization of the matrix whose non-zero locations were previously specified by a call to dss_define_structure and whose non-zero values are given in the array *rValues* or *cValues*. The arrays *rValues* and *cValues* are assumed to be of length *nNonZeros* as defined in a previous call to dss_define_structure.

The *opt* argument should contain one of the following options: CXML_DSS_POSITIVE_DEFINITE, CXML_DSS_INDEFINITE, CXML_DSS_HERMITIAN_POSITIVE_DEFINITE or CXML_DSS_HERMITIAN_INDEFINITE - depending on whether the non-zero values in *rValues* and *cValues* describe a positive definite, indefinite, or Hermitian matrix.

Default Options

CXML_DSS_POSITIVE_DEFINITE

Return Values

CXML_DSS_SUCCESS
CXML_DSS_STATE_ERR
CXML_DSS_INVALID_OPTION
CXML_DSS_OPTION_CONFLICT
CXML_DSS_OUT_OF_MEMORY
CXML_DSS_ZERO_PIVOT

dss_solve_real
dss_solve_complex

Format

dss_solve_real (handle, opt, rRhsValues, nRhs, rSolValues)

dss_solve_complex (handle, opt, cRhsValues, nRhs, cSolValues)

Arguments

handle : INPUT : CXML_DSS_HANDLE
opt : INPUT : INTEGER
Rhs : INPUT : INTEGER
rRhsValues : INPUT : DOUBLE PRECISION (see 1)
rSolValues : OUTPUT : DOUBLE PRECISION (see 2)
cRhsValues : INPUT : DOUBLE COMPLEX (see 1)
cSolValues : OUTPUT : DOUBLE COMPLEX (see 2)

1. Two dimensional array of size *nRows* by *nRhs*.
2. Two dimensional array of size *nCols* by *nRhs*.

Description

For each right hand side column vector defined in *xRhsValues* (where *x* is one of *r* or *c*), these routines compute the corresponding solutions vector and place it in the array *xSolValues*.

The lengths of the lengths of the right-hand side and solution vectors, *nCols* and *nRows* respectively, are assumed to have been defined in a previous call to dss_define_structure.

Default Options

None

Return Values

CXML_DSS_SUCCESS
CXML_DSS_STATE_ERR
CXML_DSS_INVALID_OPTION
CXML_DSS_OUT_OF_MEMORY

VLIB Routines

This section provides descriptions of the VLIB subprograms.

VCOS
Vector Cosine

Format

VCOS (x, incx, y, incy, n)

Arguments

x
real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
On exit, **incx** is unchanged.

y
real*8
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$.
On exit, if $n \leq 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; y_i is replaced by $\cos(x_i)$.

incy
integer*4
On entry, the increment for the array Y.
On exit, **incy** is unchanged.

n
integer*4
On entry, the number of elements to process.
On exit, **n** is unchanged.

Description

The VCOS function computes the cosine of n elements of a vector as follows:

$$y_i \leftarrow \cos x_i$$

where x and y are vectors.

Example

```
INTEGER*4 N, INCX, INCY
REAL*8 X(20), Y(20)
INCX = 1
INCY = 1
N = 20
CALL VCOS(X,INCX,Y,INCY, N)
```

This Fortran code shows how the cosine of all elements of the real vector x is obtained and set equal to the corresponding elements of the vector y.

VCOS_SIN
Vector Cosine and Sine

Format

VCOS_SIN (x, incx, y, incy, z, incz, n)

Arguments

x
real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
On exit, **incx** is unchanged.

y
real*8
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$.
On exit, if $n \leq 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; y_i is replaced by $\cos(x_i)$.

incy
integer*4
On entry, the increment for the array Y.
On exit, **incy** is unchanged.

z
real*8
On entry, a one-dimensional array Z of length at least $(1 + (n - 1) * |incz|)$.
On exit, if $n \leq 0$, **z** is unchanged. If $n > 0$, **z** is overwritten; z_i is replaced by $\sin(x_i)$.

incz
integer*4
On entry, the increment for the array Z.
On exit, **incz** is unchanged.

n
integer*4
On entry, the number of elements to process.
On exit, **n** is unchanged.

Description

The VCOS_SIN function computes the cosine and sine of n elements of a vector as follows:

$$y_i \leftarrow \cos x_i$$

$$z_i \leftarrow \sin x_i$$

where x, y and z are vectors. If both the sine and cosine of a vector are required, this routine is faster than calling VCOS and VSIN separately.

Example

```
INTEGER*4 N, INCX, INCY
REAL*8 X(20), Y(20), Z(20)
INCX = 1
INCY = 1
INCZ = 1
N = 20
CALL VCOS_SIN(X,INCX,Y,INCY,Z,INCZ, N)
```

This Fortran code shows how the cosine and sine of all elements of the real vector x is obtained and set equal to the corresponding elements of the vectors y and z, respectively.

VEXP
Vector Exponential

Format

VEXP (x, incx, y, incy, n)

Arguments

x
real*8
On entry, a one-dimensional array X of length at least $(1 + (n-1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
On exit, **incx** is unchanged.

y
real*8
On entry, a one-dimensional array Y of length at least $(1 + (n-1) * |incy|)$.
On exit, if $n \leq 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; y_i is replaced by $\exp(x_i)$.

incy
integer*4
On entry, the increment for the array Y.
On exit, **incy** is unchanged.

n
integer*4
On entry, the number of elements to process.
On exit, **n** is unchanged.

Description

The VEXP function computes the exponential of n elements of a vector as follows:

$$y_i \leftarrow \exp x_i$$

where x and y are vectors.

Example

```
INTEGER*4 N, INCX, INCY
REAL*8 X(20), Y(20)
INCX = 1
INCY = 1
N = 20
CALL VEXP(X,INCX,Y,INCY, N)
```

This Fortran code shows how the exponential of all elements of the real vector x is obtained and set equal to the corresponding elements of the vector y.

VLOG
Vector Logarithm

Format

VLOG (x, incx, y, incy, n)

Arguments

x
real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
On exit, **incx** is unchanged.

y
real*8
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$.
On exit, if $n \leq 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; y_i is replaced by $\log(x_i)$.

incy
integer*4
On entry, the increment for the array Y.
On exit, **incy** is unchanged.

n
integer*4
On entry, the number of elements to process.
On exit, **n** is unchanged.

Description

The VLOG function computes the natural logarithm of n elements of a vector as follows:

$$y_i \leftarrow \log x_i$$

where x and y are vectors.

Example

```
INTEGER*4 N, INCX, INCY
REAL*8 X(20), Y(20)
INCX = 1
INCY = 1
N = 20
CALL VLOG(X,INCX,Y,INCY, N)
```

This Fortran code shows how the natural logarithm of all elements of the real vector x is obtained and set equal to the corresponding elements of the vector y.

VRECIP
Vector Reciprocal

Format

VRECIP (x, incx, y, incy, n)

Arguments

x
real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
On exit, **incx** is unchanged.

y
real*8
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$.
On exit, if $n \leq 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; y_i is replaced by $\frac{1}{x_i}$.

incy
integer*4
On entry, the increment for the array Y.
On exit, **incy** is unchanged.

n
integer*4
On entry, the number of elements to process.
On exit, **n** is unchanged.

Description

The VRECIP function computes the reciprocal of n elements of a vector as follows:

$$y_i \leftarrow \frac{1}{x_i}$$

where x and y are vectors.

Example

```
INTEGER*4 N, INCX, INCY
REAL*8 X(20), Y(20)
INCX = 1
INCY = 1
N = 20
CALL VRECIP(X,INCX,Y,INCY, N)
```

This Fortran code shows how the reciprocal of all elements of the real vector x is obtained and set equal to the corresponding elements of the vector y.

VSIN
Vector Sine

Format

VSIN (x, incx, y, incy, n)

Arguments

x
real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
On exit, **incx** is unchanged.

y
real*8
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$.
On exit, if $n \leq 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; y_i is replaced by $\sin(x_i)$.

incy
integer*4
On entry, the increment for the array Y.
On exit, **incy** is unchanged.

n
integer*4
On entry, the number of elements to process.
On exit, **n** is unchanged.

Description

The VSIN function computes the sine of n elements of a vector as follows:

$$y_i \leftarrow \sin x_i$$

where x and y are vectors.

Example

```
INTEGER*4 N, INCX, INCY
REAL*8 X(20), Y(20)
INCX = 1
INCY = 1
N = 20
CALL VSIN(X,INCX,Y,INCY, N)
```

This Fortran code shows how the sine of all elements of the real vector x is obtained and set equal to the corresponding elements of the vector y.

VSQRT
Vector Square Root

Format

VSQRT (x, incx, y, incy, n)

Arguments

x
real*8
On entry, a one-dimensional array X of length at least $(1 + (n - 1) * |incx|)$, containing the elements of the vector x.
On exit, **x** is unchanged.

incx
integer*4
On entry, the increment for the array X.
On exit, **incx** is unchanged.

y
real*8
On entry, a one-dimensional array Y of length at least $(1 + (n - 1) * |incy|)$.
On exit, if $n \leq 0$, **y** is unchanged. If $n > 0$, **y** is overwritten; y_i is replaced by $\sqrt{x_i}$.

incy
integer*4
On entry, the increment for the array Y.
On exit, **incy** is unchanged.

n
integer*4
On entry, the number of elements to process.
On exit, **n** is unchanged.

Description

The VSQRT function computes the square root of n elements of a vector as follows:

$$y_i \leftarrow \sqrt{x_i}$$

where x and y are vectors.

Example

```
INTEGER*4 N, INCX, INCY
REAL*8 X(20), Y(20)
INCX = 1
INCY = 1
N = 20
CALL VSQRT(X,INCX,Y,INCY, N)
```

This Fortran code shows how the square root of all elements of the real vector x is obtained and set equal to the corresponding elements of the vector y.

Random Number Generator Subprograms

This section provides descriptions of the random number generator (RNG) subroutines.

RANL
Random Number Generator Based on L'Ecuyer Method

Format

RANL (s1, s2, v, n)

Arguments

s1
integer*4
On entry, **s1**≥1, the first part of the two-integer seed.
On exit, **s1** is changed according to **n** steps of the L'Ecuyer method.

s2
integer*4
On entry, **s2**≥1, the second part of the two-integer seed.
On exit, **s2**, is changed according to **n** steps of the L'Ecuyer method.

v
real*4
On entry, a one-dimensional vector of **n** elements. **v** can be a scalar variable if **n**=1.
On exit, contains n pseudorandom uniform[0,1] random numbers generated according to the L'Ecuyer algorithm.

n
integer*4
On entry, a positive integer specifying the number of random numbers to store in v(1),...,v(**n**).
On exit, unchanged.

Description

The RANL routine returns a vector of uniform[0,1] random numbers. After you give arguments **s1** and **s2** initial values, you need not change these, except to restart the sequence or to skip to a new subsequence.

For parallel applications using the RANL routine, CXML provides two auxiliary input programs. Refer to the descriptions of RANL_SKIP64 and RANL_SKIP2.

Example

```
c     Monte Carlo Method
      integer n,ndim,m
      parameter ( m = 10 )
      integer*4 s1,s2,i,k
      real*4 pt(m),vol,sum,r,vol_all
      print*,'nr. pts to use: '
      read*,n
      print*,' n= ',n
      print*,'       vol(10-d sphere)    vol(10-d cube) '
      sum=0.0
      s1=12345
      s2=67890
      do k=1,n
         call ranl(s1,s2,pt ,m)
          r=0.0
          do i=1,m
          r=r+pt(i)*pt(i)
          end do
      if(r.le.1.0)sum=sum+1.0
      end do
      vol = sum/n
      vol_all = 2**m*vol
      write(6,900)vol_all,2.0**m
 900  format(1x,2x,f14.2,4x,f14.0)
      end
```

This example computes the volume of a 10-dimensional sphere, using a Monte Carlo technique. The program generates `n` points in the 10-dimensional unit quadrant and then counts the number of these `n` points inside the 10-dimensional unit sphere to yield a value for `sum`. Next, the program divides `sum`, by the total `n` points inside the unit quadrant to approximate the volume of the spherical quadrant, `vol`. There are 2^{10} such quadrants. Therefore, the program multiplies `vol` by 2^{10} to approximate the total volume, `vol_all`, of the 10-dimensional sphere.

The exact value of `vol_all` is 2.55 to 2 decimals. With 10 million points, this program yields 2.56. This is in marked contrast to the case in lower dimensions where the volume of the unit sphere is nearly equal to the volume of the containing cube.

See also the example for RANL_SKIP2.

RANL_SKIP2
Routine to Skip Forward a Given Number of Seeds for the RANL and RANL_NORMAL Random Number Generators

Format

RANL_SKIP2   (d, s1, s2, s1_new, s2_new)

Arguments

d
integer*4
On entry, an integer **d**>0 specifying the number 2^d of seeds to skip starting at (s1,s2) in the L'Ecuyer algorithm.

s1
integer*4
On entry, a starting seed **s1**$\geq$1.

s2
integer*4
On entry, a starting seed **s2**$\geq$1.

s1_new
integer*4
On exit, a new starting seed 2^d iterations away from **s1**.

s2_new
integer*4
On exit, a new starting seed 2^d iterations away from **s2**.

Description

The RANL_SKIP2 routine is used to get starting seeds for parallel, independent streams of random numbers. The new starting seeds are computed using the following algorithms:

$$\mathbf{s1_new} = a1^{2^d} * s1 \quad mod\ m1$$
$$\mathbf{s2_new} = a2^{2^d} * s2 \quad mod\ m2$$

Where $a1, a2, m1, m2$ are the constants defining the L'Ecuyer method.

Example

```
      integer nprocs,n,hop
      parameter (nprocs=4)
      parameter (n=16384,hop=14)
      integer*4 j,k
      real*4 v(n,nprocs)
      integer*4 s1val(nprocs),s2val(nprocs)
      real*4 sum1(nprocs)

c     get seeds (2**hop apart) for separate streams
      s1val(1)=1
      s2val(1)=1
      do j=2,nprocs
      call ranl_skip2(hop,s1val(j-1),s2val(j-1),s1val(j),s2val(j))
      end do

c     parallel calls to ranl can be done, for example, with KAP directives:
C*$*  ASSERT CONCURRENT CALL
C*$*  ASSERT DO (CONCURRENT)
      do j=1,nprocs
         call ranl(s1val(j),s2val(j),v(1,j),n)
         sum1(j)=0.0
         do k=1,n
            sum1(j)=sum1(j)+v(k,j)
         end do
      end do

      print*,' per-stream averages'
      do j=1,nprocs
         print*,sum1(j)/n
      end do
```

```
end
```

This example calls RANL_SKIP2 to set up separate seeds for 4 streams, (`nprocs=4`), from RANL. It computes the averages per stream.

RANL_SKIP64

Routine to Skip Forward a Given Number of Seeds for the RANL and RANL_NORMAL Random Number Generators

Note

The RANL_SKIP64 subprogram is currently available on Alpha platforms only.

Format

RANL_SKIP64   (d, s1, s2, s1_new, s2_new)

Arguments

d
integer*8
On entry, an integer **d** ≥0 specifying the number **d** of seeds to skip starting at (s1,s2) in the L'Ecuyer algorithm.

s1
integer*4
On entry, a starting seed **s1**≥1.

s2
integer*4
On entry, a starting seed **s2**≥1.

s1_new
integer*4
On exit, a new starting seed **d** iterations away from **s1**.

s2_new
integer*4
On exit, a new starting seed **d** iterations away from **s2**.

Description

The RANL_SKIP64 routine is used to get starting seeds for parallel, independent streams of random numbers. The new starting seeds are computed using the following algorithms:

s1_new = $a1^d * s1 \quad mod\ m1$
s2_new = $a2^d * s2 \quad mod\ m2$

Where $a1, a2, m1, m2$ are the constants defining the L'Ecuyer method.

Example

```
      integer nprocs,n
      integer*8 hop
      parameter (nprocs=4)
      parameter (n=16384,hop=1000000)
      integer*4 j,k,nsum
      real*4 v(n,nprocs)
      integer*4 s1val(nprocs),s2val(nprocs)
      real*4 sum1(nprocs)

c     get seeds (hop apart) for separate streams
      s1val(1)=1
      s2val(1)=1
      nsum=12
      do j=2,nprocs
      call ranl_skip64(hop,s1val(j-1),s2val(j-1),s1val(j),s2val(j))
      end do

c     parallel calls to ranl_normal can be done, for example, with KAP directives:
C*$*  ASSERT CONCURRENT CALL
C*$*  ASSERT DO (CONCURRENT)
      do j=1,nprocs
         call ranl_normal(s1val(j),s2val(j),nsum,v(1,j),n)
         sum1(j)=0.0
         do k=1,n
            sum1(j)=sum1(j)+v(k,j)
         end do
      end do

      print*,' per-stream averages'
      do j=1,nprocs
         print*,sum1(j)/n
      end do

      end
```

This example calls RANL_SKIP64 to set up separate seeds for 4 streams, (`nprocs=4`), from RANL_NORMAL. It computes the averages per stream.

RANL_NORMAL
Routine to Generate Normally Distributed Random Numbers Using Summation of Uniformly Distributed Random Numbers

Format

RANL_NORMAL (s1, s2, nsum, vnormal, n)

Arguments

s1
integer*4
On entry, **s1**$\geq$1, the first part of the two-integer seed.
On exit, **s1** is changed according to **n** times **nsum** steps of the L'Ecuyer method.

s2
integer*4
On entry, **s2**$\geq$1, the second part of the two-integer seed.
On exit, **s2** is changed according to **n**$*$**nsum** steps of the L'Ecuyer method.

nsum
integer*4
On entry, number of uniform[0,1] numbers to sum to get each N(0,1) output.

vnormal
real*4
On exit, a vector **vnormal**(1),...,**vnormal**(**n**) of N(0,1) normally distributed numbers.

n
integer*4
On entry **n**≥1 specifies the number of N(0,1) results to return in **vnormal**(1),...,**vnormal**(**n**).

Description

The RANL_NORMAL routine returns a vector of N(0,1) normally distributed random numbers.

For parallel applications using the RANL_NORMAL routine, CXML provides two auxiliary input programs. Refer to the descriptions of RANL_SKIP64 and RANL_SKIP2.

Example

See the example for RANL_SKIP64.

RAN69069
Routine to Generate Single Precision Random Numbers Using a=69069 and $m = 2^{32}$

Format

RAN69069 (s)

Function Value

ran69069
real*4

The uniform[0,1] value returned.

Arguments

s
integer*4
On input, a seed **s** being set initially or left unchanged from a previous iteration. On exit, the updated seed.

Description

The RAN69069 routine computes updated seeds using the linear multiplicative algorithm as follows:

$$\mathbf{s} = 69069 * s + 1, \quad mod\ 2^{32}$$

Returns $s * 2.0^{(-32)}$, as its uniform[0,1] output.

Example

```
      integer ix,iy,i,j,iseed,nsteps,nwalks
      real*4 x
c     random walk: go N E S W each with probability 0.25
      nsteps = 1000000
      nwalks = 10
      iseed = 1234

      do j=1,nwalks
      ix=0
      iy=0
      do i = 1, nsteps
      x=ran69069(iseed)
      if(x.le.0.25)then
         ix=ix+1
      else if(x.le.0.5)then
         iy=iy+1
      else if(x.le.0.75)then
         ix=ix-1
      else
         iy=iy-1
      end if
      end do

      print*,'final position ',ix,iy
      end do
      end
```

This example simulates a random walk using RAN69069. A particle starts at (0,0) and proceeds N, E, S, or W. with probability 0.25 each.

RAN16807
Routine to Generate Single Precision Random Numbers Using a=16807 and $m = 2^{31} - 1$

Format

RAN16807 (s)

Function Value

ran16807
real*4

The uniform[0,1] value returned.

Arguments

s
integer*4
On entry, the seed **s**≥1.
On exit, the updated seed.

Description

The RAN16807 routine implements the “minimal standard” or Lehmer multiplicative generator to compute updated seeds using $a = 16807$, $m = 2^{31} - 1$, as follows:

$$\mathbf{s} = 16807 * s \quad mod \; 2^{31} - 1)$$

Returns $s * (1.0/m)$ as its uniform[0,1] output.

Example

```
      integer ix,iy,i,j,iseed,nsteps,nwalks
      real*4 x
c     random walk: go N E S W each with probability 0.25
      nsteps = 1000000
      nwalks = 10
      iseed = 1234

      do j=1,nwalks
      ix=0
      iy=0
      do i = 1, nsteps
      x=ran16807(iseed)
      if(x.le.0.25)then
         ix=ix+1
      else if(x.le.0.5)then
         iy=iy+1
      else if(x.le.0.75)then
         ix=ix-1
      else
         iy=iy-1
      end if
      end do

      print*,'final position ',ix,iy
      end do
      end
```

This example simulates a random walk using RAN16807. A particle starts at (0,0) and proceeds N, E, S, or W. with probability 0.25 each.

Sort Subprograms

This section provides descriptions of the Sort subprograms.

ISORTQ SSORTQ DSORTQ
Sorts the Elements of a Vector

Format

{I,S,D}SORTQ (order, n, x, incx)

Arguments

order
character*4
On entry, **order** specifies the operation to be performed as follows:

If **order** = 'A' or 'a', **x** is sorted in ascending sequence.
If **order** = 'D' or 'd', **x** is sorted in descending sequence.

On exit, **order** is unchanged.

n
integer*4
On entry, the length of vector **x**.
On exit, **n** is unchanged.

x
integer*4 | real*4 | real*8
On entry, a length **n** vector of data to be sorted.
On exit, **x** is overwritten by a length **n** vector of sorted data.

incx
integer*4
On entry, **incx** specifies the distance between elements of vector **x**. The argument **incx** must be positive.
On exit, **incx** is unchanged.

Description

The _SORTQ routines sort a vector of data using the quick sort algorithm. Data is sorted in ascending order if **order** is 'A' or 'a' and in descending order if **order** is 'D' or 'd'. The quick sort algorithm is implemented by recursing until the partition size is less than 16. At that point, a simple replacement sort is used to sort the elements of the partition.

Example

```
REAL*4 DATA( 100 )
N = 100
CALL SSORTQ( 'A',N,DATA,1 )
```

This Fortran code sorts a 100 element single real vector.

ISORTQX SSORTQX DSORTQX
Performs an Indexed Sort of a Vector

Format

{I,S,D}SORTQX (order, n, x, incx, index)

Arguments

order
character*1
On entry, **order** specifies the operation to be performed as follows:

If **order** = 'A' or 'a', **x** is sorted in ascending sequence.
If **order** = 'D' or 'd', **x** is sorted in descending sequence.

On exit, **order** is unchanged.

n
integer*4
On entry, the length of vector **x**.
On exit, **n** is unchanged.

x
integer*4 | real*4 | real*8
On entry, a length **n** vector of data to be sorted.
On exit, **x** is unchanged.

incx
integer*4
On entry, **incx** specifies the distance between elements of vector **x**. The argument **incx** must be positive.
On exit, **incx** is unchanged.

index
integer*4
On entry, the content of **index** is ignored.
On exit, **index** contains a permuted vector of indices that may be used to access data vector **x** in the sorted order specified by **order**.

Description

The _SORTQX routines sort an indexed vector of data using the quick sort algorithm. Data is sorted in ascending order if **order** is 'A' or 'a' and in descending order if **order** is 'D' or 'd'. The quick sort algorithm is implemented by recursing until the partition size is less than 16. At that point, a modified insertion sort is used to sort the elements of the partition. Only elements of the index vector are permuted, the data vector is left unchanged.

Example

```
REAL*4 DATA( 100 )
INTEGER*4 INDEX( 100 )
N = 100
CALL SSORTQX( 'A',N,DATA,1,INDEX )
DO I=1,N
   PRINT *,DATA( INDEX(I) )
ENDDO
```

This Fortran code sorts a 100 element single real vector and prints its contents in sorted order.

GEN_SORT
Sorts the Elements of a Vector

Format

GEN_SORT (order, type, size, n, x, incx, y, incy)

Arguments

order
character*1
On entry, **order** specifies the operation to be performed as follows:

If **order** = 'A' or 'a', **x** is sorted in ascending sequence.
If **order** = 'D' or 'd', **x** is sorted in descending sequence.

On exit, **order** is unchanged.

type
character*1
On entry, **type** specifies the data type of vectors **x** and **y**. The following types are valid:

If **type** = 'B' or 'b', binary (unsigned integer)
If **type** = 'C' or 'c', character string
If **type** = 'I' or 'i', integer (signed)
If **type** = 'L' or 'l', logical - Fortran .TRUE. or .FALSE.
If **type** = 'R' or 'r', IEEE floating point
If **type** = 'V' or 'v', VAXG floating point

On exit, **type** is unchanged.

size
integer*4
On entry, **size** specifies the size, in bytes, of each element of data vectors **x** and **y**. Valid combinations of **type** and **size** include:

If **type** = 'B' or 'b' - **size** = { 1,2,4,8 }
If **type** = 'C' or 'c' - **size** = { 0 < **size** < 65536 }
If **type** = 'I' or 'i' - **size** = { 1,2,4,8 }
If **type** = 'L' or 'l' - **size** = { 1,2,4,8 }
If **type** = 'R' or 'r' - **size** = { 4,8,16 }
If **type** = 'V' or 'v' - **size** = { 4,8 }

On exit, **size** is unchanged.

n
integer*4
On entry, the length of the **x** and **y** vectors.
On exit, **n** is unchanged.

x
data vector
On entry, a length **n** vector of data to be sorted. Each element of vector **x** is of **type** and **size** specified.
On exit, vector **x** is unchanged, unless it overlaps vector **y**.

incx
integer*4
On entry, **incx** specifies the distance between elements of vector **x**. The argument **incx** must be positive.
On exit, **incx** is unchanged.

y
data vector
On entry, **y** is ignored.
On exit, vector **y** is overwritten with sorted data. Each element of vector **y** is of **type** and **size** specified.

incy
integer*4
On entry, vector **incy** specifies the distance between elements of vector **y**. The argument **incy** must be positive.
On exit, **incy** is unchanged.

Description

GEN_SORT is a general purpose, in memory, sort routine. GEN_SORT accepts the following Fortran data types:

INTEGER*1, INTEGER*2, INTEGER*4, INTEGER*8
LOGICAL*1, LOGICAL*2, LOGICAL*4, LOGICAL*8
REAL*4, REAL*8, REAL*16
CHARACTER(*)

GEN_SORT also accepts unsigned “binary” integers of 1, 2, 4, or 8 byte sizes.

A radix algorithm is employed to sort the data. For all data types except REAL*16 and CHARACTER*(*), an N*16 byte work space is aquired from heap storage. For REAL*16 data, a work space of N*24 bytes is taken from heap storage. Heap work space required for CHARACTER data is N*((SIZE-1)/8+3)*8 bytes in size.

Note

The data provided to GEN_SORT must be of a type that is valid for the platform. GEN_SORT cannot be used to sort REAL*16 on Windows NT Alpha or Windows NT Intel. GEN_SORT cannot be used to sort INTEGER*8 or LOGICAL*8 on Windows NT Intel. The use of *type/bold* = b,l or i, and *size/bold* = 8, is prohibited on Windows NT Intel.

Example

```
REAL*4 DATA( 100 )
N = 100
CALL GEN_SORT( 'A','R',4,N,DATA,1,DATA,1 )
```

This Fortran code sorts a 100 element single-precision real vector in place.

GEN_SORTX
Sorts the Elements of an Indexed Vector

Format

GEN_SORTX (order, status, type, size, n, x, incx, index)

Arguments

order
character*1
On entry, **order** specifies the operation to be performed as follows:

If **order** = 'A' or 'a', **x** is sorted in ascending sequence.
If **order** = 'D' or 'd', **x** is sorted in descending sequence.

On exit, **order** is unchanged.

status
character*1
On entry, **status** specifies the operation to be performed as follows:

If **status** = 'N' or 'n', the **index** vector is new (empty) on input. Elements of data vector **x** are initially accessed in sequential order.
If **status** = 'O' or 'o', the **index** vector is old (full) on input. Elements of data vector **x** are initially accessed in the order specified by the **index** vector.

On exit, **status** is unchanged.

type
character*1
On entry, **type** specifies the data type of vectors **x** and **y**. The following types are valid:

If **type** = 'B' or 'b', binary (unsigned integer)
If **type** = 'C' or 'c', character string
If **type** = 'I' or 'i', integer (signed)
If **type** = 'L' or 'l', logical - Fortran .TRUE. or .FALSE.
If **type** = 'R' or 'r', IEEE floating point
If **type** = 'V' or 'v', VAXG floating point

On exit, **type** is unchanged.

size
integer*4
On entry, **size** specifies the size, in bytes, of each element of data vector **x**. Valid combinations of **type** and **size** include:

If **type** = 'B' or 'b' - **size** = { 1,2,4,8 }
If **type** = 'C' or 'c' - **size** = { 0 < **size** < 65536 }

If **type** = 'I' or 'i' - **size** = { 1,2,4,8 }
If **type** = 'L' or 'l' - **size** = { 1,2,4,8 }
If **type** = 'R' or 'r' - **size** = { 4,8,16 }
If **type** = 'V' or 'v' - **size** = { 4,8 }

On exit, **size** is unchanged.

n
integer*4
On entry, the length of the **x** vector.
On exit, **n** is unchanged.

x
data vector
On entry, a length **n** vector of data to be sorted. Each element of vector **x** is of **type** and **size** specified.
On exit, vector **x** is unchanged.

incx
integer*4
On entry, **incx** specifies the distance between elements of vector **x**. The argument **incx** must be positive.
On exit, **incx** is unchanged.

index
integer*4
On entry, vector **index** is ignored if **status** is 'N' or 'n', and used as an index vector for data vector **x** if **status** is 'O' or 'o'.
On exit, vector **index** is overwritten by a permuted vector of indices that may be used to access data vector **x** in the sorted order specified by **order**.

Description

GEN_SORTX is a general purpose, in memory, indexed sort routine. GEN_SORTX accepts the following Fortran data types:

INTEGER*1, INTEGER*2, INTEGER*4, INTEGER*8
LOGICAL*1, LOGICAL*2, LOGICAL*4, LOGICAL*8
REAL*4, REAL*8, REAL*16
CHARACTER(*)

GEN_SORTX also accepts unsigned "binary" integers of 1, 2, 4, or 8 byte sizes.

An indexed radix algorithm is employed to sort the data. For all data types except REAL*16 and CHARACTER*(*), an N*16 byte work space is aquired from heap storage. For REAL*16 data, a work space of N*24 bytes is taken from heap storage. Heap work space required for CHARACTER data is N*((SIZE-1)/8+3)*8 bytes in size.

GEN_SORTX is stable and may be used to perform multikey record sorts.

Note

The data provided to GEN_SORTX must be of a type that is valid for the platform. GEN_SORTX cannot be used to sort REAL*16 on Windows NT Alpha or Windows NT Intel. GEN_SORTX cannot be used to sort

INTEGER*8 or LOGICAL*8 on Windows NT Intel. The use of *type/bold* = b,l or i, and *size/bold* = 8, is prohibited on Windows NT Intel.

Example

```
REAL    DATA( 100 )
INTEGER INDEX( 100 )
N = 100
CALL GEN_SORTX( 'Descend','New','Real',SIZEOF(DATA(1)),N,DATA,1,INDEX )
DO I=1,N
   PRINT *,DATA(I),DATA( INDEX(I) )
ENDDO
```

This Fortran code sorts a 100 element single-precision real vector by index, leaving the data unchanged. Unsorted and sorted data are printed in adjacent columns.

Part 4—Appendices

This section contains appendices that provide supplemental information about using CXML.

The following major topics are addressed:

- Things to consider when using CXML on the Compaq Tru64 UNIX Platform - Appendix A
- Things to consider when using CXML on the Windows NT Platform - Appendix B
- Things to consider when using CXML on the OpenVMS Alpha Platform - Appendix C
- Things to consider when using CXML on the Linux Platform - Appendix D
- Things to consider when using CXML with C and C++ - Appendix E
- Retired LAPACK Functionality - Appendix F
- A bibliography of where you can find more information on areas related to CXML - Appendix G

A Compaq Tru64 UNIX Considerations

This appendix discusses any special considerations that you need to be aware of when using CXML on a Compaq Tru64 UNIX platform.

A.1 Using the Parallel Library

CXML includes a parallel library for the Compaq Tru64 UNIX platform that can yield dramatic performance improvements on symmetric multiprocessing (SMP) systems.

The CXML parallel library contains the same set of subprograms as the serial library, except a subset of the subprograms has been parallelized. The parallel subprograms have names and calling parameters that are identical to the serial versions. Currently, the parallel library is available only on Tru64 UNIX systems.

You do not have to make any changes in your source code to use the parallel library. Simply link your source code with the parallel library, and CXML automatically supplies the parallel subprograms.

At run time you declare the number of processors on your SMP system with environment variables. For complete information on the procedure, see Section 3.1.3.

The following subcomponents of the CXML library contain key subprograms that have been modified to execute in parallel if run on SMP hardware:

- Level 2 BLAS
- Level 3 BLAS
- LAPACK
- Signal Processing
- Iterative Solvers
- Direct Sparse Solvers

See Section A.1.2 for a list of the parallel subprograms.

In some cases, a parallel subprogram in one subcomponent of the library benefits the subprograms in another subcomponent. For example, LAPACK subprograms that call the parallel versions of Level 2 or Level 3 BLAS subprograms show performance improvement. See Section A.1.3.3 for details. Additionally, some Level 2 and Level 3 serial BLAS subprograms benefit by calling other BLAS subprograms that are parallel. See Section A.1.3.2 for details.

A.1.1 Setting Environment Variables for Parallel Execution

Before you can run programs compiled and linked with the parallel version of CXML, you must set one or more of the following environment variables:

OMP_NUM_THREADS <integer>
The OMP_NUM_THREADS <integer> environment variable specifies the number of threads to use during program execution. The value assigned to this environment variable is the maximum number of threads that can be used. The default value is the number of processors in the current system.

OMP_SCHEDULE
This variable applies only to DO and PARALLEL DO directives that have the schedule type of RUNTIME. You can set the schedule type and an optional chunk size for these loops at run time.

MP_STACK_SIZE
Specifies how many bytes of stack space the runtime system allocates for each thread when creating it.

MP_SPIN_COUNT
Specifies how many times the runtime system spins while waiting for a condition to become true.

MP_YIELD_COUNT
Specifies how many times the runtime system alternates between calling sched_ yield and testing the condition before going to sleep by waiting for a thread condition variable.

Refer to the "Using Parallel Compiler Directives" section of the DIGITAL Fortran 90 *User Manual for DIGITAL UNIX Systems* documentation for full information about using these environment variables.

Example:

To run a program on a multiprocessor system with three parallel threads, you would set the environment variables as follows:

```
setenv OMP_NUM_THREADS 3
```

A.1.2 CXML Parallel Subprograms

Table A–1 lists the parallel subprograms that are available. Refer to the reference section for information about each subprogram.

Table A–1 Parallel Subprograms

Name	Subcomponent Group
{S,D,C,Z}GEMV	Level 2 BLAS (Chapter 6)
{S,D,C,Z}GEMM	Level 3 BLAS (Chapter 7)
{S,D,C,Z}GETRF	LAPACK manpage computational routines
{S,D,C,Z}POTRF	"

(continued on next page)

Table A–1 (Cont.) Parallel Subprograms

Name	Subcomponent Group
{S,D,C,Z}FFT	Signal Processing (Chapter 9)
{S,D,C,Z}FFT_INIT	"
{S,D,C,Z}FFT_APPLY	"
{S,D,C,Z}FFT_EXIT	"
{S,D,C,Z}FFT_2D	"
{S,D,C,Z}FFT_INIT_2D	"
{S,D,C,Z}FFT_APPLY_2D	"
{S,D,C,Z}FFT_EXIT_2D	"
{S,D,C,Z}FFT_3D	"
{S,D,C,Z}FFT_INIT_3D	"
{S,D,C,Z}FFT_APPLY_3D	"
{S,D,C,Z}FFT_EXIT_3D	"
DITSOL_DRIVER	Iterative Solver (Chapter 10)
DMATVEC_DRIVER	"
DPCONDL_DRIVER	"
DPCONDR_DRIVER	"
DITSOL_PBCG	"
DITSOL_PCG	"
DITSOL_PCGS	"
DITSOL_PGMRES	"
DITSOL_PLSCG	"
DITSOL_PTFQMR	"
DMATVEC_GENR	"
DMATVEC_SDIA	"
DMATVEC_UDIA	"
DCREATE_DIAG_GENR	"
DCREATE_DIAG_SDIA	"
DCREATE_DIAG_UDIA	"
DAPPLY_DIAG_ALL	"
DCREATE_POLY_GENR	"
DCREATE_POLY_SDIA	"
DCREATE_POLY_UDIA	"
DAPPLY_POLY_GENR	"
DAPPLY_POLY_SDIA	"
DAPPLY_POLY_UDIA	"
dss_create	Direct Sparse Solvers (NEW) (Chapter 11)

(continued on next page)

Table A–1 (Cont.) Parallel Subprograms

Name	Subcomponent Group
dss_define_structure	"
dss_reorder	"
dss_factor_real	"
dss_factor_complex	"
dss_solve_real	"
dss_solve_complex	"
dss_delete	"

A.1.3 Performance Considerations for Parallel Execution

The following sections point out considerations about performance improvement using parallel subprograms.

A.1.3.1 Single Processor Systems

The parallel version of a subprogram may not run as quickly as the serial version on a single processor system. Overhead due to either the parallel processing software or changes in the implementation of the algorithm to make it parallelizable can cause reduced performance.

A.1.3.2 Level 2 and Level 3 BLAS Subprograms

Some Level 2 and most Level 3 BLAS serial subprograms use other subprograms that have parallel versions. For example, most Level 3 BLAS subprograms use the corresponding parallelized {S,D,C,Z}GEMM subprograms. Specifically, DSYMM uses DGEMM, CTRMM uses CGEMM, and STRSM uses both SGEMM and SGEMV. Moreover, some Level 3 BLAS subprograms use the corresponding parallelized {S,D,C,Z}GEMV subprograms.

In the case of Level 2 BLAS, many subprograms use {S,D,C,Z}GEMV. For example, ZTRSV uses ZGEMV. To the extent serial subprograms use parallel versions of other subprograms, they will run faster in a multi-processor environment, if you have linked your application to the parallel library.

A.1.3.3 LAPACK Subprograms

LAPACK subprograms that call the parallel versions of {S,D,C,Z}GEMM or {S,D,C,Z}GEMV will run faster in a multi-processor environment. For example, if you are using DGESV to solve a system of linear equations, linking your application to the parallel library results in improved performance.

A.1.3.4 Signal Processing Subprograms

All the Fast Fourier Transform subprograms in the signal processing subcomponent of the CXML library have parallel versions. The parallel versions run faster than the serial versions primarily when you use them with large input data arrays, where the "cost" of parallel initialization is small in comparison to the computations involved.

For example, using the parallel version of a one-dimensional FFT subprogram with an input array containing 8K or more elements generally results in a faster run time. When the input array contains less than 8K elements, the serial version often gives better results on an SMP system. Compaq recommends that you link your application with both libraries and compare the results.

A.1.3.5 Iterative Solver Subprograms

The performance improvement obtained by the use of parallel iterative solver subprograms is dependent not only on the system characteristics, but also on the properties of the linear system, such as the size of the matrix, the preconditioner used, and so on. In some cases, the performance can be improved by considering other options. For example, in the case of a symmetric matrix with few diagonals stored in the SDIA storage scheme, the parallel version may not yield the expected performance improvement. In this case, using the UDIA storage scheme, and trading off the extra memory required with the better parallelization properties of the UDIA scheme, may result in an overall reduction in the execution time.

B

Windows NT Considerations

This appendix discusses any special considerations that you need to be aware of when using CXML on a Windows NT platform.

B.1 Setting Environment Variables

If you build programs from the command console, you need to set CXML environment variables to access the library. Environment variables are defined in DFFORS.BAT.

C
OpenVMS Considerations

This appendix discusses any special considerations that you need to be aware of when using CXML on a Compaq OpenVMS platform.

C.1 Data Format Notes

Don't mix formats - Although OpenVMS Alpha supports calculation using either IEEE format or VAX format, you cannot mix them. Floating point numbers in one format will be misinterpreted in the other format. Therefore, programs that mix the formats will not work.

Compile for the correct format - When you compile your program, you must compile it for either IEEE float or VAX float. VAX float is the default. If you want to compile for IEEE, you must specify `/float=IEEE_floating`. Be sure to compile your program for the format that is appropriate.

Link to the correct library - A CXML library is provided for both IEEE and VAX floating point formats. Entrynames are independent of format, so when you link your program it can be linked with either the IEEE or VAX version of the CXML library. Each CXML library has a different name - you must specify the name of library to which you want to link. You must link your program to the library for which it was compiled.

Check CXML installation documentation for specific information about library names and how to set up a default link.

D
Linux Considerations

This appendix discusses any special considerations that you need to be aware of when using CXML on a Linux platform.

D.1 Linking with CXML

To compile and link a Fortran program that contains calls to CXML routines, use the following command:

```
fort my_prog.f -lcxml
```

To compile and link a C program that contains calls to CXML routines, use the following command:

```
ccc my_prog.c -lcxml
```

Notes: my_prog.f is an example Fortran program. my_prog.c is an example C program.

E

Using CXML From C and C++

Traditionally, the programming language of choice for scientific and numerical applications has been Fortran. Consequently, the interface to CXML is targeted toward ease of use in Fortran environments. However, CXML can be called from C or C++ provided you understand the calling conventions of both the C/C++ and Fortran compilers on their particular platforms.

Here are some of the things of which you need to be aware:

- Fortran uses "pass-by-reference" semantics while C and C++ use "pass-by-value" semantics. Generally this means that when calling CXML routines from C or C++, non-array arguments should be prefixed with an '&' to pass the address of the scalar rather than the value of the scalar.
- Many Fortran compilers use some form of "name decoration" for externally visible symbols, and that decoration varies from platform to platform. In the following paragraphs we discuss the name decoration for Tru64 UNIX and Linux. Note that VMS systems do not decorate the external symbols, so that VMS users can ignore this discussion.
  - For Tru64 UNIX systems, external symbols have an '_' character appended to them. So, for example, if C users on Tru64 UNIX want to call the CXML entry point saxpy, then C and C++ users should call the entry point saxpy_.
  - For Linux systems, external symbols have an '_' character appended to them unless the symbol contains an '_', in which case a double '_' is appended to them. So on Linux systems, saxpy becomes saxpy_, but cfft_init becomes cfft_init_.
- The last issue is dealing with functions that return complex results. On Compaq systems, the calling convention for returning complex results requires that the return value is in the floating point registers f0 and f1. There is currently no direct way to access a Fortran complex return value from a standard C or C++ program. The fundamental problem is that the complex type in C and C++ is essentially a structure class, and hence a complex type must be returned indirectly through a pointer.

  The Compaq C compiler provides a work around for this problem by using linkage pragmas. For the sake of example, consider the CXML function zsum which returns the sum of the elements of a complex vector. Assuming that we are on a Tru64 UNIX platform, C users would invoke the zsum function as:

```
typedef struct { double real, imag } dComplex;

#pragma linkage complex_linkage = (result (f0,f1))
#pragma use_linkage complex_linkage (zsum_)

extern dComplex zsum_(int *, dComplex *, int *);

main() {

int n = 10;
int incr = 1;
dComplex a[10], ret;
...
ret = zsum_(&n, a, &incr);
}
```

Since Compaq C++ does not support the pragma linkage directives, there is currently no way for C++ users to directly call CXML routines that return complex results. C++ users must write C jacket routines using the above linkage mechanism and use the jacket routine to obtain the result. Continuing the above example, C++ users could define the jacket routine c_zsum as follows:

```
typedef struct { double real, imag } dComplex;

#pragma linkage complex_linkage = (result (f0,f1))
#pragma use_linkage complex_linkage (zsum_)

void c_zsum( dComplex *ret, int *n, Complex *a, int *incr) {

extern dComplex zsum_(int *, dComplex *, int *);
*ret = zsum_(n, a, incr);
}
```

Assuming that the entry point c_zsum is contained in a separate object module, then a C++ routine could invoke the jacket routine as:

```
typedef std:complex<double> Complex;
extern "C" Complex c_zsum(const int *, const Complex *, const int *);
Complex sum, a[];
int n, incr;
sum = c_zsum(&n, a, &incr);
```

F

Retired LAPACK Functionality - Performance Tuning

Note: This is Retired Functionality

This section describes retired CXML functionality which is no longer recommended for use.

While this retired functionality will still be supported for a short time, it is highly recommended that you remove it from your programs immediately.

F.1 Performance Tuning

In the public release of LAPACK, the routine ILAENV provides default values for blocksizes, crossover points, and other performance-tuning parameters for use with specified routines. These values are generally sufficient for routine use of LAPACK, and are invisible to the top-level user of the package. Certain lower-level LAPACK routines call ILAENV to obtain the value of a parameters of interest.

In this CXML release, LAPACK includes the routine XLAENV which enables experimentation with blocksizes, crossover points, and other performance-tuning parameters. Use of XLAENV is of interest to expert users familiar with LAPACK source code.

Thus, you can either use the default values or experiment with the parameters to tune the performance. The descriptions of ILAENV and XLAENV specify how to switch between these modes, and how to set custom parameter values. The following sample code segment sets a custom blocksize (in this case, 32) for DGESV:

```
CALL XLAENV(100,1)
IBLK=32
CALL XLAENV(1,IBLK)
...
CALL DGESV( ... )
CALL XLAENV(100,0)
```

The final call to XLAENV reverts subsequent code back to the normal mode of using the hard-coded parameters in ILAENV. The other calls are equally straightforward, and are explained in the header and comments for the ILAENV routine, and the entire source for the XLAENV routine, as displayed in Examples F–1 and F–2.

Example F–1 ILAENV

```
      INTEGER          FUNCTION ILAENV( ISPEC, NAME, OPTS, N1, N2, N3,
     $                 N4 )
*
*  -- LAPACK auxiliary routine --
*  Modified to allow expert user modifications of
*  blocksize and other parameters using the XLAENV routine,
*  via a common block shared by ILAENV and XLAENV.
*
*  Purpose
*  =======
*
*  ILAENV returns problem-dependent parameters for the local
*  environment.  See ISPEC for a description of the parameters.
*
*  In this version, the problem-dependent parameters are either:
*   (a.) contained in the integer array IPARMS in the common block CLAENV
*        and the value with index ISPEC is copied to ILAENV.
*   (b.) hard coded in the code below. (normal use).
*   Common block initializaton forces IPARMS(100)=0 and thus
*   option (b.) is the default.
*
*   Option a.) is used if IPARMS(100)=1. (set by calling XLAENV)
*   This option is provided for parameter-tuning and testing purposes.
*   In this case values in IPARMS must be set to the desired values
*   by calling XLAENV.
*
*   Option b.) is used if IPARMS(100)=0:
*  This version provides a set of parameters which should give good,
*  but not optimal, performance on many of the currently available
*  computers.
*
*  Arguments
*  =========
*
*  ISPEC   (input) INTEGER
*          Specifies the parameter to be returned as the value of
*          ILAENV.
*          = 1: the optimal blocksize; if this value is 1, an unblocked
*               algorithm will give the best performance.
*          = 2: the minimum block size for which the block routine
*               should be used; if the usable block size is less than
*               this value, an unblocked routine should be used.
*          = 3: the crossover point (in a block routine, for N less
*               than this value, an unblocked routine should be used)
*          = 4: the number of shifts, used in the nonsymmetric
*               eigenvalue routines
*          = 5: the minimum column dimension for blocking to be used;
*               rectangular blocks must have dimension at least k by m,
*               where k is given by ILAENV(2,...) and m by ILAENV(5,...)
*          = 6: the crossover point for the SVD (when reducing an m by n
*               matrix to bidiagonal form, if max(m,n)/min(m,n) exceeds
*               this value, a QR factorization is used first to reduce
*               the matrix to a triangular form.)
*          = 7: the number of processors
```

(continued on next page)

Example F–1 (Cont.) ILAENV

```
*          = 8: the crossover point for the multishift QR and QZ methods
*               for nonsymmetric eigenvalue problems.
*
*  NAME    (input) CHARACTER*(*)
*          The name of the calling subroutine, in either upper case or
*          lower case.
*
*  OPTS    (input) CHARACTER*(*)
*          The character options to the subroutine NAME, concatenated
*          into a single character string.  For example, UPLO = 'U',
*          TRANS = 'T', and DIAG = 'N' for a triangular routine would
*          be specified as OPTS = 'UTN'.
*
*  N1      (input) INTEGER
*  N2      (input) INTEGER
*  N3      (input) INTEGER
*  N4      (input) INTEGER
*          Problem dimensions for the subroutine NAME; these may not all
*          be required.
*
* (ILAENV) (output) INTEGER
*          >= 0: the value of the parameter specified by ISPEC
*          < 0:  if ILAENV = -k, the k-th argument had an illegal value.
*
*  Further Details
*  ===============
*
*  The following conventions have been used when calling ILAENV from the
*  LAPACK routines:
*  1)  OPTS is a concatenation of all of the character options to
*      subroutine NAME, in the same order that they appear in the
*      argument list for NAME, even if they are not used in determining
*      the value of the parameter specified by ISPEC.
*  2)  The problem dimensions N1, N2, N3, N4 are specified in the order
*      that they appear in the argument list for NAME.  N1 is used
*      first, N2 second, and so on, and unused problem dimensions are
*      passed a value of -1.
*  3)  The parameter value returned by ILAENV is checked for validity in
*      the calling subroutine.  For example, ILAENV is used to retrieve
*      the optimal blocksize for STRTRI as follows:
*
*      NB = ILAENV( 1, 'STRTRI', UPLO // DIAG, N, -1, -1, -1 )
*      IF( NB.LE.1 ) NB = MAX( 1, N )
*
*  =====================================================================
*     ..
*     .. Arrays in Common ..
      INTEGER            IPARMS( 100 ) /100*0/
*     ..
*     .. Common blocks ..
      COMMON             / CLAENV / IPARMS
```

Example F–2 XLAENV

```
      SUBROUTINE XLAENV( ISPEC, NVALUE )
*
*  -- LAPACK auxiliary routine --
*  (shared common block with ILAENV)
*     .. Scalar Arguments ..
      INTEGER            ISPEC, NVALUE
*     ..
*
*  Purpose
*  =======
*
*  XLAENV sets certain machine- and problem-dependent quantities
*  which will later be retrieved by ILAENV.
*
*  Arguments
*  =========
*
*  ISPEC   (input) INTEGER
*          Specifies the parameter to be set in the COMMON array IPARMS.
*          = 1: the optimal blocksize; if this value is 1, an unblocked
*               algorithm will give the best performance.
*          = 2: the minimum block size for which the block routine
*               should be used; if the usable block size is less than
*               this value, an unblocked routine should be used.
*          = 3: the crossover point (in a block routine, for N less
*               than this value, an unblocked routine should be used)
*          = 4: the number of shifts, used in the nonsymmetric
*               eigenvalue routines
*          = 5: the minimum column dimension for blocking to be used;
*               rectangular blocks must have dimension at least k by m,
*               where k is given by ILAENV(2,...) and m by ILAENV(5,...)
*          = 6: the crossover point for the SVD (when reducing an m by n
*               matrix to bidiagonal form, if max(m,n)/min(m,n) exceeds
*               this value, a QR factorization is used first to reduce
*               the matrix to a triangular form)
*          = 7: the number of processors
*          = 8: another crossover point, for the multishift QR and QZ
*               methods for nonsymmetric eigenvalue problems.
*          = 100: with NVALUE=1, subsequent calls to ILAENV will fetch
*                 a requested value directly from the common block (rather
*                 than use the hard-coded values in ILAENV). With NVALUE=0,
*                 subsequent calls to ILAENV will use the hard-coded values.
*
*  NVALUE  (input) INTEGER
*          The value of the parameter specified by ISPEC.
*
*     .. Arrays in Common ..
      INTEGER            IPARMS( 100 )
*     ..
*     .. Common blocks ..
      COMMON             / CLAENV / IPARMS
*     ..
*     .. Save statement ..
      SAVE               / CLAENV /
```

(continued on next page)

Example F–2 (Cont.) XLAENV

```
*     ..
*     .. Executable Statements ..
*
      IF( ISPEC.GE.1 .AND. ISPEC.LE.100 ) THEN
         IPARMS( ISPEC ) = NVALUE
      END IF
*
      RETURN
*
*     End of XLAENV
*
      END
```

G Bibliography

This bibliography lists books and articles related to CXML computations. The list is divided into categories with appropriate headings.

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