# sgi

Scientific Computing Software Library (SCSL) User's Guide

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# **About This Guide**

This publication describes the SGI Scientific Computing Software Library (SCSL) which runs on SGI IRIX and Linux systems. The information in this manual supplements the man pages provided with the SCSL release.

This document is a user's guide for programmers. Readers should have a working knowledge of the IRIX and Linux operating systems, have an understanding of the Fortran and C programming languages, and have a working familiarity with scientific and mathematical theories.

# **Related publications**

The following publications provide information that can supplement the information in this document.

Release notes for Linux systems are stored in /usr/share/doc/sgi-scsl-versionnumber/README.relnotes.

#### **Related Operating System Documentation**

The following documents provide information about IRIX and Linux implementations on SGI systems:

- Linux Installation and Getting Started
- Linux Resource Administration Guide
- IRIX Admin: Resource Administration
- SGI ProPack for Linux Start Here
- Message Passing Toolkit: MPI Programmer's Manual

#### **Tuning and Application Guides**

The following documents provide information about the applications used on IRIX and Linux systems and about tuning issues on those systems:

Origin 2000 and Onyx2 Performance Tuning and Optimization Guide

- Linux Application Tuning Guide
- MIPSpro Fortran 77 Programmer's Guide
- MIPSpro Fortran 90 Commands and Directives Reference Manual
- C++ Programmer's Guide
- Guide to SGI Compilers and Compiling Tools
- ProDev WorkShop: Overview

The following documentation is provided for the compilers and performance tools which run on SGI Linux systems:

- http://sources.redhat.com/gdb/onlinedocs/gdb\_toc.html
- http://intel.com/software/perflib; documentation for Intel compiler products can be downloaded from this website.
- http://developer.intel.com/software/products/vtune/vtune61/index.htm/
- Information about the OpenMP Standard can be found at http://www.openmp.org/specs.

#### **Third Party Documentation**

The following publications provide detailed information about the topics discussed in this manual. In many cases, these documents are referenced specifically in this manual.

- Anderson, E., Z. Bai, et al. *LAPACK User's Guide*. Philadelphia SIAM, 1999. This manual is available online at http://www.netlib.org/lapack/lug/index.html.
- Anderson, Edward, Jack Dongarra, and Susan Blackford. Installation guide for LAPACK. LAPACK Working Note 41, Technical Report CS-91-138. University of Tennessee (Feb. 1992).
- Argham, Nicolas J. *Accuracy and Stability of Numeric Algorithms*. Philadelphia SIAM, 1996.
- Arioli, M., J. W. Demmel, and I. S. Duff. Solving sparse linear systems with sparse backward error. *SIAM J. Matrix Anal. Appl.* 10 (1989).

- Ashcraft, Cleve. A vector implementation of the multifrontal method for large sparse, symmetric positive definite linear systems. Technical Report ETA-TR-51. Boeing Computer Services, 1987.
- Duff, I. S., A. M. Erisman, and J. K. Reid. *Direct Methods for Sparse Matrices*. Monographs on Numerical Analysis. New York: Oxford University Press, 1986.
- George, Alan and Joseph W-H Liu. Computer Solution of Large Sparse Positive Definite Systems. Prentice-Hall Series in Computational Mathematics. Englewood Cliffs, NJ: Prentice-Hall, Inc., 1981.
- Golub, Gene and James M. Ortega. *Scientific Computing: An Introduction with Parallel Computing*. Boston: Academic Press, 1993.
- Golub, Gene H. and Charles F. Van Loan. *Matrix Computations*. 2nd edition. Baltimore, Maryland: Johns Hopkins University Press, 1989.
- Hageman, Louis A. and David M. Young. *Applied Iterative Methods*. Computer Science and Applied Mathematics. New York and London: Academic Press, 1981.
- Heroux, Michael A. A reverse communication interface for "matrix-free" preconditioned iterative solvers. Edited by C.A. Brebbia, D. Howard, and A. Peters *In Applications of Supercomputers in Engineering II*, 207-213. Boston: Computational Mechanics Publications, 1991.
- Heroux, Michael A., Phuong Vu, and Chao Wu Yang. A parallel preconditioned conjugate gradient package for solving sparse linear systems on a Cray Y-MP. *Applied Numerical Mathematics*, 8 (1991).
- Hestenes, M. R. and E. Stiefel. Methods of conjugate gradients for solving linear systems. *J. Res. National Bureau of Standards* 49 (1952): 409-436.
- Kincaid, David R., Thomas C. Oppe, John R. Respess, and David M. Young. *ITPACKV 2C User's Guide*. Technical Report CNA-191. The University of Texas at Austin: Center for Numerical Analysis, (Nov. 1984).
- Manteuffel, T. A. An incomplete factorization technique for positive definite linear systems. *Math. Comp.* 34 (1980): 473-497.
- Oppe, Thomas C., Wayne D. Joubert, and David R. Kincaid. *NSPCG User's Guide*. The University of Texas at Austin: Center for Numerical Analysis, (Dec. 1988).
- Reid, J. K., editor. On the Method of Conjugate Gradients for the Solution of Large Sparse Systems of Linear Equations. *Large Sparse Sets of Linear Equations*, Academic Press, 1971.

- Saad, Youcef. Practical use of polynomial preconditionings for the conjugate gradient method., 6(4) (Oct. 1985): 865-881.
- Saad, Youcef and Martin H. Schultz. GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems. *SIAM Journal of Scientific and Statistical Computing*, 7(3) (Jul. 1986): 856-869.
- Sonneveld, Peter. CGS, a fast lanczos-type solver for nonsymmetric linear systems. *SIAM Journal of Scientific and Statistical Computing*, 10(1) (Jan. 1989): 36-52.
- Stewart, G. W. Introduction to Matrix Computations. Orlando, Florida: Academic Press, 1973.
- Wilkinson, J. H. *The Algebraic Eigenvalue Problem*. Oxford, England: Oxford University Press, 1965.
- Yang, Chao W. A parallel multifrontal method for sparse symmetric definite linear systems on the Cray Y-MP. Proceedings of the Fifth SIAM Conference on Parallel Processing for Scientific Computing. Houston, Texas (Apr. 1992).

You can find a good general reference on the solution of sparse linear systems in Golub and Van Loan. You can find a good introduction to direct and iterative methods, as well as methods for special linear systems, in these texts. See the special section of the November 1989 issue of the *SIAM Journal of Scientific and Statistical Computing*, pages 1135-1232 for an updated general reference.

See George and Liu, Duff and Erisman, and Reid for classical references that give a thorough and in-depth treatment of sparse direct solvers. Another common reference is Ashcraft.

The original conjugate gradient algorithm was presented in Hestenes and Stiefel; however, Reid presented the first practical application. A classical text in iterative methods is that of Hageman and Young. You can find good discussions of the biconjugate gradient and biconjugate gradient squared methods in Sonneveld. GMRES is presented by Saad and Schultz.

# Conventions

The following conventions are used throughout this documentation:

command

This fixed-space font denotes literal items, such as pathnames, man page names, commands, and programming language structures.

variable	Italic typeface denotes variable entries and words or concepts being defined.
[]	Brackets enclose optional portions of a command line.

## **Obtaining Publications**

You can obtain SGI documentation as follows:

- See the SGI Technical Publications Library at http://docs.sgi.com. Various formats are available. This library contains the most recent and most comprehensive set of online books, release notes, man pages, and other information.
- If it is installed on your SGI system, you can use InfoSearch, an online tool that provides a more limited set of online books, release notes, and man pages. With an IRIX system, enter infosearch at a command line or select Help > InfoSearch from the Toolchest.
- On IRIX systems, you can view release notes by entering either grelnotes or relnotes at a command line.
- On Linux systems, you can view release notes on your system by accessing the README.txt file for the product. This is usually located in the /usr/share/doc/*productname* directory, although file locations may vary.
- You can view man pages by typing man *title* at a command line.

## **Reader Comments**

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# Introduction

This manual describes the SGI Scientific Computer Software Library, which runs on SGI IRIX and Linux systems. The information in this manual supplements the man pages provided with SCSL and provides details about the implementation and usage of these library routines.

SCSL contains the following groups of routines:

- Vector-vector linear algebra subprograms (Level 1 BLAS routines).
- Matrix-vector linear algebra subprograms (Level 2 BLAS routines).
- Matrix-matrix linear algebra subprograms (Level 3 BLAS routines).
- LAPACK routines for the solution of dense linear systems of equations, linear least-squares problems, eigenvalue problems and singular value decomposition.
- Direct linear solvers for real and complex sparse systems with symmetric non-zero structure, and iterative solvers for real sparse systems with arbitrary structure.
- Signal processing routines, which include Fast Fourier Transform (FFT) routines, convolution routines, and correlation routines.
- 64-bit thread-safe parallel random number generators.

The SCSL routines are loaded by using the *-lscs* option or the *-lscs\_mp* options to the compiler command line. The *-lscs\_mp* option directs the linker to use the multi-processor version of the library.

When linking with SCSL, the default integer size is 4 bytes (32 bits). Another version of SCSL is available in which integers are 8 bytes (64 bits). This version allows the users access to larger memory sizes. It can be loaded by using the <code>-lscs\_i8</code> option or the <code>-lscs\_i8\_mp</code> option. A program can use only one of the two versions; 4–byte integer and 8–byte integer library calls cannot be mixed.

Many SCSL routines are multitasked or multithreaded; this means that a program that calls a multitasked routine will run in parallel mode and take advantage of multiple processors whenever possible, even if the program has not specifically requested multitasking. If a significant percentage of time is spent in the routine, this feature can significantly reduce wall-clock time. Note that most LAPACK routines do not perform multiprocessing, but almost all LAPACK routines call Level 2 BLAS and Level 3 BLAS that do multiprocessing.

This manual includes the following sections:

- Chapter 2, "Basic Linear Algebra Subprogram (BLAS) Routines" on page 5, discusses the Basic Linear Algebra Subprogram (BLAS) routines.
- Chapter 3, "LAPACK" on page 13, discusses the LAPACK routines and their implementation on SGI Linux systems.
- Chapter 4, "Using Sparse Linear Equation Solvers" on page 41, discusses sparse matrices and solution techniques for sparse linear systems.
- Chapter 5, "Signal Processing Routines" on page 47, discusses the Fast Fourier Transform (FFT) routines.

#### **Parallel Processing Issues**

Parallel processing is a method of splitting a computational task into subtasks, and then simultaneously performing the subtasks. In many cases, the use of specialized libraries, such as SCSL, is a key component of parallel processing.

Parallel processing can eliminate idle CPU time because the workload is divided among all CPUs; therefore, the amount of work performed per unit time (the *throughput*) increases. However, parallel processing also introduces some overhead into program execution. In some cases, you may be able to reduce wall-clock time, but at the cost of extra CPU time which increases because more machine resources are used.

By using parallel processing, you can alleviate some of the following common problems:

- Maximum-memory jobs: if the memory is occupied by a few large-memory jobs, one or more of the CPUs might be idle even though there are other jobs to run.
- Dedicated machine: if the computer is running a single job, then all other CPUs are idle.
- Light workload: if the amount of jobs waiting for a CPU is less than the total number of CPUs, then one or more of the CPUs becomes idle.

With parallel processing, the additional CPUs reduce the wall-clock time instead of sitting idle. Even when very little idle time exists, using additional CPUs can still lead to benefits.

Parallel processing introduces some overhead into program execution. This subsection discusses some of the common types of overhead introduced by parallel processing:

- Multitasked programs require more memory than unitasked programs, and they
  can contain more code, more temporary variables, and can require additional stack
  space.
- Multitasked jobs can be swapped more often, and remain swapped longer, on a heavily loaded production system.
- Processors are forced to wait on semaphores during the process of synchronization.
- Overhead is incurred when slave processors are acquired (on entry to a parallel region) and at synchronization points within parallel regions. Tests show that the overhead of executing extra autotasking code adds a nominal 0% to 5% to the overall execution time.
- If inner-loop autotasking is used, vector performance can decrease because of shorter vector lengths and more vector loop startups.
- Processors are sometimes held for the next parallel region to improve efficiency. While holding a processor can save time, it also costs time to acquire and hold them.

Because overhead is associated with work distribution, jobs with large granularity have less partitioning than smaller jobs. Large jobs, however, may have problems with load balancing.

Parallel processing implementation strategies are discussed in detail in the following books:

- Linux Application Tuning Guide
- Origin 2000 and Onyx2 Performance Tuning and Optimization Guide

In addition to these books, other documents in the MIPSpro compiler documentation set discuss parallel processing issues that are specific to compiler use. See the *Guide to SGI Compilers and Compiling Tools* for information about those books.

# Basic Linear Algebra Subprogram (BLAS) Routines

The SCSL BLAS routines are a library of routines that perform basic operations involving matrices and vectors. The BLAS are used in a wide range of software, including LINPACK, LAPACK, and many other algorithms commonly in use today. They have become a de facto standard for elementary vector and matrix operations.

There are three 'levels' of BLAS routines:

- Level 1: these routines perform vector-vector operations such as dot-product and the adding of a multiple of one vector to another.
- Level 2: these routines perform matrix-vector operations that occur frequently in the implementation of many of the most common linear algebra algorithms. Note that algorithms that use Level 2 BLAS can be very efficient on vector computers, but are not well suite to computers with a hierarchy of memory (that is, cache memory).
- Level 3: these routines are used for matrix-matrix operations.

See the remaining subsections in this chapter for details about each type of BLAS.

BLAS 2 and BLAS 3 modules in SCSL are optimized and parallelized to take advantage of SGI's hardware architecture. Best performance is achieved with BLAS 3 routines where outer-loop unrolling and blocking techniques have been applied to take advantage of the memory cache.

SCSL's LAPACK algorithms make extensive use of BLAS 3 modules and are more efficient than the older, BLAS 1–based LINPACK algorithms.

## **Data Types**

The BLAS routines use the following data types:

- Single precision: Fortran "real" data types, C/C++ "float" data types, 32–bit floating point. These routine names begin with S.
- Single precision complex: Fortran "complex" data type, C/C++ "scsl\_complex" data type (defined in <scsl\_blas.h>), C++ STL "complex<float>" data type

(defined in <complex.h>), two 32-bit floating point reals. These routine names begin with C.

- Double precision: Fortran "double precision" data type, C/C++ "double" data type, 64–bit floating point. These routine names begin with D.
- Double precision complex: Fortran "double complex" data type, C/C++
   "scsl\_zomplex" data type (defined in <scsl\_blas.h>), C++ STL
   "complex<double>" data type (defined in <complex.h>), two 64-bit floating
   point doubles. These routine names begin with Z.

The man(1) command can find a man page online by either the single precision, single precision complex, double precision, or double precision complex name, as shown in the following table:

	Single Precision	Double Precision	Single Precision Complex	Double Precision Complex
form:	Sname	Dname	Cname	Zname
example:	SGEMM	DGEMM	CGEMM	ZGEMM

### C Interface to the BLAS Routines

SCSL supports two different C interfaces to the BLAS:

- The C interface described in individual BLAS man pages follows the same conventions used for the C interface to the SCSL signal processing library.
- SCSL also supports the C interface to the legacy BLAS set forth by the BLAS Technical Forum. This interface supports row-major storage of multidimensional arrays; see the INTRO\_CBLAS(3S) man page for details.

By default, the integer arguments are 4 bytes (32 bits) in size; this is the size obtained when the SCSL library is linked with <code>-lscs</code> or <code>lscs\_mp</code>. Another version of SCSL is available, however, in which integers are 8 bytes (64 bits). This version allows the user access to larger memory sizes and helps when porting legacy Cray codes. It can be loaded by using either the <code>-lscs\_i8</code> or <code>-lscs\_i8\_mp</code> link option. Any program may use only one of the two versions; 4-byte integer and8-byte integer library calls cannot be mixed.

C/C++ function prototypes for Level 1 BLAS routines are provided in <scsl\_blas.h>, when using the default 4-byte integers, and in <scsl\_blas\_i8.h> when using 8-byte integers. These header files define the complex types scsl\_complex and scsl\_zomplex, which are used in the prototypes. Alternatively, C++ programs may declare arguments using the types complex<float> and complex<double> from the standard template library. But if these types are used, <complex.h> must be included before <scsl\_blas.h> (or <scsl\_blas\_i8.h>). Both complex types are equivalent: they simply represent (real, imaginary) pairs of floating point numbers stored contiguously in memory. With the proper casts, you can simply pass arrays of floating point data to the routines where complex arguments are expected.

Casts, however, can be avoided. The header files <scsl\_blas.h> and <scsl\_blas\_i8.h> directly support the use of user-defined complex types or disabling prototype checking for complex arguments completely. By defining the symbol SCSL\_VOID\_ARGS before including <scsl\_blas.h> or <scsl\_blas\_i8.h> all complex arguments will be prototyped as void \*. To define the symbol SCSL\_VOID\_ARGS at compile time use the -D compiler option (for example, -DSCSL\_VOID\_ARGS) or use an explicit #define SCSL\_VOID\_ARGS in the source code. This allows the use of any complex data structure without warnings from the compiler, provided the structure is the following:

1. The real and imaginary components must be contiguous in memory.

2. Sequential array elements must also be contiguous in memory

While this allows the use of non-standard complex types without generating compiler warnings, it has the disadvantage that the compiler does not catch type mismatches.

Strong type checking can be enabled employing user-defined complex types instead of SCSL's standard complex types. To do this, define

SCSL\_USER\_COMPLEX\_T=my\_complex and SCSL\_USER\_ZOMPLEX\_T=my\_zomplex, where my\_complex and my\_zomplex are the names of user-defined complex types. These complex types must be defined before including the <scsl\_blas.h> or <scsl\_blas\_i8.h> header file.

Fortran 90 users on IRIX systems can perform compile-time checking of SCSL BLAS subroutine and function calls by adding USE SCSL\_BLAS (for 4-byte integer arguments) or USE SCSL\_BLAS\_I8 (for 8-byte integer arguments) to the source code from which the BLAS calls are made. Alternatively, the compile-time checking can be invoked without any source code modifications by using the <code>-auto\_use compiler</code> option, as in the following example:

```
% f90 -auto_use SCSL_BLAS test.f -lscs
% f90 -auto_use SCSL_BLAS_I8 -i8 test.f -lscs_i8
```

#### Increment Arguments

A vector's description consists of the name of the array (x or y) followed by the storage spacing (increment) in the array of vector elements (*incx* or *incy*). The increment can be positive or negative. When a vector x consists of n elements, the corresponding actual array arguments must be of a length at least 1+(n-1)\*|incx|. For a negative increment, the first element of x is assumed to be x(1+(n-1)\*|incx|) for Fortran arrays, x[(n-1)\*|incx|] for C/C++ arrays. The standard specification of \_SCAL, \_NRM2, \_ASUM, and I\_AMAX does not define the behavior for negative increments, so this functionality is an extension to the standard BLAS.

Note that setting an increment argument to 0 can cause unpredictable results.

# Array Storage (BLAS 2 and BLAS 3)

Multidimensional arrays passed as arguments to BLAS routines must be stored in column-major order, the storage convention used in Fortran programs. C and C++ users must explicitly store multidimensional arrays column-by-column.

One way to do this is to reverse the order of array dimensions with respect to the Fortran declaration (for example., x(ldx, n) in Fortran versus x[n][ldx] in C/C++). Because of the prototypes used in  $<scsl_blas.h>$ , the array should be cast as a pointer to the appropriate type when passed as an argument to a BLAS routine in order to avoid potential compiler type mismatch errors or warning messages.

C and C++ users who want to employ row-major storage for multidimensional arrays when calling the BLAS routines should see the INTRO\_CBLAS(3S)man page for details.

## Level 1 BLAS Routines

The Level 1 BLAS routines perform vector-vector linear algebra operations. The following types of vector-vector operations are available:

- Dot products and various vector norms
- Scaling, copying, swapping, and computing linear combinations of vectors

• Generating or applying plane or modified plane rotations.

You should use Fortran type declarations for functions. Declaring the data type of the complex Level 1 BLAS functions is important because, based on the first letter of the name of the routine and the Fortran data typing rules, the default implied data type would be REAL.

Fortran type declarations for function names are as follows:

Туре	Function Name
REAL	SASUM, SCASUM, SCNRM2, SDOT, SNRM2, SSUM
COMPLEX	CDOTC, CDOTU, CSUM
DOUBLE PRECISION	DASUM, DZASUM, DDOT, DNRM2, DZNRM2, DSUM
DOUBLE COMPLEX	ZDOTC, ZDOTU, ZSUM
INTEGER	ISAMAX, IDAMAX, ICAMAX, IZAMAX, ISAMIN, IDAMIN, ISMAX, IDMAX, ISMIN, IDMIN

The following routines are available in the SCSL BLAS 1:

- SASUM, DASUM: Sums the absolute values of the elements of a real vector (also called the l norm).
- SCASUM, DZASUM: Sums the absolute values of the real and imaginary parts of the elements of a complex vector.
- SAXPBY\*, DAXPBY\*, CAXPBY\*, ZAXPBY\*: Adds a scalar multiple of a real or complex vector to a scalar multiple of another vector.
- SAXPY, DAXPY, CAXPY, ZAXPY: Adds a scalar multiple of a real or complex vector to another vector.
- SCOPY, DCOPY, CCOPY, ZCOPY: Copies a real or complex vector into another vector.
- CDOTC, ZDOTC: Computes a dot product of the conjugate of a complex vector and another complex vector.
- SHAD\*, DHAD\*, CHAD\*, ZHAD\*: Computes the Hadamard product of two vectors.
- SNRM2, DNRM2: Computes the Euclidean norm (also called l<sub>2</sub> norm) of a real vector.
- SCNRM2, DZNRM2: Computes the Euclidean norm (1<sub>2</sub> norm) of a complex vector. 2
- CSROT\*, ZDROT\*, CROT\*, ZROT\*: Applies a real plane rotation to a pair of complex vectors.

- SROT, DROT: Applies an orthogonal plane rotation.
- SROTG, DROTG, CROTG\*, ZROTG\*: Constructs a Givens plane rotation.
- SROTM, DROTM: Applies a modified Givens plane rotation.
- SROTMG, DROTMG: Constructs a modified Givens plane rotation.
- SSCAL, DSCAL, CSCAL, ZSCAL, CSSCAL, ZDSCAL: Scales a real or complex vector.
- SSUM\*, DSUM\*, CSUM\*, ZSUM\*: Sums the elements of a real or complex vector.
- SSWAP, DSWAP, CSWAP, ZSWAP: Swaps two real or two complex vectors.
- ISAMAX, IDAMAX, ICAMAX, IZAMAX: Searches a vector for the first occurrence of the maximum absolute value.
- ISAMIN\*, IDAMIN\*: Searches a vector for the first occurrence of the minimum absolute value.
- ISMAX\*, IDMAX\*: Searches a vector for the first occurrence of the maximum value.
- ISMIN\*, IDMIN\*: Searches a vector for the first occurrence of the minimum value.

## Level 2 BLAS Routines

The Level 2 BLAS routines perform matrix-vector linear algebra operations. The following routines are available:

- CHBMV, ZHBMV: Multiplies a complex vector by a complex Hermitian band matrix.
- CHEMV, ZHEMV: Multiplies a complex vector by a complex Hermitian matrix.
- CHER, ZHER: Performs Hermitian rank 1 update of a complex Hermitian matrix.
- CHER2, ZHER2: Performs Hermitian rank 2 update of a complex Hermitian matrix.
- CHPMV, ZHPMV: Multiplies a complex vector by a packed complex Hermitian matrix.
- CHPR, ZHPR: Performs Hermitian rank 1 update of a packed complex Hermitian matrix.
- CHPR2, ZHPR2: Performs Hermitian rank 2 update of a packed complex Hermitian matrix.

- SGBMV, DGBMV, CGBMV, ZGBMV: Multiplies a real or complex vector by a real or complex general band matrix.
- SGEMV, DGEMV, CGEMV, ZGEMV: Multiplies a real or complex vector by a real or complex general matrix.
- SGER, DGER: Performs rank 1 update of a real general matrix.
- CGERC, ZGERC: Performs conjugated rank 1 update of a complex general matrix.
- CGERU, ZGERU: Performs unconjugated rank 1 update of a complex general matrix.
- SGESUM\*, DGESUM\*, CGESUM\*, ZGESUM\*: Adds a scalar multiple of a real or complex matrix to a scalar multiple of another real or complex matrix.
- SSBMV, DSBMV: Multiplies a real vector by a real symmetric band matrix.
- SSPMV, DSPMV, CSPMV\*, ZSPMV\*: Multiplies a real or complex vector by a real or complex symmetric packed matrix.
- SSPR, DSPR, CSPR\*, ZSPR\*: Performs symmetric rank 1 update of a real or complex symmetric packed matrix.
- SSPR2, DSPR2: Performs symmetric rank 2 update of a real symmetric packed matrix.
- SSYMV, DSYMV, CSYMV\*, ZSYMV\*: Multiplies a real or complex vector by a real or complex symmetric matrix.
- SSYR, DSYR, CSYR\*, ZSYR\*: Performs symmetric rank 1 update of a real or complex symmetric matrix.
- SSYR2, DSYR2: Performs symmetric rank 2 update of a real symmetric matrix.
- STBMV, DTBMV, CTBMV, ZTBMV: Multiplies a real or complex vector by a real or complex triangular band matrix.
- STBSV, DTBSV, CTBSV, ZTBSV: Solves a real or complex triangular band system of equations.
- STPMV, DTPMV, CTPMV, ZTPMV: Multiplies a real or complex vector by a real or complex triangular packed matrix.
- STPSV, DTPSV, CTPSV, ZTPSV: Solves a real or complex triangular packed system of equations.

- STRMV, DTRMV, CTRMV, ZTRMV: Multiplies a real or complex vector by a real or complex triangular matrix.
- STRSV, DTRSV, CTRSV, ZTRSV: Solves a real or complex triangular system of equations.

## Level 3 BLAS Routines

The Level 3 BLAS routines perform matrix-matrix linear algebra operations. The following routines are available:

- SGEMM, DGEMM, CGEMM, ZGEMM: Multiplies a real or complex general matrix by a real or complex general matrix.
- CGEMM3M\*, ZGEMM3M\*: Multiplies a complex general matrix by a complex general matrix, using 3 real matrix multiplications and 5 matrix additions.
- DGEMMS\*: Multiplies a double precision general matrix by a double precision general matrix, using a variation of Strassen's algorithm.
- SSYMM, DSYMM, CSYMM, ZSYMM: Multiplies a real or complex general matrix by a real or complex symmetric matrix.
- CHEMM, ZHEMM: Multiplies a complex general matrix by a Hermitian matrix.
- SSYR2K, DSYR2K, CSYR2K, ZSYR2K: Performs symmetric rank 2k update of a real or complex symmetric matrix.
- CHER2K, ZHER2K: Performs Hermitian rank 2k update of a complex Hermitian matrix.
- SSYRK, DSYRK, CSYRK, ZSYRK: Performs symmetric rank k update of a real or complex symmetric matrix.
- CHERK, ZHERK: Performs Hermitian rank k update of a complex Hermitian matrix.
- STRMM, DTRMM, CTRMM, ZTRMM: Multiplies a real or complex general matrix by a real or complex triangular matrix.

# LAPACK

LAPACK is a public domain library of subroutines for solving dense linear algebra problems, including systems of linear equations, linear least squares problems, eigenvalue problems, and singular value decomposition problems. It has been designed for efficiency on high-performance computers.

LAPACK is the successor to LINPACK and EISPACK. It uses today's high-performance computers more efficiently than the older packages and it extends the functionality of these packages by including equilibration, iterative refinement, error bounds, and driver routines for linear systems. It also includes routines for computing and reordering the Schur factorization, and condition estimation routines for eigenvalue problems.

Performance issues are addressed by implementing the most computationally-intensive algorithms using the Level 2 and 3 Basic Linear Algebra Subprograms (BLAS). Because most of the BLAS were optimized in single and multiple-processor environments, these algorithms give near optimal performance.

# LAPACK and SCSL

All routines from LAPACK 3.0 are included in SCSL. This includes driver routines, computational routines, and auxiliary routines for solving linear systems, least squares problems, and eigenvalue and singular value problems. See the INTRO\_LAPACK(3S) man page for details about the routines that are available in the current release of SCSL.

Online man pages are available for individual LAPACK subroutines. For example, to view a description of the calling sequence for the subroutine to perform the LU factorization of a real matrix, see the DGETRF(3S) man page. The user interface to all supported LAPACK routines is the same as the standard LAPACK interface.

Several enhancements improve the performance of the LAPACK routines on SGI systems. For example, the LU, Cholesky, and QR factorization routines are redesigned for better performance and scalability when running multiple processes.

Tuning parameters for the block algorithms provided in SCSL are set within the ILAENV LAPACK routine. ILAENV is an integer function subprogram that accepts information about the problem type and problem dimensions and returns a single integer parameter such as the optimal block size, the minimum block size for which a

block algorithm should be used, or the crossover point (the problem size at which it becomes more efficient to switch to an unblocked algorithm). Setting tuning parameters occurs without user intervention, but users can call ILAENV directly to check the values to be used.

## Naming Scheme for Individual Routines

The name of each LAPACK routine is a coded specification of its function. All driver and computational routines have five or six character names of the form XYYZZ or XYYZZZ. The first letter, X, indicates the data type:

• S: real

BD

- D: double precision
- C: complex
- Z: double complex

The next two letters, YY, indicate the type of matrix or the most significant matrix type. Most of these two letter codes apply to both real and complex matrices, but some apply specifically to only one or the other. The following list shows all matrix types:

BiDiagonal DI Diagonal GB General Band GΕ GEneral (nonsymmetric) GG General matrices, Generalized problem GT General Tridiagonal ΗB Hermitian Band (complex only) HErmitian (possibly indefinite) (complex only) HE Hessenberg matrix, Generalized problem HG ΗP Hermitian Packed (possibly indefinite) (complex only) HS upper HeSsenberg Orthogonal Packed (real only) OP OR ORthogonal (real only) Positive definite Band (symmetric or Hermitian) ΡB ΡO POsitive definite (symmetric or Hermitian) ΡP Positive definite Packed (symmetric or Hermitian) РΤ Positive definite Tridiagonal (symmetric or Hermitian) SB Symmetric Band (real only) SP Symmetric Packed (possibly indefinite)

```
ST
       Symmetric Tridiagonal
SY
       SYmmetric (possibly indefinite)
ТΒ
       Triangular Band
       Triangular matrices, Generalized problem
ΤG
ΤP
       Triangular Packed
      TRiangular
TR
TZ
      TrapeZoidal
       UNitary (complex only)
UN
       Unitary Packed (complex only)
UΡ
```

The last letters, ZZ or ZZZ, indicate the computation performed. For example, TRF is a Triangular Factorization.

See the INTRO\_LAPACK(3s) man page for details about the types of computations performed and a list of supported routines.

## Types of Problems Solved by LAPACK

LAPACK routines can solve systems of linear equations, linear least squares problems, eigenvalue problems, and singular value problems. LAPACK routines can also handle many associated computations such as matrix factorizations and estimating condition numbers. Dense and banded matrices are provided for, but not general sparse matrices.

This subsection discusses the LAPACK routines for solving the following two basic problems:

- Computing the unique solution to a linear system *AX* = *B*, where the coefficient matrix *A* is dense, banded, triangular, or tridiagonal, and the matrix *B* may contain one or more right-hand sides.
- Computing a least squares solution to an overdetermined system AX = B, where A is  $m \times n$  with  $m \ge n$ , or a minimum norm solution to an underdetermined system AX = B, where A is  $m \times n$  with m < n.

See "Solving Linear Systems" on page 16, and "Solving Least Squares Problems" on page 34, for a discussion of the software used to solve these problems. The orthogonal transformation routines described in "Solving Least Squares Problems" on page 34, also have application in eigenvalue and singular value computations.

There are three classes of LAPACK routines: LAPACK *driver routines* solve a complete problem; LAPACK *computational routines* perform one step of the computation; and LAPACK *auxiliary routines* perform certain subtask or low-lvel computation.

The driver routines generally call the computational routines to do their work, and offer a more convenient interface; therefore, LAPACK users are advised to use a driver routine if there is one that meets their requirements.

Man pages for both driver and computational routines are available with SCSL. A list of the auxiliary routines, with a brief description, can be found in the LAPACK User's Guide.

#### Solving Linear Systems

Finding the solution of a system of simulataneous linear equations is one of the most frequently encountered problems in scientific computing.

A linear system of equations (*n* equations with *n* unknowns) can be written as follows:

 $a_{11} x_{11} + a_{12} x_2 + \dots + a_{1n} x_n = b_1$   $a_{12} x_1 + a_{22} x_2 + \dots + a_{2n} x_n = b_2$ ......  $a_{n1} x_1 + a_{n2} x_2 + \dots + a_{nn} x_n = b_n$ 

#### Equation 3-1

This system can also be written in the form Ax = b where A is a square matrix of order n, b is a given column vector of n components and x is an unknown column vector of n components.

For example, the following linear equations:

$$2x + y = 4$$
$$-x + y = 1$$

Equation 3-2

can be written in matrix/vector notation as the following:

```
\begin{bmatrix} 2 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 4 \\ 1 \end{bmatrix}
```

#### **Equation 3-3**

The solution to this system of equations is the set of vectors  $[x, y]^T$  that satisfy both equations. The physical interpretation of this system of equations is that it represents two lines in the (x,y) plane, which may intersect in one point, no points (if they are parallel), or an infinite number of points (if the two equations are multiples of each other).

To solve the system, it is helpful to simply the system as much as possible. A standard method for doing this (Gaussian elimination) is to use the following elementary operations:

- interchange any two equations
- multiply an equation by a nonzero constant
- add a multiple of one equation to any other one

This reduces the system to a triangular form. The system obtained after each operation will be equivalent to the original system and therefore have the same solution.

For illustration consider the following system of linear equations:

$$x + y + z = 0$$
  

$$x + 2y + 4z = -1$$
  

$$x + 3y + 9z = 2$$

#### **Equation 3-4**

Subtract the first equation from the second equation and subtract the first equation from the third one. The result is the following system:

$$x + y + z = 0$$
  

$$y + 3z = -1$$
  

$$2y + 8z = 2$$

#### Equation 3-5

Note the first variable x no longer appears in the second or third equation. Similarly, the second variable y can be eliminated from the third equation by subtracting 2 times the second equation from the third equation to obtain the following:

$$x + y + z = 0$$
$$y + 3z = -1$$
$$2z = 4$$

#### **Equation 3-6**

The resulting system is upper triangular and it can easily be deduced that:

$$2z = 4 \Rightarrow z = 2$$
  

$$y + 3z = -1 \Rightarrow y = (-1 - 3 \times 2) = -7$$
  

$$x + y + z = 0 \Rightarrow x = 7 - 2 = 5$$

#### **Equation 3-7**

To represent these steps in matrix form, let *A*=A1, A2, and A3 represent the matrices of the systems (Equation 3-4, Equation 3-5, Equation 3-6, respectively), for example:

$$A2 = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 2 & 8 \end{bmatrix}$$

#### Equation 3-8

Then A2 is obtained from A1 by subtracting the first row from the second row and subtracting the first row from the third row. This means that A2 can be obtained by pre-multiplying A1 by a suitable matrix, and in this example, it is easy to verify that

$$A2 = M1 \times A1$$

**Equation 3-9** 

that is:

 $\begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 2 & 8 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \end{bmatrix}$ 

Equation 3-10

In a similar way

$$A3 = M2 \times A2$$

or

[1	1	1		[1	0	0	[1	1	1	
0	1	3	=	0	1	0	0	1	3	
0	0	2		0	$\begin{array}{c} 0 \\ 1 \\ -2 \end{array}$	1	0	<b>2</b>	8	
-		-		-		-	_		_	

Equation 3-12

Combining Equation 3-9 and Equation 3-11 we have

$$A3 = M2 \times M1 \times A$$

### Equation 3-13

Therefore, to solve the system *Ax*=*b*, we only need to calculate the following:

$$c = M2 \times M1 \times b$$

Equation 3-14

and solve the upper triangular system

$$A3 \times x = M2 \times M1 \times A \times x = M2 \times M1 \times b = c$$

Equation 3-15

Moreover, M1 and M2 are nonsingular matrices so:

$$A = M1^{-1} \times M2^{-1} \times A3$$

### Equation 3-16

Because *M*1 and *M*2 are unit lower triangular, so is the product of their inverses. Therefore, *A* can be written as the product of a lower triangular matrix  $L=M1^{-1} \times M2^{-1}$  and an upper triangular matrix U=A3. Equation 3-16 becomes A=LU, which is the factorization of the coefficient matrix *A*.

The LAPACK routines for solving linear systems assume the system is already in a matrix form. The data type (real or complex), characteristics of the coefficient matrix (general or symmetric, and positive definite or indefinite if symmetric), and the storage format of the matrix (dense, band, or packed), determine the routines that should be used.

### Factoring a Matrix

Most of the techniques in LAPACK are based on a matrix factorization as the first step. There are two main types of factorization forms:

- explicit: The actual factors are returned. For example, the Cholesky factorization routine DPOTRF(3S), with UPLO = 'L', returns a matrix L such that  $A = LL^T$ .
- factored form: The factorization is returned as a product of permutation matrices and triangular matrices that are low-rank modifications of the identity. For example, the diagonal pivoting factorization routine DSYTRF(3S), with UPLO = 'L', computes a factorization of the following form:

$$A = (P_1 L_1 P_2 L_2 \dots P_n L_n) D (P_1 L_1 P_2 L_2 \dots P_n L_n)^T$$

### Equation 3-17

where each  $P_i$  is a rank-1 permutation, each  $L_i$  is a rank-1 or rank-2 modification of the identity, and D is a diagonal matrix with 1-by-1 and 2-by–2 diagonal blocks.

Generally, users do not have to know the details of how the factorization is stored, because other LAPACK routines manipulate the factored form.

Regardless of the form of the factorization, it reduces the solution phase to one that requires only permutations and the solution of triangular systems. For example, the LU factorization of a general matrix, A = PLU, is used to solve for X in the system of equations AX = B by successively applying the inverses of *P*, *L*, and *U* to the right-hand side:

- 1.  $X \leftarrow PB$
- 2.  $X \leftarrow L^{-1}X$
- 3.  $X \leftarrow U^{-1}X$

In the last two steps, the inverse of the triangular factors is not computed, but triangular systems of the form LY = Z and UX = Y are solved instead.

The following table lists the factorization forms for each of the factorization routines for real matrices. The factorization forms differ for DGETRF and DGBTRF, even though both compute an *LU* factorization with partial pivoting. You can also obtain the same factorizations through the LAPACK driver routines (for instance, DGESV or DGESVX).

Name	Form	Equation	Notes		
DGBTRF	Factored form	A = LU	L is a product of permutations		
DGTTRF	Factored form	A = LU	and unit lower triangular matrices $L_i$ ; $L_i$ differs from the identity matrix only in column <i>i</i> .		
DGETRF	Explicit	A = PLU			
DPBTRF	Explicit	$A = LL^T$ or $A = U^T U$			
DPOTRF	Explicit	$A = LL^T$ or $A = U^T U$			
DPPTRF	Explicit	$A = LL^T$ or $A = U^T U$			
DPTTRF	Explicit	$A = LDL^T$ or $A = U^T DU$			
DSPTRF	Factored form	$A = LDL^T$ or $A = UDU^T$	L (or $U$ ) is a product of		
DSYTRF	Factored form	$A = LDL^T$ or $A = UDU^T$	permutations and block unit lower (upper) triangular matrices $L_i(U_i)$ ; $L_i(U_i)$ differs from the identity matrix only in the one or two columns that correspond to the 1-by-1 or 2-by-2 diagonal block $D_i$ .		

 Table 3-1 Factorization forms

### Example 3-1 LU factorization

The DGETRF subroutine performs an LU factorization with partial pivoting (A = PLU) as the first step in solving a general system of linear equations AX = B. If DGETRF is called with the following:

$$A = \begin{bmatrix} 4. & 9. & 2. \\ 3. & 5. & 7. \\ 8. & 1. & 6. \end{bmatrix}$$

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details of the factorization are returned, as follows:

$$A = \begin{bmatrix} 8. & 1. & 6. \\ 0.5 & 8.5 & -1.0 \\ 0.375 & 0.5441 & 5.294 \end{bmatrix}$$
$$IPIV = [3, 3, 3]$$

# Equation 3-19

Matrices *L* and *U* are given explicitly in the lower and upper triangles, respectively, of *A*:

$$L = \begin{bmatrix} 1. & & \\ 0.5 & 1. & \\ 0.375 & 0.5441 & 1. \end{bmatrix}, U = \begin{bmatrix} 8. & 1. & 6. \\ & 8.5 & -1.0 \\ & & 5.4294 \end{bmatrix}$$

### Equation 3-20

The IPIV vector specifies the row interchanges that were performed. IPIV(1) = 3 implies that the first and third rows were interchanged when factoring the first column; IPIV(2) = 3 implies that the second and third rows were interchanged when factoring the second column. In this case, IPIV(3) must be 3 because there are only three rows. Thus, the permutation matrix is the following:

 $P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$ 

### Equation 3-21

Generally, the pivot information is used directly from IPIV without constructing matrix *P*.

Example 3-2 Symmetric indefinite matrix factorization

DSYTRF factors a symmetric indefinite matrix A into one of the forms  $A = LDL^T$  or  $A = UDU^T$ , where L and U are lower triangular and upper triangular matrices, respectively, in factored form, and D is a diagonal matrix with 1-by-1 and 2-by-2

diagonal blocks. To illustrate this factorization, choose a symmetric matrix that requires both 1-by-1 and 2-by-2 pivots:

$$A = \begin{bmatrix} 9. & & \\ 5. & 7. & \\ -16. & 12. & 3. \\ 4. & -2. & 10. & 8. \end{bmatrix}$$

### Equation 3-22

Only the lower triangle of *A* is specified because the matrix is symmetric, but you could have specified the upper triangle instead. The output from DSYTRF is the following:

$$A = \begin{bmatrix} 9. \\ -16. & 3. \\ -0.9039 & -0.8210 & 21.37 \\ -0.7511 & -0.6725 & 0.4597 & 13.21 \end{bmatrix}$$
$$IPIV = [-3, -3, 3, 4]$$

### Equation 3-23

The signs of the indices in the IPIV vector indicate that a 2-by-2 pivot block was used for the first two columns, and 1-by-1 pivots were used for the third and fourth columns. Therefore, *D* must be the following:

$$D = \begin{bmatrix} 9. & & \\ -16. & 3. & & \\ & 21.37 & \\ & & 13.21 \end{bmatrix}$$

### Equation 3-24

Matrix *L* is supplied in factored form as  $L = P_1L_1P_2L_2$ , where the parts of each  $L_i$  that differ from the identity are stored in *A* below their corresponding blocks  $D_i$ :

$$P_{1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, L_{1} = \begin{bmatrix} 1. \\ 0. \\ -0.9039 & -0.8210 & 1 \\ -0.7511 & -0.6725 & 0.0 & 1.0 \end{bmatrix}$$

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$$P_2 = I, L_2 = \begin{bmatrix} 1 & & \\ 0 & 1 & & \\ 0 & 0 & 1.0 & \\ 0 & 0 & 0.4597 & 1 \end{bmatrix}$$

Equation 3-26

# **Error Codes**

The LAPACK routines always check the arguments on entry for incorrect values. If an illegal argument value is detected, the error-handling subroutine XERBLA is called. XERBLA prints a message similar to the following to standard error, and then it aborts:

\*\* On entry to DGETRF parameter number 4 had an illegal value

All other errors in the LAPACK routines are described by error codes returned in *info*, the last argument. The values returned in *info* are routine-specific, except for *info* = 0, which always means that the requested operation completed successfully.

For example, an error code of *info* > 0 from DGETRF means that one of the diagonal elements of the factor U from the factorization A = PLU is exactly 0. This indicates that one of the rows of A is a linear combination of the other rows, and the linear system does not have a unique solution.

Example 3-3 Error conditions

If DGETRF is given the matrix

$$A = \begin{bmatrix} 1. & 4. & 7. \\ 2. & 5. & 8. \\ 3. & 6. & 9. \end{bmatrix}$$

Equation 3-27

it returns

$$A = \begin{bmatrix} 3. & 6. & 9\\ 0.3333 & 2. & 4\\ 0.6667 & 0.5 & 0 \end{bmatrix}$$
$$IPIV = [3, 3, 3]$$

which corresponds to the factorization

0			1.0				3.	6.	9.
			0.3333			, U =		2.	4.
1	0	0	0.6667	0.5	1.		L		0.

### Equation 3-29

On exit from DGETRF, *info* = 3, indicating that U(3,3) is exactly 0. This is not an error condition for the factorization because the factors that were computed satisfy A = PLU, but the factorization cannot be used to solve the system.

# Solving from the Factored Form

In LAPACK, the solution step is generally separated from the factorization. This allows the matrix factorization to be reused if the same coefficient matrix appears in several systems of equations with different right-hand sides. If the number of right-hand sides is also large, it is often more efficient to separate the solve from the factorization. The typical usage is found in the driver routine DGESV, which solves a general system of equations AX = B by using two subroutine calls, the first to factor the matrix A and the second to solve the system, using the factored form:

```
CALL DGETRF( N, N, A, LDA, IPIV, INFO )
IF( INFO.EQ.0 ) THEN
CALL DGETRS( 'No transpose', N, NRHS, A, LDA,
$ IPIV, B, LDB, INFO )
END IF
```

As shown, you should always check the return code from the factorization to see whether it completed successfully and did not produce any singular factors. To obtain further information about proceeding with the solve, estimate the condition number (see "Condition Estimation" on page 26, for details). Because most of the LAPACK driver routines do their work in the LAPACK computational routines, a call to a driver routine gives the same performance as separate calls to the computational routines. The exceptions are the simple driver routines used for solving tridiagonal systems: SGTSV, SPTSV, CGTSV, and CPTSV. These routines compute the solution while performing the factorization for certain numbers of right-hand sides. Because the amount of work in each loop is small, some reloading of constants and loop overhead is saved by combining the factorization with part of the solve.

# **Condition Estimation**

A return code of info = 0 from a factorization routine indicates that the triangular factors have nonzero diagonals. The linear system still may be too ill-conditioned to give a meaningful solution.

One indicator that you can examine before computing the solution is the reciprocal condition number, RCOND. The condition number, defined as  $\kappa(A) = ||A|| ||A^{-1}||$ , tells how much the relative errors in A and b are magnified in the solution x. DGECON and the other condition estimation routines compute  $\texttt{RCOND} = 1/\kappa(A)$  by using the exact 1-norm or infinity-norm of A and an estimate for the norm of  $A^{-1}$ , because computing the inverse explicitly would be very expensive, and the inverse may not even exist. By convention, if  $A^{-1}$  does not exist,  $\kappa(A) = \infty$  and RCOND should be computed as 0 or a small number on the order of  $\epsilon$ , the machine epsilon.

If the condition number is large (that is, if RCOND is small), small errors in *A* and *b* may lead to large errors in the solution *x*. The rule of thumb is that the solution loses one digit of accuracy for every power of 10 in the condition number, assuming that the elements of *A* all have about the same magnitude. For example, a condition number of 100 (RCOND = 0.01) implies that the last 2 digits are inaccurate; a condition number of  $1/\epsilon$  (RCOND <  $\epsilon$ , the machine epsilon which is approximately  $1.1 \times 10^{-14}$  on Altix systems) implies that all of the digits have been lost. This value for the machine epsilon assumes a model of rounded floating-point arithmetic with base  $\beta = 2$  and t = 53 mantissa digits, and  $\epsilon = \beta^{(1-t)}$ .

The expert driver routine DGESVX uses this rule of thumb to decide whether the solution and error bounds should be computed. If RCOND is less than the machine epsilon, DGESVX returns *info* = N+1, indicating that the matrix A is singular to working precision, and it does not compute the solution.

Example 3-4 Roundoff errors

The matrix

$$A = \begin{bmatrix} 1. & 2. & 3. \\ 4. & 5. & 6. \\ 7. & 8. & 9. \end{bmatrix}$$

is singular in exact arithmetic, but on Altix systems, DGETRF returns

$$A = \begin{bmatrix} 7. & 8. & 9.\\ 0.1429 & 0.8571 & 1.714\\ 0.5714 & 0.5 & -1.586. \times 10^{-16} \end{bmatrix}$$

### Equation 3-31

where *IPIV*=[3,3,3] and *info* = 0. In exact arithmetic, A(3,3) would have been 0, but roundoff error has made this entry  $-1.586 \times 10^{-16}$  instead. The reciprocal condition number computed by DGECON is  $2.20 \times 10^{-18}$ , which is less than the machine epsilon of  $1.11 \times 10^{-16}$ . Therefore, DGESVX returns *info*= 4 and does not try to solve any systems with this *A*.

### **Use in Error Bounds**

You can use the condition number to compute a simple bound on the relative error in the computed solution to a system of equations Ax = b (see *Introduction to Matrix Computations*, by Stewart). If x is the exact solution and  $\hat{x}$  is the computed solution, let r be the residual  $r = b - Ax = A(x - \hat{x})$ . If A is nonsingular:

$$x - \hat{x} = A^{-1}r$$

Equation 3-32

and

$$||x - \hat{x}|| \le ||A^{-1}|| ||r||$$

### Equation 3-33

From Equation 3-33 we can already see that if ||A|| is large, then the error in  $\hat{x}$  may be significantly greater than the residual *r*.

Since Ax = b, it follows that  $||x|| \ge ||b|| / ||A||$ , therefore

$$\frac{\|x - \hat{x}\|}{\|x\|} \le \|A\| \|A - 1\| \frac{\|r\|}{\|b\|}$$

Define the condition number  $\kappa(A) = ||A|| ||A - 1||$ . This gives the bound

$$\frac{||x - \hat{x}||}{||x||} \le \kappa (A) \frac{||r||}{||b||}$$

### Equation 3-35

For a description of a more precise error bound based on a component-wise error analysis, see "Error Bounds" on page 32.

Another application of the condition number is to consider the computed solution  $\hat{x} = x + \Delta x$  to be the exact solution of a slightly perturbed linear system:

$$(A + \Delta A) (x + \Delta x) = (b + \Delta b)$$

#### Equation 3-36

where  $\Delta A$  is small in norm with respect to A, and  $\Delta b$  is small in norm with respect to b. For Gaussian elimination with partial pivoting, it has been shown that  $||\Delta A|| \leq \omega ||A||$  and  $||\Delta b|| \leq \omega ||b||$ , where  $\omega$  is the product of  $\varepsilon$  and a slowly growing function of n (see *The Algebraic Eigenvalue Problem*, by Wilkinson). Proving that an algorithm has this property is the stuff of backward error analysis, and it ensures that, if the problem is well-conditioned, the computed solution is near the exact solution of the original problem. Because Ax = b (Equation 3-34) simplifies to

$$A\Delta x = \Delta b - \Delta A \left( x + \Delta x \right)$$

Equation 3-37

Assuming A is nonsingular,

$$\Delta x = A^{-1} \left( \Delta b - \Delta A \left( x + \Delta x \right) \right)$$

Equation 3-38

Taking norms and dividing by ||x||,

$$\frac{\|\Delta x\|}{\|x\|} \le \|A^{-1}\| \left(\frac{\|\Delta b\|}{\|x\|} + \|\Delta A\| + \frac{\|\Delta A\|}{\|x\|}\right)$$

Using the inequality  $||b|| \leq ||A|| ||x||$ ,

$$\frac{\|\Delta x\|}{\|x\|} \le \|A\| \|A^{-1}\| \left(\frac{\|\Delta b\|}{\|b\|} + \frac{\|\Delta A\|}{\|A\|} + \frac{\|\Delta A\| \|\Delta x\|}{\|A\| \|x\|}\right)$$

Equation 3-40

and substituting  $\kappa(A) = ||A|| ||A^{-1}||$ ,

$$\frac{\left\|\Delta x\right\|}{\left\|x\right\|} \le \kappa\left(A\right) \left(\frac{\frac{\left\|\Delta b\right\|}{\left\|b\right\|} + \frac{\left\|\Delta A\right\|}{\left\|A\right\|}}{1 - \kappa\left(A\right) \frac{\left\|\Delta A\right\|}{\left\|A\right\|}}\right)$$

### Equation 3-41

provided  $\kappa(A) \|\Delta A\| / \|A\| < 1$ . In terms of the relative backward error  $\omega$ ,

$$\frac{\left\|\Delta x\right\|}{\left\|x\right\|} \le \frac{2\omega\kappa\left(A\right)}{1 - \omega\kappa\left(A\right)}$$

### Equation 3-42

In "Error Bounds" on page 32, the backward error is defined slightly differently to obtain a component-wise error bound.

# Equilibration

The condition number defined in the last section is sensitive to the scaling of *A*. For example, the matrix

$$A = \begin{bmatrix} 1. & 1\\ 0 & 1. \times 10^{16} \end{bmatrix}$$

Equation 3-43

has as its inverse

$$A^{-1} = \begin{bmatrix} 1. & -1 \times 10^{-16} \\ 0 & 1. \times 10^{-16} \end{bmatrix}$$

and so RCOND=1/  $(||A|| ||A^{-1}||) = 1. \times 10^{-16}$ . If this value of RCOND is less than the machine epsilon on a system, DGESVX (with FACT = 'N') does not try to solve a system with this matrix. However, *A* has elements that vary widely in magnitude, so the bounds on the relative error in the solution may be pessimistic. For example, if the right-hand side in Ax = b is the following:

$$b = \begin{bmatrix} 2.0\\ 1.0 \times 10^{16} \end{bmatrix}$$

### Equation 3-45

DGETRF followed by DGETRS produces the exact answer,  $x = [1., 1.]^T$ .

You can improve the condition of this example by a simple row scaling. Scaling a problem before computing its solution is known as *equilibration*, and it is an option to some of the expert driver routines (those for general or positive definite matrices). Enabling equilibration does not necessarily mean it will be done; the driver routine will choose to do row scaling, column scaling, both row and column scaling, or no scaling, depending on the input data. The usage of this option is as follows:

CALL DGESVX('E', 'N', N, NRHS, A, LDA, AF, LDAF, IPIV, EQUED, R, C, B, LDB, X, LDX, RCOND, FERR, BERR, WORK, IWORK, INFO)

The 'E' in the first argument enables equilibration. For this example, EQUED = 'R' on return, indicating that only row scaling was done, and the vector *R* contains the scaling constants:

$$R = \begin{bmatrix} 1.0\\ 1.0 \times 10^{-16} \end{bmatrix}$$

Equation 3-46

The form of the equilibrated problem is:

$$(diag(R) \land diag(C)) (diag(C)^{-1}X) = diag(R) B$$

or  $A_E X_E = B_E$ , where  $A_E$  is returned in A:

$$A \leftarrow \begin{bmatrix} 1. & 0. \\ 0. & 1.0 \times 10^{-16} \end{bmatrix} \begin{bmatrix} 1. & .1 \\ 0. & 1.0 \times 10^{-16} \end{bmatrix} = \begin{bmatrix} 1. & 1. \\ 0. & 1. \end{bmatrix}$$

Equation 3-48

and  $B_E$  is returned in B:

$$B \leftarrow \begin{bmatrix} 1. & 0. \\ 0. & 1.0 \times 10^{-16} \end{bmatrix} \begin{bmatrix} 2. \\ 1.0 \times 10^{16} \end{bmatrix} = \begin{bmatrix} 2. \\ 1. \end{bmatrix}$$

### Equation 3-49

The factored form, AF, returns the same matrix as A in this example, because A is upper triangular, and RCOND = 0.3, which is the estimated reciprocal condition number for the equilibrated matrix. The only output quantity that pertains to the original problem before equilibration is the solution matrix X. In this example, X is also the solution to the equilibrated problem because no column scaling was done, but if EQUED had returned 'C' or 'B' and the solution to the equilibrated system were desired, it could be computed from  $X_E = diag (C)^{-1} X$ .

# **Iterative Refinement**

Iterative refinement in LAPACK uses all same-precision arithmetic, a recent innovation, because it was long believed that a successful algorithm would require the residual to be computed in double precision. The following example illustrates the results of iterative refinement; "Error Bounds" on page 32, discusses the error bounds computed in the course of the algorithm.

One possible use of iterative refinement is to smooth out numerical differences between floating-point number representations. For example, a result computed on a system, which has about 13 digits of accuracy, may be improved on IEEE system, which has about 15 digits of accuracy, through the  $0(n^2)$  process of iterative refinement, instead of the  $0(n^3)$  process of recomputing the solution.

### Example 3-5 Hilbert matrix

The classic example of an ill-conditioned matrix is the Hilbert matrix, defined by  $A_{i,j} = 1/(i + j - 1)$ . For example, the 5-by-5 Hilbert matrix is

$\begin{bmatrix} 1 \end{bmatrix}$	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$
$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$
$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{7}$
$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{7}$	$\frac{1}{8}$
$\left[ \frac{1}{5} \right]$	$\frac{1}{6}$	$\frac{1}{7}$	$\frac{1}{8}$	$\frac{1}{9}$

which has a condition number of  $4.77 \times 10^5$ . A rule of thumb ("Condition Estimation" on page 26) suggests almost 8 digits of accuracy in the solution are possible on systems, because  $\epsilon = 1.4 \times 10^{-13}$  and  $\epsilon \kappa (A) \approx 0.5 \times 10^{-8}$ . If the matrix is factored using DGETRF and DGETRS is used to solve Ax = b, where  $b = [1, 0, 0, 0, 0]^T$ .

**Error Bounds** 

In addition to performing iterative refinement on each column of the solution matrix, DGERFS and the other *xxx*RFS routines also compute error bounds for each column of the solution. These bounds are returned in the real arrays FERR (forward error) and BERR (backward error), both of length NRHS. For a computed solution  $\hat{x}$  to the system of equations Ax = b, the forward error bound *f* is the following:

$$\frac{\|x - \hat{x}\|}{\|x\|} \le f$$

#### Equation 3-51

and the backward error bound  $\omega$  bounds the relative errors in each component of *A* and *b* in the perturbed equation 2 from "Use in Error Bounds" on page 27.

$$\|\Delta A_{i,j}\| \le \omega \|A_{i,j}\|, \|\Delta b_i\| \le \omega \|b_i\|$$

### Equation 3-52

In Example 3-5 on page 31, the first column of the inverse of the Hilbert matrix of order 5 is computed by solving  $H_5 x = e_1$ , and DGERFS computed error bounds of  $f \approx 1.4 \times 10^{-8}$  and  $\omega \approx 9.1 \times 10^{-16}$  on systems. This provides direct information about the solution; its relative error is at most  $0(10^{-8})$ ; therefore, the largest components of the solution should exhibit about 8 digits of accuracy, and the system for which this

solution is an exact solution is within a factor of epsilon ( $\epsilon \approx 1.4 \times 10^{-14}$ ) from the system whose solution was attempted, so the solution is as good as the data warrants.

The component-wise relative backward error bound (equation 3) is more restrictive than the classical backward error bound  $||\Delta A|| \le \omega ||A||$ , because it assumes  $||\Delta A||$  has the same sparsity structure as ||A||, because if  $A_{i,j}$  is 0, so must be  $\Delta A_{i,j}$ . The backward error for the solution  $\hat{x}$  is computed from the equation

$$\omega = \max_{i} \frac{|r|_{i}}{(|A| |\hat{x}| + |b|)_{i}}$$

### Equation 3-53

where  $r = b - A\hat{x}$ , and the forward error bound is computed from the equation

$$f = \frac{\left\| \left| A^{-1} \right| \left( \left| r \right| + \left( \gamma + 1 \right) \epsilon \left( \left| A \right| \left| x \right| + \left| b \right| \right) \right) \right\|}{\left\| x \right\|}$$

#### Equation 3-54

where  $\gamma$  is the maximum number of nonzeros in any row of *A*. To avoid computing  $A^{-1}$  an approximation is used for  $|||A^{-1}|g||$ , where *g* is the nonnegative vector in parentheses (see Arioli, et al., for details).

### **Inverting a Matrix**

Subroutines to compute a matrix inverse are provided in LAPACK, but they are not used in the driver routines. The inverse routines sometimes use extra workspace and always require more operations than the solve routines. For example, if there is one right-hand side in the equation Ax = b, where A is a square general matrix, the solves following the factorization require  $2n^2$  operations, while inverting the matrix A requires  $4/3n^3$  operations, plus another  $2n^2$  to multiply b by  $A^{-1}$ . The inverse must be computed only once, however, and the cost can be amortized over the number of right-hand sides. Because multiplying by the inverse may be more efficient than doing a triangular solve, the extra cost to compute the inverse may be overcome if the number of right-hand sides is large.

# Solving Least Squares Problems

In some applications, the best solution to a system of equations AX = B that does not have a unique solution is required. If *A* is overdetermined, that is, *A* is  $m \times n$  with  $m \ge n$  and rank at least *n*, the system does not have a solution, but the linear least squares problem may have to be solved:

$$minimize \|B - AX\|_2$$

### Equation 3-55

If *A* is underdetermined, that is, *A* is  $m \times n$  with m < n, generally many solutions exist, and you may want to find the solution *X* with minimum 2-norm. Solving these problems requires that you first obtain a basis for the range of *A*, and several orthogonal factorization routines are provided in LAPACK for this purpose.

An orthogonal factorization decomposes a general  $m \times n$  matrix A into a product of an orthogonal matrix Q and a triangular or trapezoidal matrix. A real matrix Q is orthogonal if  $Q^T Q = I$ , and a complex matrix Q is unitary if  $Q^H Q = I$ . The key property of orthogonal matrices for least squares problems is that multiplying a vector by an orthogonal matrix does not change its 2-norm, because

$$\|Qx\|_{2} = \sqrt{x^{T}Q^{T}Qx} = \sqrt{x^{T}x} = \|x\|_{2}$$

Equation 3-56

# **Orthogonal Factorizations**

LAPACK provides four different orthogonal factorizations for each data type. For real data, they are as follows:

- DGELQF: LQ factorization
- DGEQLF: QL factorization
- DGEQRF: QR factorization
- DGERQF: *RQ* factorization

Each of these factorizations can be done regardless of whether *m* or *n* is larger, but the *QR* and *QL* factorizations are most often used when  $m \ge n$ , and the *LQ* and *RQ* factorizations are most often used when  $m \le n$ .

The *QR* factorization of an *m*-by-*n* matrix *A* for  $m \ge n$  has the form

$$A = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$$

### Equation 3-57

where *Q* is an *m*-by-*m* orthogonal matrix, and *R* is an *n*-by-*n* upper triangular matrix. If m > n, it is convenient to write the factorization as

$$A = \left(Q^{(1)} \ Q^{(2)}\right) \begin{pmatrix} R\\ 0 \end{pmatrix}$$

Equation 3-58

or simply

$$A - Q^{(1)}R$$

# Equation 3-59

where  $Q^{(1)}$  consists of the first *n* columns of *Q*, and  $Q^{(2)}$  consists of the remaining *m*–*n* columns. The LAPACK routine SGEQRF computes this factorization. See the *LAPACK User's Guide* for details.

# Example 3-6 Orthogonal factorization

The result of calling DGEQRF with the matrix A equal to

$$A = \begin{bmatrix} 1. & 2. & 3. \\ -3. & 2. & 1. \\ 2. & 0. & -1. \\ 3. & -1. & 2. \end{bmatrix}$$

Equation 3-60

is a compact representation of Q and R consisting of

$$A = \begin{bmatrix} -4.796 & 1.460 & -0.8341 \\ -0.5176 & -2.621 & -2.754 \\ 0.3451 & -0.03805 & 2.593 \\ 0.5176 & -0.2611 & -0.3223 \end{bmatrix}$$
$$TAU = \begin{bmatrix} 1.2085, 1.8698, 1.8118 \end{bmatrix}$$

The matrix *R* appears in the upper triangle of *A* explicitly:

 $R = \begin{bmatrix} -4.796 & 1.460 & -0.8341 \\ 0. & -2.621 & -2.754 \\ 0. & 0. & 2.593 \end{bmatrix}$ 

### Equation 3-62

while the matrix Q is stored in a factored form  $Q = Q_3 Q_2 Q_1$  where each  $Q_i$  is an elementary Householder transformation of the following form:  $Q_i = I - \tau_i v_i v_i^T$ . Each vector  $v_i$  has  $v_i [0 : i - 1] = 0$ ,  $v_i [i] = 1$ , and v [i + 1 : n] is stored below the diagonal in the  $i^{ih}$  column of A. Therefore,

$$Q_1 = I - 1.2085 \begin{bmatrix} 1.\\ -0.5176\\ 0.3451\\ 0.5176 \end{bmatrix} [1. -0.5176 \ 0.3451 \ 0.5176]$$

Equation 3-63

$$Q_2 = I - 1.8698 \begin{bmatrix} 0.\\ 1.\\ -0.03805\\ -0.2611 \end{bmatrix} \begin{bmatrix} 0 & 1. & -0.03805 & -0.2611 \end{bmatrix}$$

Equation 3-64

$$Q_3 = I - 1.8118 \begin{bmatrix} 0.\\ 0.\\ 1.\\ -0.3223 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 & -0.3223 \end{bmatrix}$$

Each transformation is orthogonal (to machine precision) because  $\tau$  is chosen to have the value  $2/(v^T v)$ , so that

$$(I - \tau \upsilon \upsilon^T) (I - \tau \upsilon \upsilon^T) = I - 2\tau \upsilon \upsilon^T + \tau^2 (\upsilon^T \upsilon) \upsilon \upsilon^T = I$$

Equation 3-66

# Multiplying by the Orthogonal Matrix

In the example of the last subsection, the elementary orthogonal matrices  $Q_i$  were expressed in terms of the scalar  $\tau$  and the vector v that defines them, without multiplying out the expression. This was done to make the point that the elementary transformation is most often used in its factored form. This subsection describes one application in which multiplication by the orthogonal matrix Q is required. An alternative interface for this application is the LAPACK driver routine DGELS.

Given the *QR* factorization of a  $m \times n$  matrix *A* with m > n (Equation 3-57), if *R* has rank *n*, the solution to the linear least squares problem (Equation 3-55) is obtained by the following steps:

$$\begin{bmatrix} X \\ Y \end{bmatrix} \leftarrow Q^T B$$
$$X \leftarrow R^{-1} X$$

#### Equation 3-67

The LAPACK routine DORMQR is used in step 1 to multiply the right-hand side matrix by the transpose of the orthogonal matrix *Q*, using *Q* in its factored form. The triangular system solution in step 2 can be done using the LAPACK routine DTRTRS.

Continuing the example of "Orthogonal Factorizations" on page 34, suppose the right-hand side vector is  $b = [1, 2, 3, 4]^T$ . Multiplying *b* by  $Q^T$  by using the LAPACK routine DORMQR, you get

$$\begin{bmatrix} x \\ y \end{bmatrix} = Q^T b = \begin{bmatrix} -2.711 \\ -2.273 \\ 0.5712 \\ 4.143 \end{bmatrix}$$

and after solving the triangular system with the 3-by-3 matrix *R*,

$$x = \begin{bmatrix} 0.7203 \\ 0.6356 \\ 0.2203 \end{bmatrix}$$

### Equation 3-69

The last *m*–*n* elements of  $Q^T b$  can be used to compute the 2-norm of the residual, because  $||r||_2 \approx ||y||_2$ . Here,  $||r||_2 = 4.143$ .

# **Generating the Orthogonal Matrix**

The DORM*xx* routines described in the previous subsection are useful for operating with the orthogonal matrix Q in its factored form, but sometimes it is the matrix Q itself that is of interest.

For example, the first step in the computational procedure for the generalized eigenvalue problem  $AX = \Lambda BX$  is to find orthogonal matrices U and Z such that  $U^T AZ$  is upper Hessenberg and  $U^T BZ$  is upper triangular (see Golub and Van Loan for details). First, the matrix B is reduced to upper triangular form by the QR factorization, and A is overwritten by  $Q^T A$ , using the subroutines of the previous section for multiplying by the orthogonal matrix.

Next, the updated *A* is reduced to Hessenberg form while preserving the triangular structure of *B* by applying Givens rotations to *A* and *B*, alternately from the left and the right. In order to obtain the orthogonal matrices *U* and *Z* that reduce the original problem, it is necessary to keep a copy of the matrix *Q* from B = QR and continually update it. This requires that *Q* be generated after the *QR* factorization.

The DORG*xx* routines generate the orthogonal matrix Q as a full matrix by expanding its factored form. Using the example of "Orthogonal Factorizations" on page 34, Q can be generated from its factored form by using the following Fortran code:

```
DO J = 1, N
    DO I = J+1, M
        Q(I,J) = A(I,J)
        END DO
END DO
CALL GORGQR(M,M,N,Q,LDQ,TAU,WORK,LWORK,INFO)
```

where the data from the QR factorization of A has been copied into a separate matrix Q because DORGQR overwrites its input data with the expanded matrix. The orthogonal matrix is returned in Q:

Q =	-0.2085	-0.8792	0.1562	-0.3989
	0.6255	-0.4147	0.1465	0.6444
	-0.4170	-0.2322	-0.7665	0.4296
	-0.6255	0.03318	0.6054	0.4910

### Equation 3-70

The matrix  $Q^{(1)}$ , consisting of only the first *n* columns of *Q*, could be generated by specifying *N*, rather than *M*, as the second argument in the call to DORGQR.

# Comparing Answers

The results obtained by LAPACK routines should be deterministic; that is, if the same input is provided to the same subroutine in the same system environment, the output should be the same. However, because all computers operate in finite-precision arithmetic, a different order of operations may produce a different set of rounding errors, so results of the same operation obtained from different subroutines, or from the same subroutine with different numbers of processors, are not guaranteed to agree to the last decimal place.

In testing LAPACK, the test ratios in the following table were used to verify the correctness of different operations. All of these ratios give a measure of relative error. Residual tests are scaled by  $1/\varepsilon$ , the reciprocal of the machine precision, to make the test ratios O(1), and results that are sensitive to conditioning are scaled by  $1/\kappa$ , where  $\kappa = ||A|| ||A^{-1}||$  is the condition number of the matrix A, as computed from the norms of A and its computed inverse  $A^{-1}$ . If a given result has a test ratio less than 30, it is judged to be as accurate as the machine precision and the conditioning of the problem will allow. See the *Installation Guide for LAPACK* for further details on the testing strategy used for LAPACK.

**Table 3-2** Verification tests for LAPACK (all should be O(1))

Operation or result	Test ratio		
Factorization $A = LU$	$\left\ LU - A\right\  / (n \left\ A\right\  \epsilon)$		
Solution $\hat{x}$ to $Ax = b$	$  b-A\hat{x}  $ / ( $  A  $ $  \hat{x}  $ $\epsilon$ )		
Compared to exact soln <i>x</i>	$  x-\hat{x}   / (  \hat{x}  \kappa\epsilon)$		
Reciprocal condition number RCOND	$\max(\text{RCOND}, \kappa) / \min(\text{RCOND}, \kappa)$		
Forward error bound $f$	$  x-\hat{x}  /(  \hat{x}  f)$		
Backward error bound $\omega$	$\omega/\varepsilon$		
Computation a $A^{-1}$	$\left\ I - AA^{-1}\right\  / \left(n \left\ A\right\  \left\ A^{-1}\right\  \epsilon\right)$		
Orthogonality check for Q	$\left\ I-Q^{H}Q\right\ /\left(n\epsilon\right)$		
$\varepsilon$ = Machine epsilon n = Order of matrices $\kappa = \kappa =   A     A^{-1}  $			

# **Using Sparse Linear Equation Solvers**

Many techniques exist for solving sparse linear systems. The appropriate technique depends on many factors, including the mathematical and structural properties of matrix *A*, the dimension of *A*, and the number of right-hand sides *b*.

SGI provides two direct solvers, PSLDLT and PSLDU, and one iterative solver, DITERATIVE, for sparse linear systems of equations. These solvers are optimized and parallelized for SGI platforms.

Direct solvers of dense linear systems of equations are described on the INTRO\_LAPACK(3s) man page.

This section describes some of the properties that are useful in determining a good solution technique, with some common sources of matrices with these properties.

# Sparse Matrices

A *linear system* can be described as Ax = b, where A is an n-by-n matrix, and x and b are n dimensional vectors. A system of this kind is considered *sparse* if the matrix A has a small percentage of nonzero terms (less than 10%, often less than 1%). Large sparse linear systems occur frequently in engineering and scientific applications, and the solution of these systems (finding x given A and b) is an important and costly step.

If matrix *A* has a regular pattern, such as a banded or block structure, good performance can easily be obtained when solving the linear system. Good performance is much more difficult to obtain in problems in which *A* has no discernible pattern. The goal of the routines described in this section is to solve sparse linear systems efficiently, especially those where matrix *A* has no known regular pattern.

The following list defines the different types of sparse matrices:

• symmetric positive definite matrix: A matrix A is symmetric if  $A = A^T$  (that is, if the coefficients of A are such that  $a_{ij} = a_{ji}$  for all *i* and *j*).

A matrix *A* is defined to be *symmetric positive definite (SPD)* if *A* is symmetric and  $y^T A y > 0$  for all vectors  $y \neq 0$ . It is usually difficult to directly verify that a matrix is SPD; however, it can often be determined by considering the problem source. For example, many finite difference or finite volume approximations of *partial* 

*differential equations* (PDEs) with Dirichlet or mixed boundary conditions and other mild assumptions generate SPD matrices. Also, finite element approximations with a symmetric bilinear form and equivalent test and basis functions generate SPD matrices.

SPD matrices occur frequently in applications. Optimal techniques exist to solve the related linear systems. Common sources of SPD matrices are finite element analysis of structures, the pressure correction phase of a segregated fluid dynamics simulation, and the analysis of electrical networks.

- Diagonally dominant matrix: A matrix A is (*strictly*) diagonally dominant if
   |a<sub>ij</sub>| > ∑<sub>i≠j</sub> |a<sub>ij</sub>| for all *i*. If A is diagonally dominant, operations that involve A
   are often numerically stable. Common sources of diagonally-dominant matrices
   are simple reservoir simulation models and the velocity equations of a segregated
   fluid dynamics solver.
- Structurally symmetric matrix: If the nonzero pattern of A is symmetric, a matrix A is *structurally symmetric*; that is,  $a_{ij} \neq 0$  if and only if  $a_{ji} \neq 0$ . The integer complexity of a solver for a structurally symmetric matrix is greatly reduced compared to a more general solver. If A is diagonally dominant, many of the optimal solution techniques for SPD matrices can be used. Common sources of these matrices are the same as those for diagonally dominant matrices.
- Banded matrix: If  $a_{ij} = 0$  for |i j| > k, matrix *A* is *banded*. If *k* is small in relation to the problem dimension *n*, special techniques exist for solving the related linear systems. Systems of this form usually occur in special domains with a particular ordering of the grid or node points.
- Tridiagonal matrix: If  $a_{ij} = 0$  for |i j| > 1, matrix A is *tridiagonal*. Tridiagonal matrices occur frequently in fluid dynamics and reservoir simulation.

During a simulation, an application often generates many sparse linear systems that must be solved. These are usually related to some linear approximation of a nonlinear function or some time-marching scheme for a time-dependent problem. In these cases, the linear systems are often related and information from the previous solution can be used to solve the next linear system.

For example, consider Newton's method for a nonlinear PDE. In this case, the linear system  $A_n$  is generated by evaluating the Jacobian at a certain point. A subsequent matrix,  $A_{n+1}$ , is generated using the Jacobian at a nearby point. Thus, the two matrices  $A_n$  and  $A_{n+1}$  are close to each other, and this fact is used in the solver technique. The structure of  $A_n$  and  $A_{n+1}$  is usually identical and all structural preprocessing can be done once for all related matrices.

# Solution Techniques

Solution techniques for sparse linear systems can usually be divided into two broad classes: *direct methods* and *iterative methods*. The following subsections provide an overview of both classes and provide brief algorithmic descriptions.

# **Direct Methods**

The DPSLDLT and ZPSLDLT routines solve sparse symmetric linear systems of the form AX=b where A is a symmetric input matrix, b is an input vector of length n, and x is a vector of unknowns of length n. This solver uses a direct method. A is factored into  $A = L D^{LT}$  where L is a lower triangular matrix with unit diagonal and D is a diagonal matrix.

This solver supports both real and complex double precision data types and is available in the multi-processing versions of SCSL. See the man pages for details.

DPSLDU and ZPSLDU solve sparse unsymmetric linear systems of the form Ax=b where A is an input matrix with symmetric non-zero pattern but unsymmetric non-zero values, b is an input vector of length n, and x is a vector of unknowns of length n.

The unsymmetric solver uses a direct method. *A* is factored into A = L D U where *L* is a lower triangular matrix with unit diagonal, *D* is a diagonal matrix, and *U* is an upper triangular matrix with unit diagonal.

The unsymmetric solver supports both real and complex double precision data types and is available in the multi-processing versions of SCSL. See the man pages for details.

# How Direct Solvers Work

Direct solution methods transform matrix A into a product of several other operators so that each of the resulting operators is easy to invert for a given right-hand side b. For example, the LU factorization of A generates lower and upper triangular matrices, L and U, respectively, such that A = LU.

To find  $x = A^{-1}b$ , compute  $y = L^{-1}b$  followed by  $x = U^{-1}y$ , both of which are straightforward computations. Direct methods are usually popular because they are considered to be very reliable. This is true if the problem dimension and the condition number of *A* are not too large. See *Matrix Computations*, by Golub and Van Loan for details about error bounds.

Direct methods for dense, tridiagonal, and banded matrices are quite straightforward to implement and use the three basic steps of LU factorization as mentioned previously; they may also solve for a given right-hand side without factorization. However, for general sparse matrices, the situation is considerably more complicated; in particular, the factors L and U can become extremely dense. If pivoting is required, implementing sparse factorization can use a lot of time searching lists of numbers and creating a great deal of computational overhead.

Efficient implementations can be developed, especially for SPD and symmetric pattern, positive definite matrices. See *Computer Solution of Large Sparse Positive Definite Systems*, by George and Liu, for details.

The following algorithm shows the basic steps of the sparse Cholesky solver:

Structural preprocessing phase:

- 1. Find *P* so that  $\overline{A} = PAP^T$  has factor *L* with near minimal fill.
- 2. Compute symbolic factorization, that is, find structure of *L*.
- 3. Find optimal memory use and node execution sequence.

Numerical factorization phase:

4. Compute *L* such that  $\overline{A} = LDL^T$ .

Solution phase:

5. Given *b*, compute  $y = L^{-1}b$ ,  $z = D^{-1}y$ ,  $x = L^{-T}z$ .

In this case, *A* is SPD, and *L* and *D* can be found such that  $A = LDL^T$ , where *L* is a lower triangle with unit diagonal, and *D* is diagonal.

Steps 1 through 3 require only the nonzero structure of *A*. Therefore, if two matrices  $A_1$  and  $A_2$  have the same structure, these steps can be skipped for  $A_2$ . Furthermore, if the same matrix *A* is used for more than one right-hand side *b*, step 5 can be repeated (or if all right-hand sides are available at once, they can be solved for simultaneously).

# **Iterative Solvers**

The DITERATIVE solver solves sparse linear systems of the form Ax=b where A is a sparse input matrix in Compressed Sparse Column (CSC) format or Compressed Sparse Row (CSR) format, b is an input vector of length n, and x is a vector of unknowns in length n.

The iterative solver uses one of four preconditioned iterative methods:

- conjugate gradient (CG) and conjugate residual (CR) for symmetric systems
- conjugate gradient squared (CGS) and BiCGSTAB, a variant of CGS with smoother convergence properties, for unsymmetric systems.

Four different types of preconditioners are available:

- Jacobi
- symmetric successive over-relaxation (SSOR)
- ILDLT (incomplete LDLT) by pattern
- ILDLT by value

The ILDLT preconditioners are only available for symmetric matrices and ILDLT by value is currently not parallelized.

Note that the iterative solver supports only real double precision data. See the ITERATIVE(3s) man page for details.

### How Iterative Methods Work

Iterative solution methods comprise a wide variety of techniques. The solvers presented in this subsection are all in the general class of preconditioned conjugate gradient (CG) methods. These methods attempt to solve Ax = b by solving an equivalent system  $M^{-1}Ax = M^{-1}b$ , where *M* is some approximation to *A* which is inexpensive to construct and can be easily used to compute *z* such that  $z = M^{-1}r$ .

This is left preconditioning. It is also possible to apply the preconditioner on the right side of A or on both sides. After the preconditioner is constructed and an initial approximation,  $x_0$  to x is given, the iterative method generates a sequence of vectors  $\{x_i\}$  such that  $x_i$  converges to x. Each  $x_i$  is chosen to satisfy some orthogonality or minimization condition, or both.

Unlike direct methods, iterative methods are more special-purpose. No general, effective iterative algorithms exist for an arbitrary sparse linear system. However, for certain classes of problems, an appropriate iterative method can be used to yield an approximate solution significantly faster than direct methods. Also, iterative methods usually require less memory than direct methods, thus making them the only feasible approach for large problems. See *Matrix Computations*, by Golub and Van Loan, for an introduction to these methods.

The standard preconditioned CG method, shown in the following algorithm, illustrates the basic phases common to all CG type methods used in the solvers:

Preprocessing phase:

- 1. Compute structure of preconditioner M.
- 2. Compute values of preconditioner *M*.
- 3. Analyze structure of A to optimize performance of sparse matrix vector product, q = Ap.

Iterative phase:

4. 
$$r^{o} = b - Ax^{o}$$
  
Do  $k=0$ , ...  
5.  $z^{k} = Mr^{k}$   
6.  $\gamma_{k} = (r^{k}, z^{k})$   
7.  $\beta_{k} = \gamma_{k}/\gamma_{k-1}, \beta_{0} = 0$   
8.  $p^{k} = z^{k} + \beta_{k}p^{k-1}$   
9.  $q^{k} = Ap^{k}$   
10.  $\delta_{k} = (q^{k}, p^{k})$   
11.  $\alpha_{k} = \gamma_{k}/\delta_{k}$   
12.  $x^{k+1} = x^{k} + \alpha_{k}p^{k}$   
13.  $r^{k+1} = r^{k} - \alpha_{k}p^{k}$   
End Do

Iterative methods are very flexible. Like direct solvers, if two matrices  $A_1$  and  $A_2$  have the same structure, the structural preprocessing needs to be done only once. If there are multiple right-hand sides, Steps 1 through 3 can be skipped after the first right-hand side.

*Chapter 5* 

# **Signal Processing Routines**

SCSL provides three types of signal processing routines:

- Fast Fourier Transform (FFT) routines
- Convolution routines
- Correlation routines

The SCSL FFT interfaces are incompatible with those of the IRIX CHALLENGEcomplib scientific library, which has been superseded by SCSL. See the release notes that are provided with your SCSL distribution for details about converting CHALLENGEcomplib FFT calls to SCSL FFT calls.

# **FFT Routines**

The FFT routines have been highly optimized for single-processor use. The two-dimensional, three-dimensional, and one-dimentional multiple routines are also multitasked (multithreaded) for all sizes for which there is a performance benefit. The one-dimensional routines are multitasked if the data size exceeds the size of the largest processor cache. Each routine can compute either a forward or an inverse Fourier transform.

# **Data Types**

The following data types are used in these routines:

- Single precision: Fortran "real" data type, C/C++ "float" data type, 32-bit floating point; these routine names begin with S.
- Single precision complex: Fortran "complex" data type, C/C++ "scsl\_complex" data type (defined in <scsl\_ft.h>), C++ STL "complex float>" data type (defined in <complex.h>, two 32-bit floating point reals; these routine names begin with C.
- Double precision: Fortran "double precision" data type, C/C++ "double" data type, 64-bit floating point; these routine names begin with D.
- Double precision complex: Fortran "double complex" data type, C/C++ "scsl\_zomplex" data type (defined in <scsl\_ft.h>), C++ STL

"complex\_double>" data type (defined in <complex.h>), two 64-bit floating point doubles; these routine names begin with Z.

When using the C++ Standard Template Library (STL) to define complex types, the include files must be used in the following order:

#include <complex.h>
#include <scsl\_fft.h>

# Implementation Details

Often little or no difference exists between these versions, other than the data types of some inputs and outputs. In this case, the routines are described on the same man page, and that man page is named after the real or complex routine.

The man(1) command can find a man page online by either the real, complex, double precision, or double complex name.

The data types for the *scale*, *table*, and *work* arguments in these routines vary, depending on the function which is called. In the CC, SC, and CS routines, the arguments are single precision. In the ZZ, DZ and ZD routines, the arguments are double precision.

By default, the integer arguments are 4 bytes (32 bits) in size; this is the size obtained when one links to the SCSL library with <code>-lscs or -lscs\_mp</code>. Another version of SCSL is available, however, in which integers are 8 bytes (64 bits). This version allows the user access to larger memory sizes and helps when porting legacy codes. It can be loaded by using either the <code>-lscs\_i8 or -lscs\_i8\_mp link</code> option. Note that any program may use only one of the two versions; 4-byte integer and 8-byte integer library calls cannot be mixed.

C/C++ function prototypes for the signal processing routines are provided in <scsl\_fft.h>, when using the default 4-byte integers, and <scsl\_fft\_i8.h> when using 8-byte integers. These header files define the complex types scsl\_complex and scsl\_zomplex, which are used in the prototypes. Alternatively, C++ programs may declare arguments using the types complex<float> and complex<double> from the standard template library (STL). But if these types are used, <complex.h> must be included before <scsl\_fft.h> (or <scsl\_fft\_i8.h>). Note, though, that both complex types are equivalent: they simply represent (real, imaginary) pairs of floating point numbers stored contiguously in memory. With the proper casts, you can simply pass arrays of floating point data to the routines where complex arguments are expected.

Casts, however, can be avoided. The header files <scsl\_fft.h> and <scsl\_fft\_i8.h> directly support the use of user-defined complex types or disabling prototype checking for complex arguments completely. By defining the symbol SCSL\_VOID\_ARGS before including <scsl\_fft.h> or <scsl\_fft\_i8.h> all complex arguments will be prototyped as void \*. To define the symbol SCSL\_VOID\_ARGS at compile time use the -D compiler option (for example, -DSCSL\_VOID\_ARGS) or use an explicit #define SCSL\_VOID\_ARGS in the source code. This allows the use of any complex data structure without warnings from the compiler, provided the structure is as described above:

1. The real and imaginary components must be contiguous in memory.

2. Sequential array elements must also be contiguous in memory.

While this allows the use of non-standard complex types without generating compiler warnings, it has the disadvantage that the compiler will not catch type mismatches.

Strong type checking can be enabled employing user-defined complex types instead of SCSL's standard complex types. To do this, define

SCSL\_USER\_COMPLEX\_T=my\_complex and SCSL\_USER\_ZOMPLEX\_T=my\_complex, where my\_complex and my\_complex are the names of user-defined complex types. These complex types must be defined before including the <scsl\_fft.h> (or <scsl\_fft\_i8.h>) header file.

Fortran 90 users on IRIX systems can perform compile-time checking of SCSL FFT subroutine calls by adding USE SCSL\_FFT (for 4-byte integer arguments) or USE SCSL\_FFT\_I8 (for 8-byte integer arguments) to the source code from which the FFT calls are made. Alternatively, the compile-time checking can be invoked without any source code modifications by using the <code>-auto\_use</code> compiler option. For example:

% f90 -auto\_use SCSL\_FFT test.f -lscs
% f90 -auto\_use SCSL\_FFT\_I8 -i8 test.f -lscs\_i8

Fortran 90 users on SGI Altix systems can also perform compile-time argument checking, but in this case the USE statements must be explicitly incorporated into the source code.

# **Supported Routines**

The following list describes the supported FFT routines. Rows of the table represent input and output data types for the routines in each column:

• C->C implies 32-bit complex input and output.

- Z->Z implies 64-bit double complex input and output. Each routine in this row is documented with the complex routine in the prior row.
- S->C implies 32-bit real input and 32-bit complex output.
- D->Z implies 64-bit double precision real input and 64-bit double precision complex output. Each routine in this row is documented with the real-to-complex routine in the prior row.
- C->S implies 32-bit complex input and 32-bit real output.
- Z->D implies 64-bit double complex input and 64-bit double precision output. Each routine named in this row is documented with the complex-real routine in the prior row.

Columns of the table represent the number of dimensions for which the FFT is calculated for the routines in each row:

- One-dimensional (single) calculates one FFT in one dimension.
- One-dimensional (multiple) calculates an FFT in one dimension for each column (FFTM) or row (FFTMR) of a two-dimensional matrix.
- Two-dimensional calculates one FFT in two dimensions.
- Three-dimensional calculates one FFT in three dimensions.

	1-dimensional (single)	1-dimensional (multiple)		2-dimensional	3-dimensional	
C->C	CCFFT	CCFFTM	CCFFTMR	CCFFT2D	CCFFT3D	
Z->Z	ZZFFT	ZZFFTM	ZZFFTMR	ZZFFT2D	ZZFFT3D	
S->C	SCFFT	SCFFTM		SCFFT2D	SCFFT3D	
D->Z	DZFFT	DZFFTM		DZFFT2D	DZFFT3D	
C->S	CSFFT	CSFFTM		CSFFT2D	CSFFT3D	
Z->D	ZDFFT	ZDFFTM		ZDFFT2D	ZDFFT3D	

### Implementation Notes: work and table arrays

The FFT routines were designed so that they can be implemented efficiently on many different architectures. The calling sequence is the same in any implementation. Certain details, however, depend on the particular implementation.

One area of difference is the size of the *table* and *work* arrays. Different systems may need different sizes. The subroutine call requires no change, but you may have to change array sizes in the DIMENSION or type statements that declare the arrays. The following are the required array sizes for the Origin and Altix series (n, n1, n2, and n3 are transform sizes; the values of *NF* and *NFR* are explained below):

• CCFFT

```
table: 2n + NF REAL
work: 2n REAL WORDS
```

• ZZFFT

table: 2n + NF DBL PREC WORDS
work: 2n DBL PREC WORDS

• CCFFTMR

table: 2n + NF REAL WORDS
work: 2n REAL WORDS

• ZZFFTMR

table: 2n + NF DBL PREC WORDS
work: 2n DBL PREC WORDS

• CCFFT2D

table: (2\*n1+NF) + (2\*n2+NF) REAL WORDS
work: 2\*MAX(n1,n2) REAL WORDS

• ZZFFT2D

table: (2\*n1+NF) + (2\*n2+NF) DBL PREC WORDS work: 2\*MAX(n1,n2) DBL PREC WORDS

• CCFFT3D

table: (2\*n1+NF) + (2\*n2+NF) + (2\*n3+NF) REAL WORDS
work: 2\*MAX(n1,n2,n3) REAL WORDS

```
• ZZFFT3D
  table: (2*n1+NF) + (2*n2+NF) + (2*n3+NF) DBL PREC WORDS
  work: 2*MAX(n1,n2,n3) DBL PREC WORDS
• CCFFTM
  table: (NF + 2 * n) REAL
  work: 2n REAL WORDS
• ZZFFTM
  table: (NF + 2 * n) DBL PREC
  work: 2n DBL PREC WORDS
• SCFFT, CSFFT
  table: (n+NFR) REAL
  work: n+2 REAL WORDS
• DZFFT, ZDFFT
  table: (n+NFR) DBL PREC
  work: n + 2 DBL PREC WORDS
• SCFFT2D, CSFFT2D
  table: (n+NFR) + (2*n2+NF) REAL
  work: n1+4*n2 REAL WORDS
• DZFFT2D, ZDFFT2D
  table: (n1+NFR) + (2*n2+NF) DBL PREC WORDS
  work: n1 + 4 * n2 DBL PREC WORDS
• SCFFT3D, CSFFT3D
  table: (n1+NFR) + (2*n2+NF) + (2*n3+NF) REAL WORDS
  work: n1 + 4 * n3 REAL WORDS
• DZFFT3D, ZDFFT3D
  table: (n1+NFR) + (2*n2+NF) + (2*n3+NF) DBL PREC WORDS
  work: n1 + 4 * n3 DBL PREC WORDS
```

• SCFFTM, CSFFTM

table: (n+NFR) REAL WORDS
work: n + 2 REAL WORDS

• DZFFTM, ZDFFTM

table: (n+NFR) DBL PREC work: n + 2 DBL PREC WORDS

## Implementation Notes: *isys* Parameter Array

The second area of difference is the isys parameter array, an array that gives certain implementation-specific information. All features and functions of the FFT routines specific to any particular implementation are confined to this *isys* array. On any implementation, you can use the default values by using an argument value of 0.

In the Origin and Altix series implementations, isys(0) = 0 and isys(0) = 1 are supported. In SCSL versions prior to 1.3, only isys(0) = 0 was allowed. For isys(0) = 0, NF=30 and NFR=15, and for isys(0) = 1, NF=NFR=256. The NF(R) words of storage in the *table* array contain a factorization of the length of the transform.

The smaller values of *NF* and *NFR* for isys(0)=0 are historical. They are too small to store all the required factors for the highest performing FFT, so when isys(0)=0, extra space is allocated when the *table* array is initialized. To avoid memory leaks, this extra space must be deallocated when the *table* array is no longer needed. The routines CCFFTF, CCFFTMF, etc., are used to release this memory. Due to the potential for memory leaks, the use of *isys*(0)=0 should be avoided.

For *isys* (0) =1, the values of *NF* and *NFR* are large enough so that no extra memory needs to be allocated, and there is no need to call CCFFTF, etc. to release memory. (If called, these routines do nothing.) *isys* (0) = 1 means that *isys* is an integer array with two elements. The second element, *isys* (1), will not be accessed.

## Implementation Notes: Scratch Space

Finally, in addition to the *work* array, the FFT routines also dynamically allocate scratch space from the stack. The amount of space allocated can be slightly bigger than the size of the largest processor cache. For single processor runs, the default stack size is large enough that these allocations generally cause no problems. But for parallel runs, you need to ensure that the stack size of slave threads is big enough to hold this scratch space. Failure to reserve sufficient stack space will cause programs to dump core due to stack overflows. The stack size of MP library slave threads on

Origin systems is controlled via the MP\_SLAVE\_STACKSIZE environment variable or the mp\_set\_slave\_stacksize() library routine. See the mp(3c), mp(3F) and pe\_environ(5)man pages for more information on controlling the slave stack size.

On Altix systems, the OpenMP thread stack size is controlled by the KMP\_STACKSIZE environment variable or by the kmp\_set\_stacksize\_s() library routine; see the Intel compiler documentation for additional details. SCSL versions 1.4.1, or later, will automatically attempt to increase the OpenMP thread stack size limit to a safe value if the library detects an initial setting that is too low. Because this action is performed at DSO initialization time, it is not possible for the library to detect subsequent kmp\_set\_stacksize\_s() calls within user code that may be below the recommended threshold.

For pthreads applications, the thread's stack size is specified as one of many creation attributes provided in the *pthread\_attr\_t* argument to pthread\_create(3P). The stacksize attribute should be set explicitly to a non-default value using the pthread\_attr\_setstacksize(3P) call, described in the pthread\_attr\_init(3P) man page.

# **Convolution and Correlation Routines**

The convolution routines feature convolution for Finite Impulse Response (FIR) filters, as well as, correlations. Each routine is highly optimized for single-processor use. The routines which use two-dimensional input sequences are multitasked (multi-threaded).

The convolution and correlation routines are very general. To achieve this generality and maximum flexibility, one-dimensional sequences are defined by 3 parameters. Six parameters are necessary for two-dimensional sequences. One drawback of this generality is the long subroutine argument list.

The following table contains a summary of the filter and correlation routines. In this table, rows of the table represent data types for the routines in each column:

- C implies 32-bit complex data.
- Z implies 64-bit double complex data
- S implies 32-bit real data.
- D implies 64-bit double precision real data.

Columns of the table represent the type of computation as well as the number of dimensions for which the convolution or correlation is calculated for the routines in each row:

- One-dimensional FIR applies a Finite Impulse Response filter to one-dimensional signals.
- One-dimensional (multiple) FIR applies a Finite Impulse Response filter to multiple one-dimensional signals.
- Two-dimensional FIR applies a Finite Impulse Response filter to two-dimensional signals.
- One-dimensional COR calculates the correlation of one-dimensional sequences.
- One-dimensional (multiple) COR calculates the correlation of multiple one-dimensional sequences.

Туре	1D (single)	1D (multiple)	2D
C	CFIR1D	CFIRM1D	CFIR2D
Z	ZFIR1D	ZFIRM1D	ZFIR2D
S	SFIR1D	SFIRM1D	SFIR2D
D	DFIR1D	DFIRM1D	DFIR2D
C	CCOR1D	CCORM1D	CCOR2D
Z	ZCOR1D	ZCORM1D	ZCOR2D
S	SCOR1D	SCORM1D	SCOR2D
D	DCOR1D	DCORM1D	DCOR2D

• Two-dimensional COR calculates the correlation of two-dimensional sequences.

# Supported SCSL Routines

This appendix lists all supported SCSL routines and a brief description of each.

For details, see the individual man pages.

#### **Introductory Man Pages**

The following man pages provide and introduction to the different types of routines supported in SCSL.

- INTRO\_BLAS1 Introduction to vector-vector linear algebra subprograms
- INTRO\_BLAS2 Introduction to matrix-vector linear algebra subprograms
- INTRO\_BLAS3 Introduction to matrix-matrix linear algebra subprograms
- INTRO\_BLAS Introduction to SCSL Basic Linear Algebra Subprograms
- INTRO\_CBLAS Introduction to the C interface to Fortran 77 Basic Linear Algebra Subprograms (legacy BLAS)
- INTRO\_FFT Introduction to signal processing routines
- INTRO\_LAPACK Introduction to LAPACK solvers for dense linear systems
- INTRO\_SCSL Introduction to Scientific Computing Software Library (SCSL) routines
- INTRO\_SOLVERS Introduction to SGI-developed linear equation solvers

### **BLAS Routines**

The following is a list of all BLAS 1, BLAS 2, and BLAS 3 supported routines.

- CGEMM3M, ZGEMM3M Multiplies a complex general matrix by a complex general matrix
- CHBMV, ZHBMV Multiplies a complex vector by a complex Hermitian band matrix

- CHEMM, ZHEMM Multiplies a complex general matrix by a complex Hermitian matrix
- CHEMV, ZHEMV Multiplies a complex vector by a complex Hermitian matrix
- CHER2, ZHER2 Performs Hermitian rank 2 update of a complex Hermitian matrix
- CHER2K, ZHER2K Performs Hermitian rank 2k update of a complex Hermitian matrix
- CHER, ZHER Performs Hermitian rank 1 update of a complex Hermitian matrix
- CHERK, ZHERK Performs Hermitian rank k update of a complex Hermitian matrix
- CHPMV, ZHPMV Multiplies a complex vector by a packed complex Hermitian matrix
- CHPR2, ZHPR2 Performs Hermitian rank 2 update of a packed complex Hermitian matrix
- CHPR, ZHPR Performs Hermitian rank 1 update of a packed complex Hermitian matrix
- CSROT, ZDROT applies a real plane rotation to a pair of complex vectors
- DGEMMS Multiplies a real general matrix by a real general matrix, using Strassen's algorithm
- ISAMAX, IDAMAX, ICAMAX, IZAMAX Searches a vector for the first occurrence of the maximum absolute value
- ISAMIN, IDAMIN Searches a vector for the first occurrence of the minimum absolute value
- ISMAX, IDMAX Searches a real vector for the first occurrence of the maximum value
- ISMIN, IDMIN Searches a real vector for the first occurrence of the minimum value
- SASUM, DASUM, SCASUM, DZASUM Sums the absolute value of elements in a real or complex vector
- SAXPBY, DAXPBY, CAXPBY, ZAXPBY Adds a scalar multiple of a Single precision or complex vector x to a scalar multiple of another Single precision or complex vector y

- SAXPY, CAXPY, DAXPY, ZAXPY Adds a scalar multiple of a real or complex vector to another real or complex vector
- SCOPY, DCOPY, CCOPY, ZCOPY Copies a real or complex vector into another real or complex vector
- SDOT, DDOT, CDOTC, ZDOTC, CDOTU, ZDOTU Computes a dot product (inner product) of two real or complex vectors
- SGBMV, DGBMV, CGBMV, ZGMBV Multiplies a real or complex vector by a real or complex general band matrix
- SGEMM, DGEMM, CGEMM, ZGEMM Multiplies a real or complex general matrix by a real or complex general matrix
- SGEMV, DGEMV, CGEMV, ZGEMV Multiplies a real or complex vector by a real or complex general matrix
- SGER, DGER, CGERC, ZGERC, CGERU, ZGERU Performs rank 1 update of a real or complex general matrix
- SGESUM, DGESUM, CGESUM, ZGESUM Adds a scalar multiple of a real or complex matrix to a scalar multiple of another real or complex matrix
- SHAD, DHAD, CHAD, ZHAD Computes the Hadamard product of two vectors
- SNRM2, DNRM2, SCNRM2, DZNRM2 Computes the Euclidean norm of a vector
- SROT, DROT, CROT, ZROT applies a real plane rotation or complex coordinate rotation
- SROTG, DROTG, CROTG, ZROTG Constructs a Givens plane rotation
- SROTM, DROTM applies a modified Givens plane rotation
- SROTMG, DROTMG Constructs a modified Givens plane rotation
- SSBMV, DSBMV Multiplies a real vector by a real symmetric band matrix
- SSCAL, DSCAL, CSSCAL, ZDSCAL, CSCAL, ZSCAL Scales a real or complex vector
- SSPMV, DSPMV, CSPMV, ZSPMV Multiplies a real or complex symmetric packed matrix by a real or complex vector
- SSPR2, DSPR2 Performs symmetric rank 2 update of a real symmetric packed matrix

- SSPR, DSPR, CSPR, ZSPR Performs symmetric rank 1 update of a real or complex symmetric packed matrix
- SSUM, DSUM, CSUM, ZSUM Sums the elements of a real or complex vector
- SSWAP, DSWAP, CSWAP, ZSWAP Swaps two real or complex vectors
- SSYMM, DSYMM, CSYMM, ZSYMM Multiplies a real or complex general matrix by a real or complex symmetric matrix
- SSYMV, DSYMV, CSYMV, ZSYMV Multiplies a real or complex vector by a real or complex symmetric matrix
- SSYR2, DSYR2 Performs symmetric rank 2 update of a real symmetric matrix
- SSYR2K, DSYR2K, CSYR2K, ZSYR2K Performs symmetric rank 2k update of a real or complex symmetric matrix
- SSYR, DSYR, CSYR, ZSYR Performs symmetric rank 1 update of a real or complex symmetric matrix
- SSYRK, DSYRK, CSYRK, ZSYRK Performs symmetric rank k update of a real or complex symmetric matrix
- STBMV, DTBMV, CTBMV, ZTBMV Multiplies a real or complex vector by a real or complex triangular band matrix
- STBSV, DTBSV, CTBSV, ZTBSV Solves a real or complex triangular banded system of equations
- STPMV, DTPMV, CTPMV, ZTPMV Multiplies a real or complex vector by a real or complex triangular packed matrix
- STPSV, DTPSV, CTPSV, ZTPSV Solves a real or complex triangular packed system of equations
- STRMM, DTRMM, CTRMM, ZTRMM Multiplies a real or complex general matrix by a real or complex triangular matrix
- STRMV, DTRMV, CTRMV, ZTRMV Multiplies a real or complex vector by a real or complex triangular matrix
- STRSM, DTRSM, CTRSM, ZTRSM Solves a real or complex triangular system of equations with multiple right-hand sides

• STRSV, DTRSV, CTRSV, ZTRSV - Solves a real or complex triangular system of equations

## **FFT Routines**

The following is a list of all supported Fast Fourier Transform (FFT) routines.

- CCFFT2D, ZZFFT2D applies a two-dimensional complex-to-complex Fast Fourier Transform (FFT)
- CCFFT3D, ZZFFT3D applies a three-dimensional complex-to-complex Fast Fourier Transform (FFT)
- CCFFT, ZZFFT applies a complex-to-complex Fast Fourier Transform (FFT)
- CCFFTF, CCFFTMF, CCFFTMRF, CCFFT2DF, CCFFT3DF, ZZFFTF, ZZFFTMF, ZZFFTMRF, ZZFFT2DF, ZZFFT3DF deallocates memory tacked on to the table array during initialization
- CCFFTM, ZZFFTM applies multiple complex-to-complex Fast Fourier Transforms (FFTs)
- CCFFTMR, ZZFFTMR applies multiple complex-to-complex Fast Fourier Transforms (FFTs) to the rows of a two-dimensional (2D) array
- CCOR1D, ZCOR1D, SCOR1D, DCOR1D computes the one-dimensional (1D) correlation of two sequences.
- CCOR2D, ZCOR2D, SCOR2D, DCOR2D computes the two-dimensional (2D) correlation of two two-dimensional (2D) arrays
- CCORM1D, ZCORM1D, SCORM1D, DCORM1D computes multiple 1D correlations
- CFIR1D, ZFIR1D, SFIR1D, DFIR1D -computes the 1D convolution of a sequence
- CFIR2D, ZFIR2D, SFIR2D, DFIR2D computes the two-dimensional (2D) convolution of two 2D arrays
- CFIRM1D, ZFIRM1D, SFIRM1D, DFIRM1D computes multiple 1D convolutions
- SCFFT2D, DZFFT2D, CSFFT2D, ZDFFT2D applies a two-dimensional real-to-complex or complex-to-real Fast Fourier Transform (FFT)

- SCFFT3D, DZFFT3D, CSFFT3D, ZDFFT3D applies a three-dimensional real-to-complex Fast Fourier Transform (FFT)
- SCFFT, DZFFT, CSFFT, ZDFFT computers a real-to-complex or complex-to-real Fast Fourier Transform (FFT)
- SCFFTF, SCFFTMF, SCFFT2DF, SCFFT3DF, DZFFTF, DZFFTMF, DZFFT2DF, DZFFT3DF - Deallocate memory tacked on to the table array during initialization
- SCFFTM, DZFFTM, CSFFTM, ZDFFTM applies multiple real-to-complex or complex-to-real Fast Fourier Transforms (FFTs)

## LAPACK Routines

The following is a list of all supported LAPACK routines.

- CBDSQR computes the singular value decomposition (SVD) of a real N-by-N (upper or lower) bidiagonal matrix B
- CGBBRD reduces a complex general m-by-n band matrix A to real upper bidiagonal form B by a unitary transformation
- CGBCON estimates the reciprocal of the condition number of a complex general band matrix A
- CGBEQU computes row and column scalings intended to equilibrate an M-by-N band matrix A and reduce its condition number
- CGBRFS improves the computed solution to a system of linear equations when the coefficient matrix is banded
- CGBSV computes the solution to a complex system of linear equations
- CGBSVX uses the LU factorization to compute the solution to a complex system of linear equations
- CGBTF2 computes an LU factorization of a complex m-by-n band matrix A using partial pivoting with row interchanges
- CGBTRF computes an LU factorization of a complex m-by-n band matrix A using partial pivoting with row interchanges
- CGBTRS solves a system of linear equations with a general band matrix A using the LU factorization computed by CGBTRF

- CGEBAK forms the right or left eigenvectors of a complex general matrix by backward transformation on the computed eigenvectors of the balanced matrix output by CGEBAL
- CGEBAL balances a general complex matrix A
- CGEBD2 reduces a complex general m by n matrix A to upper or lower real bidiagonal form B by a unitary transformation
- CGEBRD reduces a general complex M-by-N matrix A to upper or lower bidiagonal form B by a unitary transformation
- CGECON estimates the reciprocal of the condition number of a general complex matrix A using the LU factorization computed by CGETRF
- CGEEQU computes row and column scalings intended to equilibrate an M-by-N matrix A and reduce its condition number
- CGEES computes the eigenvalues, the Schur form T, and, optionally, the matrix of Schur vectors Z
- CGEESX computes the eigenvalues, the Schur form T, and, optionally, the matrix of Schur vectors Z
- CGEEV computes the eigenvalues and, optionally, the left and/or right eigenvectors
- CGEEVX computes the eigenvalues and, optionally, the left and/or right eigenvectors
- CGEGS routine is deprecated and has been replaced by routine CGGES
- CGEGV routine is deprecated and has been replaced by routine CGGEV
- CGEHD2 reduces a complex general matrix A to upper Hessenberg form H by a unitary similarity transformation
- CGEHRD reduces a complex general matrix A to upper Hessenberg form H by a unitary similarity transformation
- CGELQ2 computes an LQ factorization of a complex m by n matrix A
- CGELQF computes an LQ factorization of a complex M-by-N matrix A
- CGELS solves overdetermined or underdetermined complex linear systems

- CGELSD computes the minimum-norm solution to a real linear least squares problem
- CGELSS computes the minimum norm solution to a complex linear least squares problem
- CGELSX routine is deprecated and has been replaced by routine CGELSY
- CGELSY computes the minimum-norm solution to a complex linear least squares problem
- CGEQL2 computes a QL factorization of a complex m by n matrix A
- CGEQLF computes a QL factorization of a complex M-by-N matrix A
- CGEQP3 computes a QR factorization with column pivoting of a matrix A
- CGEQPF routine is deprecated and has been replaced by routine CGEQP3
- CGEQR2 computes a QR factorization of a complex m by n matrix A
- CGEQRF computes a QR factorization of a complex M-by-N matrix A
- CGERFS improves the computed solution to a system of linear equations
- CGERQ2 computes an RQ factorization of a complex m by n matrix A
- CGERQF computes an RQ factorization of a complex M-by-N matrix A
- CGESC2 solves a system of linear equations with a general N-by-N matrix A using the LU factorization with complete pivoting computed by CGETC2
- CGESDD computes the singular value decomposition (SVD) of a complex M-by-N matrix A
- CGESV computes the solution to a complex system of linear equations
- CGESVD computes the singular value decomposition (SVD) of a complex M-by-N matrix A, optionally computing the left and/or right singular vectors
- CGESVX uses the LU factorization to compute the solution to a complex system of linear equations
- CGETC2 computes an LU factorization, using complete pivoting, of the n-by-n matrix A

- CGETF2 computes an LU factorization of a general m-by-n matrix A using partial pivoting with row interchanges
- CGETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges
- CGETRI computes the inverse of a matrix using the LU factorization computed by CGETRF
- CGETRS solves a system of linear equations with a general N-by-N matrix A using the LU factorization computed by CGETRF
- CGGBAK forms the right or left eigenvectors of a complex generalized eigenvalue problem by backward transformation on the computed eigenvectors of the balanced pair of matrices output by CGGBAL
- CGGBAL balances a pair of general complex matrices (A,B)
- CGGES computes the generalized eigenvalues, the generalized complex Schur form (S, T), and optionally left and/or right Schur vectors (VSL and VSR)
- CGGESX computes the generalized eigenvalues, the complex Schur form (S,T),
- CGGEV computes the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
- CGGEVX computes the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
- CGGGLM solves a general Gauss-Markov linear model (GLM) problem
- CGGHRD reduces a pair of complex matrices (A,B) to generalized upper Hessenberg form using unitary transformations, where A is a general matrix and B is upper triangular
- CGGLSE solves the linear equality-constrained least squares (LSE) problem
- CGGQRF computes a generalized QR factorization of an N-by-M matrix A and an N-by-P matrix B
- CGGRQF computes a generalized RQ factorization of an M-by-N matrix A and a P-by-N matrix B
- CGGSVD computes the generalized singular value decomposition (GSVD) of an M-by-N complex matrix A and P-by-N complex matrix B

- CGGSVP computes unitary matrices
- CGTCON estimates the reciprocal of the condition number of a complex tridiagonal matrix A using the LU factorization as computed by CGTTRF
- CGTRFS improves the computed solution to a system of linear equations when the coefficient matrix is tridiagonal
- CGTSV solves the equation AX = B,
- CGTSVX uses the LU factorization to compute the solution to a complex system of linear equations
- CGTTRF computes an LU factorization of a complex tridiagonal matrix A using elimination with partial pivoting and row interchanges
- CGTTRS solves systems of equations
- CGTTS2 solves systems of equations
- CHBEV computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix A
- CHBEVD computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix A
- CHBEVX computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix A
- CHBGST reduces a complex Hermitian-definite banded generalized eigenproblem
- CHBGV computes all the eigenvalues and optionally, the eigenvectors of a complex generalized Hermitian-definite banded eigenproblem
- CHBGVD computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite banded eigenproblem
- CHBGVX computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite banded eigenproblem
- CHBTRD reduces a complex Hermitian band matrix A to real symmetric tridiagonal form T by a unitary similarity transformation
- CHECON estimates the reciprocal of the condition number of a complex Hermitian matrix A

- CHEEV computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A
- CHEEVD computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A
- CHEEVR computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix T
- CHEEVX computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A
- CHEGS2 reduces a complex Hermitian-definite generalized eigenproblem to standard form
- CHEGST reduces a complex Hermitian-definite generalized eigenproblem to standard form
- CHEGV computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
- CHEGVD computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
- CHEGVX computes selected eigenvalues, and optionally, eigenvectors of a complex generalized Hermitian-definite eigenproblem
- CHERFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian indefinite
- CHESV computes the solution to a complex system of linear equations
- CHESVX uses the diagonal pivoting factorization to compute the solution to a complex system of linear equations
- CHETD2 reduces a complex Hermitian matrix A to real symmetric tridiagonal form T by a unitary similarity transformation
- CHETF2 computes the factorization of a complex Hermitian matrix A using the Bunch-Kaufman diagonal pivoting method
- CHETRD reduces a complex Hermitian matrix A to real symmetric tridiagonal form T by a unitary similarity transformation
- CHETRF computes the factorization of a complex Hermitian matrix A using the Bunch-Kaufman diagonal pivoting method

- CHETRI computes the inverse of a complex Hermitian indefinite matrix A using the factorization computed by CHETRF
- CHETRS solves a system of linear equations with a complex Hermitian matrix A using the factorization computed by CHETRF
- CHGEQZ implements a single-shift version of the QZ method for finding the generalized eigenvalues
- CHPCON estimates the reciprocal of the condition number of a complex Hermitian packed matrix A using the factorization computed by CHPTRF
- CHPEV computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix in packed storage
- CHPEVD computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A in packed storage
- CHPEVX computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A in packed storage
- CHPGST reduces a complex Hermitian-definite generalized eigenproblem to standard form, using packed storage
- CHPGV computes all the eigenvalues and, optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
- CHPGVD computes all the eigenvalues and, optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
- CHPGVX computes selected eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian-definite eigenproblem
- CHPRFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian indefinite and packed
- CHPSV computes the solution to a complex system of linear equations
- CHPSVX uses diagonal pivoting factorization to compute the solution to a complex system of linear equations
- CHPTRD reduces a complex Hermitian matrix A stored in packed form to real symmetric tridiagonal form T by a unitary similarity transformation
- CHPTRF computes the factorization of a complex Hermitian packed matrix A using the Bunch-Kaufman diagonal pivoting method

- CHPTRI computes the inverse of a complex Hermitian indefinite matrix A in packed storage using the factorization computed by CHPTRF
- CHPTRS solves a system of linear equations with a complex Hermitian matrix A stored in packed format using the factorization computed by CHPTRF
- CHSEIN uses inverse iteration to find specified right and/or left eigenvectors of a complex upper Hessenberg matrix H
- CHSEQR computes the eigenvalues of a complex upper Hessenberg matrix H, and, optionally, the matrices T and Z from the Schur decomposition
- CLABRD reduces the first NB rows and columns of a complex general m by n matrix A to upper or lower real bidiagonal form
- CLACGV conjugates a complex vector of length N
- CLACON estimates the 1-norm of a square, complex matrix A
- CLACP2 copies all or part of a real two-dimensional matrix A to a complex matrix B
- CLACPY copies all or part of a two-dimensional matrix A to another matrix B
- CLACRM performs a very simple matrix-matrix multiplication
- CLACRT perform the operation (c s)(x)>= (x)(-s c)(y)(y) where c and s are complex and the vectors x and y are complex
- CLADIV := X / Y, where X and Y are complex
- CLAED0 computes all eigenvalues of a symmetric tridiagonal matrix which is one diagonal block
- CLAED7 computes the updated eigensystem of a diagonal matrix after modification by a rank-one symmetric matrix
- CLAED8 merges the two sets of eigenvalues together into a single sorted set
- CLAEIN uses inverse iteration to find a right or left eigenvector corresponding to the eigenvalue W of a complex upper Hessenberg matrix H
- CLAESY computes the eigendecomposition of a 2-by-2 symmetric matrix
- CLAEV2 computes the eigendecomposition of a 2-by-2 Hermitian matrix
- CLAGS2 computes 2-by-2 unitary matrices U, V and Q

- CLAGTM performs a matrix-vector product
- CLAHEF computes a partial factorization of a complex Hermitian matrix A using the Bunch-Kaufman diagonal pivoting method
- CLAHQR an auxiliary routine called by CHSEQR to update the eigenvalues and Schur decomposition already computed by CHSEQR
- CLAHRD reduces the first NB columns of a complex general matrix so that elements below the k-th subdiagonal are zero
- CLAIC1 applies one step of incremental condition estimation in its simplest version
- CLALSO applies back the multiplying factors of either the left or the right singular vector matrix of a diagonal matrix
- CLALSA an itermediate step in solving the least squares problem by computing the SVD of the coefficient matrix in compact form
- CLALSD uses the singular value decomposition of A to solve the least squares problem of finding X to minimize the Euclidean norm of each column of AX-B
- CLANGB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n band matrix A
- CLANGE returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex matrix A
- CLANGT returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex tridiagonal matrix A
- CLANHB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n hermitian band matrix A, with k super-diagonals
- CLANHE returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex hermitian matrix A
- CLANHP returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex hermitian matrix A, supplied in packed form
- CLANHS returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a Hessenberg matrix A

- CLANHT returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex Hermitian tridiagonal matrix A
- CLANSB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n symmetric band matrix A, with k super-diagonals
- CLANSP returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex symmetric matrix A, supplied in packed form
- CLANSY returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex symmetric matrix A
- CLANTB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n triangular band matrix A, with (k + 1) diagonals
- CLANTP returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a triangular matrix A, supplied in packed form
- CLANTR returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a trapezoidal or triangular matrix A
- CLAPLL computes the QR factorization of A=QR
- CLAPMT rearranges the columns of the M by N matrix X
- CLAQGB equilibrates a general M by N band matrix A
- CLAQGE equilibrates a general M by N matrix A using the row and scaling factors in the vectors R and C
- CLAQHB equilibrates a symmetric band matrix A using the scaling factors in the vector S
- CLAQHE equilibrates a Hermitian matrix A using the scaling factors in the vector S
- CLAQHP equilibrates a Hermitian matrix A using the scaling factors in the vector S
- CLAQP2 computes a QR factorization with column pivoting

- CLAQPS computes a step of QR factorization with column pivoting of a complex M-by-N matrix A
- CLAQSB equilibrates a symmetric band matrix A using the scaling factors in the vector S
- CLAQSP equilibrates a symmetric matrix A using the scaling factors in the vector S
- CLAQSY equilibrates a symmetric matrix A using the scaling factors in the vector S
- CLAR1V computes the (scaled) r<sup>th</sup> column of the inverse of the sumbmatrix in rows B1 through BN of a tridiagonal matrix
- CLAR2V applies a vector of complex plane rotations with real cosines from both sides to a sequence of 2-by-2 complex Hermitian matrices,
- CLARCM performs a very simple matrix-matrix multiplication
- CLARF applies a complex elementary reflector H to a complex M-by-N matrix C, from either the left or the right
- CLARFB applies a complex block reflector H or its transpose H' to a complex M-by-N matrix C, from either the left or the right
- CLARFG generates a complex elementary reflector H of order n
- CLARFT forms the triangular factor T of a complex block reflector H of order n, which is defined as a product of k elementary reflectors
- CLARFX applies a complex elementary reflector H to a complex m by n matrix C, from either the left or the right
- CLARGV generates a vector of complex plane rotations with real cosines, determined by elements of the complex vectors x and y
- CLARNV returns a vector of n random complex numbers from a uniform or normal distribution
- CLARRV computes the eigenvectors of a tridiagonal matrix
- CLARTG generates a plane rotation
- CLARTV applies a vector of complex plane rotations with real cosines to elements of the complex vectors x and y

- CLARZ applies a complex elementary reflector H to a complex M-by-N matrix C, from either the left or the right
- CLARZB applies a complex block reflector H or its transpose to a complex distributed M-by-N C from the left or the right
- CLARZT forms the triangular factor T of a complex block reflector H
- CLASCL multiplies the M by N complex matrix A by the real scalar CTO/CFROM
- CLASET initializes a 2-D array A to BETA on the diagonal and ALPHA on the offdiagonals
- CLASR performs a transformation A := PA
- CLASSQ returns the values scl and ssq
- CLASWP performs a series of row interchanges on the matrix A
- CLASYF computes a partial factorization of a complex symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- CLATBS solves a triangular system
- CLATDF computes the contribution to the reciprocal Dif-estimate
- CLATPS solves a triangular system
- CLATRD reduces NB rows and columns of a complex Hermitian matrix A
- CLATRS solves a triangular system
- CLATRZ factors a M-by-(M+L) complex upper trapezoidal matrix
- CLATZM routine is deprecated and has been replaced by routine CUNMRZ
- CLAUU2 computes the product U × U' or L' × L
- CLAUUM computes the product U × U' or L' × L, where the triangular factor U or L is stored in the upper or lower triangular part of the array A
- CPBCON estimates the reciprocal of the condition number (in the 1-norm) of a complex Hermitian positive definite band matrix using the Cholesky factorization computed by CPBTRF

- CPBEQU computes row and column scalings intended to equilibrate a Hermitian positive definite band matrix A and reduce its condition number (with respect to the two-norm)
- CPBRFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian positive definite and banded
- CPBSTF computes a split Cholesky factorization of a complex Hermitian positive definite band matrix A
- CPBSV computes the solution to a complex system of linear equations
- CPBSVX uses the Cholesky factorization to compute the solution to a complex system of linear equations
- CPBTF2 computes the Cholesky factorization of a complex Hermitian positive definite band matrix A
- CPBTRF computes the Cholesky factorization of a complex Hermitian positive definite band matrix A
- CPBTRS solves a system of linear equations with a Hermitian positive definite band matrix A
- CPOCON estimates the reciprocal of the condition number (in the 1-norm) of a complex Hermitian positive definite matrix
- CPOEQU computes row and column scalings intended to equilibrate a Hermitian positive definite matrix A and reduce its condition number (with respect to the two-norm)
- CPORFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian positive definite
- CPOSV computes the solution to a complex system of linear equations
- CPOSVX uses the Cholesky factorization to compute the solution to a complex system of linear equations
- CPOTF2 computes the Cholesky factorization of a complex Hermitian positive definite matrix A
- CPOTRF computes the Cholesky factorization of a complex Hermitian positive definite matrix A
- CPOTRI computes the inverse of a complex Hermitian positive definite matrix A

- CPOTRS solves a system of linear equations with a Hermitian positive definite matrix A
- CPPCON estimates the reciprocal of the condition number (in the 1-norm) of a complex Hermitian positive definite packed matrix
- CPPEQU computes row and column scalings intended to equilibrate a Hermitian positive definite matrix A in packed storage and reduce its condition number (with respect to the two-norm)
- CPPRFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian positive definite and packed, and provides error bounds and backward error estimates for the solution
- CPPSV computes the solution to a complex system of linear equations
- CPPSVX uses the Cholesky factorization to compute the solution to a complex system of linear equations
- CPPTRF computes the Cholesky factorization of a complex Hermitian positive definite matrix A stored in packed format
- CPPTRI computes the inverse of a complex Hermitian positive definite matrix A using the Cholesky factorization computed by CPPTRF
- CPPTRS solves a system of linear equations with a Hermitian positive definite matrix A in packed storage using the Cholesky factorization computed by CPPTRF
- CPTCON computes the reciprocal of the condition number (in the 1-norm) of a complex Hermitian positive definite tridiagonal matrix using the factorization computed by CPTTRF
- CPTEQR computes all eigenvalues and, optionally, eigenvectors of a symmetric positive definite tridiagonal matrix
- CPTRFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian positive definite and tridiagonal
- CPTSV computes the solution to a complex system of linear equations
- CPTSVX computes the solution to a complex system of linear equations
- CPTTRF computes the factorization of a complex Hermitian positive definite tridiagonal matrix A
- CPTTRS solves a tridiagonal system using the factorization computed by CPTTRF

- CPTTS2 solves a tridiagonal system using the factorization computed by CPTTRF
- CSPCON estimates the reciprocal of the condition number (in the 1-norm) of a complex symmetric packed matrix A
- CSPRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric indefinite and packed
- CSPSV computes the solution to a complex system of linear equations
- CSPSVX uses diagonal pivoting factorization to compute the solution to a complex system of linear equations
- CSPTRF computes the factorization of a complex symmetric matrix A stored in packed format using the Bunch-Kaufman diagonal pivoting method
- CSPTRI computes the inverse of a complex symmetric indefinite matrix A in packed storage using the factorization computed by CSPTRF
- CSPTRS solves a system of linear equations with a complex symmetric matrix A stored in packed format using the factorization computed by CSPTRF
- CSRSCL multiplies an n-element complex vector x by the real scalar 1/a
- CSTEDC computes all eigenvalues and, optionally, eigenvectors of a symmetric tridiagonal matrix using the divide and conquer method
- CSTEGR computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix T
- CSTEIN computes the eigenvectors of a real symmetric tridiagonal matrix T corresponding to specified eigenvalues, using inverse iteration
- CSTEQR computes all eigenvalues and, optionally, eigenvectors of a symmetric tridiagonal matrix using the implicit QL or QR method
- CSYCON estimates the reciprocal of the condition number (in the 1-norm) of a complex symmetric matrix A using the factorization computed by CSYTRF
- CSYRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric indefinite, and provides error bounds and backward error estimates for the solution
- CSYSV computes the solution to a complex system of linear equations

- CSYSVX uses the diagonal pivoting factorization to compute the solution to a complex system of linear equations
- CSYTF2 computes the factorization of a complex symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- CSYTRF computes the factorization of a complex symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- CSYTRI computes the inverse of a complex symmetric indefinite matrix A using the factorization computed by CSYTRF
- CSYTRS solves a system of linear equations with a complex symmetric matrix A using the factorization computed by CSYTRF
- CTBCON estimates the reciprocal of the condition number of a triangular band matrix A, in either the 1-norm or the infinity-norm
- CTBRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular band coefficient matrix
- CTBTRS solves a triangular system
- CTGEVC computes some or all of the right and/or left generalized eigenvectors of a pair of complex upper triangular matrices (A,B)
- CTGEX2 swaps adjacent diagonal 1 by 1 blocks (A11,B11) and (A22,B22)
- CTGEXC reorders the generalized Schur decomposition of a complex matrix pair (A,B), using a unitary equivalence transformation
- CTGSEN reorders the generalized Schur decomposition of a complex matrix pair (A, B)
- CTGSJA computes the generalized singular value decomposition (GSVD) of two complex upper triangular (or trapezoidal) matrices A and B
- CTGSNA estimates reciprocal condition numbers for specified eigenvalues and/or eigenvectors of a matrix pair (A, B)
- CTGSY2 solves the generalized Sylvester equation using Level 1 and 2 BLAS
- CTGSYL solves the generalized Sylvester equation
- CTPCON estimates the reciprocal of the condition number of a packed triangular matrix A, in either the 1-norm or the infinity-norm

- CTPRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular packed coefficient matrix
- CTPTRI computes the inverse of a complex upper or lower triangular matrix A stored in packed format
- CTPTRS solves a triangular system
- CTRCON estimates the reciprocal of the condition number of a triangular matrix A, in either the 1-norm or the infinity-norm
- CTREVC computes some or all of the right and/or left eigenvectors of a complex upper triangular matrix T
- CTREXC reorders the Schur factorization of a complex matrix so that the diagonal element of T with row index IFST is moved to row ILST
- CTRID computes the solution to a complex system of linear equations
- CTRRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular coefficient matrix
- CTRSEN reorders the Schur factorization of a complex matrix
- CTRSNA estimates reciprocal condition numbers for specified eigenvalues and/or right eigenvectors of a complex upper triangular matrix T
- CTRSYL solves the complex Sylvester matrix equation
- CTRTI2 computes the inverse of a complex upper or lower triangular matrix
- CTRTRI computes the inverse of a complex upper or lower triangular matrix A
- CTRTRS solves a triangular system
- CTZRQF routine is deprecated and has been replaced by routine CTZRZF
- CTZRZF reduces the M-by-N ( M $\leftarrow$ N )complex upper trapezoidal matrix A to upper triangular form by means of unitary transformations
- CUNG2L generates an m by n complex matrix Q with orthonormal columns,
- CUNG2R generates an m by n complex matrix Q with orthonormal columns,
- CUNGBR generates one of the complex unitary matrices Q or P<sup>H</sup> determined by CGEBRD when reducing a complex matrix A to bidiagonal form

- CUNGHR generates a complex unitary matrix Q which is defined as the product of IHI-ILO elementary reflectors of order N, as returned by CGEHRD
- CUNGL2 generates an m-by-n complex matrix Q with orthonormal rows,
- CUNGLQ generates an M-by-N complex matrix Q with orthonormal rows,
- CUNGQL generates an M-by-N complex matrix Q with orthonormal columns,
- CUNGQR generates an M-by-N complex matrix Q with orthonormal columns,
- CUNGR2 generates an m by n complex matrix Q with orthonormal rows,
- CUNGRQ generates an M-by-N complex matrix Q with orthonormal rows,
- CUNGTR generates a complex unitary matrix Q which is defined as the product of n-1 elementary reflectors of order N, as returned by CHETRD
- CUNM2L overwrites the general complex m-by-n matrix C
- CUNM2R overwrites the general complex m-by-n matrix C
- CUNMBR overwrites the general complex M-by-N matrix C
- CUNMHR overwrites the general complex M-by-N matrix C
- CUNML2 overwrites the general complex m-by-n matrix C
- CUNMLQ overwrites the general complex M-by-N matrix C
- CUNMQL overwrites the general complex M-by-N matrix C
- CUNMQR overwrites the general complex M-by-N matrix C
- CUNMR2 overwrites the general complex m-by-n matrix C
- CUNMR3 overwrites the general complex m by n matrix C
- CUNMRQ overwrites the general complex M-by-N matrix C
- CUNMRZ overwrites the general complex M-by-N matrix C
- CUNMTR overwrites the general complex M-by-N matrix C
- CUPGTR generates a complex unitary matrix Q
- CUPMTR overwrites the general complex M-by-N matrix C

- DBDSDC computes the singular value decomposition (SVD) of a real N-by-N (upper or lower) bidiagonal matrix B
- DBDSQR computes the singular value decomposition (SVD) of a real N-by-N (upper or lower) bidiagonal matrix B
- DDISNA computes the reciprocal condition numbers for the eigenvectors of a real symmetric or complex Hermitian matrix or for the left or right singular vectors of a general m-by-n matrix
- DGBBRD reduces a real general m-by-n band matrix A to upper bidiagonal form B by an orthogonal transformation
- DGBCON estimates the reciprocal of the condition number of a real general band matrix A
- DGBEQU computes row and column scalings intended to equilibrate an M-by-N band matrix A and reduce its condition number
- DGBRFS improves the computed solution to a system of linear equations when the coefficient matrix is banded
- DGBSV computes the solution to a real system of linear equations
- DGBSVX uses the LU factorization to compute the solution to a real system of linear equations
- DGBTF2 computes an LU factorization of a real m-by-n band matrix A using partial pivoting with row interchanges
- DGBTRF computes an LU factorization of a real m-by-n band matrix A using partial pivoting with row interchanges
- DGBTRS solves a system of linear equations with a general band matrix A using the LU factorization computed by DGBTRF
- DGEBAK forms the right or left eigenvectors of a real general matrix by backward transformation on the computed eigenvectors of the balanced matrix output by DGEBAL
- DGEBAL balances a general real matrix A
- DGEBD2 reduces a real general m by n matrix A to upper or lower bidiagonal form B by an orthogonal transformation

- DGEBRD reduces a general real M-by-N matrix A to upper or lower bidiagonal form B by an orthogonal transformation
- DGECON estimates the reciprocal of the condition number of a general real matrix A, in either the 1-norm or the infinity-norm, using the LU factorization computed by DGETRF
- DGEEQU computes row and column scalings intended to equilibrate an M-by-N matrix A and reduce its condition number
- DGEES computes for an N-by-N real nonsymmetric matrix A, the eigenvalues, the real Schur form T, and, optionally, the matrix of Schur vectors Z
- DGEESX computes for an N-by-N real nonsymmetric matrix A, the eigenvalues, the real Schur form T, and, optionally, the matrix of Schur vectors Z
- DGEEV computes for an N-by-N real nonsymmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors
- DGEEVX computes for an N-by-N real nonsymmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors
- DGEGS routine is deprecated and has been replaced by routine DGGES
- DGEGV routine is deprecated and has been replaced by routine DGGEV
- DGEHD2 reduces a real general matrix A to upper Hessenberg form H by an orthogonal similarity transformation
- DGEHRD reduces a real general matrix A to upper Hessenberg form H by an orthogonal similarity transformation
- DGELQ2 computes an LQ factorization of a real m by n matrix A
- DGELQF computes an LQ factorization of a real M-by-N matrix A
- DGELS solves overdetermined or underdetermined real linear systems involving an M-by-N matrix A, or its transpose, using a QR or LQ factorization of A
- DGELSD computes the minimum-norm solution to a real linear least squares problem
- DGELSS computes the minimum norm solution to a real linear least squares problem
- DGELSX routine is deprecated and has been replaced by routine DGELSY

- DGELSY computes the minimum-norm solution to a real linear least squares problem
- DGEQL2 computes a QL factorization of a real m by n matrix A
- DGEQLF computes a QL factorization of a real M-by-N matrix A
- DGEQP3 computes a QR factorization with column pivoting of a matrix A
- DGEQPF routine is deprecated and has been replaced by routine DGEQP3
- DGEQR2 computes a QR factorization of a real m by n matrix A
- DGEQRF computes a QR factorization of a real M-by-N matrix A
- DGERFS improves the computed solution to a system of linear equations and provides error bounds and backward error estimates for the solution
- DGERQ2 computes an RQ factorization of a real m by n matrix A
- DGERQF computes an RQ factorization of a real M-by-N matrix A
- DGESC2 solves a system of linear equations with a general N-by-N matrix A using the LU factorization with complete pivoting computed by DGETC2
- DGESDD computes the singular value decomposition (SVD) of a real M-by-N matrix A
- DGESV computes the solution to a real system of linear equations
- DGESVD computes the singular value decomposition (SVD) of a real M-by-N matrix A
- DGESVX uses the LU factorization to compute the solution to a real system of linear equations
- DGETC2 computes an LU factorization with complete pivoting of the n-by-n matrix A
- DGETF2 computes an LU factorization of a general m-by-n matrix A using partial pivoting with row interchanges
- DGETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges
- DGETRI computes the inverse of a matrix using the LU factorization computed by DGETRF

- DGETRS solves a system of linear equations with a general N-by-N matrix A using the LU factorization computed by DGETRF
- DGGBAK forms the right or left eigenvectors of a real generalized eigenvalue problem by backward transformation on the computed eigenvectors of the balanced pair of matrices output by DGGBAL
- DGGBAL balances a pair of general real matrices (A,B)
- DGGES computes for a pair of N-by-N real nonsymmetric matrices (A,B),
- DGGESX computes for a pair of N-by-N real nonsymmetric matrices (A,B), the generalized eigenvalues and the real Schur form (S,T)
- DGGEV computes for a pair of N-by-N real nonsymmetric matrices (A,B) the generalized eigenvalues
- DGGEVX computes for a pair of N-by-N real nonsymmetric matrices (A,B) the generalized eigenvalues
- DGGGLM solves a general Gauss-Markov linear model (GLM) problem
- DGGHRD reduces a pair of real matrices (A,B) to generalized upper Hessenberg form using orthogonal transformations, where A is a general matrix and B is upper triangular
- DGGLSE solves the linear equality-constrained least squares (LSE) problem
- DGGQRF computes a generalized QR factorization of an N-by-M matrix A and an N-by-P matrix B
- DGGRQF computes a generalized RQ factorization of an M-by-N matrix A and a P-by-N matrix B
- DGGSVD computes the generalized singular value decomposition (GSVD) of an M-by-N real matrix A and P-by-N real matrix B
- DGGSVP computes orthogonal matrices U, V and Q
- DGTCON estimates the reciprocal of the condition number of a real tridiagonal matrix A using the LU factorization as computed by DGTTRF
- DGTRFS improves the computed solution to a system of linear equations when the coefficient matrix is tridiagonal
- DGTSV solves the equation AX = B

- DGTSVX uses the LU factorization to compute the solution to a real system of linear equations
- DGTTRF computes an LU factorization of a real tridiagonal matrix A using elimination with partial pivoting and row interchanges
- DGTTRS solves one of the systems of equations AX = B or A'X = B
- DGTTS2 solves one of the systems of equations AX = B or A'X = B
- DHGEQZ implements a single-/double-shift version of the QZ method for finding generalized eigenvalues
- DHSEIN uses inverse iteration to find specified right and/or left eigenvectors of a real upper Hessenberg matrix H
- DHSEQR computes the eigenvalues of a real upper Hessenberg matrix H
- DLABAD returns the square root of values
- DLABRD reduces the first NB rows and columns of a real general m by n matrix A to upper or lower bidiagonal form by an orthogonal transformation
- DLACON estimates the 1-norm of a square, real matrix A
- DLACPY copies all or part of a two-dimensional matrix A to another matrix B
- DLADIV performs complex division in real arithmetic
- DLAE2 computes the eigenvalues of a 2-by-2 symmetric matrix
- DLAEBZ contains the iteration loops which compute and use the function N(w)
- DLAED0 computes all eigenvalues and corresponding eigenvectors of a symmetric tridiagonal matrix using the divide and conquer method
- DLAED1 computes the updated eigensystem of a diagonal matrix after modification by a rank-one symmetric matrix
- DLAED2 merges the two sets of eigenvalues together into a single sorted set
- DLAED3 finds the roots of the secular equation, as defined by the values in D, W, and RHO, between 1 and K
- DLAED4 computes the I-th updated eigenvalue of a symmetric rank-one modification to a diagonal matrix

- DLAED5 computes the I-th eigenvalue of a symmetric rank-one modification of a 2-by-2 diagonal matrix
- DLAED6 computes the positive or negative root (closest to the origin)
- DLAED7 computes the updated eigensystem of a diagonal matrix after modification by a rank-one symmetric matrix
- DLAED8 merges the two sets of eigenvalues together into a single sorted set
- DLAED9 finds the roots of the secular equation, as defined by the values in D, Z, and RHO, between KSTART and KSTOP
- DLAEDA computes the Z vector corresponding to the merge step in the CURLVL<sup>th</sup> step of the merge process with TLVLS steps for the CURPBMth problem
- DLAEIN uses inverse iteration to find a right or left eigenvector corresponding to the eigenvalue (WR,WI) of a real upper Hessenberg matrix H
- DLAEV2 computes the eigendecomposition of a 2-by-2 symmetric matrix
- DLAEXC swaps adjacent diagonal blocks T11 and T22 of order 1 or 2 in an upper quasi-triangular matrix T by an orthogonal similarity transformation
- DLAG2 computes the eigenvalues of a 2 x 2 generalized eigenvalue problem with scaling as necessary to avoid over-/underflow
- DLAGS2 computes 2-by-2 orthogonal matrices U, V and Q
- DLAGTF factorizes a matrix
- DLAGTM performs a matrix-vector product
- DLAGTS solves one of two systems of equations
- DLAGV2 computes the Generalized Schur factorization of a real 2-by-2 matrix pencil (A,B) where B is upper triangular
- DLAHQR updates the eigenvalues and Schur decomposition already computed by DHSEQR
- DLAHRD reduces the first NB columns of a real general n-by-(n-k+1) matrix A so that elements below the k<sup>th</sup> subdiagonal are zero
- DLAIC1 applies one step of incremental condition estimation in its simplest version

- DLALN2 solves a system with possible scaling and perturbation of A
- DLALSO applies back the multiplying factors of either the left or the right singular vector matrix of a diagonal matrix appended by a row to the right hand side matrix B in solving the least squares problem using the divide-and-conquer SVD approach
- DLALSA an itermediate step in solving the least squares problem by computing the SVD of the coefficient matrix in compact form
- DLALSD uses the singular value decomposition of A to solve the least squares problem
- DLAMCH determines double precision machine parameters
- DLAMRG creates a permutation list which merges the elements of A
- DLANGB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n band matrix A
- DLANGE returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real matrix A
- DLANGT returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real tridiagonal matrix A
- DLANHS returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a Hessenberg matrix A
- DLANSB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n symmetric band matrix A, with k super-diagonals
- DLANSP returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real symmetric matrix A, supplied in packed form
- DLANST returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real symmetric tridiagonal matrix A
- DLANSY returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real symmetric matrix A

- DLANTB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n triangular band matrix A, with ( k + 1 )diagonals
- DLANTP returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a triangular matrix A, supplied in packed form
- DLANTR returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a trapezoidal or triangular matrix A
- DLANV2 computes the Schur factorization of a real 2-by-2 nonsymmetric matrix in standard form
- DLAPLL computers the QR factorization of A=QR
- DLAPMT rearranges the columns of the M by N matrix X
- DLAPY2 returns  $sqrt(x^2 + y^2)$  without causing unnecessary overflow
- DLAPY3 returns  $sqrt(x^2+y^2+z^2)$  without causing unnecessary overflow
- DLAQGB equilibrates a general M by N band matrix A with KL subdiagonals and KU superdiagonals using the row and scaling factors in the vectors R and C
- DLAQGE equilibrates a general M by N matrix A using the row and scaling factors in the vectors R and C
- DLAQP2 computes a QR factorization with column pivoting of the block A(OFFSET+1:M,1:N)
- DLAQPS computes a step of QR factorization with column pivoting of a real M-by-N matrix A by using Blas-3
- DLAQSB equilibrates a symmetric band matrix A using the scaling factors in the vector S
- DLAQSP equilibrates a symmetric matrix A using the scaling factors in the vector S
- DLAQSY equilibrates a symmetric matrix A using the scaling factors in the vector S
- DLAQTR solves a real quasi-triangular system

- DLAR1V computes the (scaled) r<sup>th</sup> column of the inverse of a sumbmatrix
- DLAR2V applies a vector of real plane rotations from both sides to a sequence of 2-by-2 real symmetric matrices, defined by the elements of the vectors x, y and z
- DLARF applies a real elementary reflector H to a real m by n matrix C, from either the left or the right
- DLARFB applies a real block reflector H or its transpose H' to a real m by n matrix C, from either the left or the right
- DLARFG generates a real elementary reflector H of order n
- DLARFT forms the triangular factor T of a real block reflector H of order n, which is defined as a product of k elementary reflectors
- DLARFX applies a real elementary reflector H to a real m by n matrix C, from either the left or the right
- DLARGV generates a vector of real plane rotations, determined by elements of the real vectors x and y
- DLARNV returns a vector of n random real numbers from a uniform or normal distribution
- DLARRB does limited bisection to locate eigenvalues
- DLARRE sets "small" off-diagonal elements to zero
- DLARRF finds a robust representation of input values
- DLARRV computes the eigenvectors of the tridiagonal matrix
- DLARTG generates a plane rotation
- DLARTV applies a vector of real plane rotations to elements of the real vectors x and y
- DLARUV returns a vector of n random real numbers from a uniform (0,1)
- DLARZ applies a real elementary reflector H to a real M-by-N matrix C, from either the left or the right
- DLARZB applies a real block reflector H or its transpose to a real distributed M-by-N C from the left or the right

- DLARZT forms the triangular factor T of a real block reflector H of order > n, which is defined as a product of k elementary reflectors
- DLAS2 computes the singular values of the 2-by-2 matrix
- DLASCL multiplies the M by N real matrix A by the real scalar CTO/CFROM
- DLASD0 computes the singular value decomposition (SVD) of a real upper bidiagonal N-by-M matrix B
- DLASD1 computes the SVD of an upper bidiagonal N-by-M matrix B
- DLASD2 merges the two sets of singular values together into a single sorted set
- DLASD3 finds all the square roots of the roots of the secular equation, as defined by the values in D and Z
- DLASD4 computes the square root of the I<sup>th</sup> updated eigenvalue of a positive symmetric rank-one modification to a positive diagonal matrix
- DLASD5 computes the square root of the I<sup>th</sup> eigenvalue of a positive symmetric rank-one modification of a 2-by-2 diagonal matrix
- DLASD6 computes the SVD of an updated upper bidiagonal matrix B obtained by merging two smaller ones by appending a row
- DLASD7 merges the two sets of singular values together into a single sorted set
- DLASD8 finds the square roots of the roots of the secular equation,
- DLASD9 finds the square roots of the roots of the secular equation,
- DLASDA computes the singular value decomposition (SVD) of a real upper bidiagonal N-by-M matrix B with diagonal D and offdiagonal E
- DLASDQ computes the singular value decomposition (SVD) of a real (upper or lower) bidiagonal matrix with diagonal D and offdiagonal E, accumulating the transformations if desired
- DLASDT creates a tree of subproblems for bidiagonal divide and conquer
- DLASET initializes an m-by-n matrix A to BETA on the diagonal and ALPHA on the offdiagonals
- DLASQ1 computes the singular values of a real N-by-N bidiagonal matrix with diagonal D and off-diagonal E

- DLASQ2 computes all the eigenvalues of the symmetric positive definite tridiagonal matrix
- DLASQ3 computes a shift (TAU)
- DLASQ4 computes an approximation TAU to the smallest eigenvalue using values of d from the previous transform
- DLASQ5 computes one dqds transform in ping-pong form, one version for IEEE machines another for non IEEE machines
- DLASQ6 computes one dqd (shift equal to zero) transform in ping-pong form, with protection against underflow and overflow
- DLASR perform a transformation where A is an m by n real matrix and P is an orthogonal matrix,
- DLASRT sorts numbers
- DLASSQ returns the values scl and smsq
- DLASV2 computes the singular value decomposition of a 2-by-2 triangular matrix
- DLASWP performs a series of row interchanges on the matrix A
- DLASY2 solves for the N1 by N2 matrix X
- DLASYF computes a partial factorization of a real symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- DLATBS solves one of two triangular systems with scaling to prevent overflow, where A is an upper or lower triangular band matrix
- DLATDF uses the LU factorization of the n-by-n matrix Z computed by DGETC2
- DLATPS solves a triangular system with scaling to prevent overflow
- DLATRD reduces NB rows and columns of a real symmetric matrix A to symmetric tridiagonal form
- DLATRS solves a triangular system with scaling to prevent overflow
- DLATRZ factors the M-by-(M+L) real upper trapezoidal matrix by means of orthogonal transformations
- DLATZM routine is deprecated and has been replaced by routine DORMRZ

- DLAUU2 computes the product U × U' or L' × L, where the triangular factor U or L is stored in the upper or lower triangular part of the array A
- DLAUUM computes the product U × U' or L' × L, where the triangular factor U or L is stored in the upper or lower triangular part of the array A
- DOPGTR generates a real orthogonal matrix Q which is defined as the product of n-1 elementary reflectors H(i) of order n, as returned by DSPTRD using packed storage
- DOPMTR overwrites the general real M-by-N matrix C with SIDE = 'L' SIDE = 'R' TRANS = 'N'
- DORG2L generates an m by n real matrix Q with orthonormal columns
- DORG2R generates an m by n real matrix Q with orthonormal columns
- DORGBR generates one of the real orthogonal matrices Q or P<sup>T</sup> determined by DGEBRD when reducing a real matrix A to bidiagonal form
- DORGHR generates a real orthogonal matrix Q which is defined as the product of IHI-ILO elementary reflectors of order N, as returned by DGEHRD
- DORGL2 generates an m by n real matrix Q with orthonormal rows
- DORGLQ generates an M-by-N real matrix Q with orthonormal rows
- DORGQL generates an M-by-N real matrix Q with orthonormal columns
- DORGQR generates an M-by-N real matrix Q with orthonormal columns
- DORGR2 generates an m by n real matrix Q with orthonormal rows
- DORGRQ generates an M-by-N real matrix Q with orthonormal rows
- DORGTR generates a real orthogonal matrix Q as returned by DSYTRD
- DORM2L overwrites the general real m by n matrix C
- DORM2R overwrites the general real m by n matrix C
- DORMBR overwrites the general real M-by-N matrix C
- DORMHR overwrites the general real M-by-N matrix C
- DORML2 overwrites the general real m by n matrix C
- DORMLQ overwrites the general real M-by-N matrix C

- DORMQL overwrites the general real M-by-N matrix C
- DORMQR overwrites the general real M-by-N matrix C
- DORMR2 overwrites the general real m by n matrix C
- DORMR3 overwrites the general real m by n matrix C
- DORMRQ overwrites the general real M-by-N matrix C
- DORMRZ overwrites the general real M-by-N matrix C
- DORMTR overwrites the general real M-by-N matrix C
- DPBCON estimates the reciprocal of the condition number (in the 1-norm) of a real symmetric positive definite band matrix using the Cholesky factorization computed by DPBTRF
- DPBEQU computes row and column scalings intended to equilibrate a symmetric positive definite band matrix A and reduce its condition number (with respect to the two-norm)
- DPBRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric positive definite and banded, and provides error bounds and backward error estimates for the solution
- DPBSTF computes a split Cholesky factorization of a real symmetric positive definite band matrix A
- DPBSV computes the solution to a real system of linear equations
- DPBSVX uses the Cholesky factorization to compute the solution to a real system of linear equations
- DPBTF2 computes the Cholesky factorization of a real symmetric positive definite band matrix A
- DPBTRF computes the Cholesky factorization of a real symmetric positive definite band matrix A
- DPBTRS solves a system of linear equations with a symmetric positive definite band matrix A using the Cholesky factorization computed by DPBTRF
- DPOCON estimates the reciprocal of the condition number (in the 1-norm) of a real symmetric positive definite matrix using the Cholesky factorization computed by DPOTRF

- DPOEQU computes row and column scalings intended to equilibrate a symmetric positive definite matrix A and reduce its condition number (with respect to the two-norm)
- DPORFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric positive definite
- DPOSV computes the solution to a real system of linear equations
- DPOSVX uses the Cholesky factorization to compute the solution to a real system of linear equations
- DPOTF2 computes the Cholesky factorization of a real symmetric positive definite matrix A
- DPOTRF computes the Cholesky factorization of a real symmetric positive definite matrix A
- DPOTRI computes the inverse of a real symmetric positive definite matrix A using the Cholesky factorization computed by DPOTRF
- DPOTRS solves a system of linear equations with a symmetric positive definite matrix A using the Cholesky factorization computed by DPOTRF
- DPPCON estimates the reciprocal of the condition number (in the 1-norm) of a real symmetric positive definite packed matrix using the Cholesky factorization computed by DPPTRF
- DPPEQU computes row and column scalings intended to equilibrate a symmetric positive definite matrix A in packed storage and reduce its condition number (with respect to the two-norm)
- DPPRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric positive definite and packed
- DPPSV computes the solution to a real system of linear equations
- DPPSVX uses the Cholesky factorization to compute the solution to a real system of linear equations
- DPPTRF computes the Cholesky factorization of a real symmetric positive definite matrix A stored in packed format
- DPPTRI computes the inverse of a real symmetric positive definite matrix A using the Cholesky factorization computed by DPPTRF

- DPPTRS solves a system of linear equations with a symmetric positive definite matrix A in packed storage using the Cholesky factorization computed by DPPTRF
- DPTCON computes the reciprocal of the condition number (in the 1-norm) of a real symmetric positive definite tridiagonal matrix using the factorization computed by DPTTRF
- DPTEQR computes all eigenvalues and, optionally, eigenvectors of a symmetric positive definite tridiagonal matrix
- DPTRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric positive definite and tridiagonal
- DPTSV computes the solution to a real system of linear equations
- DPTSVX computes the solution to a real system of linear equations where A is an N-by-N symmetric positive definite tridiagonal matrix and X and B are N-by-NRHS matrices
- DPTTRF computes the factorization of a real symmetric positive definite tridiagonal matrix A
- DPTTRS solves a tridiagonal system using the factorization of A computed by DPTTRF
- DPTTS2 solves a tridiagonal system using the factorization of A computed by DPTTRF
- DRSCL multiplies an n-element real vector x by the real scalar 1/a
- DSBEV computes all the eigenvalues and, optionally, eigenvectors of a real symmetric band matrix A
- DSBEVD computes all the eigenvalues and, optionally, eigenvectors of a real symmetric band matrix A
- DSBEVX computes selected eigenvalues and, optionally, eigenvectors of a real symmetric band matrix A
- DSBGST reduces a real symmetric-definite banded generalized eigenproblem
- DSBGV computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite banded eigenproblem
- DSBGVD computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite banded eigenproblem

- DSBGVX computes selected eigenvalues, and optionally, eigenvectors of a real generalized symmetric-definite banded eigenproblem
- DSBTRD reduces a real symmetric band matrix A to symmetric tridiagonal form T by an orthogonal similarity transformation
- DSECND returns the user time for a process in seconds
- DSPCON estimates the reciprocal of the condition number (in the 1-norm) of a real symmetric packed matrix A
- DSPEV computes all the eigenvalues and, optionally, eigenvectors of a real symmetric matrix A in packed storage
- DSPEVD computes all the eigenvalues and, optionally, eigenvectors of a real symmetric matrix A in packed storage
- DSPEVX computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix A in packed storage
- DSPGST reduces a real symmetric-definite generalized eigenproblem to standard form, using packed storage
- DSPGV computes all the eigenvalues and, optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
- DSPGVD computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
- DSPGVX computes selected eigenvalues, and optionally, eigenvectors of a real generalized symmetric-definite eigenproblem
- DSPRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric indefinite and packed
- DSPSV computes the solution to a real system of linear equations
- DSPSVX uses the diagonal pivoting factorization to compute the solution to a real system of linear equations where A is an N-by-N symmetric matrix stored in packed format and X and B are N-by-NRHS matrices
- DSPTRD reduces a real symmetric matrix A stored in packed form to symmetric tridiagonal form T by an orthogonal similarity transformation
- DSPTRF computes the factorization of a real symmetric matrix A stored in packed format using the Bunch-Kaufman diagonal pivoting method

- DSPTRI computes the inverse of a real symmetric indefinite matrix A in packed storage using a factorization computed by DSPTRF
- DSPTRS solves a system of linear equations with a real symmetric matrix A stored in packed format using a factorization computed by DSPTRF
- DSTEBZ computes the eigenvalues of a symmetric tridiagonal matrix T
- DSTEDC computes all eigenvalues and, optionally, eigenvectors of a symmetric tridiagonal matrix using the divide and conquer method
- DSTEGR computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix T
- DSTEIN computes the eigenvectors of a real symmetric tridiagonal matrix T corresponding to specified eigenvalues, using inverse iteration
- DSTEQR computes all eigenvalues and, optionally, eigenvectors of a symmetric tridiagonal matrix using the implicit QL or QR method
- DSTERF computes all eigenvalues of a symmetric tridiagonal matrix using the Pal-Walker-Kahan variant of the QL or QR algorithm
- DSTEV computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix A
- DSTEVD computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix
- DSTEVR computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix T
- DSTEVX computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix A
- DSYCON estimates the reciprocal of the condition number (in the 1-norm) of a real symmetric matrix A using a factorization computed by DSYTRF
- DSYEV computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix A
- DSYEVD computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix A
- DSYEVR computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix T

- DSYEVX computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix A
- DSYGS2 reduces a real symmetric-definite generalized eigenproblem to standard form
- DSYGST reduces a real symmetric-definite generalized eigenproblem to standard form
- DSYGV computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
- DSYGVD computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
- DSYGVX computes selected eigenvalues, and optionally, eigenvectors of a real generalized symmetric-definite eigenproblem
- DSYRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric indefinite, and provides error bounds and backward error estimates for the solution
- DSYSV computes the solution to a real system of linear equations
- DSYSVX uses the diagonal pivoting factorization to compute the solution to a real system of linear equations
- DSYTD2 reduces a real symmetric matrix A to symmetric tridiagonal form T by an orthogonal similarity transformation
- DSYTF2 computes the factorization of a real symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- DSYTRD reduces a real symmetric matrix A to real symmetric tridiagonal form T by an orthogonal similarity transformation
- DSYTRF computes the factorization of a real symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- DSYTRI computes the inverse of a real symmetric indefinite matrix A using a factorization computed by DSYTRF
- DSYTRS solves a system of linear equations with a real symmetric matrix A using a factorization computed by DSYTRF

- DTBCON estimates the reciprocal of the condition number of a triangular band matrix A, in either the 1-norm or the infinity-norm
- DTBRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular band coefficient matrix
- DTBTRS solves a triangular system
- DTGEVC computes some or all of the right and/or left generalized eigenvectors of a pair of real upper triangular matrices (A,B)
- DTGEX2 swaps adjacent diagonal blocks (A11, B11) and (A22, B22)
- DTGEXC reorders the generalized real Schur decomposition of a real matrix pair (A,B)
- DTGSEN reorders the generalized real Schur decomposition of a real matrix pair (A, B)
- DTGSJA computes the generalized singular value decomposition (GSVD) of two real upper triangular (or trapezoidal) matrices A and B
- DTGSNA estimates reciprocal condition numbers for specified eigenvalues and/or eigenvectors of a matrix pair (A, B) in generalized real Schur canonical form
- DTGSY2 solves the generalized Sylvester equation
- DTGSYL solves the generalized Sylvester equation
- DTPCON estimates the reciprocal of the condition number of a packed triangular matrix A, in either the 1-norm or the infinity-norm
- DTPRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular packed coefficient matrix
- DTPTRI computes the inverse of a real upper or lower triangular matrix A stored in packed format
- DTPTRS solves a triangular system
- DTRCON estimates the reciprocal of the condition number of a triangular matrix A, in either the 1-norm or the infinity-norm
- DTREVC computes some or all of the right and/or left eigenvectors of a real upper quasi-triangular matrix T

- DTREXC reorders the real Schur factorization of a real matrix so that the diagonal block of T with row index IFST is moved to row ILST
- DTRID computes the solution to a real system of linear equations where A is an N-by-N tridiagonal matrix, and x and b are vectors of length N
- DTRRFS provide serror bounds and backward error estimates for the solution to a system of linear equations with a triangular coefficient matrix
- DTRSEN reorders the real Schur factorization of a real matrix so that a selected cluster of eigenvalues appears in the leading diagonal blocks of the upper quasi-triangular matrix T
- DTRSNA estimates reciprocal condition numbers for specified eigenvalues and/or right eigenvectors of a real upper quasi-triangular matrix T
- DTRSYL solves the real Sylvester matrix equation
- DTRTI2 computes the inverse of a real upper or lower triangular matrix
- DTRTRI computes the inverse of a real upper or lower triangular matrix A
- DTRTRS solves a triangular system
- DTZRQF routine is deprecated and has been replaced by routine DTZRZF
- DTZRZF reduces the M-by-N real upper trapezoidal matrix A to upper triangular form by means of orthogonal transformations
- DZSUM1 takes the sum of the absolute values of a complex vector and returns a double precision result
- ICMAX1 finds the index of the element whose real part has maximum absolute value
- ILAENV called from the LAPACK routines to choose problem-dependent parameters for the local environment
- IZMAX1 finds the index of the element whose real part has maximum absolute value
- LSAME return .TRUE
- LSAMEN tests if the first N letters of CA are the same as the first N letters of CB, regardless of case

- SBDSDC computes the singular value decomposition (SVD) of a real N-by-N (upper or lower) bidiagonal matrix B
- SBDSQR computes the singular value decomposition (SVD) of a real N-by-N (upper or lower) bidiagonal matrix B
- SCSUM1 take the sum of the absolute values of a complex vector and returns a single precision result
- SDISNA computes the reciprocal condition numbers for the eigenvectors of a real symmetric or complex Hermitian matrix or for the left or right singular vectors of a general m-by-n matrix
- SECOND returns the user time for a process in seconds
- SGBBRD reduces a real general m-by-n band matrix A to upper bidiagonal form B by an orthogonal transformation
- SGBCON estimates the reciprocal of the condition number of a real general band matrix A, in either the 1-norm or the infinity-norm,
- SGBEQU computes row and column scalings intended to equilibrate an M-by-N band matrix A and reduce its condition number
- SGBRFS improves the computed solution to a system of linear equations when the coefficient matrix is banded
- SGBSV computes the solution to a real system of linear equations where A is a band matrix of order N with KL subdiagonals and KU superdiagonals, and X and B are N-by-NRHS matrices
- SGBSVX uses the LU factorization to compute the solution to a real system of linear equations
- SGBTF2 computes an LU factorization of a real m-by-n band matrix A using partial pivoting with row interchanges
- SGBTRF computes an LU factorization of a real m-by-n band matrix A using partial pivoting with row interchanges
- SGBTRS solves a system of linear equations with a general band matrix A using the LU factorization computed by SGBTRF
- SGEBAK forms the right or left eigenvectors of a real general matrix by backward transformation on the computed eigenvectors of the balanced matrix output by SGEBAL

- SGEBAL balances a general real matrix A
- SGEBD2 reduces a real general m by n matrix A to upper or lower bidiagonal form B by an orthogonal transformation
- SGEBRD reduces a general real M-by-N matrix A to upper or lower bidiagonal form B by an orthogonal transformation
- SGECON estimates the reciprocal of the condition number of a general real matrix A, in either the 1-norm or the infinity-norm, using the LU factorization computed by SGETRF
- SGEEQU computes row and column scalings intended to equilibrate an M-by-N matrix A and reduce its condition number
- SGEES computes for an N-by-N real nonsymmetric matrix A, the eigenvalues, the real Schur form T, and, optionally, the matrix of Schur vectors Z
- SGEESX computes for an N-by-N real nonsymmetric matrix A, the eigenvalues, the real Schur form T, and, optionally, the matrix of Schur vectors Z
- SGEEV computes for an N-by-N real nonsymmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors
- SGEEVX computes for an N-by-N real nonsymmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors
- SGEGS routine is deprecated and has been replaced by routine SGGES
- SGEGV routine is deprecated and has been replaced by routine SGGEV
- SGEHD2 reduces a real general matrix A to upper Hessenberg form H by an orthogonal similarity transformation
- SGEHRD reduces a real general matrix A to upper Hessenberg form H by an orthogonal similarity transformation
- SGELQ2 computes an LQ factorization of a real m by n matrix A
- SGELQF computes an LQ factorization of a real M-by-N matrix A
- SGELS solves overdetermined or underdetermined real linear systems involving an M-by-N matrix A, or its transpose, using a QR or LQ factorization of A
- SGELSD computes the minimum-norm solution to a real linear least squares problem

- SGELSS computes the minimum norm solution to a real linear least squares problem
- SGELSX routine is deprecated and has been replaced by routine SGELSY
- SGELSY computes the minimum-norm solution to a real linear least squares problem
- SGEQL2 computes a QL factorization of a real m by n matrix A
- SGEQLF computes a QL factorization of a real M-by-N matrix A
- SGEQP3 computes a QR factorization with column pivoting of a matrix A
- SGEQPF routine is deprecated and has been replaced by routine SGEQP3
- SGEQR2 computes a QR factorization of a real m by n matrix A
- SGEQRF computes a QR factorization of a real M-by-N matrix A
- SGERFS improves the computed solution to a system of linear equations and provides error bounds and backward error estimates for the solution
- SGERQ2 computes an RQ factorization of a real m by n matrix A
- SGERQF computes an RQ factorization of a real M-by-N matrix A
- SGESC2 solves a system of linear equations with a general N-by-N matrix A using the LU factorization with complete pivoting computed by SGETC2
- SGESDD computes the singular value decomposition (SVD) of a real M-by-N matrix A
- SGESV computes the solution to a real system of linear equations
- SGESVD computes the singular value decomposition (SVD) of a real M-by-N matrix A
- SGESVX uses the LU factorization to compute the solution to a real system of linear equations
- SGETC2 computes an LU factorization with complete pivoting of the n-by-n matrix A
- SGETF2 computes an LU factorization of a general m-by-n matrix A using partial pivoting with row interchanges

- SGETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges
- SGETRI computes the inverse of a matrix using the LU factorization computed by SGETRF
- SGETRS solves a system of linear equations with a general N-by-N matrix A using the LU factorization computed by SGETRF
- SGGBAK forms the right or left eigenvectors of a real generalized eigenvalue problem by backward transformation on the computed eigenvectors of the balanced pair of matrices output by SGGBAL
- SGGBAL balances a pair of general real matrices (A,B)
- SGGES computes for a pair of N-by-N real nonsymmetric matrices (A,B),
- SGGESX computes for a pair of N-by-N real nonsymmetric matrices (A,B), the generalized eigenvalues, the real Schur form (S,T), and,
- SGGEV computes for a pair of N-by-N real nonsymmetric matrices (A,B)
- SGGEVX computes for a pair of N-by-N real nonsymmetric matrices (A,B)
- SGGGLM solves a general Gauss-Markov linear model (GLM) problem
- SGGHRD reduces a pair of real matrices (A,B) to generalized upper Hessenberg form using orthogonal transformations, where A is a general matrix and B is upper triangular
- SGGLSE solves the linear equality-constrained least squares (LSE) problem
- SGGQRF computes a generalized QR factorization of an N-by-M matrix A and an N-by-P matrix B
- SGGRQF computes a generalized RQ factorization of an M-by-N matrix A and a P-by-N matrix B
- SGGSVD computes the generalized singular value decomposition (GSVD) of an M-by-N real matrix A and P-by-N real matrix B
- SGGSVP computes orthogonal matrices U, V and Q
- SGTCON estimates the reciprocal of the condition number of a real tridiagonal matrix A using the LU factorization as computed by SGTTRF

- SGTRFS improves the computed solution to a system of linear equations when the coefficient matrix is tridiagonal
- SGTSV solves the equation AX = B,
- SGTSVX uses the LU factorization to compute the solution to a real system of linear equations
- SGTTRF computes an LU factorization of a real tridiagonal matrix A using elimination with partial pivoting and row interchanges
- SGTTRS solves one of two systems of equations
- SGTTS2 solves one of two systems of equations
- SHGEQZ implements a single-/double-shift version of the QZ method for finding generalized eigenvalues
- SHSEIN uses inverse iteration to find specified right and/or left eigenvectors of a real upper Hessenberg matrix H
- SHSEQR computes the eigenvalues of a real upper Hessenberg matrix H and, optionally, the matrices T and Z from the Schur decomposition
- SLABAD takes as input the values computed by SLAMCH for underflow and overflow, and returns the square root of each of these values if the log of LARGE is sufficiently large
- SLABRD reduces the first NB rows and columns of a real general m by n matrix A to upper or lower bidiagonal form by an orthogonal transformation
- SLACON estimates the 1-norm of a square, real matrix A
- SLACPY copies all or part of a two-dimensional matrix A to another matrix B
- SLADIV performs complex division in real arithmetic
- SLAE2 computes the eigenvalues of a 2-by-2 symmetric matrix
- SLAEBZ contains the iteration loops which compute and use the function N(w)
- SLAED0 computes all eigenvalues and corresponding eigenvectors of a symmetric tridiagonal matrix using the divide and conquer method
- SLAED1 computes the updated eigensystem of a diagonal matrix after modification by a rank-one symmetric matrix

- SLAED2 merges the two sets of eigenvalues together into a single sorted set
- SLAED3 finds the roots of the secular equation, as defined by the values in D, W, and RHO, between 1 and K
- SLAED4 computes the I<sup>th</sup> updated eigenvalue of a symmetric rank-one modification to a diagonal matrix
- SLAED5 computes the I<sup>th</sup> eigenvalue of a symmetric rank-one modification of a 2-by-2 diagonal matrix
- SLAED6 computes the positive or negative root (closest to the origin)
- SLAED7 computes the updated eigensystem of a diagonal matrix after modification by a rank-one symmetric matrix
- SLAED8 merges the two sets of eigenvalues together into a single sorted set
- SLAED9 finds the roots of the secular equation, as defined by the values in D, Z, and RHO, between KSTART and KSTOP
- SLAEDA computes the Z vector corresponding to the merge step in the CURLVL<sup>th</sup> step of the merge process with TLVLS steps for the CURPBMth problem
- SLAEIN uses inverse iteration to find a right or left eigenvector corresponding to the eigenvalue (WR,WI) of a real upper Hessenberg matrix H
- SLAEV2 computes the eigendecomposition of a 2-by-2 symmetric matrix
- SLAEXC swaps adjacent diagonal blocks T11 and T22 of order 1 or 2 in an upper quasi-triangular matrix T by an orthogonal similarity transformation
- SLAG2 computes the eigenvalues of a 2 x 2 generalized eigenvalue problem with scaling as necessary
- SLAGS2 computes 2-by-2 orthogonal matrices
- SLAGTF factorizes the matrix where T is an n by n tridiagonal matrix and lambda is a scalar
- SLAGTM performs a matrix-vector product
- SLAGTS solves one of twi systems of equations
- SLAGV2 computes the Generalized Schur factorization of a real 2-by-2 matrix pencil (A,B) where B is upper triangular

- SLAHQR an auxiliary routine called by SHSEQR to update the eigenvalues and Schur decomposition already computed by SHSEQR
- SLAHRD reduces the first NB columns of a real general n-by-(n-k+1) matrix A so
  that elements below the k<sup>th</sup> subdiagonal are zero
- SLAIC1 applies one step of incremental condition estimation in its simplest version
- SLALN2 solves a system with possible scaling ("s") and perturbation of A
- SLALSO applies back the multiplying factors of either the left or the right singular vector matrix of a diagonal matrix
- SLALSA an itermediate step in solving the least squares problem by computing the SVD of the coefficient matrix in compact form
- SLALSD uses the singular value decomposition of A to solve the least squares problem
- SLAMCH determines single precision machine parameters
- SLAMRG creates a permutation list that merges the elements of A (which is composed of two independently sorted sets) into a single set which is sorted in ascending order
- SLANGB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n band matrix A
- SLANGE returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real matrix A
- SLANGT returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real tridiagonal matrix A
- SLANHS returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a Hessenberg matrix A
- SLANSB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n symmetric band matrix A, with k super-diagonals
- SLANSP returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real symmetric matrix A, supplied in packed form

- SLANST returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real symmetric tridiagonal matrix A
- SLANSY returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real symmetric matrix A
- SLANTB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n triangular band matrix A
- SLANTP returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a triangular matrix A
- SLANTR returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a trapezoidal or triangular matrix A
- SLANV2 computes the Schur factorization of a real 2-by-2 nonsymmetric matrix in standard form
- SLAPLL computes the QR factorization of A=QR
- SLAPMT rearranges the columns of the M by N matrix X
- SLAPY2 returns  $sqrt(x^2+y^2)$  without causing unnecessary overflow
- SLAPY3 returns sqrt( $x^2+y^2+z^2$ ) without causing unnecessary overflow
- SLAQGB equilibrates a general M by N band matrix A with KL subdiagonals and KU superdiagonals
- SLAQGE equilibrates a general M by N matrix A using the row and scaling factors in the vectors R and C
- SLAQP2 computes a QR factorization with column pivoting of the block A(OFFSET+1:M,1:N)
- SLAQPS computes a step of QR factorization with column pivoting of a real M-by-N matrix A by using Blas3
- SLAQSB equilibrates a symmetric band matrix A using the scaling factors in the vector S
- SLAQSP equilibrates a symmetric matrix A using the scaling factors in the vector S

- SLAQSY equilibrates a symmetric matrix A using the scaling factors in the vector S
- SLAQTR solves a real quasi-triangular system
- SLAR1V computes the (scaled) r<sup>th</sup> column of the inverse of the sumbmatrix of a tridiagonal matrix
- SLAR2V applies a vector of real plane rotations from both sides to a sequence of 2-by-2 real symmetric matrices, defined by the elements of the vectors x, y and z
- SLARF applies a real elementary reflector H to a real m by n matrix C, from either the left or the right
- SLARFB applies a real block reflector H or its transpose H' to a real m by n matrix C, from either the left or the right
- SLARFG generates a real elementary reflector H of order n
- SLARFT forms the triangular factor T of a real block reflector H of order n, which is defined as a product of k elementary reflectors
- SLARFX applies a real elementary reflector H to a real m by n matrix C, from either the left or the right
- SLARGV generates a vector of real plane rotations, determined by elements of the real vectors x and y
- SLARNV returns a vector of n random real numbers from a uniform or normal distribution
- SLARRB does limited bisection to locate eigenvalues
- SLARRE sets "small" off-diagonal elements to zero
- SLARRF finds a robust representation of input values.
- SLARRV computes the eigenvectors of the tridiagonal matrix
- SLARTG generates a plane rotation
- SLARTV applies a vector of real plane rotations to elements of the real vectors x and y
- SLARUV returns a vector of n random real numbers from a uniform (0,1)

- SLARZ applies a real elementary reflector H to a real M-by-N matrix C, from either the left or the right
- SLARZB applies a real block reflector H or its transpose to a real distributed M-by-N C from the left or the right
- SLARZT forms the triangular factor T of a real block reflector H
- SLAS2 computes the singular values of the 2-by-2 matrix
- SLASCL multiplie the M by N real matrix A by the real scalar CTO/CFROM
- SLASD0 computes the singular value decomposition (SVD) of a real upper bidiagonal N-by-M matrix B
- SLASD1 computes the SVD of an upper bidiagonal N-by-M matrix B,
- SLASD2 merges the two sets of singular values together into a single sorted set
- SLASD3 finds all the square roots of the roots of the secular equation, as defined by the values in D and Z
- SLASD4 computes the square root of the I<sup>th</sup> updated eigenvalue of a positive symmetric rank-one modification to a positive diagonal matrix
- SLASD5 -computes the square root of the I<sup>th</sup> eigenvalue of a positive symmetric rank-one modification of a 2-by-2 diagonal matrix
- SLASD6 computes the SVD of an updated upper bidiagonal matrix B obtained by merging two smaller ones by appending a row
- SLASD7 merges the two sets of singular values together into a single sorted set
- SLASD8 finds the square roots of the roots of the secular equation,
- SLASD9 finds the square roots of the roots of the secular equation,
- SLASDA computes the singular value decomposition (SVD) of a real upper bidiagonal N-by-M matrix B with diagonal D and offdiagonal E
- SLASDQ computes the singular value decomposition (SVD) of a real (upper or lower) bidiagonal matrix with diagonal D and offdiagonal E, accumulating the transformations if desired
- SLASDT creates a tree of subproblems for bidiagonal divide and conquer

- SLASET initializes an m-by-n matrix A to BETA on the diagonal and ALPHA on the offdiagonals
- SLASQ1 computes the singular values of a real N-by-N bidiagonal matrix with diagonal D and off-diagonal E
- SLASQ2 computes all the eigenvalues of the symmetric positive definite tridiagonal matrix associated with the qd array Z
- SLASQ3 checks for deflation, computes a shift (TAU) and calls dqds
- SLASQ4 computes an approximation TAU to the smallest eigenvalue using values of d from the previous transform
- SLASQ5 computes sone dqds transform in ping-pong form, one version for IEEE machines another for non IEEE machines
- SLASQ6 computes one dqd (shift equal to zero) transform in ping-pong form, with protection against underflow and overflow
- SLASR performs a transformation
- SLASRT sorts numbers
- SLASSQ returns the values scl and smsq
- SLASV2 computes the singular value decomposition of a 2-by-2 triangular matrix
- SLASWP performs a series of row interchanges on the matrix A
- SLASY2 solves for the N1 by N2 matrix X
- SLASYF computes a partial factorization of a real symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- SLATBS solves one of two triangular systems with scaling to prevent overflow
- SLATDF computes a contribution to the reciprocal Dif-estimate
- SLATPS solves one of two triangular systems with scaling to prevent overflow
- SLATRD reduces NB rows and columns of a real symmetric matrix A to symmetric tridiagonal form
- SLATRS solves one of two triangular systems with scaling to prevent overflow

- SLATRZ factors the M-by-(M+L) real upper trapezoidal matrix by means of orthogonal transformations
- SLATZM routine is deprecated and has been replaced by routine SORMRZ
- SLAUU2 computes the product U × U' or L' × L
- SLAUUM computes the product U × U' or L' × L, where the triangular factor U
  or L is stored in the upper or lower triangular part of the array A
- SOPGTR generates a real orthogonal matrix Q as returned by SSPTRD using packed storage
- SOPMTR overwrites the general real M-by-N matrix C
- SORG2L generates an m by n real matrix Q with orthonormal columns,
- SORG2R generates an m by n real matrix Q with orthonormal columns,
- SORGBR generates one of the real orthogonal matrices determined by SGEBRD when reducing a real matrix A to bidiagonal form
- SORGHR generates a real orthogonal matrix Q as returned by SGEHRD
- SORGL2 generates an m by n real matrix Q with orthonormal rows
- SORGLQ generates an M-by-N real matrix Q with orthonormal rows
- SORGQL generates an M-by-N real matrix Q with orthonormal columns
- SORGQR generates an M-by-N real matrix Q with orthonormal columns
- SORGR2 generates an m by n real matrix Q with orthonormal rows
- SORGRQ generates an M-by-N real matrix Q with orthonormal rows
- SORGTR generates a real orthogonal matrix Q as returned by SSYTRD
- SORM2L overwrites the general real m by n matrix C
- SORM2R overwrites the general real m by n matrix C with Q
- SORMBR VECT = 'Q', SORMBR overwrites the general real M-by-N matrix C with SIDE = 'L' SIDE = 'R' TRANS = 'N'
- SORMHR overwrites the general real M-by-N matrix C
- SORML2 overwrites the general real m by n matrix C

- SORMLQ overwrites the general real M-by-N matrix C
- SORMQL overwrites the general real M-by-N matrix C
- SORMQR overwrites the general real M-by-N matrix C
- SORMR2 overwrites the general real m by n matrix C
- SORMR3 overwrites the general real m by n matrix C
- SORMRQ overwrites the general real M-by-N matrix C
- SORMRZ overwrites the general real M-by-N matrix C
- SORMTR overwrites the general real M-by-N matrix C
- SPBCON estimates the reciprocal of the condition number (in the 1-norm) of a real symmetric positive definite band matrix using the Cholesky factorization computed by SPBTRF
- SPBEQU computes row and column scalings intended to equilibrate a symmetric positive definite band matrix A and reduce its condition number (with respect to the two-norm)
- SPBRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric positive definite and banded
- SPBSTF computes a split Cholesky factorization of a real symmetric positive definite band matrix A
- SPBSV computes the solution to a real system of linear equations
- SPBSVX uses the Cholesky factorization to compute the solution to a real system of linear equations
- SPBTF2 computes the Cholesky factorization of a real symmetric positive definite band matrix A
- SPBTRF computes the Cholesky factorization of a real symmetric positive definite band matrix A
- SPBTRS solves a system of linear equations with a symmetric positive definite band matrix A using the Cholesky factorization computed by SPBTRF
- SPOCON estimates the reciprocal of the condition number (in the 1-norm) of a real symmetric positive definite matrix using the Cholesky factorization computed by SPOTRF

- SPOEQU computes row and column scalings intended to equilibrate a symmetric positive definite matrix A and reduce its condition number (with respect to the two-norm)
- SPORFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric positive definite
- SPOSV computes the solution to a real system of linear equations
- SPOSVX uses the Cholesky factorization to compute the solution to a real system of linear equations
- SPOTF2 computes the Cholesky factorization of a real symmetric positive definite matrix A
- SPOTRF computes the Cholesky factorization of a real symmetric positive definite matrix A
- SPOTRI computes the inverse of a real symmetric positive definite matrix A using the Cholesky factorization computed by SPOTRF
- SPOTRS solves a system of linear equations with a symmetric positive definite matrix A using the Cholesky factorization computed by SPOTRF
- SPPCON estimates the reciprocal of the condition number (in the 1-norm) of a real symmetric positive definite packed matrix using the Cholesky factorization computed by SPPTRF
- SPPEQU computes row and column scalings intended to equilibrate a symmetric positive definite matrix A in packed storage and reduce its condition number (with respect to the two-norm)
- SPPRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric positive definite and packed, and provides error bounds and backward error estimates for the solution
- SPPSV computes the solution to a real system of linear equations
- SPPSVX uses the Cholesky factorization to compute the solution to a real system of linear equations
- SPPTRF computes the Cholesky factorization of a real symmetric positive definite matrix A stored in packed format
- SPPTRI computes the inverse of a real symmetric positive definite matrix A using the Cholesky factorization computed by SPPTRF

- SPPTRS solves a system of linear equations with a symmetric positive definite matrix A in packed storage using the Cholesky factorization computed by SPPTRF
- SPTCON computes the reciprocal of the condition number (in the 1-norm) of a real symmetric positive definite tridiagonal matrix using the factorization computed by SPTTRF
- SPTEQR computes all eigenvalues and, optionally, eigenvectors of a symmetric positive definite tridiagonal matrix by first factoring the matrix using SPTTRF, and then calling SBDSQR to compute the singular values of the bidiagonal factor
- SPTRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric positive definite and tridiagonal, and provides error bounds and backward error estimates for the solution
- SPTSV computes the solution to a real system of linear equations
- SPTSVX uses a factorization to compute the solution to a real system of linear equations
- SPTTRF computes the factorization of a real symmetric positive definite tridiagonal matrix A
- SPTTRS solves a tridiagonal system
- SPTTS2 solves a tridiagonal system using the factorization of A computed by SPTTRF
- SRSCL multiplies an n-element real vector x by the real scalar 1/a
- SSBEV computes all the eigenvalues and, optionally, eigenvectors of a real symmetric band matrix A
- SSBEVD computes all the eigenvalues and, optionally, eigenvectors of a real symmetric band matrix A
- SSBEVX computes selected eigenvalues and, optionally, eigenvectors of a real symmetric band matrix A
- SSBGST reduces a real symmetric-definite banded generalized eigenproblem
- SSBGV computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite banded eigenproblem
- SSBGVD computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite banded eigenproblem

- SSBGVX computes selected eigenvalues, and optionally, eigenvectors of a real generalized symmetric-definite banded eigenproblem
- SSBTRD reduces a real symmetric band matrix A to symmetric tridiagonal form T by an orthogonal similarity transformation
- SSPCON estimates the reciprocal of the condition number (in the 1-norm) of a real symmetric packed matrix A
- SSPEV computes all the eigenvalues and, optionally, eigenvectors of a real symmetric matrix A in packed storage
- SSPEVD computes all the eigenvalues and, optionally, eigenvectors of a real symmetric matrix A in packed storage
- SSPEVX computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix A in packed storage
- SSPGST reduces a real symmetric-definite generalized eigenproblem to standard form, using packed storage
- SSPGV computes all the eigenvalues and, optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
- SSPGVD computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
- SSPGVX computes selected eigenvalues, and optionally, eigenvectors of a real generalized symmetric-definite eigenproblem
- SSPRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric indefinite and packed
- SSPSV computes the solution to a real system of linear equations
- SSPSVX uses the diagonal pivoting factorization to compute the solution to a real system of linear equations
- SSPTRD reduces a real symmetric matrix A stored in packed form to symmetric tridiagonal form T by an orthogonal similarity transformation
- SSPTRF computes the factorization of a real symmetric matrix A stored in packed format using the Bunch-Kaufman diagonal pivoting method
- SSPTRI computes the inverse of a real symmetric indefinite matrix A in packed storage using the factorization computed by SSPTRF

- SSPTRS solves a system of linear equations with a real symmetric matrix A stored in packed format using the factorization computed by SSPTRF
- SSTEBZ computes the eigenvalues of a symmetric tridiagonal matrix T
- SSTEDC computes all eigenvalues and, optionally, eigenvectors of a symmetric tridiagonal matrix using the divide and conquer method
- SSTEGR computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix T
- SSTEIN computes the eigenvectors of a real symmetric tridiagonal matrix T corresponding to specified eigenvalues, using inverse iteration
- SSTEQR computes all eigenvalues and, optionally, eigenvectors of a symmetric tridiagonal matrix using the implicit QL or QR method
- SSTERF computes all eigenvalues of a symmetric tridiagonal matrix using the Pal-Walker-Kahan variant of the QL or QR algorithm
- SSTEV computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix A
- SSTEVD computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix
- SSTEVR computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix T
- SSTEVX computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix A
- SSYCON estimates the reciprocal of the condition number (in the 1-norm) of a real symmetric matrix A using the factorization computed by SSYTRF
- SSYEV computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix A
- SSYEVD computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix A
- SSYEVR computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix T
- SSYEVX computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix A

- SSYGS2 reduces a real symmetric-definite generalized eigenproblem to standard form
- SSYGST reduces a real symmetric-definite generalized eigenproblem to standard form
- SSYGV computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
- SSYGVD computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
- SSYGVX computes selected eigenvalues, and optionally, eigenvectors of a real generalized symmetric-definite eigenproblem
- SSYRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric indefinite
- SSYSV computes the solution to a real system of linear equations
- SSYSVX uses the diagonal pivoting factorization to compute the solution to a real system of linear equations
- SSYTD2 reduces a real symmetric matrix A to symmetric tridiagonal form T by an orthogonal similarity transformation
- SSYTF2 computes the factorization of a real symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- SSYTRD reduces a real symmetric matrix A to real symmetric tridiagonal form T by an orthogonal similarity transformation
- SSYTRF computes the factorization of a real symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- SSYTRI computes the inverse of a real symmetric indefinite matrix A using the factorization computed by SSYTRF
- SSYTRS solves a system of linear equations with a real symmetric matrix A using the factorization computed by SSYTRF
- STBCON estimates the reciprocal of the condition number of a triangular band matrix A, in either the 1-norm or the infinity-norm
- STBRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular band coefficient matrix

- STBTRS solves a triangular system of the form
- STGEVC computes some or all of the right and/or left generalized eigenvectors of a pair of real upper triangular matrices (A,B)
- STGEX2 swaps adjacent diagonal blocks (A11, B11) and (A22, B22) of size 1-by-1 or 2-by-2 in an upper (quasi) triangular matrix pair (A, B) by an orthogonal equivalence transformation
- STGEXC reorders the generalized real Schur decomposition of a real matrix pair (A,B) using an orthogonal equivalence transformation
- STGSEN reorders the generalized real Schur decomposition of a real matrix pair (A, B)
- STGSJA computes the generalized singular value decomposition (GSVD) of two real upper triangular (or trapezoidal) matrices A and B
- STGSNA estimates reciprocal condition numbers for specified eigenvalues and/or eigenvectors of a matrix pair
- STGSY2 solves the generalized Sylvester equation
- STGSYL solves the generalized Sylvester equation
- STPCON estimates the reciprocal of the condition number of a packed triangular matrix A, in either the 1-norm or the infinity-norm
- STPRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular packed coefficient matrix
- STPTRI computes the inverse of a real upper or lower triangular matrix A stored in packed format
- STPTRS solves a triangular system
- STRCON estimates the reciprocal of the condition number of a triangular matrix A, in either the 1-norm or the infinity-norm
- STREVC computes some or all of the right and/or left eigenvectors of a real upper quasi-triangular matrix T
- STREXC reorders the real Schur factorization of a real matrix
- STRID computes the solution to a real system of linear equations

- STRRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular coefficient matrix
- STRSEN reorders the real Schur factorization of a real matrix
- STRSNA estimates reciprocal condition numbers for specified eigenvalues and/or right eigenvectors of a real upper quasi-triangular matrix T
- STRSYL solves the real Sylvester matrix equation
- STRTI2 computes the inverse of a real upper or lower triangular matrix
- STRTRI computes the inverse of a real upper or lower triangular matrix A
- STRTRS solves a triangular system
- STZRQF routine is deprecated and has been replaced by routine STZRZF
- STZRZF reduces the M-by-N real upper trapezoidal matrix A to upper triangular form by means of orthogonal transformations
- XERBLA error handler for the LAPACK routines
- ZBDSQR computes the singular value decomposition (SVD) of a real N-by-N (upper or lower) bidiagonal matrix B
- ZDRSCL multiplies an n-element complex vector x by the real scalar 1/a
- ZGBBRD reduces a complex general m-by-n band matrix A to real upper bidiagonal form B by a unitary transformation
- ZGBCON estimates the reciprocal of the condition number of a complex general band matrix A, in either the 1-norm or the infinity-norm,
- ZGBEQU computes row and column scalings intended to equilibrate an M-by-N band matrix A and reduce its condition number
- ZGBRFS improves the computed solution to a system of linear equations when the coefficient matrix is banded, and provides error bounds and backward error estimates for the solution
- ZGBSV computes the solution to a complex system of linear equations where A is a band matrix of order N with KL subdiagonals and KU superdiagonals, and X and B are N-by-NRHS matrices
- ZGBSVX uses the LU factorization to compute the solution to a complex system of linear equations

- ZGBTF2 computes an LU factorization of a complex m-by-n band matrix A using partial pivoting with row interchanges
- ZGBTRF computes an LU factorization of a complex m-by-n band matrix A using partial pivoting with row interchanges
- ZGBTRS solves a system of linear equations with a general band matrix A using the LU factorization computed by ZGBTRF
- ZGEBAK forms the right or left eigenvectors of a complex general matrix by backward transformation on the computed eigenvectors of the balanced matrix output by ZGEBAL
- ZGEBAL balances a general complex matrix A
- ZGEBD2 reduces a complex general m by n matrix A to upper or lower real bidiagonal form B by a unitary transformation
- ZGEBRD reduces a general complex M-by-N matrix A to upper or lower bidiagonal form B by a unitary transformation
- ZGECON estimates the reciprocal of the condition number of a general complex matrix A, in either the 1-norm or the infinity-norm, using the LU factorization computed by ZGETRF
- ZGEEQU computes row and column scalings intended to equilibrate an M-by-N matrix A and reduce its condition number
- ZGEES computes for an N-by-N complex nonsymmetric matrix A, the eigenvalues, the Schur form T, and, optionally, the matrix of Schur vectors Z
- ZGEESX computes for an N-by-N complex nonsymmetric matrix A, the eigenvalues, the Schur form T, and, optionally, the matrix of Schur vectors Z
- ZGEEV computes for an N-by-N complex nonsymmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors
- ZGEEVX computes for an N-by-N complex nonsymmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors
- ZGEGS routine is deprecated and has been replaced by routine ZGGES
- ZGEGV routine is deprecated and has been replaced by routine ZGGEV
- ZGEHD2 reduces a complex general matrix A to upper Hessenberg form H by a unitary similarity transformation

- ZGEHRD reduces a complex general matrix A to upper Hessenberg form H by a unitary similarity transformation
- ZGELQ2 computes an LQ factorization of a complex m by n matrix A
- ZGELQF computes an LQ factorization of a complex M-by-N matrix A
- ZGELS solves overdetermined or underdetermined complex linear systems involving an M-by-N matrix A, or its conjugate-transpose, using a QR or LQ factorization of A
- ZGELSD computes the minimum-norm solution to a real linear least squares problem
- ZGELSS computes the minimum norm solution to a complex linear least squares problem
- ZGELSX routine is deprecated and has been replaced by routine ZGELSY
- ZGELSY computes the minimum-norm solution to a complex linear least squares problem
- ZGEQL2 computes a QL factorization of a complex m by n matrix A
- ZGEQLF computes a QL factorization of a complex M-by-N matrix A
- ZGEQP3 computes a QR factorization with column pivoting of a matrix A
- ZGEQPF routine is deprecated and has been replaced by routine ZGEQP3
- ZGEQR2 computes a QR factorization of a complex m by n matrix A
- ZGEQRF computes a QR factorization of a complex M-by-N matrix A
- ZGERFS improves the computed solution to a system of linear equations and provides error bounds and backward error estimates for the solution
- ZGERQ2 computes an RQ factorization of a complex m by n matrix A
- ZGERQF computes an RQ factorization of a complex M-by-N matrix A
- ZGESC2 solves a system of linear equations with a general N-by-N matrix A using the LU factorization with complete pivoting computed by ZGETC2
- ZGESDD computes the singular value decomposition (SVD) of a complex M-by-N matrix A

- ZGESV computes the solution to a complex system of linear equations
- ZGESVD computes the singular value decomposition (SVD) of a complex M-by-N matrix A
- ZGESVX uses the LU factorization to compute the solution to a complex system of linear equations
- ZGETC2 computes an LU factorization, using complete pivoting, of the n-by-n matrix A
- ZGETF2 computes an LU factorization of a general m-by-n matrix A using partial pivoting with row interchanges
- ZGETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges
- ZGETRI computes the inverse of a matrix using the LU factorization computed by ZGETRF
- ZGETRS solves a system of linear equations with a general N-by-N matrix A using the LU factorization computed by ZGETRF
- ZGGBAK forms the right or left eigenvectors of a complex generalized eigenvalue problem by backward transformation on the computed eigenvectors of the balanced pair of matrices output by ZGGBAL
- ZGGBAL balances a pair of general complex matrices (A,B)
- ZGGES computes for a pair of N-by-N complex nonsymmetric matrices (A,B), the generalized eigenvalues, the generalized complex Schur form (S, T), and optionally left and/or right Schur vectors (VSL and VSR)
- ZGGESX computes for a pair of N-by-N complex nonsymmetric matrices (A,B), the generalized eigenvalues, the complex Schur form (S,T),
- ZGGEV computes for a pair of N-by-N complex nonsymmetric matrices (A,B), the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
- ZGGEVX computes for a pair of N-by-N complex nonsymmetric matrices (A,B) the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
- ZGGGLM solves a general Gauss-Markov linear model (GLM) problem

- ZGGHRD reduces a pair of complex matrices (A,B) to generalized upper Hessenberg form using unitary transformations, where A is a general matrix and B is upper triangular
- ZGGLSE solves the linear equality-constrained least squares (LSE) problem
- ZGGQRF computes a generalized QR factorization of an N-by-M matrix A and an N-by-P matrix B
- ZGGRQF computes a generalized RQ factorization of an M-by-N matrix A and a P-by-N matrix B
- ZGGSVD computes the generalized singular value decomposition (GSVD) of an M-by-N complex matrix A and P-by-N complex matrix B
- ZGGSVP computes unitary matrices U, V and Q
- ZGTCON estimates the reciprocal of the condition number of a complex tridiagonal matrix A using the LU factorization as computed by ZGTTRF
- ZGTRFS improves the computed solution to a system of linear equations when the coefficient matrix is tridiagonal, and provides error bounds and backward error estimates for the solution
- ZGTSV solves the equation AX = B
- ZGTSVX uses the LU factorization to compute the solution to a complex system of linear equations
- ZGTTRF computes an LU factorization of a complex tridiagonal matrix A using elimination with partial pivoting and row interchanges
- ZGTTRS solves one of the systems of equations
- ZGTTS2 solves one of the systems of equations
- ZHBEV computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix A
- ZHBEVD computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix A
- ZHBEVX computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix A

- ZHBGST reduces a complex Hermitian-definite banded generalized eigenproblem to standard form
- ZHBGV computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite banded eigenproblem
- ZHBGVD computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite banded eigenproblem
- ZHBGVX computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite banded eigenproblem
- ZHBTRD reduces a complex Hermitian band matrix A to real symmetric tridiagonal form T by a unitary similarity transformation
- ZHECON estimates the reciprocal of the condition number of a complex Hermitian matrix A using the factorization computed by ZHETRF
- ZHEEV computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A
- ZHEEVD computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A
- ZHEEVR computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix T
- ZHEEVX computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A
- ZHEGS2 reduces a complex Hermitian-definite generalized eigenproblem to standard form
- ZHEGST reduces a complex Hermitian-definite generalized eigenproblem to standard form
- ZHEGV computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
- ZHEGVD computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
- ZHEGVX computes selected eigenvalues, and optionally, eigenvectors of a complex generalized Hermitian-definite eigenproblem

- ZHERFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian indefinite, and provides error bounds and backward error estimates for the solution
- ZHESV computes the solution to a complex system of linear equations
- ZHESVX uses the diagonal pivoting factorization to compute the solution to a complex system of linear equations
- ZHETD2 reduces a complex Hermitian matrix A to real symmetric tridiagonal form T by a unitary similarity transformation
- ZHETF2 computes the factorization of a complex Hermitian matrix A using the Bunch-Kaufman diagonal pivoting method
- ZHETRD reduces a complex Hermitian matrix A to real symmetric tridiagonal form T by a unitary similarity transformation
- ZHETRF computes the factorization of a complex Hermitian matrix A using the Bunch-Kaufman diagonal pivoting method
- ZHETRI computes the inverse of a complex Hermitian indefinite matrix A using the factorization computed by ZHETRF
- ZHETRS solves a system of linear equations with a complex Hermitian matrix A using the factorization computed by ZHETRF
- ZHGEQZ implements a single-shift version of the QZ method for finding generalized eigenvalues
- ZHPCON estimates the reciprocal of the condition number of a complex Hermitian packed matrix A using the factorization computed by ZHPTRF
- ZHPEV computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix in packed storage
- ZHPEVD computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A in packed storage
- ZHPEVX computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A in packed storage
- ZHPGST reduces a complex Hermitian-definite generalized eigenproblem to standard form, using packed storage

- ZHPGV computes all the eigenvalues and, optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
- ZHPGVD computes all the eigenvalues and, optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
- ZHPGVX computes selected eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian-definite eigenproblem
- ZHPRFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian indefinite and packed, and provides error bounds and backward error estimates for the solution
- ZHPSV computes the solution to a complex system of linear equations
- ZHPSVX uses the diagonal pivoting factorization to compute the solution to a complex system of linear equations
- ZHPTRD reduces a complex Hermitian matrix A stored in packed form to real symmetric tridiagonal form T by a unitary similarity transformation
- ZHPTRF computes the factorization of a complex Hermitian packed matrix A using the Bunch-Kaufman diagonal pivoting method
- ZHPTRI computes the inverse of a complex Hermitian indefinite matrix A in packed storage using the factorization computed by ZHPTRF
- ZHPTRS solves a system of linear equations with a complex Hermitian matrix A stored in packed format using the factorization computed by ZHPTRF
- ZHSEIN uses inverse iteration to find specified right and/or left eigenvectors of a complex upper Hessenberg matrix H
- ZHSEQR computes the eigenvalues of a complex upper Hessenberg matrix H, and, optionally, the matrices T and Z from the Schur decomposition
- ZLABRD reduces the first NB rows and columns of a complex general m by n matrix A to upper or lower real bidiagonal form by a unitary transformation
- ZLACGV conjugates a complex vector of length N
- ZLACON estimatse the 1-norm of a square, complex matrix A
- ZLACP2 copies all or part of a real two-dimensional matrix A to a complex matrix B

- ZLACPY copies all or part of a two-dimensional matrix A to another matrix B
- ZLACRM performs a very simple matrix-matrix multiplication
- ZLACRT performs the operation (c s)(x)==> (x)(-s c)(y)(y) where c and s are complex and the vectors x and y are complex
- ZLADIV := X / Y, where X and Y are complex
- ZLAED0 computes all eigenvalues of a symmetric tridiagonal matrix
- ZLAED7 computes the updated eigensystem of a diagonal matrix after modification by a rank-one symmetric matrix
- ZLAED8 merges the two sets of eigenvalues together into a single sorted set
- ZLAEIN uses inverse iteration to find a right or left eigenvector corresponding to the eigenvalue W of a complex upper Hessenberg matrix H
- ZLAESY computes the eigendecomposition of a 2-by-2 symmetric matrix
- ZLAEV2 computes the eigendecomposition of a 2-by-2 Hermitian matrix
- ZLAGS2 computes 2-by-2 unitary matrices U, V and Q
- ZLAGTM performs a matrix-vector product
- ZLAHEF computes a partial factorization of a complex Hermitian matrix A using the Bunch-Kaufman diagonal pivoting method
- ZLAHQR called by ZHSEQR to update the eigenvalues and Schur decomposition already computed by ZHSEQR
- ZLAHRD reduces the first NB columns of a complex general n-by-(n-k+1) matrix A so that elements below the k<sup>th</sup> subdiagonal are zero
- ZLAIC1 applies one step of incremental condition estimation in its simplest version
- ZLALSO applies back the multiplying factors of either the left or the right singular vector matrix of a diagonal matrix appended by a row to the right hand side matrix B in solving the least squares problem using the divide-and-conquer SVD approach
- ZLALSA an itermediate step in solving the least squares problem by computing the SVD of the coefficient matrix in compact form

- ZLALSD uses the singular value decomposition of A to solve the least squares problem of finding X to minimize the Euclidean norm
- ZLANGB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n band matrix A,
- ZLANGE returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex matrix A
- ZLANGT returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex tridiagonal matrix A
- ZLANHB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n hermitian band matrix A, with k super-diagonals
- ZLANHE returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex hermitian matrix A
- ZLANHP returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex hermitian matrix A, supplied in packed form
- ZLANHS returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a Hessenberg matrix A
- ZLANHT returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex Hermitian tridiagonal matrix A
- ZLANSB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n symmetric band matrix A, with k super-diagonals
- ZLANSP returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex symmetric matrix A, supplied in packed form
- ZLANSY returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex symmetric matrix A
- ZLANTB returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n by n triangular band matrix A, with (k + 1) diagonals

- ZLANTP returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a triangular matrix A, supplied in packed form
- ZLANTR returns the value of the one norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a trapezoidal or triangular matrix A
- ZLAPLL computes the QR factorization of A=QR
- ZLAPMT rearranges the columns of the M by N matrix X
- ZLAQGB equilibrates a general M by N band matrix A with KL subdiagonals and KU superdiagonals using the row and scaling factors in the vectors R and C
- ZLAQGE equilibrates a general M by N matrix A using the row and scaling factors in the vectors R and C
- ZLAQHB equilibrates a symmetric band matrix A using the scaling factors in the vector S
- ZLAQHE equilibrates a Hermitian matrix A using the scaling factors in the vector S
- ZLAQHP equilibrates a Hermitian matrix A using the scaling factors in the vector S
- ZLAQP2 computes a QR factorization with column pivoting
- ZLAQPS computes a step of QR factorization with column pivoting of a complex M-by-N matrix A by using Blas-3
- ZLAQSB equilibrates a symmetric band matrix A using the scaling factors in the vector S
- ZLAQSP equilibrates a symmetric matrix A using the scaling factors in the vector S
- ZLAQSY equilibrates a symmetric matrix A using the scaling factors in the vector S
- ZLARIV computes the (scaled) r<sup>th</sup> column of the inverse of the sumbmatrix
- ZLAR2V applies a vector of complex plane rotations with real cosines from both sides to a sequence of 2-by-2 complex Hermitian matrices,
- ZLARCM performs a very simple matrix-matrix multiplication

- ZLARF applies a complex elementary reflector H to a complex M-by-N matrix C, from either the left or the right
- ZLARFB applies a complex block reflector H or its transpose H' to a complex M-by-N matrix C, from either the left or the right
- ZLARFG generates a complex elementary reflector H o
- ZLARFT forms the triangular factor T of a complex block reflector H of order n, which is defined as a product of k elementary reflectors
- ZLARFX applies a complex elementary reflector H to a complex m by n matrix C, from either the left or the right
- ZLARGV generates a vector of complex plane rotations with real cosines, determined by elements of the complex vectors x and y
- ZLARNV returns a vector of n random complex numbers from a uniform or normal distribution
- ZLARRV computes the eigenvectors of a tridiagonal matrix
- ZLARTG generates a plane rotation
- ZLARTV applies a vector of complex plane rotations with real cosines to elements of the complex vectors x and y
- ZLARZ applies a complex elementary reflector H to a complex M-by-N matrix C, from either the left or the right
- ZLARZB applies a complex block reflector H or its transpose to a complex distributed M-by-N C from the left or the right
- ZLARZT forms the triangular factor T of a complex block reflector which is defined as a product of k elementary reflectors
- ZLASCL multiplies the M by N complex matrix A by the real scalar CTO/CFROM
- ZLASET initializes a 2-D array A to BETA on the diagonal and ALPHA on the offdiagonals
- ZLASR performs a transformation where A is an m by n complex matrix and P is an orthogonal matrix
- ZLASSQ returns the values scl and ssq
- ZLASWP performs a series of row interchanges on the matrix A

- ZLASYF computes a partial factorization of a complex symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- ZLATBS solves triangular systems
- ZLATDF computes the contribution to the reciprocal Dif-estimate
- ZLATPS solves triangular systems
- ZLATRD reduces NB rows and columns of a complex Hermitian matrix A to Hermitian tridiagonal form
- ZLATRS solves triangular systems
- ZLATRZ factors the M-by-(M+L) complex upper trapezoidal matrix
- ZLATZM routine is deprecated and has been replaced by routine ZUNMRZ
- ZLAUU2 computes the product  $U \times U'$  or  $L' \times L$
- ZLAUUM computes the product U × U' or L' × L
- ZPBCON estimates the reciprocal of the condition number (in the 1-norm) of a complex Hermitian positive definite band matrix
- ZPBEQU computes row and column scalings intended to equilibrate a Hermitian positive definite band matrix A
- ZPBRFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian positive definite and banded
- ZPBSTF computes a split Cholesky factorization of a complex Hermitian positive definite band matrix A
- ZPBSV computes the solution to a complex system of linear equations
- ZPBSVX uses the Cholesky factorization to compute the solution to a complex system of linear equations
- ZPBTF2 computes the Cholesky factorization of a complex Hermitian positive definite band matrix A
- ZPBTRF computes the Cholesky factorization of a complex Hermitian positive definite band matrix A
- ZPBTRS solves a system of linear equations with a Hermitian positive definite band matrix A using the Cholesky factorization computed by ZPBTRF

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- ZPOCON estimates the reciprocal of the condition number (in the 1-norm) of a complex Hermitian positive definite matrix using the Cholesky factorization computed by ZPOTRF
- ZPOEQU computes row and column scalings intended to equilibrate a Hermitian positive definite matrix A and reduce its condition number (with respect to the two-norm)
- ZPORFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian positive definite,
- ZPOSV computes the solution to a complex system of linear equations
- ZPOSVX uses the Cholesky factorization to compute the solution to a complex system of linear equations
- ZPOTF2 computes the Cholesky factorization of a complex Hermitian positive definite matrix A
- ZPOTRF computes the Cholesky factorization of a complex Hermitian positive definite matrix A
- ZPOTRI computes the inverse of a complex Hermitian positive definite matrix A using the Cholesky factorization computed by ZPOTRF
- ZPOTRS solves a system of linear equations with a Hermitian positive definite matrix A using the Cholesky factorization computed by ZPOTRF
- ZPPCON estimates the reciprocal of the condition number (in the 1-norm) of a complex Hermitian positive definite packed matrix using the Cholesky factorization computed by ZPPTRF
- ZPPEQU computes row and column scalings intended to equilibrate a Hermitian positive definite matrix A in packed storage and reduce its condition number (with respect to the two-norm)
- ZPPRFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian positive definite and packed, and provides error bounds and backward error estimates for the solution
- ZPPSV computes the solution to a complex system of linear equations
- ZPPSVX use the Cholesky factorization to compute the solution to a complex system of linear equations

- ZPPTRF computes the Cholesky factorization of a complex Hermitian positive definite matrix A stored in packed format
- ZPPTRI computes the inverse of a complex Hermitian positive definite matrix A using the Cholesky factorization computed by ZPPTRF
- ZPPTRS solves a system of linear equations with a Hermitian positive definite matrix A in packed storage using the Cholesky factorization computed by ZPPTRF
- ZPTCON computes the reciprocal of the condition number (in the 1-norm) of a complex Hermitian positive definite tridiagonal matrix using the factorization computed by ZPTTRF
- ZPTEQR computes all eigenvalues and, optionally, eigenvectors of a symmetric positive definite tridiagonal matrix
- ZPTRFS improves the computed solution to a system of linear equations when the coefficient matrix is Hermitian positive definite and tridiagonal, and provides error bounds and backward error estimates for the solution
- ZPTSV computes the solution to a complex system of linear equations where A is an N-by-N Hermitian positive definite tridiagonal matrix, and X and B are N-by-NRHS matrices
- ZPTSVX uses the factorization to compute the solution to a complex system of linear equations where A is an N-by-N Hermitian positive definite tridiagonal matrix and X and B are N-by-NRHS matrices
- ZPTTRF computes the factorization of a complex Hermitian positive definite tridiagonal matrix A
- ZPTTRS solves a tridiagonal system of the form using the factorization computed by ZPTTRF
- ZPTTS2 solves a tridiagonal system of the form using the factorization computed by ZPTTRF
- ZSPCON estimates the reciprocal of the condition number (in the 1-norm) of a complex symmetric packed matrix A using the factorization computed by ZSPTRF
- ZSPRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric indefinite and packed, and provides error bounds and backward error estimates for the solution
- ZSPSV computes the solution to a complex system of linear equations

- ZSPSVX uses the diagonal pivoting factorization to compute the solution to a complex system of linear equations
- ZSPTRF computes the factorization of a complex symmetric matrix A stored in packed format using the Bunch-Kaufman diagonal pivoting method
- ZSPTRI computes the inverse of a complex symmetric indefinite matrix A in packed storage using the factorization computed by ZSPTRF
- ZSPTRS solves a system of linear equations with a complex symmetric matrix A stored in packed format using the factorization computed by ZSPTRF
- ZSTEDC computes all eigenvalues and, optionally, eigenvectors of a symmetric tridiagonal matrix using the divide and conquer method
- ZSTEGR computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix T
- ZSTEIN computes the eigenvectors of a real symmetric tridiagonal matrix T corresponding to specified eigenvalues, using inverse iteration
- ZSTEQR computes all eigenvalues and, optionally, eigenvectors of a symmetric tridiagonal matrix using the implicit QL or QR method
- ZSYCON estimates the reciprocal of the condition number (in the 1-norm) of a complex symmetric matrix A using the factorization computed by ZSYTRF
- ZSYRFS improves the computed solution to a system of linear equations when the coefficient matrix is symmetric indefinite, and provides error bounds and backward error estimates for the solution
- ZSYSV computes the solution to a complex system of linear equations
- ZSYSVX uses the diagonal pivoting factorization to compute the solution to a complex system of linear equations
- ZSYTF2 computes the factorization of a complex symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- ZSYTRF computes the factorization of a complex symmetric matrix A using the Bunch-Kaufman diagonal pivoting method
- ZSYTRI computes the inverse of a complex symmetric indefinite matrix A using the factorization computed by ZSYTRF

- ZSYTRS solves a system of linear equations with a complex symmetric matrix A using the factorization computed by ZSYTRF
- ZTBCON estimates the reciprocal of the condition number of a triangular band matrix A, in either the 1-norm or the infinity-norm
- ZTBRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular band coefficient matrix
- ZTBTRS solves a triangular system
- ZTGEVC computes some or all of the right and/or left generalized eigenvectors of a pair of complex upper triangular matrices (A,B)
- ZTGEX2 swaps adjacent diagonal 1 by 1 blocks (A11,B11) and (A22,B22)
- ZTGEXC reorders the generalized Schur decomposition of a complex matrix pair (A,B)
- ZTGSEN reorders the generalized Schur decomposition of a complex matrix pair (A, B)
- ZTGSJA computes the generalized singular value decomposition (GSVD) of two complex upper triangular (or trapezoidal) matrices A and B
- ZTGSNA estimates reciprocal condition numbers for specified eigenvalues and/or eigenvectors of a matrix pair (A, B)
- ZTGSY2 solves the generalized Sylvester equation
- ZTGSYL solves the generalized Sylvester equation
- ZTPCON estimates the reciprocal of the condition number of a packed triangular matrix A, in either the 1-norm or the infinity-norm
- ZTPRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular packed coefficient matrix
- ZTPTRI computes the inverse of a complex upper or lower triangular matrix A stored in packed format
- ZTPTRS solves a triangular system
- ZTRCON estimates the reciprocal of the condition number of a triangular matrix A, in either the 1-norm or the infinity-norm

- ZTREVC computes some or all of the right and/or left eigenvectors of a complex upper triangular matrix T
- ZTREXC reorders the Schur factorization of a complex matrix so that the diagonal element of T with row index IFST is moved to row ILST
- ZTRID computes the solution to a complex system of linear equations where A is an N-by-N tridiagonal matrix, and x and b are vectors of length N
- ZTRRFS provides error bounds and backward error estimates for the solution to a system of linear equations with a triangular coefficient matrix
- ZTRSEN reorders the Schur factorization of a complex matrix
- ZTRSNA estimates reciprocal condition numbers for specified eigenvalues and/or right eigenvectors of a complex upper triangular matrix T
- ZTRSYL solves the complex Sylvester matrix equation
- ZTRTI2 computes the inverse of a complex upper or lower triangular matrix
- ZTRTRI computes the inverse of a complex upper or lower triangular matrix A
- ZTRTRS solves a triangular system
- ZTZRQF routine is deprecated and has been replaced by routine ZTZRZF
- ZTZRZF reduces the M-by-N complex upper trapezoidal matrix A to upper triangular form by means of unitary transformations
- ZUNG2L generates an m by n complex matrix Q with orthonormal columns,
- ZUNG2R generates an m by n complex matrix Q with orthonormal columns,
- ZUNGBR generates one of the complex unitary matrices determined by ZGEBRD when reducing a complex matrix A to bidiagonal form
- ZUNGHR generates a complex unitary matrix Q
- ZUNGL2 generates an m-by-n complex matrix Q with orthonormal rows,
- ZUNGLQ generates an M-by-N complex matrix Q with orthonormal rows,
- ZUNGQL generates an M-by-N complex matrix Q with orthonormal columns,
- ZUNGQR generates an M-by-N complex matrix Q with orthonormal columns,
- ZUNGR2 generates an m by n complex matrix Q with orthonormal rows,

- ZUNGRQ generates an M-by-N complex matrix Q with orthonormal rows,
- ZUNGTR generates a complex unitary matrix Q which is defined as the product of n-1 elementary reflectors of order N, as returned by ZHETRD
- ZUNM2L overwrites the general complex m-by-n matrix C
- ZUNM2R overwrites the general complex m-by-n matrix C
- ZUNMBR overwrites the general complex M-by-N matrix C
- ZUNMHR overwrites the general complex M-by-N matrix C
- ZUNML2 overwrites the general complex m-by-n matrix C
- ZUNMLQ overwrites the general complex M-by-N matrix C
- ZUNMQL overwrites the general complex M-by-N matrix C
- ZUNMQR overwrites the general complex M-by-N matrix C
- ZUNMR2 overwrites the general complex m-by-n matrix C
- ZUNMR3 overwrites the general complex m by n matrix C
- ZUNMRQ overwrites the general complex M-by-N matrix C
- ZUNMRZ overwrites the general complex M-by-N matrix C
- ZUPGTR generates a complex unitary matrix Q
- ZUPMTR overwrites the general complex M-by-N matrix C

# Glossary

## Basic Linear Algebra Subprogram

A set of commonly used algebraic equations defined by C. L. Lawson, and J. J. Dongerra, in a series of papers (see bibliography of *LAPACK User's Guide*, publication TPD–0003, pp. 112–115, entries [16], [17], [18], [19], and [38].

## BCG

See Bi-Conjugate Gradient Method.

## **Bi-Conjugate Gradient Method**

One of the iterative methods provided through the DITERATIVE package of optimized precondtioned iterative methods.

## BLAS

See Basic Linear Algebra Subprogram.

# CGM

See Conjugate Gradient Method.

# CGS

See Bi-Conjugate Gradient Squared Method.

## computational routines

Term used to define LAPACK routines that perform a distinct computational task.

# **Conjugate Gradient Method**

One of the iterative methods provided through the DITERATIVE package of optimized preconditioned iterative methods.

#### dedicated environment

A parallel processing environment in which the NCPUS environment variable is equal to the number of available processors.

#### direct solution methods

Direct solution methods for sparse linear systems transform the matrix *A* into a product of several other operators so that each of the resulting operators is easy to invert for a given right-hand side *b*.

#### driver routines

Term used to define LAPACK routines used for solving standard types of problems.

#### equilibration

The process of scaling a problem before computing its solution.

#### Fourier analysis

The mathematical process of resolving a given function, f(x), into its frequency components, which means finding the sequence of constant amplitudes to plug into a Fourier series to reconstruct the original function.

#### Hermitian matrix

A complex matrix which is equal to the conjugate of its transpose, with either the lower or upper triangle being stored.

#### iterative solution methods

Iterative solution methods for sparse linear systems attempt to solve Ax = b by solving an equivalent system  $M^{-1}Ax = M^{-1}b$ , where M is some approximation to A which is inexpensive to construct and can be easily used to compute z. Unlike direct methods, iterative methods are more special-purpose. There are no general, effective iterative algorithms for an arbitrary sparse linear system.

# LAPACK

A public domain library of subroutines for solving dense linear algebra problems, including systems of linear equations, linear least squares problems, eigenvalue problems, and singular value problems. It has been designed for efficiency on high-performance computers.

## linear system

A set of simultaneous linear algebraic equations.

## load balancing

The process of dividing work done by each available processor into approximately equal amounts.

## multiuser environment

A parallel processing environment in which users do not know how many processors will be available to a job during run time.

#### out-of-core technique

A term that refers to algorithms that combine input and output with computation to solve problems in which the data resides on disk or some other secondary random-access storage device.

#### packed storage

A triangular or symmetric matrix in which the full matrix representation is retained while storing only half the matrix elements.

## parallel instruction execution

The execution of one instruction per clock period, even those instructions that take several clock periods to complete execution.

#### Pipelining

A method of execution which allows each step of an operation to pass its result to the next step after only one clock period.

#### single-threaded code segments

A section of a program that must use a single processor.

#### small parallel/vector problem

A class of problem size in which problems are large enough for vector and parallel processing, but for which parallel processing degrades vector performance.

#### sparse matrix

A linear system which can be described as Ax = b, where A is an n-by-n matrix, and x and b are n dimensional vectors. A system of this kind is considered *sparse* if the matrix A has a small percentage of nonzero terms (less than 10%, often less than 1%).

## SPD

See Symmetric Positive Definite Matrix.

## SPVP

See Small Paralell/Vector Problem.

#### Strassen's algorithm

A recursive algorithm that is slightly faster than the ordinary inner product algorithm. Strassen's algorithm performs the floating-point operations for matrix multiplication in an order differently from the vector method; this can cause round-off problems.

#### supernodes

A collection of columns that have the same nonzero pattern.

#### time slicing

A method of execution in which the system works on several jobs or processes simultaneously.

#### vectorization

A form of parallel processing that uses instruction segmenting and vector registers.

## virtual matrices

A virtual matrix is similar to a Fortran array, but it cannot be accessed directly from a program. It can only be accessed with calls to specific subroutines. Users do not do any explicit input or output to read from or write to a virtual matrix.

## VP

See Vector Problem.

# well-conditioned matrix

The condition number of a matrix is defined as  $\kappa(A) = ||A|| \cdot ||A^{-1}||$ . A *well-conditioned* matrix is one for which  $\kappa(A)$  is small. Although small is relative, if  $\kappa(A) < 10^3$ , A can be considered well-conditioned.

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