

List of Contents

The contains two categories of routines which can be called by users. They are listed separately in the two sections below.

Fully Documented Routines

87 routines, for each of which an individual routine document is provided. These are regarded as the primary contents of the .

Fundamental Support Routines

15 comparatively simple routines which are documented in compact form in the relevant Chapter Introductions (X01, X02).

Note: all the routines in the above categories have either six-character names ending in 'F' or seven-character names ending in 'FP'.

Fully Documented Routines

Chapter A00: Library Identification

A00AAFP Prints details of the NAG Parallel Library implementation

Chapter D01: Quadrature

D01ATFP 1-d quadrature, adaptive, finite interval, allowing for badly behaved integrands
 D01AUFP 1-d quadrature, adaptive, finite interval, suitable for oscillating functions
 D01AXFP 1-d quadrature, adaptive, finite interval, weight functions $\cos(\omega x)$ or $\sin(\omega x)$
 D01DAFP 2-d quadrature, finite region
 D01FAFP Multi-dimensional quadrature, hyper-rectangle, adaptive
 D01GCFP Multi-dimensional quadrature, general product region, number-theoretic method

Chapter E04: Minimising or Maximising a Function

E04FDFP Unconstrained minimum of a sum of squares, Gauss–Newton algorithm using function values only (easy-to-use)
 E04JBFP Minimum of a general nonlinear function with unconstrained, Gauss–Newton algorithm using function values only (easy-to-use)

Chapter F01: Matrix Operations and Distribution

F01YAFP Cyclic row block distribution routine for real sparse matrices stored in coordinate storage format
 F01YEFP Distribution routine for real dense vectors distributed conformally to sparse matrices
 F01ZPPF Gathering of a block distributed real vector used for F07 and F08 ScaLAPACK routines
 F01ZQFP Real matrix generation and distribution in cyclic 2-d block fashion, used for F07 and F08 ScaLAPACK routines
 F01ZRFP Real matrix generation and distribution in block column fashion, used for F02 routines
 F01ZSFP Real matrix generation and distribution in cyclic 2-d block fashion, used for F04 (Black Box) routines
 F01ZVFP Complex matrix generation and distribution in cyclic 2-d block fashion, used for F07 and F08 ScaLAPACK routines
 F01ZWFP Complex matrix generation and distribution in block column fashion, used for F02 routines
 F01ZXFP Complex matrix generation and distribution in cyclic 2-d block fashion, used for F04 (Black Box) routines

Chapter F02: Eigenvalues and Eigenvectors

F02FQFP Eigenvalues and eigenvectors of a real symmetric matrix, one-sided Jacobi method
 F02FRFP Eigenvalues and eigenvectors of a complex Hermitian matrix, one-sided Jacobi method
 F02WQFP Singular Value Decomposition (SVD) of a real matrix, one-sided Jacobi method
 F02WRFP Singular Value Decomposition (SVD) of a complex matrix, one-sided Jacobi method

Chapter F04: Simultaneous Linear Equations

F04EBFP	Solution of real simultaneous linear equations with multiple right-hand sides (Black Box)
F04ECFP	Solution of complex simultaneous linear equations with multiple right-hand sides (Black Box)
F04FBFP	Solution of real symmetric positive-definite simultaneous linear equations with multiple right-hand sides (Black Box)
F04FCFP	Solution of complex Hermitian positive-definite simultaneous linear equations with multiple right-hand sides (Black Box)
F04GBFP	Solution of a real linear least-squares problem multiple right-hand sides (Black Box)

Chapter F07: Linear Equations (ScaLAPACK)

F07ADFP	LU factorization of a real general matrix (PDGETRF)
F07AEFP	Solution of a real system of linear equations, multiple right-hand sides, matrix already factorized by F07ADFP (PDGETRF)
F07ARFP	LU factorization of a complex general matrix (PZGETRF)
F07ASFP	Solution of a complex system of linear equations, multiple right-hand sides, matrix already factorized by F07ARFP (PZGETRF)
F07FDFP	Cholesky factorization of a real symmetric positive-definite matrix (PDPOTRF)
F07FEFP	Solution of a real symmetric positive-definite system of linear equations, multiple right-hand sides, matrix already factorized by F07FDFP (PDPOTRF)
F07FRFP	Cholesky factorization of a complex Hermitian positive-definite matrix (PZPOTRF)
F07FSFP	Solution of a complex Hermitian positive-definite system of linear equations, multiple right-hand sides, matrix already factorized by F07FRFP (PZPOTRF)
F07TGFP	Estimate the condition number of a real triangular matrix (PDTRCON)

Chapter F08: Least-squares Problems (ScaLAPACK)

F08AEFP	QR factorization of a real general rectangular matrix (PDGEQRF)
F08AFFP	Form all or part of an orthogonal Q from QR factorization determined by F08AEFP (PDGEQRF)
F08AGFP	Apply the orthogonal transformation determined by F08AEFP (PDORMQR)
F08ASFP	QR factorization of a complex general rectangular matrix (PZGEQRF)
F08ATFP	Form all or part of a unitary Q from QR factorization determined by F08ASFP (PZGEQRF)
F08AUFP	Apply the unitary transformation determined by F08ASFP (PZUNMQR)
F08FEFP	Orthogonal reduction of a real symmetric matrix to tridiagonal form (PDSYTRD)
F08JJFP	All or selected eigenvalues of a real symmetric tridiagonal matrix by bisection (PDSTEBZ)

Chapter F11: Sparse Linear Algebra

F11BAFP	Set-up for F11BBFP and F11BCFP, iterative solution of real (unsymmetric) system of simultaneous linear equations, Restarted Generalised Minimal Residual method (RGMRES)
F11BBFP	Main solver, iterative solution of a general (unsymmetric) system of simultaneous linear equations, Restarted Generalised Minimal Residual method (RGMRES)
F11BCFP	Information about the computations carried out by F11BBFP, iterative solution of a general (unsymmetric) system of simultaneous linear equations, Restarted Generalised Minimal Residual method (RGMRES)
F11DAFP	Incomplete <i>LU</i> factorization of the local diagonal blocks of a real sparse matrix, represented in coordinate storage format, distributed on a logical grid of processors in cyclic row block form
F11DBFP	Solution of real system of linear equations, involving a real block diagonal sparse matrix, represented in coordinate storage format, distributed on a logical grid of processors in cyclic row block form
F11DCFP	Black-box routine for sparse system of linear equations
F11GAFP	Set-up for F11GBFP and F11GCFP, iterative solution of a symmetric system of simultaneous linear equations, Conjugate Gradient method or a Lanczos method based on SYMMLQ
F11GBFP	Main solver, iterative solution of a symmetric system of simultaneous linear equations, Conjugate Gradient method or a Lanczos method based on SYMMLQ
F11GCFP	Information about the computations carried out by F11GBFP, iterative solution of a symmetric system of simultaneous linear equations, Conjugate Gradient method or a Lanczos method based on SYMMLQ
F11XAFP	Set-up for F11XBFP, matrix-vector or transposed matrix-vector product involving a real sparse matrix, represented in coordinate storage format, distributed on a logical grid of processors in cyclic row block form
F11XBFP	Computes a matrix-vector or transposed matrix-vector product involving a real sparse matrix, represented in coordinate storage format, distributed on a logical grid of processors in cyclic row block form
F11ZAFP	General set-up routine for real sparse matrices, represented in coordinate storage format, distributed on a logical grid of processors in cyclic row block form

Chapter G05: Random Number Generators

G05AAFP	Pseudo-random real numbers, uniform distribution over $(0, 1)$, Wichmann–Hill generator
G05ABFP	Select a random number generator and initialise seeds to give repeatable sequence

Chapter X04: Input/Output Utilities

X04AAF	Returns or sets a unit number for error message
X04ABF	Returns or sets a unit number for advisory messages
X04BCFP	Reads a real general matrix from an external file (stored in its natural, non-distributed form) into an array in a cyclic 2-d block distribution on 2-d logical processor grid, used for the F07 and F08 ScaLAPACK routines
X04BDFP	Outputs a real general matrix stored in a cyclic 2-d block distribution on a 2-d logical processor grid to an external file (in its natural, non-distributed form), used with the F07 and F08 ScaLAPACK routines
X04BFFP	Outputs a set of real general matrices distributed on a 2-d logical processor grid, used with the F02 routines
X04BGFP	Reads a general real matrix from an external file (stored in its natural, non-distributed form) into an array in a cyclic 2-d block distribution on a 2-d logical processor grid, used for the F04 (Black Box) routines
X04BHFP	Outputs a general real matrix stored in a cyclic 2-d block distribution on a 2-d logical processor grid to an external file (in its natural, non-distributed form), used with the F04 (Black Box) routines
X04BRFP	Reads a complex general matrix from an external file (stored in its natural, non-distributed form) into an array in a cyclic 2-d block distribution on 2-d logical processor grid, used for the F07 and F08 ScaLAPACK routines
X04BSFP	Outputs a complex general matrix stored in a cyclic 2-d block distribution on a 2-d logical processor grid to an external file (in its natural, non-distributed form), used with the F07 and F08 ScaLAPACK routines
X04BUFP	Outputs a set of complex general matrices distributed on a 2-d logical processor grid, used with the F02 routines
X04BVFP	Reads a general complex matrix from an external file (stored in its natural, non-distributed form) into an array in a cyclic 2-d block distribution on a 2-d logical processor grid, used for the F04 (Black Box) routines
X04BWFP	Outputs a general complex matrix stored in a cyclic 2-d block distribution on a 2-d logical processor grid to an external file (in its natural, non-distributed form), used with the F04 (Black Box) routines
X04YAFP	Outputs a real dense vector, distributed conformally to a sparse matrix on a logical grid of processors, to an external file

Chapter Z01: Library Utilities

Z01AAFP	Defines a 2-d logical processor grid (Library Grid) and returns the BLACS context
Z01ABFP	Undefines the logical processor grid and invalidates the BLACS context initialised by Z01AAFP
Z01ACFP	Root processor identifier
Z01ADFP	Used in creating processes outside the default library mechanism, allows multigriding, used in more advanced applications (PVM-based version only)
Z01AEFP	Used in creating processes outside the default library mechanism, allows multigriding, used in more advanced applications (MPI-based version only)
Z01BAFP	Row and column indices of the root processor within the logical grid
Z01BBFP	Identifies logical processors in context in the 2-d grid declared by Z01AAFP
Z01BDFP	Information about PVM tasks (PVM-based version only)
Z01BEFP	Topology to be used by BLACS for broadcasting and global operations
Z01BFFP	Enables debugging (PVM-based version only)
Z01BGFP	Information about MPI tasks (MPI-based version only)
Z01CAFP	Number of rows or columns of a matrix held locally on a given processor when the matrix is distributed in the cyclic 2-d block fashion (NUMROC)
Z01CBFP	Length of the workspace for F08AEFP and F08AFFP
Z01CCFP	Length of the workspace for F08AGFP
Z01CDFP	Process coordinate which possesses the entry of a distributed matrix specified by a global index (INDXG2P)
Z01CEFP	Length of the workspace for F08FEFP (PDSYTRD)

Fundamental Support Routines

Chapter X01: Mathematical Constants

X01AAF	π
X01ABF	Euler's constant, γ

Chapter X02: Machine Constants

X02AHF	Largest permissible argument for sin and cos
X02AJF	Machine precision
X02AKF	Smallest positive model number
X02ALF	Largest positive model number
X02AMF	Safe range of real floating-point arithmetic
X02ANF	Safe range of complex floating-point arithmetic
X02BBF	Largest representable integer
X02BEF	Maximum number of decimal digits that can be represented
X02BHF	Parameter of floating-point arithmetic model, b
X02BJF	Parameter of floating-point arithmetic model, p
X02BKF	Parameter of floating-point arithmetic model, e_{\min}
X02BLF	Parameter of floating-point arithmetic model, e_{\max}
X02DJF	Parameter of floating-point arithmetic model, ROUNDS
