

NAG Parallel Library, Release 3 Library Contents

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

Fully Documented Routines

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

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'.

Chapter A00 – Library Identification

A00AAFP Prints details of the NAG Parallel Library implementation

Chapter C06 – Summation of Series

C06FUFP Direct or inverse two-dimensional Fourier transform of a complex sequence
 C06GXFP Factorizes a positive integer n as $n = n_1 \times n_2$. This routine may be used in conjunction with C06MCFP
 C06MCFP Direct or inverse one-dimensional discrete Fourier transform of a complex sequence
 C06MXFP Direct or inverse three-dimensional discrete Fourier transform of a complex sequence

Chapter D01 – Quadrature

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

Chapter E04 – Minimizing or Maximizing 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

F01CPFP Element-wise maximum or minimum in absolute value of integer matrices
 F01WAFFP Gather real matrix, regarded as submatrix of matrix distributed in cyclic two-dimensional block format, used with routines from Chapters F07 and F08
 F01WBFP Gather real matrix distributed in cyclic two-dimensional block format, used with routines from Chapter F04
 F01WGFP Gather complex matrix distributed in cyclic two-dimensional block format, used with routines from Chapters F07 and F08
 F01WHFP Gather complex matrix distributed in cyclic two-dimensional block format, used with routines from Chapter F04
 F01WNFP Scatter real matrix from the root processor to the Library Grid using cyclic two-dimensional block format, used with routines from Chapters F07 and F08
 F01WPFP Scatter real matrix from the root processor to the Library Grid using cyclic two-dimensional block format, used with routines from Chapter F04
 F01WUFP Scatter complex matrix from the root processor to the Library Grid using cyclic two-dimensional block format, used with routines from Chapters F07 and F08
 F01WVFP Scatter complex matrix from the root processor to the Library Grid using cyclic two-dimensional block format, used with routines from Chapter F04
 F01XAFP Scatter real sparse matrix, stored in coordinate storage format, using cyclic row block distribution
 F01XEFP Scatter real vector distributed conformally to sparse matrix, used with routines from Chapter F11
 F01XFFP Gather real vector distributed conformally to sparse matrix, used with routines from Chapter F11
 F01XGFP Scatter integer vector distributed conformally to sparse matrix, used with routines from Chapter F11
 F01XHFP Gather integer vector distributed conformally to sparse matrix, used with routines from Chapter F11
 F01XPFP Scatter complex sparse matrix, stored in coordinate storage format, using cyclic row block distribution, used with routines from Chapter F11
 F01XTFP Scatter complex vector distributed conformally to sparse matrix, used with routines from Chapter F11
 F01XUFP Gather complex vector distributed conformally to sparse matrix, used with routines from Chapter F11
 F01YAFFP In-place generation of real sparse matrix using cyclic row block distribution
 F01YBFP In-place generation of real sparse matrix using cyclic row block distribution (suitable for repeated sparsity pattern), used with routines from Chapter F11
 F01YEFP In-place generation of real dense vector distributed conformally to sparse matrix
 F01YFPFP In-place generation of complex sparse matrix according to cyclic row block distribution, used with routines from Chapter F11

- F01YQFP In-place generation of complex sparse matrix according to cyclic row block distribution (suitable for repeated sparsity pattern)
- F01YTFP In-place generation of complex dense vector distributed conformally to sparse matrix, used with routines from Chapter F11
- F01YWFP In-place generation of complex Hermitian banded matrix in column block fashion, used with routines from Chapter F07
- F01YXFP In-place generation of real symmetric banded matrix in column block fashion, used with routines from Chapter F07
- F01YYFP In-place generation of real matrix in row block fashion on a one-dimensional grid of processors, used with routines from Chapter F07
- F01YZFP In-place generation of complex matrix in row block fashion on a one-dimensional grid of processors, used with routines from Chapter F07
- F01ZHFP Generates an l by m by n three-dimensional array $A(i, j, k)$ on a grid of processors in i -block form
- F01ZMFP In-place generation of real matrix in row block fashion, used with routines from Chapters C06 and F04
- F01ZNFP In-place generation of complex matrix in row block fashion, used with routines from Chapter F04
- F01ZPPF Gather real vector distributed conformally to matrix, used with routines from Chapters F07 and F08
- F01ZQFP In-place generation of real matrix in cyclic two-dimensional block fashion, used with routines from Chapters F07 and F08
- F01ZRFP In-place generation of real matrix in column block fashion, used with routines from Chapters F02 and F04
- F01ZSFP In-place generation of real matrix in cyclic two-dimensional block fashion, used with routines from Chapter F04 (Black Box)
- F01ZVFP In-place generation of complex matrix in cyclic two-dimensional block fashion, used with routines from Chapters F07 and F08
- F01ZWFP In-place generation of complex matrix in column block fashion, used with routines from Chapters F02 and F04
- F01ZXFP In-place generation of complex matrix in cyclic two-dimensional block fashion, used with routines from Chapters F04 (Black Box)
- F01ZYFP In-place generation of complex vector in column block fashion, used with routines from Chapter F07
- F01ZZFP In-place generation of real vector in column block fashion, used with routines from Chapter F07

Chapter F02 – Eigenvalues and Eigenvectors

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

Chapter F04 – Simultaneous Linear Equations

- F04EBFP Solution of real linear system (Black Box)
- F04ECFP Solution of complex linear equations (Black Box)
- F04FBFP Solution of real symmetric positive-definite linear system (Black Box)
- F04FCFP Solution of complex Hermitian positive-definite linear system (Black Box)
- F04GBFP Solution of real linear least-squares problem (Black Box)
- F04HBFPSolution of real symmetric banded linear system (Black Box)
- F04HZFP Solution of complex Hermitian banded linear system (Black Box)
- F04JBFP Solution of real symmetric tridiagonal linear system (Black Box)
- F04JZFP Solution of complex Hermitian tridiagonal linear system (Black Box)

Chapter F07 – Linear Equations (ScaLAPACK)

- F07ADFP (PDGETRF) LU factorization of real general matrix
- F07AEFP (PDGETRS) Solution of real linear system, matrix already factorized by F07ADFP (PDGETRF)
- F07ARFP (PZGETRF) LU factorization of complex general matrix
- F07ASFP (PZGETRS) Solution of complex linear system, matrix already factorized by F07ARFP (PZGETRF)
- F07FDFP (PDPOTRF) Cholesky factorization of real symmetric positive-definite matrix
- F07FEFP (PDPOTRS) Solution of real symmetric positive-definite linear system, matrix already factorized by F07FDFP (PDPOTRF)

F07FRFP	(PZPOTRF) Cholesky factorization of complex Hermitian positive-definite matrix
F07FSFP	(PZPOTRS) Solution of complex Hermitian positive-definite linear system, matrix already factorized by F07FRFP (PZPOTRF)
F07HDFP	(PDPBTRF) Cholesky factorization of real symmetric banded matrix with no pivoting
F07HEFP	(PDPBTRS) Solution of real symmetric banded linear system, matrix already factorized by F07HDFP (PDPBTRF)
F07HRFP	(PZPBTRF) Cholesky factorization of complex Hermitian banded matrix with no-pivoting
F07HSFP	(PZPBTRS) Solution of complex Hermitian banded linear system, matrix already factorized by F07HRFP (PZPBTRF)
F07JDFP	(PDPTTRF) Cholesky factorization of real symmetric tridiagonal matrix with no-pivoting
F07JEFP	(PDPTTRS) Solution of real symmetric tridiagonal linear system, matrix already factorized by F07JDFP (PDPTTRF)
F07JRFp	(PZPTTRF) Factorization of complex Hermitian tridiagonal matrix with no-pivoting
F07JSFP	(PZPTTRS) Solution of real symmetric tridiagonal linear system, matrix already factorized by F07JRFp (PZPTTRF)
F07TGFp	(PDTRCON) Estimates condition number of real triangular matrix

Chapter F08 – Least-squares and Eigenvalue Problems (ScaLAPACK)

F08AEFP	(PDGEQRF) QR factorization of real general rectangular matrix
F08AFFP	(PDORGQR) Form all or part of an orthogonal Q from QR factorization determined by F08AEFP (PDGEQRF)
F08AGFP	(PDORMQR) Apply the orthogonal transformation determined by F08AEFP (PDORMQR)
F08ASFP	(PZGEQRF) QR factorization of complex general rectangular matrix
F08ATFP	(PZUNGQR) Form all or part of a unitary Q from QR factorization determined by F08ASFP (PZGEQRF)
F08AUFp	(PZUNMQR) Apply the unitary transformation determined by F08ASFP (PZUNMQR)
F08FEFP	(PDSYTRD) Orthogonal reduction of real symmetric matrix to tridiagonal form
F08FGFP	(PDORMTR) Apply orthogonal transformation determined by F08FEFP (PDSYTRD)
F08FSFP	(PZHETRD) Unitary reduction of complex Hermitian matrix to real symmetric tridiagonal form
F08FUFP	(PZUNMTR) Apply unitary transformation matrix determined by F08FSFP (PZHETRD)
F08JJFP	(PDSTEBZ) All or selected eigenvalues of real symmetric tridiagonal matrix by bisection
F08JKFP	(PDSTEIN) Selected eigenvectors of real symmetric tridiagonal matrix by inverse iteration, storing eigenvectors in real array
F08JXFP	(PZSTEIN) Selected eigenvectors of real symmetric tridiagonal matrix by inverse iteration, storing eigenvectors in complex array

Chapter F11 – Sparse Linear Algebra

F11BAFP	Real sparse nonsymmetric linear system, reverse-communication, set-up for F11BBFP
F11BBFP	Real sparse nonsymmetric linear system, reverse-communication, solver using preconditioned RGMRES, CGS or Bi-CGSTAB
F11BCFP	Real sparse nonsymmetric linear system, reverse-communication, diagnostic for F11BBFP
F11BRFP	Complex sparse non-Hermitian linear system, reverse-communication, set-up for F11BSFP
F11BSFP	Complex sparse non-Hermitian linear system, reverse-communication, solver using preconditioned GMRES, CGS or Bi-CGSTAB
F11BTFP	Complex sparse non-Hermitian linear system, reverse-communication, diagnostic for F11BSFP
F11DAFP	Incomplete LU 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
F11DDFP	Apply iterations of SOR method to real sparse linear system, used mostly as SOR preconditioner for real sparse matrix
F11DEFP	Solution of real sparse nonsymmetric linear system using Jacobi, SOR or no preconditioned RGMRES, CGS or Bi-CGSTAB (Black Box)
F11DFFP	Real sparse nonsymmetric linear system, reverse-communication, incomplete LU factorization of local or overlapping diagonal blocks, used mostly as incomplete LU preconditioner for real sparse matrix
F11DGFp	Real sparse nonsymmetric linear system, reverse-communication, preconditioner for real sparse matrix

F11DHFP	Solution of real sparse nonsymmetric linear system using block-Jacobi preconditioned RGMRES, CGS or Bi-CGSTAB (Black Box)
F11DKFP	Apply iterations of relaxed Jacobi iterative method to a real sparse linear system, used mostly as Jacobi preconditioner for real sparse matrix
F11DRFP	Apply iterations of SOR method to the complex sparse linear system, used mostly as SOR preconditioner for complex sparse matrix
F11DSFP	Solution of complex sparse non-Hermitian linear system using Jacobi, SOR or no preconditioned RGMRES, CGS or Bi-CGSTAB (Black Box)
F11DTFP	Computes incomplete LU factorization of local diagonal blocks of complex sparse matrix
F11DUFP	Complex sparse non-Hermitian linear system, reverse-communication, block-Jacobi preconditioner generated by F11DTFP
F11DVFP	Solution of complex sparse non-Hermitian linear system using block-Jacobi preconditioned RGMRES, CGS or Bi-CGSTAB (Black Box)
F11DXFP	Apply iterations of relaxed Jacobi iterative method to complex sparse linear system, used mostly as Jacobi preconditioner for complex sparse matrix
F11GAFP	Real sparse symmetric linear system, reverse-communication, set-up for F11GBFP
F11GBFP	Real sparse symmetric linear system, reverse-communication, solver using preconditioned CG or SYMMLQ
F11GCFP	Real sparse symmetric linear system, reverse-communication, diagnostic for F11GBFP
F11JEFP	Solution of real sparse symmetric linear system using Jacobi, SSOR or no preconditioned CG or SYMMLQ (Black Box)
F11JHFP	Solution of sparse symmetric linear system using block-Jacobi preconditioned CG or SYMMLQ (Black Box)
F11XBFP	Matrix-vector multiplication for real sparse matrix
F11XFPF	Matrix-vector multiplication for complex sparse matrix
F11YAFP	Permutation of non-zero entries of real sparse matrix with repeated sparsity pattern
F11YBFP	Permutation of real vector from distribution based order to local indexing based order
F11YCFP	Permutation of real vector from local indexing based order to distribution based order
F11YNFP	Permutation of non-zero entries of complex sparse matrix with repeated sparsity pattern
F11YFPF	Permutation of complex vector from distribution based order to local indexing based order
F11YQFP	Permutation of complex vector from local indexing based order to distribution based order
F11ZAFP	General set-up routine for real sparse matrix distributed in cyclic row block form
F11ZBFP	General set-up routine for real sparse matrix distributed in cyclic row block form (suitable for repeated sparsity pattern)
F11ZGFP	Generates multi-colour ordering for real sparse matrix with symmetric sparsity pattern, distributed in row block form
F11ZFPF	General set-up routine for complex sparse matrix, distributed in cyclic row block form (suitable for repeated sparsity pattern)
F11ZUFP	Generates multi-colour ordering for complex sparse matrix with symmetric sparsity pattern, distributed in row block form.
F11ZZFP	Release of internally allocated memory

Chapter G05 – Random Number Generators

G05AAFP	Function returning pseudo-random real number from the interval (0,1)
G05ABFP	Selects random number generator and initialises seeds to give repeatable sequence
G05ACFP	Function returning pseudo-random real number from the interval $[a,b)$, uniform distribution
G05ADFP	Function returning pseudo-random real number from the interval $[a,b)$, Normal distribution
G05AEFP	Function returning pseudo-random real number from the interval $[a,b)$, exponential distribution
G05AZFP	Function returning pseudo-random integer from the interval $[ia,ib)$, uniform distribution
G05BAFP	Pseudo-random real numbers from the interval (0,0), uniform distribution
G05BBFP	Selects random number generator and initialises seeds to give repeatable sequence
G05BCFP	Pseudo-random real numbers from the interval (a,b) , uniform distribution
G05BDFP	Pseudo-random real numbers from the interval (a,b) , Normal distribution
G05BEFP	Pseudo-random real numbers from the interval (a,b) , exponential distribution
G05BZFP	Pseudo-random integers from the interval (ia,ib) , uniform distribution

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

Chapter X04 – Input/Output Utilities

X04AAF	Returns or sets unit number for error message
X04ABF	Returns or sets unit number for advisory messages
X04BCFP	Reads real general matrix, from external file, into array distributed in cyclic two-dimensional form, used with routines from Chapters F07 and F08
X04BDFP	Outputs real general matrix, stored in cyclic two-dimensional block fashion, to an external file, used with routines from Chapters F07 and F08
X04BFFP	Outputs set of real general matrices distributed on a two-dimensional logical processor grid, used with routines from Chapter F02
X04BGFP	Reads general real matrix from external file into array distributed in cyclic two-dimensional block form, used with routines from Chapter F04 (Black Box)
X04BHFP	Outputs general real matrix, stored in cyclic two-dimensional block fashion, to external file, used with routines from Chapter F04 (Black Box)
X04BMFP	Outputs set of general integer matrices distributed on a two-dimensional logical processor grid
X04BRFP	Reads complex general matrix from an external file into array distributed in cyclic two-dimensional block form, used with routines from Chapters F07 and F08
X04BSFP	Outputs complex general matrix, stored in cyclic two-dimensional block fashion to an external file, used with routines from Chapters F07 and F08
X04BUFP	Outputs set of complex general matrices distributed on a two-dimensional logical processor grid, used with routines from Chapter F02
X04BVFP	Reads general complex matrix from an external file into an array distributed in cyclic two-dimensional block form, used with routines from Chapter F04 (Black Box)
X04BWFP	Outputs general complex matrix, stored in cyclic two-dimensional block fashion, used with routines from Chapter F04 (Black Box)
X04BXFP	Outputs real matrix stored in row block fashion
X04BZFP	Outputs complex matrix stored in row block fashion
X04YAFP	Outputs real dense vector, distributed conformally to a sparse matrix on a logical grid of processors, to an external file
X04YPFP	Outputs complex vector, distributed conformally to sparse matrix to a sequential file

Chapter Z01 – Library Utilities

Z01AAFP	Defines two-dimensional logical processor grid (Library Grid) and returns the BLACS context
Z01ABFP	Undefines logical processor grid and invalidates the BLACS context initialised by Z01AAFP
Z01ACFP	Root processor identifier
Z01AEPF	Used in creating processes outside the default library mechanism, allows multigridding, used in more advanced applications
Z01BAFP	Row and column indices of the root processor within the logical grid

Z01BBFP	Identifies logical processors in context in the two-dimensional grid declared by Z01AAFP
Z01BEFP	Topology to be used by BLACS for broadcasting and global operations
Z01BGFP	Information about MPI tasks
Z01CAFP	Number of rows or columns of matrix held locally on a given processor when the matrix is distributed in the cyclic two-dimensional block fashion (NUMROC)
Z01CBFP	Length of the workspace for F08AEFP (PDGEQRF) and F08AFFP (PDORGQR)
Z01CCFP	Length of the workspace for F08AGFP (PDORMQR)
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)
Z01CFFP	Computes number of rows of a row block distributed matrix owned by a processor
Z01ZAFP	Returns information on coordinates in Library Grid set up by Z01AAFP
Z01ZBFP	Creates an MPI communicator from a Library context

Chapter Z02 – Error Checking Mode

Z02EAFP	Specification of error checking level, can reduce the amount of checking carried out in subsequent calls to other Library routines
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