

NAG Library

Mark 24 NAG Library for SMP & Multicore News

1 Introduction

1.1 New Functionality

At Mark 24 of the NAG Library for SMP & Multicore new functionality has been introduced in addition to improvements in existing areas. The Library now contains 1784 user-callable routines of which 139 are new at this mark.

New Chapter X07 (IEEE Arithmetic) has been introduced, providing routines relating to IEEE arithmetic such as determining or creating an infinite value or a NaN (Not a Number). There have also been extensions in functionality included in the areas of statistics, wavelets, ordinary differential equations, interpolation, surface fitting, optimization, matrix operations, linear algebra, operations research, and special functions.

Chapter C06 (Summation of Series) has Fast Fourier Transforms (FFTs) for two-dimensional and three-dimensional real data.

Chapter C09 (Wavelet Transforms) has three-dimensional discrete wavelet transforms.

Chapter D01 (Quadrature) has a comprehensive one-dimensional adaptive quadrature routine and a variant for badly behaved integrands.

Chapter D02 (Ordinary Differential Equations) has threadsafe versions of the suite implementing Runge–Kutta methods.

Chapter E01 (Interpolation) has the modified Shepard's method for interpolating in dimensions greater than 5.

Chapter E02 (Curve and Surface Fitting) has a two-stage approximation method for two-dimensional scattered data.

Chapter E04 (Minimizing or Maximizing a Function) has non-negative least squares and an improved MPS data reader.

Chapter E05 (Global Optimization of a Function) has multi-start versions of general nonlinear programming and least squares routines.

Chapter F01 (Matrix Operations, Including Inversion) has greatly extended its range of matrix function routines including the calculation of condition numbers and the action on another matrix.

Chapter F02 (Eigenvalues and Eigenvectors) has a driver routine for calculating selected eigenvalues/vectors of real sparse general matrices.

Chapter F04 (Simultaneous Linear Equations) has norm estimators for rectangular matrices.

Chapter F11 (Large Scale Linear Systems) has a block diagonal (possibly overlapping) preconditioner and associated solver for real and complex nonsymmetric sparse matrices.

Chapter F12 (Large Scale Eigenproblems) has a driver for selected eigenvalues/vectors of general banded complex eigenproblems.

Chapter F16 (Further Linear Algebra Support Routines) has two additions from the BLAST set of routines.

Chapter G01 (Simple Calculations on Statistical Data) has routines for combining summary statistics from blocks of data, probabilities from a multivariate Student's t -distribution, and a large set of vectorized versions of routines for probabilities and density functions.

Chapter G02 (Correlation and Regression Analysis) has routines for weighted nearest correlation matrix and combining two sums of squares.

Chapter G03 (Multivariate Methods) has a Gaussian mixture model routine.

Chapter G05 (Random Number Generators) has Brownian bridge and random field routines.

Chapter G13 (Time Series Analysis) has moving averages for inhomogeneous time series.

Chapter H (Operations Research) has routines for computing best subsets.

Chapter S (Approximations of Special Functions) has added special functions: confluent hypergeometric, log beta and incomplete beta; additionally a large set of vectorized versions of existing special functions.

Chapter X07 (IEEE Arithmetic) has a set of IEEE routines including testing and setting Infs and NaNs.

1.2 New SMP parallelism and other optimizations

SMP parallelism has been added to new routines introduced at Mark 24 in the areas of discrete Fourier transforms, 3-D wavelets, multi-dimensional interpolation, cubic splines, global optimization, matrix functions, the mean and standard deviation of an arbitrary-sized data stream using a rolling window, Gaussian mixture model, Brownian bridge and univariate inhomogeneous time series. An existing routine for Heston's model option pricing formula with Greeks has also been parallelized.

2 New Routines

The 139 new user-callable routines included in the NAG Library at Mark 24 are as follows.

Routine Name	Purpose
C06PVF	Two-dimensional real-to-complex discrete Fourier transform
C06PWF	Two-dimensional complex-to-real discrete Fourier transform
C06PYF	Three-dimensional real-to-complex discrete Fourier transform
C06PZF	Three-dimensional complex-to-real discrete Fourier transform
C09ACF	Three-dimensional wavelet filter initialization
C09FAF	Three-dimensional discrete wavelet transform
C09FBF	Three-dimensional inverse discrete wavelet transform
C09FCF	Three-dimensional multi-level discrete wavelet transform
C09FDF	Three-dimensional inverse multi-level discrete wavelet transform
D01RAF	One-dimensional quadrature, adaptive, finite interval, multiple integrands, vectorized abscissae, reverse communication
D01RBF	Diagnostic routine for D01RAF
D01RCF	Determine required array dimensions for D01RAF
D01RGF	One-dimensional quadrature, adaptive, finite interval, strategy due to Gonnet, allowing for badly behaved integrands
D01TBF	Pre-computed weights and abscissae for Gaussian quadrature rules, restricted choice of rule
D01UAF	One-dimensional Gaussian quadrature, choice of weight functions
D01ZKF	Option setting routine
D01ZLF	Option getting routine
D02PEF	Ordinary differential equations, initial value problem, Runge-Kutta method, integration over range with output
D02PFF	Ordinary differential equations, initial value problem, Runge-Kutta method, integration over one step
D02PQF	Ordinary differential equations, initial value problem, setup for D02PEF and D02PFF
D02PRF	Ordinary differential equations, initial value problem, resets end of range for D02PFF
D02PSF	Ordinary differential equations, initial value problem, interpolation for D02PFF

D02PTF	Ordinary differential equations, initial value problem, integration diagnostics for D02PEF and D02PFF
D02PUF	Ordinary differential equations, initial value problem, error assessment diagnostics for D02PEF and D02PFF
E01ZMF	Interpolating function, modified Shepard's method, d dimensions
E01ZNF	Interpolated values, evaluate interpolant computed by E01ZMF, function and first derivatives, d dimensions
E02BFF	Evaluation of fitted cubic spline, function and optionally derivatives at a vector of points
E02JDF	Spline approximation to a set of scattered data using a two-stage approximation method
E02JEF	Evaluation at a vector of points of a spline computed by E02JDF
E02JFF	Evaluation at a mesh of points of a spline computed by E02JDF
E02ZKF	Option setting routine
E02ZLF	Option getting routine
E04MXF	Reads MPS data file defining LP, QP, MILP or MIQP problem
E04PCF	Computes the least squares solution to a set of linear equations subject to fixed upper and lower bounds on the variables. An option is provided to return a minimal length solution if a solution is not unique
E05UCF	Global optimization using multi-start, nonlinear constraints
E05USF	Global optimization of a sum of squares problem using multi-start, nonlinear constraints
F01EJF	Real matrix logarithm
F01EKF	Exponential, sine, cosine, sinh or cosh of a real matrix (Schur–Parlett algorithm)
F01ELF	Function of a real matrix (using numerical differentiation)
F01EMF	Function of a real matrix (using user-supplied derivatives)
F01FJF	Complex matrix logarithm
F01FKF	Exponential, sine, cosine, sinh or cosh of a complex matrix (Schur–Parlett algorithm)
F01FLF	Function of a complex matrix (using numerical differentiation)
F01FMF	Function of a complex matrix (using user-supplied derivatives)
F01GAF	Action of a real matrix exponential on a real matrix
F01GBF	Action of a real matrix exponential on a real matrix (reverse communication)
F01HAF	Action of a complex matrix exponential on a complex matrix
F01HBF	Action of a complex matrix exponential on a complex matrix (reverse communication)
F01JAF	Condition number for the exponential, logarithm, sine, cosine, sinh or cosh of a real matrix
F01JBF	Condition number for a function of a real matrix (using numerical differentiation)
F01JCF	Condition number for a function of a real matrix (using user-supplied derivatives)
F01KAF	Condition number for the exponential, logarithm, sine, cosine, sinh or cosh of a complex matrix
F01KBF	Condition number for a function of a complex matrix (using numerical differentiation)
F01KCF	Condition number for a function of a complex matrix (using user-supplied derivatives)
F02EKF	Selected eigenvalues and eigenvectors of a real sparse general matrix
F04YDF	Norm estimation (for use in condition estimation), real rectangular matrix
F04ZDF	Norm estimation (for use in condition estimation), complex rectangular matrix

F11DFF	Real sparse nonsymmetric linear system, incomplete LU factorization of local or overlapping diagonal blocks
F11DGF	Solution of real sparse nonsymmetric linear system, RGMRES, CGS, Bi-CGSTAB or TFQMR method, incomplete LU block diagonal preconditioner computed by F11DFF
F11DTF	Complex sparse nonsymmetric linear system, incomplete LU factorization of local or overlapping diagonal blocks
F11DUF	Solution of complex sparse nonsymmetric linear system, RGMRES, CGS, Bi-CGSTAB or TFQMR method, incomplete LU block diagonal preconditioner computed by F11DTF
F12ATF	Initialization routine for (F12AUF) computing selected eigenvalues and, optionally, eigenvectors of a complex banded (standard or generalized) eigenproblem.
F12AUF	Selected eigenvalues and, optionally, eigenvectors of complex non-Hermitian banded eigenproblem, driver
F16ECF	Real scaled vector accumulation
F16GCF	Complex scaled vector accumulation
G01ATF	Computes univariate summary information: mean, variance, skewness, kurtosis
G01AUF	Combines multiple sets of summary information, for use after G01ATF
G01HDF	Computes the probability for the multivariate Student's t -distribution
G01KKF	Computes a vector of values for the probability density function of the gamma distribution
G01KQF	Computes a vector of values for the probability density function of the Normal distribution
G01LBF	Computes a vector of values for the probability density function of the multivariate Normal distribution
G01SAF	Computes a vector of probabilities for the standard Normal distribution
G01SBF	Computes a vector of probabilities for the Student's t -distribution
G01SCF	Computes a vector of probabilities for χ^2 distribution
G01SDF	Computes a vector of probabilities for F -distribution
G01SEF	Computes a vector of probabilities for the beta distribution
G01SFF	Computes a vector of probabilities for the gamma distribution
G01SJF	Computes a vector of probabilities for the binomial distribution
G01SKF	Computes a vector of probabilities for the Poisson distribution
G01SLF	Computes a vector of probabilities for the hypergeometric distribution
G01TAF	Computes a vector of deviates for the standard Normal distribution
G01TBF	Computes a vector of deviates for Student's t -distribution
G01TCF	Computes a vector of deviates for χ^2 distribution
G01TDF	Computes a vector of deviates for F -distribution
G01TEF	Computes a vector of deviates for the beta distribution
G01TFF	Computes a vector of deviates for the gamma distribution
G01WAF	Computes the mean and standard deviation using a rolling window
G02AJF	Computes the nearest correlation matrix to a real square matrix, using element-wise weighting
G02BZF	Combines two sums of squares matrices, for use after G02BUF
G03GAF	Fits a Gaussian mixture model
G05XAF	Initializes the Brownian bridge generator

G05XBF	Generate paths for a free or non-free Wiener process using the Brownian bridge algorithm
G05XCF	Initializes the generator which backs out the increments of sample paths generated by a Brownian bridge algorithm
G05XDF	Backs out the increments from sample paths generated by a Brownian bridge algorithm
G05XEF	Creates a Brownian bridge construction order out of a set of input times
G05ZMF	Setup for simulating one-dimensional random fields, user-defined variogram
G05ZNF	Setup for simulating one-dimensional random fields
G05ZPF	Generates realisations of a one-dimensional random field
G05ZQF	Setup for simulating two-dimensional random fields, user-defined variogram
G05ZRF	Setup for simulating two-dimensional random fields, preset variogram
G05ZSF	Generates realisations of a two-dimensional random field
G05ZTF	Generates realisations of fractional Brownian motion
G13MEF	Computes the iterated exponential moving average for a univariate inhomogeneous time series
G13MFF	Computes the iterated exponential moving average for a univariate inhomogeneous time series, intermediate results are also returned
G13MGF	Computes the exponential moving average for a univariate inhomogeneous time series
H05AAF	Best m subsets of size p (reverse communication)
H05ABF	Best m subsets of size p (direct communication)
S14CBF	Logarithm of the beta function $\ln(B, a, b)$
S14CCF	Incomplete beta function $I_x(a, b)$ and its complement $1 - I_x$
S17AQF	Bessel function vectorized $Y_0(x)$
S17ARF	Bessel function vectorized $Y_1(x)$
S17ASF	Bessel function vectorized $J_0(x)$
S17ATF	Bessel function vectorized $J_1(x)$
S17AUF	Airy function vectorized $\text{Ai}(x)$
S17AVF	Airy function vectorized $\text{Bi}(x)$
S17AWF	Airy function vectorized $\text{Ai}'(x)$
S17AXF	Airy function vectorized $\text{Bi}'(x)$
S18AQF	Modified Bessel function vectorized $K_0(x)$
S18ARF	Modified Bessel function vectorized $K_1(x)$
S18ASF	Modified Bessel function vectorized $I_0(x)$
S18ATF	Modified Bessel function vectorized $I_1(x)$
S18CQF	Scaled modified Bessel function vectorized $e^x K_0(x)$
S18CRF	Scaled modified Bessel function vectorized $e^x K_1(x)$
S18CSF	Scaled modified Bessel function vectorized $e^{- x } I_0(x)$
S18CTF	Scaled modified Bessel function vectorized $e^{- x } I_1(x)$
S19ANF	Kelvin function vectorized $\text{ber } x$
S19APF	Kelvin function vectorized $\text{bei } x$
S19AQF	Kelvin function vectorized $\text{ker } x$

S19ARF	Kelvin function vectorized $\text{kei } x$
S20AQF	Fresnel integral vectorized $S(x)$
S20ARF	Fresnel integral vectorized $C(x)$
S22BAF	Real confluent hypergeometric function ${}_1F_1(a; b; x)$
S22BBF	Real confluent hypergeometric function ${}_1F_1(a; b; x)$ in scaled form
X07AAF	Determines whether its argument has a finite value
X07ABF	Determines whether its argument is a NaN (Not A Number)
X07BAF	Creates a signed infinite value.
X07BBF	Creates a NaN (Not A Number)
X07CAF	Gets current behaviour of floating point exceptions
X07CBF	Sets behaviour of floating point exceptions

3 Tuned Routines

The following is a list of user-callable routines that have been parallelized, or otherwise optimized, since the last release. There are 28 of these routines at this release in the areas of Fourier and wavelet transforms, interpolation, cubic splines, global optimization, matrix functions, simple and multivariate statistics, random number generators (RNGs), time series analysis and option pricing. See the document ‘Tuned and Enhanced Routines in the NAG Library for SMP & Multicore’ for a full list of tuned routines.

Note: on some implementations, the equivalent vendor library routines may be substituted for some of the following list – consult the Users’ Note for your implementation for further information.

Routine

Name	Purpose
C06PVF	Two-dimensional real-to-complex discrete Fourier transform
C06PWF	Two-dimensional complex-to-real discrete Fourier transform
C06PYF	Three-dimensional real-to-complex discrete Fourier transform
C06PZF	Three-dimensional complex-to-real discrete Fourier transform
C09FAF	Three-dimensional discrete wavelet transform
C09FBF	Three-dimensional inverse discrete wavelet transform
C09FCF	Three-dimensional multi-level discrete wavelet transform
C09FDF	Three-dimensional inverse multi-level discrete wavelet transform
E01ZMF	Interpolating function, modified Shepard’s method, d dimensions
E01ZNF	Interpolated values, evaluate interpolant computed by E01ZMF, function and first derivatives, d dimensions
E02BFF	Evaluation of fitted cubic spline, function and optionally derivatives at a vector of points
E05UCF	Global optimization using multi-start, nonlinear constraints
E05USF	Global optimization of a sum of squares problem using multi-start, nonlinear constraints
F01EJF	Real matrix logarithm
F01EKF	Exponential, sine, cosine, sinh or cosh of a real matrix (Schur–Parlett algorithm)
F01EMF	Function of a real matrix (using user-supplied derivatives)
F01FJF	Complex matrix logarithm
F01FKF	Exponential, sine, cosine, sinh or cosh of a complex matrix (Schur–Parlett algorithm)

F01FMF	Function of a complex matrix (using user-supplied derivatives)
G01ATF	Computes univariate summary information: mean, variance, skewness, kurtosis
G01WAF	Computes the mean and standard deviation using a rolling window
G03GAF	Fits a Gaussian mixture model
G05XBF	Generate paths for a free or non-free Wiener process using the Brownian bridge algorithm
G05XDF	Backs out the increments from sample paths generated by a Brownian bridge algorithm
G13MEF	Computes the iterated exponential moving average for a univariate inhomogeneous time series
G13MFF	Computes the iterated exponential moving average for a univariate inhomogeneous time series, intermediate results are also returned
G13MGF	Computes the exponential moving average for a univariate inhomogeneous time series
S30NBF	Heston's model option pricing formula with Greeks

4 Enhanced Routines

These routines call one or more of the tuned routines as part of their core operations and may thereby exhibit improved performance and scalability. There are 24 newly enhanced routines at this Mark; these include the areas of curve and surface fitting, matrix functions, sparse linear algebra, correlation and regression analysis and random number generators (RNGs). See the document 'Tuned and Enhanced Routines in the NAG Library for SMP & Multicore' for a full list of enhanced routines.

Routine

Name	Purpose
E02JDF	Spline approximation to a set of scattered data using a two-stage approximation method
F01ELF	Function of a real matrix (using numerical differentiation)
F01FLF	Function of a complex matrix (using numerical differentiation)
F01GAF	Action of a real matrix exponential on a real matrix
F01GBF	Action of a real matrix exponential on a real matrix (reverse communication)
F01HAF	Action of a complex matrix exponential on a complex matrix
F01HBF	Action of a complex matrix exponential on a complex matrix (reverse communication)
F01JAF	Condition number for the exponential, logarithm, sine, cosine, sinh or cosh of a real matrix
F01JBF	Condition number for a function of a real matrix (using numerical differentiation)
F01JCF	Condition number for a function of a real matrix (using user-supplied derivatives)
F01KAF	Condition number for the exponential, logarithm, sine, cosine, sinh or cosh of a complex matrix
F01KBF	Condition number for a function of a complex matrix (using numerical differentiation)
F01KCF	Condition number for a function of a complex matrix (using user-supplied derivatives)
F02EKF	Selected eigenvalues and eigenvectors of a real sparse general matrix
F11DGF	Solution of real sparse nonsymmetric linear system, RGMRES, CGS, Bi-CGSTAB or TFQMR method, incomplete <i>LU</i> block diagonal preconditioner computed by F11DFF
F11DUF	Solution of complex sparse nonsymmetric linear system, RGMRES, CGS, Bi-CGSTAB or TFQMR method, incomplete <i>LU</i> block diagonal preconditioner computed by F11DTF
F12AUF	Selected eigenvalues and, optionally, eigenvectors of complex non-Hermitian banded eigenproblem, driver

G01LBF	Computes a vector of values for the probability density function of the multivariate Normal distribution
G02AJF	Computes the nearest correlation matrix to a real square matrix, using element-wise weighting
G05ZPF	Generates realisations of a one-dimensional random field
G05ZQF	Setup for simulating two-dimensional random fields, user-defined variogram
G05ZRF	Setup for simulating two-dimensional random fields, preset variogram
G05ZSF	Generates realisations of a two-dimensional random field
G05ZTF	Generates realisations of fractional Brownian motion

5 Withdrawn Routines

The following routines have been withdrawn from the NAG Library at Mark 24. Warning of their withdrawal was included in the NAG Library Manual at Mark 23, together with advice on which routines to use instead. See the document 'Advice on Replacement Calls for Withdrawn/Superseded Routines' for more detailed guidance.

Withdrawn

Routine	Replacement Routine(s)
E04CCF	E04CBF
E04ZCF	No longer required
G05HKF	G05PDF
G05HLF	G05PEF
G05HMF	G05PFF
G05HNF	G05PGF
G05KAF	G05SAF
G05KBF	G05KFF
G05KCF	G05KGF
G05KEF	G05TBF
G05LAF	G05SKF
G05LBF	G05SNF
G05LCF	G05SDF
G05LDF	G05SHF
G05LEF	G05SBF
G05LFF	G05SJF
G05LGF	G05SQF
G05LHF	G05SPF
G05LJF	G05SFF
G05LKF	G05SMF
G05LLF	G05SJF
G05LMF	G05SSF
G05LNF	G05SLF
G05LPF	G05SRF

G05LQF	G05SGF
G05LXF	G05RYF
G05LYF	G05RZF
G05LZF	G05RZF
G05MAF	G05TLF
G05MBF	G05TCF
G05MCF	G05THF
G05MDF	G05TFF
G05MEF	G05TKF
G05MJF	G05TAF
G05MKF	G05TJF
G05MLF	G05TEF
G05MRF	G05TGF
G05MZF	G05TDF
G05NAF	G05NCF
G05NBF	G05NDF
G05PAF	G05PHF
G05PCF	G05PJF
G05QAF	G05PXF
G05QBF	G05PYF
G05QDF	G05PZF
G05RAF	G05RDF
G05RBF	G05RCF
G05YCF	G05YLF
G05YDF	G05YMF
G05YEF	G05YLF
G05YFF	G05YMF
G05YGF	G05YLF
G05YHF	G05YMF
G13DCF	G13DDF
P01ABF	No longer required
X02DAF	No longer required
X02DJF	No longer required

6 Routines Scheduled for Withdrawal

The routines listed below are scheduled for withdrawal from the NAG Library, because improved routines have now been included in the Library. You are advised to stop using routines which are scheduled for withdrawal immediately and to use recommended replacement routines instead. See the document 'Advice on Replacement Calls for Withdrawn/Superseded Routines' for more detailed guidance, including advice on how to change a call to the old routine into a call to its recommended replacement.

The following routines will be withdrawn at Mark 25.

**Routines Scheduled
for Withdrawal**

Replacement Routine(s)

C05ADF	C05AYF
C05AGF	C05AUF
C05AJF	C05AWF
C05NBF	C05QBF
C05NCF	C05QCF
C05NDF	C05QDF
C05PBF	C05RBF
C05PCF	C05RCF
C05PDF	C05RDF
C05ZAF	C05ZDF
C06DBF	C06DCF
F03AAF	F07ADF (DGETRF) and F03BAF
F03ABF	F07FDF (DPOTRF) and F03BFF
F03ACF	F07HDF (DPBTRF) and F03BHF
F03ADF	F07ARF (ZGETRF) and F03BNF
F03AEF	F07FDF (DPOTRF) and F03BFF
F03AFF	F07ADF (DGETRF) and F03BAF
F04AFF	No replacement routine required
F04AGF	No replacement routine required
F04AHF	No replacement routine required
F04AJF	No replacement routine required

The following routines have been superseded, but will not be withdrawn from the Library until Mark 26 at the earliest.

Superseded

Routine Replacement Routine(s)

C06EAF	C06PAF
C06EBF	C06PAF
C06ECF	C06PCF
C06EKF	C06FKF
C06FRF	C06PSF
C06FUF	C06PUF
C06GBF	No replacement required
C06GCF	No replacement required
C06GQF	No replacement required
C06GSF	No replacement required
C06HAF	C06RAF
C06HBF	C06RAF

C06HCF	C06RCF
C06HDF	C06RDF
D01BAF	D01UAF
D01BBF	D01TBF
D02PCF	D02PEF and associated D02P routines
D02PDF	D02PFF and associated D02P routines
D02PVF	D02PQF
D02PWF	D02PRF
D02PXF	D02PSF
D02PYF	D02PTF
D02PZF	D02PUF
E04MZF	E04MXF
F04YCF	F04YDF
F04ZCF	F04ZDF
G01AAF	G01ATF
