NAG Fortran Library

Mark 20 News

1 Introduction

At Mark 20 of the Fortran Library new functionality has been introduced in addition to improvements in existing areas. The Library now contains 1248 documented routines, of which 95 are new at this Mark. A completely new chapter on mesh generation has been introduced, and extensions have been included in the areas of zeros of polynomials, partial differential equations, eigenvalue problems (LAPACK), sparse linear algebra, random number generation, time series analysis and approximations of special functions.

In addition the provision of thread safe versions of existing routines has been significantly extended in Chapter C05 (Roots of One or More Transcendental Equations), Chapter D03 (Partial Differential Equations), Chapter E04 (Optimization) and Chapter G05 (Random Number Generators) to aid users developing multithreaded applications. Moreover, at this Mark we have produced fully thread safe libraries for several platforms.

The new chapter on Mesh Generation (Chapter D06) has routines for generating 2-D meshes together with a number of associated utility routines.

Routines for finding the roots of real and complex cubic and quartic equations have been added to Chapter C02 (Zeros of a Polynomial).

Chapter D03 (Partial Differential Equations) now includes routines for solving Black–Scholes equations.

Chapter F08 (Least-squares and Eigenvalue Problems (LAPACK)) has been extended to include routines for the solution of the generalized nonsymmetric eigenvalue problem, including the computation of the generalized Schur form.

Real and complex Jacobi preconditioners have been added to Chapter F11 (Sparse Linear Algebra).

The additions to Chapter G05 (Random Number Generation) include:

a new random number generator;

generation of univariate GARCH, asymmetric GARCH and EGARCH processes;

quasi-random number generators;

generators for further distributions.

Chapter G13 (Time Series Analysis) has been extended with routines for parameter estimation and forecasting for univariate regression GARCH, asymmetric GARCH and EGARCH processes.

Chapter S (Approximations of Special Functions) has new routines for polygamma functions, zeros of Bessel functions, Jacobian functions, elliptic integrals and Legendre and associated Legendre functions.

2 New Routines

The 95 new user-callable routines included in the NAG Fortran Library at Mark 20 are as follows.

2.1 Routines with New Functionality

C02AKF All zeros of real cubic equation
C02ALF All zeros of real quartic equation
C02AMF All zeros of complex cubic equation
C02ANF All zeros of complex quartic equation
D03NCF Finite difference solution of the Black–Scholes equations
D03NDF Analytic solution of the Black–Scholes equations
D03NEF Compute average values for D03NDF
D06AAF Generates a two-dimensional mesh using a simple incremental method

D06ABF	Generates a two-dimensional mesh using a Delaunay–Voronoi process
D06ACF	Generates a two-dimensional mesh using an Advancing-front method
D06BAF	Generates a boundary mesh
D06CAF	Uses a barycentering technique to smooth a given mesh
D06CBF	Generates a sparsity pattern of a Finite Element matrix associated with a given mesh
D06CCF	Renumbers a given mesh using Gibbs method
D06DAF	Generates a mesh resulting from an affine transformation of a given mesh
D06DBF	Joins together two given adjacent (possibly overlapping) meshes
E04USF	Minimum of a sum of squares, nonlinear constraints, sequential QP method, using function values and optionally first derivatives (comprehensive)
E04WBF	Initialization routine for E04DGA, E04MFA, E04NCA, E04NFA, E04NKA, E04UCA, E04UFA, E04UGA and E04USA
F08WEF	Orthogonal reduction of a pair of real general matrices to generalized upper Hessenberg form
F08WHF	Balance a pair of real general matrices
F08WJF	Transform eigenvectors of a pair of real balanced matrices to those of original matrix pair supplied to F08WHF (SGGBAL/DGGBAL)
F08WSF	Unitary reduction of a pair of complex general matrices to generalized upper Hessenberg form
F08WVF	Balance a pair of complex general matrices
F08WWF	Transform eigenvectors of a pair of complex balanced matrices to those of original matrix pair supplied to F08WVF (CGGBAL/ZGGBAL)
F08XEF	Eigenvalues and generalized Schur factorization of real generalized upper Hessenberg matrix reduced from a pair of real general matrices
F08XSF	Eigenvalues and generalized Schur factorization of complex generalized upper Hessenberg matrix reduced from a pair of complex general matrices
F08YKF	Left and right eigenvectors of a pair of real upper quasi-triangular matrices
F08YXF	Left and right eigenvectors of a pair of complex upper triangular matrices
F11DKF	Real sparse nonsymmetric linear systems, line Jacobi preconditioner
F11DXF	Complex sparse nonsymmetric linear systems, line Jacobi preconditioner
F11GDF	Real sparse symmetric linear systems, setup for F11GEF
F11GEF	Real sparse symmetric linear systems, preconditioned conjugate gradient or Lanczos
F11GFF	Real sparse symmetric linear systems, diagnostic for F11GEF
F11GRF	Complex sparse symmetric linear systems, setup for F11GEF
F11GSF	Complex sparse symmetric linear systems, preconditioned conjugate gradient or Lanczos
F11GTF	Complex sparse symmetric linear systems, diagnostic for F11GEF
G05HKF	Univariate time series, generate n terms of either a symmetric GARCH process or a GARCH process with asymmetry of the form $(\epsilon_{t-1}+\gamma)^2$
G05HLF	Univariate time series, generate n terms of a GARCH process with asymmetry of the form $(\lvert\epsilon_{t-1}\rvert+\gamma\epsilon_{t-1})^2$
G05HMF	Univariate time series, generate n terms of an asymmetric Glosten, Jagannathan and Runkle (GJR) GARCH process
G05HNF	Univariate time series, generate n terms of an exponential GARCH (EGARCH) process
G05KAF	Pseudo-random real numbers, uniform distribution over (0,1), seeds and generator number passed explicitly
G05KBF	Initialise seeds of a given generator for random number generating routines (that pass seeds expicitly) to give a repeatable sequence
G05KCF	Initialise seeds of a given generator for random number generating routines (that pass seeds expicitly) to give non-repeatable sequence
G05KEF	Pseudo-random logical (boolean) value, seeds and generator number passed explicitly

G05LAF Generates a vector of random numbers from a Normal distribution, seeds and generator number passed explicitly

G05LBF Generates a vector of random numbers from a Student's t-distribution, seeds and generator number passed explicitly

G05LCF Generates a vector of random numbers from a χ^2 distribution, seeds and generator number passed explicitly

G05LDF Generates a vector of random numbers from an F-distribution, seeds and generator number passed explicitly

G05LEF Generates a vector of random numbers from a β distribution, seeds and generator number passed explicitly

G05LFF Generates a vector of random numbers from a γ distribution, seeds and generator number passed explicitly

G05LGF Generates a vector of random numbers from a uniform distribution, seeds and generator number passed explicitly

G05LHF Generates a vector of random numbers from a triangular distribution, seeds and generator number passed explicitly

G05LJF Generates a vector of random numbers from an exponential distribution, seeds and generator number passed explicitly

G05LKF Generates a vector of random numbers from a lognormal distribution, seeds and generator number passed explicitly

G05LLF Generates a vector of random numbers from a Cauchy distribution, seeds and generator number passed explicitly

G05LMF Generates a vector of random numbers from a Weibull distribution, seeds and generator number passed explicitly

G05LNF Generates a vector of random numbers from a logistic distribution, seeds and generator number passed explicitly

G05LPF Generates a vector of random numbers from a Von Mises distribution, seeds and generator number passed explicitly

G05LQF Generates a vector of random numbers from an exponential mixture distribution, seeds and generator number passed explicitly

G05LZF Generates a vector of random numbers from a multivariate Normal distribution, seeds and generator number passed explicitly

G05MAF Generates a vector of random integers from a uniform distribution, seeds and generator number passed explicitly

G05MBF Generates a vector of random integers from a geometric distribution, seeds and generator number passed explicitly

G05MCF Generates a vector of random integers from a negative binomial distribution, seeds and generator number passed explicitly

G05MDF Generates a vector of random integers from a logarithmic distribution, seeds and generator number passed explicitly

G05MEF Generates a vector of random integers from a Poisson distribution with varying mean, seeds and generator number passed explicitly

G05MJF Generates a vector of random integers from a binomial distribution, seeds and generator number passed explicitly

G05MKF Generates a vector of random integers from a Poisson distribution, seeds and generator number passed explicitly

G05MLF Generates a vector of random integers from a hypergeometric distribution, seeds and generator number passed explicitly

G05MRF Generates a vector of random integers from a multinomial distribution, seeds and generator number passed explicitly

G05MZF Generates a vector of random integers from a general discrete distribution, seeds and generator number passed explicitly

G05NAF Pseudo-random permutation of an integer vector
G05NBF Pseudo-random sample from an integer vector
G05PAF Generates a realisation of a time series from an ARMA model
G05PCF Generates a realisation of a multivariate time series from a VARMA model
G05QAF Computes a random orthogonal matrix
G05QBF Computes a random correlation matrix
G05QDF Generates a random table matrix
G05YAF Multi-dimensional quasi-random number generator with a uniform probability distribution
G05YBF Multi-dimensional quasi-random number generator with a Gaussian or log-normal probability distribution
G05ZAF Selects either the basic generator or the Wichmann–Hill generator for those routines using internal communication
G13FAF Univariate time series, parameter estimation for either a symmetric GARCH process or a GARCH process with asymmetry of the form $(\epsilon_{t-1}+\gamma)^2$
G13FBF Univariate time series, forecast function for either a symmetric GARCH process or a GARCH process with asymmetry of the form $(\epsilon_{t-1}+\gamma)^2$
G13FCF Univariate time series, parameter estimation for a GARCH process with asymmetry of the form $(|\epsilon_{t-1}|+\gamma\epsilon_{t-1})^2$
G13FDF Univariate time series, forecast function for a GARCH process with asymmetry of the form $(|\epsilon_{t-1}|+\gamma\epsilon_{t-1})^2$
G13FEF Univariate time series, parameter estimation for an asymmetric Glosten, Jagannathan and Runkle (GJR) GARCH process
G13FFF Univariate time series, forecast function for an asymmetric Glosten, Jagannathan and Runkle (GJR) GARCH process
G13FGF Univariate time series, forecast function for an exponential GARCH (EGARCH) process
G13FHF Univariate time series, forecast function for an exponential GARCH (EGARCH) process
S14AEF Polygamma function $\psi^{(n)}(x)$ for real x
S14AFF Polygamma function $\psi^{(n)}(z)$ for complex z
S17ALF Zeros of Bessel functions $J_\alpha(x)$, $J'_\alpha(x)$, $Y_\alpha(x)$ or $Y'_\alpha(x)$
S21CBF Jacobian elliptic functions sn, cn and dn of complex argument
S21CCF Jacobian theta functions $\theta_k(x,q)$ of real argument
S21DAF General elliptic integral of 2nd kind $F(z,k',a,b)$ of complex argument
S22AAF Legendre functions of 1st kind $P_n^m(x)$ or $\overline{P_n^m}(x)$

2.2 Thread Safe Equivalents of Existing Routines

The thread safe versions of existing routines included in the NAG Fortran Library at Mark 20 are as follows.

C05PDA Solution of system of nonlinear equations using first derivatives (reverse communication)
D03PCA General system of parabolic PDEs, method of lines, finite differences, one space variable
D03PDA General system of parabolic PDEs, method of lines, Chebyshev C^0 collocation, one space variable
D03PHA General system of parabolic PDEs, coupled DAEs, method of lines, finite differences, one space variable
D03PJA General system of parabolic PDEs, coupled DAEs, method of lines, Chebyshev C^0 collocation, one space variable
D03PPA General system of parabolic PDEs, coupled DAEs, method of lines, finite differences, remeshing, one space variable
E04ABA Minimum, function of one variable using function values only

E04BBA Minimum, function of one variable, using first derivative
E04CCA Unconstrained minimum, simplex algorithm, function of several variables using function values only (comprehensive)
E04DGA Unconstrained minimum, preconditioned conjugate gradient algorithm, function of several variables using first derivatives (comprehensive)
E04DJA Read optional parameter values for E04DGF/E04DGA from external file
E04DKA Supply optional parameter values to E04DGF/E04DGA
E04MFA LP problem (dense)
E04MGA Read optional parameter values for E04MFF/E04MFA from external file
E04MHA Supply optional parameter values to E04MFF/E04MFA
E04NCA Convex QP problem or linearly-constrained linear least-squares problem (dense)
E04NDA Read optional parameter values for E04NCF/E04NCA from external file
E04NEA Supply optional parameter values to E04NCF/E04NCA
E04NFA QP problem (dense)
E04NGA Read optional parameter values for E04NFF/E04NFA from external file
E04NHA Supply optional parameter values to E04NFF/E04NFA
E04NKA LP or QP problem (sparse)
E04NLA Read optional parameter values for E04NKF/E04NKA from external file
E04NMA Supply optional parameter values to E04NKF/E04NKA
E04UCA Minimum, function of several variables, sequential QP method, nonlinear constraints, using function values and optionally first derivatives (forward communication, comprehensive)
E04UDA Read optional parameter values for E04UCF/E04UCA or E04UFF/E04UFA from external file
E04UEA Supply optional parameter values to E04UCF/E04UCA or E04UFF/E04UFA
E04UFA Minimum, function of several variables, sequential QP method, nonlinear constraints, using function values and optionally first derivatives (reverse communication, comprehensive)
E04UGA NLP problem (sparse)
E04UHA Read optional parameter values for E04UGF/E04UGA from external file
E04UJA Supply optional parameter values to E04UGF/E04UGA
E04UQA Read optional parameter values for E04USF/E04USA from external file
E04URA Supply optional parameter values to E04USF/E04USA
E04USA Minimum of a sum of squares, nonlinear constraints, sequential QP method, using function values and optionally first derivatives (comprehensive)
E04XAA Estimate (using numerical differentiation) gradient and/or Hessian of a function
E04ZCA Check user's routines for calculating first derivatives of function and constraints

3 Withdrawn Routines

The following routines have been withdrawn from the NAG Fortran Library at Mark 20. Warning of their withdrawal was included in the Mark 19 Library Manual, 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)**
E01SEF	E01SGF
E01SFF	E01SHF

4 Routines Scheduled for Withdrawal

The routines listed below are scheduled for withdrawal from the NAG Fortran Library, because improved routines have now been included in the Library. Users 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 21.

Routine Scheduled for Withdrawal	**Replacement Routine(s)**
F11BAF	F11BDF
F11BBF	F11BEF
F11BCF	F11BFF

The following routines have been superseded, but will not be withdrawn from the Library until Mark 22 at the earliest.

Superseded Routine	**Replacement Routine(s)**
E04UNF	E04USF/E04USA
F11GAF	F11GDF
F11GBF	F11GEF
F11GCF	F11GFF
G05CAF	G05KAF
G05CBF	G05KBF
G05CCF	G05KCF
G05CFF	F06DFF
G05CGF	F06DFF
G05DAF	G05LGF
G05DBF	G05LJF
G05DCF	G05LNF
G05DDF	G05LAF
G05DEF	G05LKF
G05DFF	G05LLF
G05DHF	G05LCF
G05DJF	G05LBF
G05DKF	G05LDF
G05DPF	G05LMF
G05DRF	G05MEF
G05DYF	G05MAF
G05DZF	G05KEF
G05EAF	G05LZF
G05EBF	G05MAF
G05ECF	G05MKF
G05EDF	G05MJF
G05EEF	G05MCF
G05EFF	G05MLF
G05EGF	G05PAF
G05EHF	G05NAF
G05EJF	G05NBF
G05EWF	G05PAF
G05EXF	G05MZF
G05EYF	G05MZF
G05EZF	G05LZF
G05FAF	G05LGF
G05FBF	G05LJF
G05FDF	G05LAF
G05FEF	G05LEF

G05FFF	G05LFF
G05FSF	G05LPF
G05GAF	G05QAF
G05GBF	G05QBF
G05HDF	G05PCF