

NAG Library

Mark 22 NAG Fortran Library News

1 Introduction

At Mark 22 of the NAG Library new functionality has been introduced in addition to improvements in existing areas. The Library now contains 1617 user-callable routines, all of which are documented, of which 129 are new at this mark.

Three new chapters have been introduced on wavelet transforms global optimization, and further linear algebra support routines; a new sub-chapter has also been introduced on option pricing formulae; and extensions have been included in the areas of statistics, optimization, linear algebra, ordinary differential equations, regression, random numbers, searching, and special functions.

The new Chapter C09 (Wavelet Transforms) has routines for performing one-dimensional discrete, single-level and multi-level, wavelet transforms and their inverses.

The new Chapter E05 (Global Optimization of a Function) has a routine for performing global optimization on a problem with simple bounds using a multi-level coordinate search, which is complemented by a number of support routines for initializing the data and setting optional parameters.

The new Chapter F16 (Further Linear Algebra Support Routines) contains various useful level-1 routines from the BLAS Technical Forum (BLAST).

Chapter C05 (Roots of One or More Transcendental Equations) has a new routine to evaluate real values of Lambert's W function.

Chapter D02 (Ordinary Differential Equations) has extended its functionality to include routines that use the integration method of DASSL; thus, implicit differential algebraic equations of index 2 can now be solved.

Chapter E04 (Minimizing or Maximizing a Function) has added a replacement routine for applying the simplex algorithm which should perform significantly faster than the original.

Chapter F01 (Matrix Operations, Including Inversion) contains a new routine for computing the matrix exponential of a real-valued matrix.

Chapter F02 (Eigenvalues and Eigenvectors) contains a new routine for obtaining leading terms in the singular value decomposition of a real general matrix.

Chapter F07 (Linear Equations (LAPACK)) contains two new routines for solving systems of linear equations using mixed single and double precision arithmetic. For well conditioned problems, these can produce results accurate to double precision while taking advantage of the higher performance of single precision routines on many computer architectures.

Chapter G01 (Simple Calculations on Statistical Data) contains a new routine for finding quantiles of an unordered vector.

Chapter G02 (Correlation and Regression Analysis) contains new routines for: computing the nearest correlation matrix to a real square matrix; computing predicted value and error from a generalized linear model; ridge regression; and partial least squares.

Chapter G03 (Multivariate Methods) contains a new routine for performing ProMax rotations.

Chapter G05 (Random Number Generators) has been overhauled to provide a consistent set of routines for: initializing pseudorandom, quasirandom and scrambled quasirandom base generators; generating vectors from distributions; generating matrices from Copula and multivariate distributions; and generating realizations from (V)ARMA models and GARCH processes. The base generators now include the Mersenne Twister and ACORN generators.

Chapter G13 (Time Series Analysis) contains new routines for exponential smoothing of a univariate time series, and fitting a VARMA model to a multivariate time series.

Chapter M01 (Sorting and Searching) is renamed from ‘Sorting’ and contains routines for searching arrays of real-valued, integer or character data.

Chapter S (Approximations of Special Functions) now includes a suite of routines for evaluating various option pricing formulae. This chapter also contains new routines for computing the scaled complement of the error function (erfcx), a scaled gamma function and computing elliptic integrals in the classical Legendre form.

Plots of example program results have been added to many routine documents. In some cases the example program has been modified slightly to produce a larger set of results giving a more representative plot of the solution profile produced.

2 New Routines

The 129 new user-callable routines included in the NAG Library at Mark 22 are as follows.

Routine Name	Purpose
A00ADF	Library identification, details of implementation, major and minor marks
C05BAF	Real values of Lambert’s W function, $W(x)$
C09AAF	Wavelet filter initialization
C09CAF	one-dimensional discrete wavelet transform
C09CBF	one-dimensional inverse discrete wavelet transform
C09CCF	one-dimensional multi-level discrete wavelet transform
C09CDF	one-dimensional inverse multi-level discrete wavelet transform
D02MCF	Implicit ordinary differential equations/DAEs, initial value problem, DASSL method continuation for D02NEF
D02MWF	Implicit ordinary differential equations/DAEs, initial value problem, setup for D02NEF
D02NEF	Implicit ordinary differential equations/DAEs, initial value problem, DASSL method integrator
D02NPF	Implicit ordinary differential equations/DAEs, initial value problem linear algebra setup routine for D02NEF
E04CBF	Unconstrained minimization using simplex algorithm, function of several variables using function values only
E05JAF	Initialization routine for E05JBF
E05JBF	Global optimization by multi-level coordinate search, simple bounds, using function values only
E05JCF	Supply optional parameter values for E05JBF from external file
E05JDF	Set a single optional parameter for E05JBF from a character string
E05JEF	Set a single optional parameter for E05JBF from an ‘ON’/‘OFF’-valued character argument
E05JFF	Set a single optional parameter for E05JBF from an integer argument
E05JGF	Set a single optional parameter for E05JBF from a real argument
E05JHF	Determine whether an optional parameter for E05JBF has been set by you or not
E05JJF	Get the setting of an ‘ON’/‘OFF’-valued character optional parameter of E05JBF
E05JKF	Get the setting of an Integer valued optional parameter of E05JBF
E05JLF	Get the setting of a real valued optional parameter of E05JBF
F01ECF	Real matrix exponential

F02WGF	Computes leading terms in the singular value decomposition of a real general matrix; also computes corresponding left and right singular vectors
F07ACF	Mixed precision real system solver
F07AQF	Mixed precision complex system solver
F16DLF	Sum elements of integer vector
F16DNF	Maximum value and location, integer vector
F16DPF	Minimum value and location, integer vector
F16DQF	Maximum absolute value and location, integer vector
F16DRF	Minimum absolute value and location, integer vector
F16EHF	Real scaled vector addition preserving input
F16ELF	Sum elements of real vector
F16GHF	Complex scaled vector addition preserving input
F16GLF	Sum elements of complex vector
F16JNF	Maximum value and location, real vector
F16JPF	Minimum value and location, real vector
F16JQF	Maximum absolute value and location, real vector
F16JRF	Minimum absolute value and location, real vector
F16JSF	Maximum absolute value and location, complex vector
F16JTF	Minimum absolute value and location, complex vector
G01AMF	Find quantiles of an unordered vector, real numbers
G02AAF	Computes the nearest correlation matrix to a real square matrix, using the method of Qi and Sun
G02GPF	Computes a predicted value and its associated standard error based on a previously fitted generalized linear model.
G02KAF	Ridge regression, optimizing a ridge regression parameter
G02KBF	Ridge regression using a number of supplied ridge regression parameters
G02LAF	Partial least-squares (PLS) regression using singular value decomposition
G02LBF	Partial least-squares (PLS) regression using Wold's iterative method
G02LCF	PLS parameter estimates following partial least-squares regression by G02LAF or G02LBF
G02LDF	PLS predictions based on parameter estimates from G02LCF
G03BDF	ProMax rotations
G05KFF	Initializes a pseudorandom number generator to give a repeatable sequence
G05KGF	Initializes a pseudorandom number generator to give a non-repeatable sequence
G05KHF	Primes a pseudorandom number generator for generating multiple streams using leap-frog
G05KJF	Primes a pseudorandom number generator for generating multiple streams using skip-ahead
G05NCF	Pseudorandom permutation of an integer vector
G05NDF	Pseudorandom sample from an integer vector
G05PDF	Generates a realization of a time series from a GARCH process with asymmetry of the form $(\epsilon_{t-1} + \gamma)^2$

G05PEF	Generates a realization of a time series from a GARCH process with asymmetry of the form $(\epsilon_{t-1} + \gamma\epsilon_{t-1})^2$
G05PFF	Generates a realization of a time series from an asymmetric Glosten, Jagannathan and Runkle (GJR) GARCH process
G05PGF	Generates a realization of a time series from an exponential GARCH (EGARCH) process
G05PHF	Generates a realization of a time series from an ARMA model
G05PJF	Generates a realization of a multivariate time series from a VARMA model
G05PMF	Generates a realization of a time series from an exponential smoothing model
G05PXF	Generates a random orthogonal matrix
G05PYF	Generates a random correlation matrix
G05PZF	Generates a random two-way table
G05RCF	Generates a matrix of pseudorandom numbers from a Student's t -copula
G05RDF	Generates a matrix of pseudorandom numbers from a Gaussian copula
G05RYF	Generates a matrix of pseudorandom numbers from a multivariate Student's t -distribution
G05RZF	Generates a matrix of pseudorandom numbers from a multivariate Normal distribution
G05SAF	Generates a vector of pseudorandom numbers from a uniform distribution over $(0, 1]$
G05SBF	Generates a vector of pseudorandom numbers from a beta distribution
G05SCF	Generates a vector of pseudorandom numbers from a Cauchy distribution
G05SDF	Generates a vector of pseudorandom numbers from a χ^2 distribution
G05SEF	Generates a vector of pseudorandom numbers from a Dirichlet distribution
G05SFF	Generates a vector of pseudorandom numbers from an exponential distribution
G05SGF	Generates a vector of pseudorandom numbers from an exponential mix distribution
G05SHF	Generates a vector of pseudorandom numbers from an F -distribution
G05SJF	Generates a vector of pseudorandom numbers from a gamma distribution
G05SKF	Generates a vector of pseudorandom numbers from a Normal distribution
G05SLF	Generates a vector of pseudorandom numbers from a logistic distribution
G05SMF	Generates a vector of pseudorandom numbers from a log-normal distribution
G05SNF	Generates a vector of pseudorandom numbers from a Student's t -distribution
G05SPF	Generates a vector of pseudorandom numbers from a triangular distribution
G05SQF	Generates a vector of pseudorandom numbers from a uniform distribution over $[a, b]$
G05SRF	Generates a vector of pseudorandom numbers from a von Mises distribution
G05SSF	Generates a vector of pseudorandom numbers from a Weibull distribution
G05TAF	Generates a vector of pseudorandom integers from a binomial distribution
G05TBF	Generates a vector of pseudorandom logical values
G05TCF	Generates a vector of pseudorandom integers from a geometric distribution
G05TDF	Generates a vector of pseudorandom integers from a general discrete distribution
G05TEF	Generates a vector of pseudorandom integers from a hypergeometric distribution
G05TFF	Generates a vector of pseudorandom integers from a logarithmic distribution
G05TGF	Generates a vector of pseudorandom integers from a multinomial distribution

G05THF	Generates a vector of pseudorandom integers from a negative binomial distribution
G05TJF	Generates a vector of pseudorandom integers from a Poisson distribution
G05TKF	Generates a vector of pseudorandom integers from a Poisson distribution with varying mean
G05TLF	Generates a vector of pseudorandom integers from a uniform distribution
G05YLF	Initializes a quasi-random number generator
G05YMF	Generates a uniform quasi-random number sequence
G05YNF	Initializes a scrambled quasi-random number generator
G13AMF	Univariate time series, exponential smoothing
G13DDF	Multivariate time series, estimation of VARMA model
M01NAF	Binary search in set of real numbers
M01NBF	Binary search in set of integer numbers
M01NCF	Binary search in set of character data
S15AGF	Scaled complement of error function, $\operatorname{erfcx}(x)$
S21BEF	Elliptic integral of 1st kind, Legendre form, $F(\phi m)$
S21BFF	Elliptic integral of 2nd kind, Legendre form, $E(\phi m)$
S21BGF	Elliptic integral of 3rd kind, Legendre form, $\Pi(n; \phi m)$
S21BHF	Complete elliptic integral of 1st kind, Legendre form, $K(m)$
S21BJF	Complete elliptic integral of 2nd kind, Legendre form, $E(m)$
S30AAF	Black–Scholes–Merton option pricing formula
S30ABF	Black–Scholes–Merton option pricing formula with Greeks
S30BAF	Floating-strike lookback option pricing formula
S30BBF	Floating-strike lookback option pricing formula with Greeks
S30CAF	Binary option: cash-or-nothing pricing formula
S30CBF	Binary option: cash-or-nothing pricing formula with Greeks
S30CCF	Binary option: asset-or-nothing pricing formula
S30CDF	Binary option: asset-or-nothing pricing formula with Greeks
S30FAF	Standard barrier option pricing formula
S30JAF	Jump-diffusion, Merton’s model, option pricing formula
S30JBF	Jump-diffusion, Merton’s model, option pricing formula with Greeks
S30NAF	Heston’s model option pricing formula
S30QCF	American option: Bjerksund and Stensland pricing formula
S30SAF	Asian option: geometric continuous average rate pricing formula
S30SBF	Asian option: geometric continuous average rate pricing formula with Greeks

3 Withdrawn Routines

The following routines have been withdrawn from the NAG Library at Mark 22. Warning of their withdrawal was included in the NAG Library Manual at Mark 21, 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)
E04UNF	E04USF/E04USA
F11GAF	F11GDF
F11GBF	F11GEF
F11GCF	F11GFF
G05CAF	G05SAF
G05CBF	G05KFF
G05CCF	G05KGF
G05CFF	F06DFF
G05CGF	F06DFF
G05DAF	G05SQF
G05DBF	G05SFF
G05DCF	G05SLF
G05DDF	G05SKF
G05DEF	G05SMF
G05DFF	G05SCF
G05DHF	G05SDF
G05DJF	G05SNF
G05DKF	G05SHF
G05DPF	G05SSF
G05DRF	G05TKF
G05DYF	G05TLF
G05DZF	G05TBF
G05EAF	G05RZF
G05EBF	G05TLF
G05ECF	G05TJF
G05EDF	G05TAF
G05EEF	G05THF
G05EFF	G05TEF
G05EGF	G05PHF
G05EHF	G05NCF
G05EJF	G05NDF
G05EWF	G05PHF
G05EXF	G05TDF
G05EYF	G05TDF
G05EZF	G05RZF
G05FAF	G05SQF
G05FBF	G05SFF

G05FDF	G05SKF
G05FEF	G05SBF
G05FFF	G05SJF
G05FSF	G05SRF
G05GAF	G05PXF
G05GBF	G05PYF
G05HDF	G05PJF
G05ZAF	No replacement routine required

4 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. Users are advised to stop using routines which are scheduled for withdrawal 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 23.

Routines Scheduled for Withdrawal

Routines Scheduled for Withdrawal	Replacement Routine(s)
F02BJF	F08WAF (DGGEV)
F02EAF	F08PAF (DGEES)
F02EBF	F08NAF (DGEEV)
F02FAF	F08FAF (DSYEV)
F02FCF	F08FBF (DSYEVX)
F02FDF	F08SAF (DSYGV)
F02FHF	F08UAF (DSBGV)
F02GAF	F08PNF (ZGEES)
F02GBF	F08NNF (ZGEEV)
F02GJF	F08WNF (ZGGEV)
F02HAF	F08FNF (ZHEEV)
F02HCF	F08FPF (ZHEEVX)
F02HDF	F08SNF (ZHEGV)
F02WEF	F08KBF (DGESVD)
F02XEF	F08KPF (ZGESVD)
F04AAF	F07AAF (DGESV)
F04ACF	F07HAF (DPBSV)
F04ADF	F07ANF (ZGESV)
F04ARF	F07AAF (DGESV)
F04EAF	F07CAF (DGTSV)
F04FAF	F07JAF (DPTSV), F07JDF (DPTTRF) and F07JEF (DPTTRS)
F04JAF	F08KAF (DGELSS)

F04JDF	F08KAF (DGELSS)
F04JLF	F08ZBF (DGGGLM)
F04JMF	F08ZAF (DGGLSE)
F04KLF	F08ZPF (ZGGGLM)
F04KMF	F08ZNF (ZGGLSE)
G05YAF	G05YLF and G05YMF
G05YBF	G05YLF and either G05YJF or G05YKF

The following routines have been superseded, but will not be withdrawn from the Library until Mark 24 at the earliest.

Superseded**Routine Replacement Routine(s)**

E04CCF	E04CBF
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
