NAG Library

Mark 25 NAG Fortran Library News

1 Introduction

At Mark 25 of the NAG Library new functionality has been introduced in addition to improvements in existing areas. The Library now contains 1844 user-callable routines, all of which are documented, of which 81 are new at this mark.

Chapter C06 (Summation of Series) has replacement routines for real symmetric discrete Fourier transforms with simplified interface.

Chapter C09 (Wavelet Transforms) has new routines for inserting coefficients into and extracting coefficients from the compact form used in the multilevel two-dimensional routines and all three-dimensional routines, which make working with the DWT functions easier as demonstrated in the examples. There are also routines for the maximal overlap discrete wavelet transform (MODWT) and its inverse in one dimension, which are useful in time series analysis.

Chapter D01 (Quadrature) has a routine for high dimensional quadrature using sparse grids.

Chapter D02 (Ordinary Differential Equations) has a threadsafe replacement for the the general nonlinear boundary value problem solver using collocation.

Chapter E01 (Interpolation) has a routine for the triangulation of a two-dimensional scattered grid, and a routine for the barycentric interpolation on function values on a triangulated scattered grid.

Chapter E02 (Curve and Surface Fitting) has a replacement routine for minimax polynomial fitting of a set of data points.

Chapter F01 (Matrix Operations, Including Inversion) has greatly extended its range of matrix routines. New and improved algorithms are available for the matrix logarithm, the matrix square root, the matrix exponential and general matrix powers. We also now have routines for computing Fréchet derivatives.

Chapter F02 (Eigenvalues and Eigenvectors) has routines for the solution of the real and complex quadratic eigenvalue problem, and a driver routine for calculating selected eigenvalues/vectors of symmetric sparse matrices.

Chapter F08 (Least Squares and Eigenvalue Problems (LAPACK)) has routines for recursive, explicitly blocked QR factorization and applying Q for general matrices and for triangular-pentagonal matrices, and has routines for the complete CS decomposition of an orthogonal or unitary matrix.

Chapter F11 (Large Scale Linear Systems) has a routine for the bandwidth reduction of a sparse symmetric matrix by reverse Cuthill–McKee reordering.

Chapter F16 (Further Linear Algebra Support Routines) has a routine for scaled accumulated dot product (BLAS_DDOT).

Chapter G01 (Simple Calculations on Statistical Data) has a routine for computing probabilities for the Dickey–Fuller unit root test.

Chapter G02 (Correlation and Regression Analysis) has routines for performing Least Angle Regression (LARS), Least Absolute Shrinkage and Selection Operator (LASSO) and forward stagewise regression. There is also an additional nearest correlation matrix routine that allows the leading principal submatrix to be preserved.

Chapter G05 (Random Number Generators) has routines for generating training and validation datasets suitable for use in cross-validation.

Chapter G10 (Smoothing in Statistics) has a thread safe replacement for kernel density estimation using a Gaussian kernel.

Chapter G13 (Time Series Analysis) has routines for computing: the Dickey–Fuller unit root test statistic; applying the unscented Kalman filter to a nonlinear state-space model with additive noise; and change point analysis using the PELT algorithm or using binary segmentation.

Chapter H (Operations Research) has a routine for solving mixed integer nonlinear programming problems; optional settings for this are supplied and interrogated via two new option routines. Additionally, there is a routine for approximating solutions to the classical travelling salesman problem.

Chapter S (Approximations of Special Functions) has routines for evaluating the Gauss hypergeometric function for real arguments and for computing the European option price from Heston's stochastic volatility model with term structure.

Chapter X06 (OpenMP Utilities) is a new chapter of routines that provide utilities for controlling the OpenMP environment for your program.

It should also be noted that we have made changes to the Essential Introduction at this mark. We have provided clarification of the term 'Direct and Reverse Communication Routines', see Section 3.2.3 in the Essential Introduction, and also taken the decision to document a number of error conditions, i.e., Dynamic Memory Allocation (see Section 3.6 in the Essential Introduction), License Management (see Section 3.7 in the Essential Introduction) and Unexpected Errors (see Section 3.8 in the Essential Introduction). The Essential Introduction is a useful document providing information advice on how to use the Library and its Documentation and how to get support from NAG.

2 New Routines

The 81 new user-callable routines included in the NAG Library at Mark 25 are as follows.

Routine Name	**Purpose**
C06REF	Multiple discrete sine transforms, simple
C06RFF	Multiple discrete cosine transforms, simple
C06RGF	Multiple discrete quarter-wave sine transforms, simple
C06RHF	Multiple discrete quarter-wave cosine transforms, simple
C09DAF	One-dimensional maximal overlap discrete wavelet transform (MODWT)
C09DBF	One-dimensional inverse maximal overlap discrete wavelet transform (IMODWT)
C09DCF	One-dimensional multi-level maximal overlap discrete wavelet transform (MODWT)
C09DDF	One-dimensional inverse multi-level maximal overlap discrete wavelet transform (IMODWT)
C09EYF	Two-dimensional discrete wavelet transform coefficient extraction
C09EZF	Two-dimensional discrete wavelet transform coefficient insertion
C09FYF	Three-dimensional discrete wavelet transform coefficient extraction
C09FZF	Three-dimensional discrete wavelet transform coefficient insertion
D01ESF	Multi-dimensional quadrature using sparse grids
D02TLF	Ordinary differential equations, general nonlinear boundary value problem, collocation technique (thread safe)
E01EAF	Triangulation of two-dimensional scattered grid, method of Renka and Cline
E01EBF	Barycentric interpolation on function values provided on a two-dimensional scattered grid
E02ALF	Minimax curve fit by polynomials
F01ENF	Real matrix square root
F01EPF	Real upper quasi-triangular matrix square root

F01EQF	General power of a real matrix
F01FNF	Complex matrix square root
F01FPF	Complex upper triangular matrix square root
F01FQF	General power of a complex matrix
F01JDF	Condition number for square root of real matrix
F01JEF	Condition number for real matrix power
F01JFF	Fréchet derivative of real matrix power
F01JGF	Condition number for real matrix exponential
F01JHF	Fréchet derivative of real matrix exponential
F01JJF	Condition number for real matrix logarithm
F01JKF	Fréchet derivative of real matrix logarithm
F01KDF	Condition number for square root of complex matrix
F01KEF	Condition number for complex matrix power
F01KFF	Fréchet derivative of complex matrix power
F01KGF	Condition number for complex matrix exponential
F01KHF	Fréchet derivative of complex matrix exponential
F01KJF	Condition number for complex matrix logarithm
F01KKF	Fréchet derivative of complex matrix logarithm
F02FKF	Selected eigenvalues and eigenvectors of a real symmetric sparse matrix
F02JCF	Solves the quadratic eigenvalue problem for real matrices
F02JQF	Solves the quadratic eigenvalue problem for complex matrices
F08ABF	Performs a QR factorization of real general rectangular matrix, with explicit blocking
F08ACF	Applies the orthogonal transformation determined by F08ABF (DGEQRT)
F08APF	Performs a QR factorization of complex general rectangular matrix using recursive algorithm
F08AQF	Applies the unitary transformation determined by F08APF (ZGEQRT)
F08BBF	QR factorization of real general triangular-pentagonal matrix
F08BCF	Applies the orthogonal transformation determined by F08BBF (DTPQRT)
F08BPF	QR factorization of complex triangular-pentagonal matrix
F08BQF	Applies the unitary transformation determined by F08BPF (ZTPQRT)
F08RAF	Computes the CS decomposition of an orthogonal matrix partitioned into four real submatrices
F08RNF	Computes the CS decomposition of a unitary matrix partitioned into four complex submatrices
F11YEF	Reverse Cuthill–McKee reordering of a sparse symmetric matrix in CCS format
F16EAF	Dot product of two vectors, allows scaling and accumulation.
G01EWF	Computes probabilities for the Dickey–Fuller unit root test
G02ANF	Computes a correlation matrix from an approximate matrix with fixed submatrix
G02MAF	Least angle regression (LARS), least absolute shrinkage and selection operator (LASSO) and forward stagewise regression

G02MBF	Least Angle Regression (LARS), Least Absolute Shrinkage and Selection Operator (LASSO) and forward stagewise regression using the cross-products matrix
G02MCF	Additional parameter calculate following Least Angle Regression (LARS), Least Absolute Shrinkage and Selection Operator (LASSO) or forward stagewise regression
G05PVF	Permutes a matrix, vector, vector triplet into a form suitable for K-fold cross validation
G05PWF	Permutes a matrix, vector, vector triplet into a form suitable for random sub-sampling validation
G10BBF	Kernel density estimate using Gaussian kernel (thread safe)
G13AWF	Computes (augmented) Dickey–Fuller unit root test statistic
G13EJF	Combined time and measurement update, one iteration of the Unscented Kalman Filter for a nonlinear state space model, with additive noise (reverse communication)
G13EKF	Combined time and measurement update, one iteration of the Unscented Kalman Filter for a nonlinear state space model, with additive noise
G13NAF	Change point detection, using the PELT algorithm
G13NBF	Change points detection using the PELT algorithm, user supplied cost function
G13NDF	Change point detection, using binary segmentation
G13NEF	Change point detection, using binary segmentation, user supplied cost function
H02DAF	Mixed integer nonlinear programming
H02ZKF	Option setting routine for H02DAF
H02ZLF	Option getting routine for H02DAF
H03BBF	Travelling Salesman Problem, simulated annealing
S22BEF	Real Gauss hypergeometric function ${}_2F_1(a,b;c;x)$
S22BFF	Real Gauss hypergeometric function ${}_2F_1(a,b;c;x)$ in scaled form.
S30NCF	Heston's model option pricing with term structure
X06AAF	Sets the number of threads for OpenMP parallel regions
X06ABF	The number of OpenMP threads in the current team
X06ACF	An upper bound on the number of threads in the next parallel region
X06ADF	The OpenMP thread number of the calling thread
X06AFF	Tests for an active OpenMP parallel region
X06AGF	Enables or disables nested OpenMP parallelism
X06AHF	Tests the status of nested OpenMP parallelism

3 Internal Changes Affecting Users

There have been no internal changes at this mark.

4 Withdrawn Routines

The following routines have been withdrawn from the NAG Library at Mark 25. Warning of their withdrawal was included in the NAG Library Manual at Mark 24, 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)
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

5 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 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 26.

Routines Scheduled for Withdrawal	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	C06REF
C06HBF	C06RFF
C06HCF	C06RGF
C06HDF	C06RHF
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
F04YCF	F04YDF
F04ZCF	F04ZDF
G01AAF	G01ATF

The following routines have been superseded, but will not be withdrawn from the Library until Mark 27 at the earliest.

Superseded Routine	**Replacement Routine(s)**
D01RBF	No replacement required
D02TKF	D02TLF
E02ACF	E02ALF
F02SDF	F12AGF and F12FGF
F02WDF	F02WUF and F08AEF (DGEQRF)
G10BAF	G10BBF