Release 2 News

1 Introduction

In this document we describe the differences between Release 1 and Release 2 of the NAG Fortran SMP Library. There are two main differences:

(i) Release 1 was based on Mark 17 of the NAG Fortran Library while Release 2 is based on Mark 19; and
(ii) in Release 2, a much larger number of routines have been specially tuned to maximize their performance on shared memory parallel systems.

From the point of view of performance and scalability there are three categories of routine in this Library.

Tuned routines: those that have been specially tuned and which therefore demonstrate near optimal performance and scalability, together with set-up and diagnostic routines. There are 101 of these routines at Release 2 in the areas of FFTs, dense and sparse linear algebra, and random number generators.

Enhanced routines: those that call one or more of the tuned routines as part of their core operations and thereby exhibit improved performance and scalability. There are 130 enhanced routines at Release 2; these include the areas of ODEs, PDEs, optimisation and multivariate statistics.

Additional routines: these provide extra functionality introduced since Mark 17 of the NAG Fortran Library. Some of these perform BLAS operations as part of their algorithm and so benefit from the performance and scalability exhibited by the particular vendor BLAS associated with your implementation of the NAG Fortran SMP Library.

2 New Routines

The 89 new routines at Release 2 of the NAG Fortran SMP Library are those routines introduced at Marks 18 and 19 of the NAG Fortran Library (other than the thirteen complex FFT routines that were already incorporated into Release 1) and a further five user callable routines that will be introduced to the NAG Fortran Library at Mark 20. These five extra routines are F11DKF, F11GDF, F11GEF, F11GFF and G05ZAF. The routine F11DKF provides an additional preconditioner for the sparse linear algebra solvers (see the F11 Chapter Introduction for details). The remaining extra Chapter F11 routines are threadsafe equivalents of the sparse linear algebra routines F11GAF, F11GBF and F11GCF respectively. G05ZAF is a new routine in the chapter concerned with random number generators; specifically it allows you to choose between using the standard algorithm (as in Mark 19 of the NAG Fortran Library) or a set of parallelized Wichmann–Hill generators for generating random numbers – the default and recommended choice for the NAG Fortran SMP Library is the set of Wichmann–Hill generators (see the Users' Note for further details).

3 Tuned Routines

C06FKF	Circular convolution or correlation of two real vectors, extra workspace for greater speed
C06FPF	Multiple one-dimensional real discrete Fourier transforms
C06FQF	Multiple one-dimensional Hermitian discrete Fourier transforms
C06FRF	Multiple one-dimensional complex discrete Fourier transforms
C06FUF	Two-dimensional complex discrete Fourier transform
C06FXF	Three-dimensional complex discrete Fourier transform
C06HAF	Discrete sine transform
C06HBF	Discrete cosine transform
C06HCF	Discrete quarter-wave sine transform
C06HDF	Discrete quarter-wave cosine transform
C06PAF	Single one-dimensional real and Hermitian complex discrete Fourier transform, using complex data format for Hermitian sequences
C06PCF	Single one-dimensional complex discrete Fourier transform, complex data format

C06PJF	Multi-dimensional complex discrete Fourier transform of multi-dimensional data (using complex data type)
C06PFF	One-dimensional complex discrete Fourier transform of multi-dimensional data (using complex data type)
C06PKF	Circular convolution or correlation of two complex vectors
C06PPF	Multiple one-dimensional real and Hermitian complex discrete Fourier transforms, using complex data format for Hermitian sequences
C06PQF	Multiple one-dimensional real and Hermitian complex discrete Fourier transforms, using complex data format for Hermitian sequences and sequences stored as columns
C06PRF	Multiple one-dimensional complex discrete Fourier transforms using complex data format
C06PSF	Multiple one-dimensional complex discrete Fourier transforms using complex data format and sequences stored as columns
C06PUF	Two-dimensional complex discrete Fourier transform, complex data format
C06PXF	Three-dimensional complex discrete Fourier transform, complex data format
C06RAF	Discrete sine transform (easy-to-use)
C06RBF	Discrete cosine transform (easy-to-use)
C06RCF	Discrete quarter-wave sine transform (easy-to-use)
C06RDF	Discrete quarter-wave cosine transform (easy-to-use)
F07ADF	(SGETRF/DGETRF) LU factorization of real m by n matrix
F07AEF	(SGETRS/DGETRS) Solution of real system of linear equations, multiple right-hand sides, matrix already factorized by F07ADF
F07ARF	(CGETRF/ZGETRF) LU factorization of complex m by n matrix
F07ASF	(CGETRS/ZGETRS) Solution of complex system of linear equations, multiple right-hand sides, matrix already factorized by F07ARF
F07FDF	(SPOTRF/DPOTRF) Cholesky factorization of real symmetric positive-definite matrix
F07FEF	(SPOTRS/DPOTRS) Solution of real symmetric positive-definite system of linear equations, multiple right-hand sides, matrix already factorized by F07FDF
F07FRF	(CPOTRF/ZPOTRF) Cholesky factorization of complex Hermitian positive-definite matrix
F07FSF	(CPOTRS/ZPOTRS) Solution of complex Hermitian positive-definite system of linear equations, multiple right-hand sides, matrix already factorized by F07FRF
F08AEF	(SGEQRF/DGEQRF) QR factorization of real general rectangular matrix
F08AFF	(SORGQR/DORGQR) Form all or part of orthogonal Q from QR factorization determined by F08AEF or F08BEF
F08AGF	(SORMQR/DORMQR) Apply orthogonal transformation determined by F08AEF or F08BEF
F08ASF	(CGEQRF/ZGEQRF) QR factorization of complex general rectangular matrix
F08ATF	(CUNGQR/ZUNGQR) Form all or part of unitary Q from QR factorization determined by F08ASF or F08BSF
F08AUF	(CUNMQR/ZUNMQR) Apply unitary transformation determined by F08ASF or F08BSF
F08FEF	(SSYTRD/DSYTRD) Orthogonal reduction of real symmetric matrix to symmetric tridiagonal form
F08FFF	(SORGTR/DORGTR) Generate orthogonal transformation matrix from reduction to tridiagonal form determined by F08FEF
F08FSF	(CHETRD/ZHETRD) Unitary reduction of complex Hermitian matrix to real symmetric tridiagonal form
F08FTF	(CUNGTR/ZUNGTR) Generate unitary transformation matrix from reduction to tridiagonal form determined by F08FSF
F08GFF	(SOPGTR/DOPGTR) Generate orthogonal transformation matrix from reduction to tridiagonal form determined by F08GEF
F08GTF	(CUPGTR/ZUPGTR) Generate unitary transformation matrix from reduction to tridiagonal form determined by F08GSF
F08JEF	(SSTEQR/DSTEQR) All eigenvalues and eigenvectors of real symmetric tridiagonal matrix, reduced from real symmetric matrix using implicit QL or QR
F08JSF	(CSTEQR/ZSTEQR) All eigenvalues and eigenvectors of real symmetric tridiagonal matrix, reduced from complex Hermitian matrix, using implicit QL or QR

F08KEF	(SGEBRD/DGEBRD) Orthogonal reduction of real general rectangular matrix to bidiagonal form
F08KSF	(CGEBRD/ZGEBRD) Unitary reduction of complex general rectangular matrix to bidiagonal form
F08MEF	(SBDSQR/DBDSQR) SVD of real bidiagonal matrix reduced from real general matrix
F08MSF	(CBDSQR/ZBDSQR) SVD of real bidiagonal matrix reduced from complex general matrix
F11BDF	Real sparse nonsymmetric linear systems, set-up for F11BEF
F11BEF	Real sparse nonsymmetric linear systems, preconditioned RGMRES, CGS, Bi-CGSTAB or TFQMR method
F11BFF	Real sparse nonsymmetric linear systems, diagnostic for F11BEF
F11DKF	Real sparse nonsymmetric linear systems, line Jacobi preconditioner
F11GDF	Real sparse symmetric linear systems, set-up for F11GEF
F11GEF	Real sparse symmetric linear systems, preconditioned conjugate gradient or Lanczos, threadsafe
F11GFF	Real sparse symmetric linear systems, diagnostic for F11GEF
F11XAF	Real sparse nonsymmetric matrix vector multiply
F11XEF	Real sparse symmetric matrix vector multiply
G05CAF	Pseudo-random real numbers, uniform distribution over (0,1)
G05CBF	Initialise random number generating routines to give repeatable sequence
G05CCF	Initialise random number generating routines to give non-repeatable sequence
G05CFF	Save state of random number generating routines
G05CGF	Restore state of random number generating routines
G05DAF	Pseudo-random real numbers, uniform distribution over (a, b)
G05DBF	Pseudo-random real numbers, (negative) exponential distribution
G05DCF	Pseudo-random real numbers, logistic distribution
G05DDF	Pseudo-random real numbers, Normal distribution
G05DEF	Pseudo-random real numbers, log-normal distribution
G05DFF	Pseudo-random real numbers, Cauchy distribution
G05DHF	Pseudo-random real numbers, χ^2 distribution
G05DJF	Pseudo-random real numbers, Student's t-distribution
G05DKF	Pseudo-random real numbers, F-distribution
G05DPF	Pseudo-random real numbers, Weibull distribution
G05DRF	Pseudo-random integer, Poisson distribution
G05DYF	Pseudo-random integer from uniform distribution
G05DZF	Pseudo-random logical (boolean) value
G05EAF	Set up reference vector for multivariate Normal distribution
G05EBF	Set up reference vector for generating pseudo-random integers, uniform distribution
G05ECF	Set up reference vector for generating pseudo-random integers, Poisson distribution
G05EDF	Set up reference vector for generating pseudo-random integers, binomial distribution
G05EEF	Set up reference vector for generating pseudo-random integers, negative binomial distribution
G05EFF	Set up reference vector for generating pseudo-random integers, hypergeometric distribution
G05EGF	Set up reference vector for univariate ARMA time series model
G05EHF	Pseudo-random permutation of an integer vector
G05EJF	Pseudo-random sample from an integer vector
G05EWF	Generate next term from reference vector for ARMA time series model
G05EXF	Set up reference vector from supplied cumulative distribution function or probability distribution function
G05EYF	Pseudo-random integer from reference vector
G05EZF	Pseudo-random multivariate Normal vector from reference vector
G05FAF	Generates a vector of random numbers from a uniform distribution
G05FBF	Generates a vector of random numbers from an (negative) exponential distribution
G05FDF	Generates a vector of random numbers from a Normal distribution
G05FEF	Generates a vector of pseudo-random numbers from a beta distribution
G05FFF	Generates a vector of pseudo-random numbers from a gamma distribution
G05FSF	Generates a vector of pseudo-random variates from von Mises distribution

G05GAF	Computes random orthogonal matrix
G05GBF	Computes random correlation matrix
G05HDF	Generates a realisation of a multivariate time series from a VARMA model
G05ZAF	Selection of basic algorithm random number generator or Wichmann–Hill algorithm generators for subsequent calls to Chapter G05 routines

4 Enhanced Routines

D01PAF	Multi-dimensional quadrature over an n-simplex
D02AGF	ODEs, boundary value problem, shooting and matching technique, allowing interior matching point, general parameters to be determined
D02EJF	ODEs, stiff IVP, BDF method, until function of solution is zero, intermediate output (simple driver)
D02HAF	ODEs, boundary value problem, shooting and matching, boundary values to be determined
D02HBF	ODEs, boundary value problem, shooting and matching, general parameters to be determined
D02NBF	Explicit ODEs, stiff IVP, full Jacobian (comprehensive)
D02NCF	Explicit ODEs, stiff IVP, banded Jacobian (comprehensive)
D02NDF	Explicit ODEs, stiff IVP, sparse Jacobian (comprehensive)
D02NGF	Implicit/algebraic ODEs, stiff IVP, full Jacobian (comprehensive)
D02NHF	Implicit/algebraic ODEs, stiff IVP, banded Jacobian (comprehensive)
D02NJF	Implicit/algebraic ODEs, stiff IVP, sparse Jacobian (comprehensive)
D02NMF	Explicit ODEs, stiff IVP (reverse communication, comprehensive)
D02NNF	Implicit/algebraic ODEs, stiff IVP (reverse communication, comprehensive)
D02SAF	ODEs, boundary value problem, shooting and matching technique, subject to extra algebraic equations, general parameters to be determined
D02TKF	ODEs, general nonlinear boundary value problem, collocation technique
D03PCF	General system of parabolic PDEs, method of lines, finite differences, one space variable
D03PDF	General system of parabolic PDEs, method of lines, Chebyshev C^0 collocation, one space variable
D03PEF	General system of first-order PDEs, method of lines, Keller box discretisation, one space variable
D03PFF	General system of convection-diffusion PDEs with source terms in conservative form, method of lines, upwind scheme using numerical flux function based on Riemann solver, one space variable
D03PHF	General system of parabolic PDEs, coupled DAEs, method of lines, finite differences, one space variable
D03PJF	General system of parabolic PDEs, coupled DAEs, method of lines, Chebyshev C^0 collocation, one space variable
D03PKF	General system of first-order PDEs, coupled DAEs, method of lines, Keller box discretisation, one space variable
D03PLF	General system of convection-diffusion PDEs with source terms in conservative form, coupled DAEs, method of lines, upwind scheme using numerical flux function based on Riemann solver, one space variable
D03PPF	General system of parabolic PDEs, coupled DAEs, method of lines, finite differences, remeshing, one space variable
D03PRF	General system of first-order PDEs, coupled DAEs, method of lines, Keller box discretisation, remeshing, one space variable
D03PSF	General system of convection-diffusion PDEs with source terms in conservative form, coupled DAEs, method of lines, upwind scheme using numerical flux function based on Riemann solver, remeshing, one space variable
D05AAF	Linear non-singular Fredholm integral equation, second kind, split kernel
D05ABF	Linear non-singular Fredholm integral equation, second kind, smooth kernel
E04FCF	Unconstrained minimum of a sum of squares, combined Gauss–Newton and modified Newton algorithm using function values only (comprehensive)
E04FYF	Unconstrained minimum of a sum of squares, combined Gauss–Newton and modified Newton algorithm using function values only (easy-to-use)

E04GBF	Unconstrained minimum of a sum of squares, combined Gauss–Newton and quasi-Newton algorithm using first derivatives (comprehensive)
E04GDF	Unconstrained minimum of a sum of squares, combined Gauss–Newton and modified Newton algorithm using first derivatives (comprehensive)
E04GYF	Unconstrained minimum of a sum of squares, combined Gauss–Newton and quasi-Newton algorithm, using first derivatives (easy-to-use)
E04GZF	Unconstrained minimum of a sum of squares, combined Gauss–Newton and modified Newton algorithm using first derivatives (easy-to-use)
E04HEF	Unconstrained minimum of a sum of squares, combined Gauss–Newton and modified Newton algorithm, using second derivatives (comprehensive)
E04HYF	Unconstrained minimum of a sum of squares, combined Gauss–Newton and modified Newton algorithm, using second derivatives (easy-to-use)
E04NCF	Convex QP problem or linearly-constrained linear least-squares problem (dense)
E04UCF	Minimum, function of several variables, sequential QP method, nonlinear constraints, using function values and optionally first derivatives (forward communication, comprehensive)
E04UFF	Minimum, function of several variables, sequential QP method, nonlinear constraints, using function values and optionally first derivatives (reverse communication, comprehensive)
E04UNF	Minimum of a sum of squares, nonlinear constraints, sequential QP method, using function values and optionally first derivatives (comprehensive)
F01ABF	Inverse of real symmetric positive-definite matrix using iterative refinement
F01ADF	Inverse of real symmetric positive-definite matrix
F02EAF	All eigenvalues and Schur factorization of real general matrix (Black Box)
F02EBF	All eigenvalues and eigenvectors of real general matrix (Black Box)
F02FAF	All eigenvalues and eigenvectors of real symmetric matrix (Black Box)
F02FCF	Selected eigenvalues and eigenvectors of real symmetric matrix (Black Box)
F02FDF	All eigenvalues and eigenvectors of real symmetric-definite generalized problem (Black Box)
F02FJF	Selected eigenvalues and eigenvectors of sparse symmetric eigenproblem (Black Box)
F02GAF	All eigenvalues and Schur factorization of complex general matrix (Black Box)
F02GBF	All eigenvalues and eigenvectors of complex general matrix (Black Box)
F02GCF	Selected eigenvalues and eigenvectors of complex nonsymmetric matrix (Black Box)
F02HAF	All eigenvalues and eigenvectors of complex Hermitian matrix (Black Box)
F02HCF	Selected eigenvalues and eigenvectors of complex Hermitian matrix (Black Box)
F02HDF	All eigenvalues and eigenvectors of complex Hermitian-definite generalized problem (Black Box)
F03AAF	Determinant of real matrix (Black Box)
F03ABF	Determinant of real symmetric positive-definite matrix (Black Box)
F03AEF	LL^T factorization and determinant of real symmetric positive-definite matrix
F04AAF	Solution of real simultaneous linear equations with multiple right-hand sides (Black Box)
F04ABF	Solution of real symmetric positive-definite simultaneous linear equations with multiple right-hand sides using iterative refinement (Black Box)
F04ARF	Solution of real simultaneous linear equations, one right-hand side (Black Box)
F04ASF	Solution of real symmetric positive-definite simultaneous linear equations, one right-hand side using iterative refinement (Black Box)
F04JAF	Minimal least-squares solution of m real equations in n unknowns, rank $\leq n$, $m \geq n$
F04JLF	Real general Gauss–Markov linear model (including weighted least-squares)
F04JMF	Equality-constrained real linear least-squares problem
F04KLF	Complex general Gauss–Markov linear model (including weighted least-squares)
F04KMF	Equality-constrained complex linear least-squares problem
F07AHF	(SGERFS/DGERFS) Refined solution with error bounds of real system of linear equations, multiple right-hand sides
F07AVF	(CGERFS/ZGERFS) Refined solution with error bounds of complex system of linear equations, multiple right-hand sides
F07FHF	(SPORFS/DPORFS) Refined solution with error bounds of real symmetric positive-definite system of linear equations, multiple right-hand sides

F07FVF	(CPORFS/ZPORFS) Refined solution with error bounds of complex Hermitian positive-definite system of linear equations, multiple right-hand sides
F08FCF	(SSYEVD/DSYEVD) All eigenvalues and optionally all eigenvectors of real symmetric matrix, using divide and conquer
F08FGF	(SORMTR/DORMTR) Apply orthogonal transformation determined by F08FEF
F08FQF	(CHEEVD/ZHEEVD) All eigenvalues and optionally all eigenvectors of complex Hermitian matrix, using divide and conquer
F08FUF	(CUNMTR/ZUNMTR) Apply unitary transformation matrix determined by F08FSF
F08GCF	(SSPEVD/DSPEVD) All eigenvalues and optionally all eigenvectors of real symmetric matrix, packed storage, using divide and conquer
F08GQF	(CHPEVD/ZHPEVD) All eigenvalues and optionally all eigenvectors of complex Hermitian matrix, packed storage, using divide and conquer
F08HCF	(SSBEVD/DSBEVD) All eigenvalues and optionally all eigenvectors of real symmetric band matrix, using divide and conquer
F08HQF	(CHBEVD/ZHBEVD) All eigenvalues and optionally all eigenvectors of complex Hermitian band matrix, using divide and conquer
F08JCF	(SSTEVD/DSTEVD) All eigenvalues and optionally all eigenvectors of real symmetric tridiagonal matrix, using divide and conquer
F08JGF	(SPTEQR/DPTEQR) All eigenvalues and eigenvectors of real symmetric positive-definite tridiagonal matrix, reduced from real symmetric positive-definite matrix
F08JUF	(CPTEQR/ZPTEQR) All eigenvalues and eigenvectors of real symmetric positive-definite tridiagonal matrix, reduced from complex Hermitian positive-definite matrix
F08KFF	(SORGBR/DORGBR) Generate orthogonal transformation matrices from reduction to bidiagonal form determined by F08KEF
F08KGF	(SORMBR/DORMBR) Apply orthogonal transformations from reduction to bidiagonal form determined by F08KEF
F08KTF	(CUNGBR/ZUNGBR) Generate unitary transformation matrices from reduction to bidiagonal form determined by F08KSF
F08KUF	(CUNMBR/ZUNMBR) Apply unitary transformations from reduction to bidiagonal form determined by F08KSF
F08NFF	(SORGHR/DORGHR) Generate orthogonal transformation matrix from reduction to Hessenberg form determined by F08NEF
F08NGF	(SORMHR/DORMHR) Apply orthogonal transformation matrix from reduction to Hessenberg form determined by F08NEF
F08NTF	(CUNGHR/ZUNGHR) Generate unitary transformation matrix from reduction to Hessenberg form determined by F08NSF
F08NUF	(CUNMHR/ZUNMHR) Apply unitary transformation matrix from reduction to Hessenberg form determined by F08NSF
G02CGF	Multiple linear regression, from correlation coefficients, with constant term
G02CHF	Multiple linear regression, from correlation-like coefficients, without constant term
G02DAF	Fits a general (multiple) linear regression model
G02DEF	Add a new variable to a general linear regression model
G02DGF	Fits a general linear regression model for new dependent variable
G02EAF	Computes residual sums of squares for all possible linear regressions for a set of independent variables
G02EEF	Fits a linear regression model by forward selection
G02GAF	Fits a generalized linear model with Normal errors
G02GBF	Fits a generalized linear model with binomial errors
G02GCF	Fits a generalized linear model with Poisson errors
G02GDF	Fits a generalized linear model with gamma errors
G02HAF	Robust regression, standard M-estimates
G02HFF	Robust regression, variance-covariance matrix following G02HDF
G03AAF	Performs principal component analysis
G03ACF	Performs canonical variate analysis
G03ADF	Performs canonical correlation analysis
G03BAF	Computes orthogonal rotations for loading matrix, generalized orthomax criterion
G03BCF	Computes Procrustes rotations
G03CAF	Computes maximum likelihood estimates of the parameters of a factor analysis model, factor loadings, communalities and residual correlations

G03DAF	Computes test statistic for equality of within-group covariance matrices and matrices for discriminant analysis
G04BBF	Analysis of variance, randomized block or completely randomized design, treatment means and standard errors
G04BCF	Analysis of variance, general row and column design, treatment means and standard errors
G08RAF	Regression using ranks, uncensored data
G08RBF	Regression using ranks, right-censored data
G11SAF	Contingency table, latent variable model for binary data
G13AEF	Univariate time series, estimation, seasonal ARIMA model (comprehensive)
G13AFF	Univariate time series, estimation, seasonal ARIMA model (easy-to-use)
G13AJF	Univariate time series, state set and forecasts, from fully specified seasonal ARIMA model
G13ASF	Univariate time series, diagnostic checking of residuals, following G13AEF or G13AFF
G13BAF	Multivariate time series, filtering (pre-whitening) by an ARIMA model
G13BBF	Multivariate time series, filtering by a transfer function model
G13BDF	Multivariate time series, preliminary estimation of transfer function model
G13BEF	Multivariate time series, estimation of multi-input model
G13BJF	Multivariate time series, state set and forecasts from fully specified multi-input model
G13DBF	Multivariate time series, multiple squared partial autocorrelations
G13DCF	Multivariate time series, estimation of VARMA model
G13DJF	Multivariate time series, forecasts and their standard errors
G13DNF	Multivariate time series, sample partial lag correlation matrices, χ^2 statistics and significance levels
G13DPF	Multivariate time series, partial autoregression matrices
G13DSF	Multivariate time series, diagnostic checking of residuals, following G13DCF
G13EBF	Combined measurement and time update, one iteration of Kalman filter, time-invariant, square root covariance filter

5 Additional Routines Introduced Since Release 1

D02BJF	ODEs, IVP, Runge–Kutta method, until function of solution is zero, integration over range with intermediate output (simple driver)
D03PWF	Modified HLL Riemann solver for Euler equations in conservative form, for use with D03PFF, D03PLF and D03PSF
D03PXF	Exact Riemann Solver for Euler equations in conservative form, for use with D03PFF, D03PLF and D03PSF
D03RAF	General system of second-order PDEs, method of lines, finite differences, remeshing, two space variables, rectangular region
D03RBF	General system of second-order PDEs, method of lines, finite differences, remeshing, two space variables, rectilinear region
D03RYF	Check initial grid data in D03RBF
D03RZF	Extract grid data from D03RBF
E01SGF	Interpolating functions, modified Shepard's method, two variables
E01SHF	Interpolated values, evaluate interpolant computed by E01SGF, function and first derivatives, two variables
E01TGF	Interpolating functions, modified Shepard's method, three variables
E01THF	Interpolated values, evaluate interpolant computed by E01TGF, function and first derivatives, three variables
E04JYF	Minimum, function of several variables, quasi-Newton algorithm, simple bounds, using function values only (easy-to-use)
E04KYF	Minimum, function of several variables, quasi-Newton algorithm, simple bounds, using first derivatives (easy-to-use)
E04KZF	Minimum, function of several variables, modified Newton algorithm, simple bounds, using first derivatives (easy-to-use)
E04LYF	Minimum, function of several variables, modified Newton algorithm, simple bounds, using first and second derivatives (easy-to-use)
E04MZF	Converts MPSX data file defining LP or QP problem to format required by E04NKF

E04NKF	LP or QP problem (sparse)
E04NLF	Read optional parameter values for E04NKF from external file
E04NMF	Supply optional parameter values to E04NKF
E04UGF	NLP problem (sparse)
E04UHF	Read optional parameter values for E04UGF from external file
E04UJF	Supply optional parameter values to E04UGF
F08LEF	(SGBBRD/DGBBRD) Reduction of real rectangular band matrix to upper bidiagonal form
F08LSF	(CGBBRD/ZGBBRD) Reduction of complex rectangular band matrix to upper bidiagonal form
F08UEF	(SSBGST/DSBGST) Reduction of real symmetric-definite banded generalized eigenproblem $Ax = \lambda Bx$ to standard form $Cy = \lambda y$, such that C has the same bandwidth as A
F08UFF	(SPBSTF/DPBSTF) Computes a split Cholesky factorization of real symmetric positive-definite band matrix A
F08USF	(CHBGST/ZHBGST) Reduction of complex Hermitian-definite banded generalized eigenproblem $Ax = \lambda Bx$ to standard form $Cy = \lambda y$, such that C has the same bandwidth as A
F08UTF	(CPBSTF/ZPBSTF) Computes a split Cholesky factorization of complex Hermitian positive-definite band matrix A
F11BAF	Real sparse nonsymmetric linear systems, set-up for F11BBF
F11BBF	Real sparse nonsymmetric linear systems, preconditioned RGMRES, CGS or Bi-CGSTAB
F11BCF	Real sparse nonsymmetric linear systems, diagnostic for F11BBF
F11BRF	Complex sparse non-Hermitian linear systems, set-up for F11BSF
F11BSF	Complex sparse non-Hermitian linear systems, preconditioned RGMRES, CGS, Bi-CGSTAB or TFQMR method
F11BTF	Complex sparse non-Hermitian linear systems, diagnostic for F11BSF
F11DAF	Real sparse nonsymmetric linear systems, incomplete LU factorization
F11DBF	Solution of linear system involving incomplete LU preconditioning matrix generated by F11DAF
F11DCF	Solution of real sparse nonsymmetric linear system, RGMRES, CGS or Bi-CGSTAB method, preconditioner computed by F11DAF (Black Box)
F11DDF	Solution of linear system involving preconditioning matrix generated by applying SSOR to real sparse nonsymmetric matrix
F11DEF	Solution of real sparse nonsymmetric linear system, RGMRES, CGS or Bi-CGSTAB method, Jacobi or SSOR preconditioner (Black Box)
F11DNF	Complex sparse non-Hermitian linear systems, incomplete LU factorization
F11DPF	Solution of complex linear system involving incomplete LU preconditioning matrix generated by F11DNF
F11DQF	Solution of complex sparse non-Hermitian linear system, RGMRES, CGS, Bi-CGSTAB or TFQMR method, preconditioner computed by F11DNF (Black Box)
F11DRF	Solution of linear system involving preconditioning matrix generated by applying SSOR to complex sparse non-Hermitian matrix
F11DSF	Solution of complex sparse non-Hermitian linear system, RGMRES, CGS, Bi-CGSTAB or TFQMR method, Jacobi or SSOR preconditioner (Black Box)
F11JNF	Complex sparse Hermitian matrix, incomplete Cholesky factorization
F11JPF	Solution of complex linear system involving incomplete Cholesky preconditioning matrix generated by F11JNF
F11JQF	Solution of complex sparse Hermitian linear system, conjugate gradient/Lanczos method, preconditioner computed by F11JNF (Black Box)
F11JRF	Solution of linear system involving preconditioning matrix generated by applying SSOR to complex sparse Hermitian matrix
F11JSF	Solution of complex sparse Hermitian linear system, conjugate gradient/Lanczos method, Jacobi or SSOR preconditioner (Black Box)
F11XNF	Complex sparse non-Hermitian matrix vector multiply
F11XSF	Complex sparse Hermitian matrix vector multiply
F11ZAF	Real sparse nonsymmetric matrix reorder routine
F11ZBF	Real sparse symmetric matrix reorder routine

F11ZNF	Complex sparse non-Hermitian matrix reorder routine
F11ZPF	Complex sparse Hermitian matrix reorder routine
G11CAF	Returns parameter estimates for the conditional analysis of stratified data
G12ZAF	Creates the risk sets associated with the Cox proportional hazards model for fixed covariates
H02CBF	Integer QP problem (dense)
H02CCF	Read optional parameter values for H02CBF from external file
H02CDF	Supply optional parameter values to H02CBF
H02CEF	Integer LP or QP problem (sparse)
H02CFF	Read optional parameter values for H02CEF from external file
H02CGF	Supply optional parameter values to H02CEF
M01EDF	Rearrange a vector according to given ranks, complex numbers
X04ACF	Open unit number for reading, writing or appending, and associate unit with named file
X04ADF	Close file associated with given unit number

6 Withdrawn Routines

The following routines have been withdrawn from the NAG Fortran SMP Library at Release 2; the list is an accumulation of the routines withdrawn at Marks 18 and 19 of the NAG Fortran Library. For detailed guidance and advice on which routines to use instead of withdrawn routines see the document 'Advice on Replacement Calls for Superseded/Withdrawn Routines'.

Withdrawn Routine	**Recommended Replacement**
D02BAF	D02PCF and associated D02P routines
D02BBF	D02PCF and associated D02P routines
D02BDF	D02PCF and associated D02P routines
D02CAF	D02CJF
D02CBF	D02CJF
D02CGF	D02CJF
D02CHF	D02CJF
D02EAF	D02EJF
D02EBF	D02EJF
D02EGF	D02EJF
D02EHF	D02EJF
D02PAF	D02PDF and associated D02P routines
D02XAF	D02PXF and associated D02P routines
D02XBF	D02PXF and associated D02P routines
D02YAF	D02PDF and associated D02P routines
E04FDF	E04FYF
E04GCF	E04GYF
E04GEF	E04GZF
E04HFF	E04HYF
E04JAF	E04JYF
E04KAF	E04KYF
E04KCF	E04KZF
E04LAF	E04LYF
E04MBF	E04MFF
E04NAF	E04NFF
E04UPF	E04UNF
F01AEF	F07FDF (SPOTRF/DPOTRF) and F08SEF (SSYGST/DSYGST)
F01AFF	F06YJF (STRSM/DTRSM)
F01AGF	F08FEF (SSYTRD/DSYTRD)
F01AHF	F08FGF (SORMTR/DORMTR)
F01AJF	F08FEF (SSYTRD/DSYTRD) and F08FFF (SORGTR/DORGTR)
F01AKF	F08NEF (SGEHRD/DGEHRD)
F01ALF	F08NGF (SORMHR/DORMHR)
F01AMF	F08NSF (CGEHRD/ZGEHRD)
F01ANF	F08NTF (CUNMHR/ZUNMHR)

F01APF	F08NFF (SORGHR/DORGHR)
F01ATF	F08NHF (SGEBAL/DGEBAL)
F01AUF	F08NJF (SGEBAK/DGEBAK)
F01AVF	F08NVF (CGEBAL/ZGEBAL)
F01AWF	F08NWF (CGEBAK/ZGEBAK)
F01AXF	F08BEF (SGEQPF/CGEQPF)
F01AYF	F08GEF (SSPTRD/DSPTRD)
F01AZF	F08GGF (SOPMTR/DOPMTR)
F01BCF	F08FSF (CHETRD/ZHETRD) and F08FTF (CUNGTR/ZUNGTR)
F01BDF	F07FDF (SPOTRF/DPOTRF) and F08SEF (SSYGST/DSYGST)
F01BEF	F06YFF (STRMM/DTRMM)
F01BTF	F07ADF (SGETRF/DGETRF)
F01BWF	F08HEF (SSBTRD/DSBTRD)
F01LBF	F07BDF (SGBTRF/DGBTRF)
F01MAF	F11JAF
F01QCF	F08AEF (SGEQRF/DGEQRF)
F01QDF	F08AGF (SORMQR/DORMQR)
F01QEF	F08AFF (SORGQR/DORGQR)
F01QFF	F08BEF (SGEQPF/DGEQPF)
F01RCF	F08ASF (CGEQRF/ZGEQRF)
F01RDF	F08AUF (CUNMQR/ZUNMQR)
F01REF	F08ATF (CUNGQR/ZUNGQR)
F01RFF	F08BSF (CGEQPF/ZGEQPF)
F02AAF	F02FAF
F02ABF	F02FAF
F02ADF	F02FDF
F02AEF	F02FDF
F02AFF	F02EBF
F02AGF	F02EBF
F02AJF	F02GBF
F02AKF	F02GBF
F02AMF	F08JEF (SSTEQR/DSTEQR)
F02ANF	F08PSF (CHSEQR/ZHSEQR)
F02APF	F08PEF (SHSEQR/DHSEQR)
F02AQF	F08PEF (SHSEQR/DHSEQR) and F08QKF (STREVC/DTREVC)
F02ARF	F08PSF (CHSEQR/ZHSEQR) and F08QXF (CTREVC/ZTREVC)
F02AVF	F08JFF (SSTERF/DSTERF)
F02AWF	F02HAF
F02AXF	F02HAF
F02AYF	F08JSF (CSTEQR/ZSTEQR)
F02BBF	F02FCF
F02BCF	F02ECF
F02BDF	F02GCF
F02BEF	F08JJF (SSTEBZ/DSTEBZ) and F08JKF (SSTEIN/DSTEIN)
F02BFF	F08JJF (SSTEBZ/DSTEBZ)
F02BKF	F08PKF (SHSEIN/DHSEIN)
F02BLF	F08PXF (CHSEIN/ZHSEIN)
F02SWF	F08KEF (SGEBRD/DGEBRD)
F02SXF	F08KFF (SORGBR/DORGBR) or F08KGF (SORMBR/DORMBR)
F02SYF	F08MEF (SBDSQR/DBDSQR)
F02UWF	F08KSF (CGEBRD/ZGEBRD)
F02UXF	F08KTF (CUNGBR/ZUNGBR) or F08KUF (CUNMBR/ZUNMBR)
F02UYF	F08MSF (CBDSQR/ZBDSQR)
F04ANF	F08AGF (SORMQR/DORMQR) and F06PJF (STRSV/DTRSV)
F04AYF	F07AEF (SGETRS/DGETRS)
F04LDF	F07BEF (SGBTRS/DGBTRS)
F04MAF	F11JCF
F04MBF	F11GAF, F11GBF and F11GCF (or F11JCF or F11JEF)
G01CEF	G01FAF

7 Routines Scheduled for Withdrawal

The routines listed below are scheduled for withdrawal from the NAG Fortran Library and hence are also scheduled for withdrawal from future releases of the NAG Fortran SMP Library that will be based on future Marks of the NAG Fortran 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 Superseded/Withdrawn 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 Release 3.

Routine Scheduled for Withdrawal	**Recommended Replacement**
E01SEF	E01SGF
E01SFF	E01SHF

The following routines have been superseded, but will not be withdrawn from the NAG Fortran Library until Mark 21 at the earliest (and consequently will not be withdrawn from the NAG Fortran SMP Library until Release 4 at the earliest).

Superseded routine	**Recommended Replacement**
F11BAF	F11BDF
F11BBF	F11BEF
F11BCF	F11BFF