Mark 21 News – SMP Library

1 Introduction

In this document we describe the differences between the last release 'Release 2' and this latest release, now named 'Mark 21', of the NAG SMP Library. There are two main differences:

(i) Release 2 was based on Mark 19 of the NAG Fortran Library while this latest release is based on Mark 21 of the NAG Fortran Library; and

(ii) in Mark 21, a larger number of routines have been specially tuned to maximize their performance on shared memory parallel systems.

1.1 New Functionality

At Mark 21 of the NAG SMP Library new functionality has been introduced in addition to improvements in existing areas. The Library now contains 1533 user-callable routines, all of which are documented, and 375 are new at this mark.

New chapters on large scale eigenproblems and mesh generation have been introduced, and extensions have been included in the areas of optimization, dense and banded linear algebra, direct solution of large scale linear systems, simple statistical calculations, regression, random numbers, zeros of polynomials, partial differential equations, time series analysis, and 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 (Minimizing or Maximizing a Function) and Chapter G05 (Random Number Generators) to aid users developing multithreaded applications.

The new Chapter D06 (Mesh Generation) has routines for generating 2-D meshes together with a number of associated utility routines and the new Chapter F12 (Large Scale Eigenproblems) has routines for the solution of symmetric and nonsymmetric standard and generalized large scale eigenvalue problems. Chapter F11 has been renamed as Large Scale Linear Systems, and new routines for the direct solution of sparse problems have been added.

Chapter E04 (Minimizing or Maximizing a Function) has been updated with new routines for the solution of LP, QP and nonlinear programming problems with sparse linear constraints.

Chapter F07 (Linear Equations (LAPACK)) and Chapter F08 (Least-squares and Eigenvalue Problems (LAPACK)) have been extended to include all the LAPACK driver routines, thus allowing the solution of most problems with a call to a single routine rather than multiple calls to LAPACK computational routines. A comprehensive suite of driver routines for the solution of dense and banded linear equations has also been added to Chapter F04 (Simultaneous Linear Equations).

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

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

Routines for Landau and Vavilov distributions have been added to Chapter G01 (Simple Calculations on Statistical Data), new routines for stepwise regression and mixed effects regression have been included in Chapter G02 (Correlation and Regression Analysis), and a number of new random number generators, including Copulas and improved quasi-random number generators, generation of univariate GARCH, asymmetric GARCH and EGARCH processes, and generators for further distributions have been added to Chapter G05 (Random Number Generators).

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. Variant routines for the log Gamma function, and Bessel function of the 1st kind have also been added.

1.2 New SMP parallelism and other optimizations

SMP Parallel versions of many of the new Chapter F11 sparse direct solvers, and Chapter F12 sparse eigenproblem are included, and parallelism has been extended to many more LAPACK routines. In addition, improvements in underlying NAG auxiliary routines improves the usage of the SMP optimized dense linear algebra by routines in the areas of optimization, ODEs and PDEs, and statistics.

1.3 Documentation

The NAG Fortran Library Manual has undergone a fundamental change since Release 2 and the Essential Introduction and the Introduction to the NAG SMP Library are ***essential*** reading for all users of the NAG Fortran Library.

2 Tuned Routines

The following is a list of user-callable routines that have been parallelized, or otherwise optimized, since the last release. There are 67 of these routines at this release in the area of dense and sparse linear algebra. See the document 'Tuned and Enhanced Routines in the NAG SMP Library' 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.

F04AFF Solution of real symmetric positive-definite simultaneous linear equations using iterative refinement (coefficient matrix already factorized by F03AEF)
F04AGF Solution of real symmetric positive-definite simultaneous linear equations (coefficient matrix already factorized by F03AEF)
F04AHF Solution of real simultaneous linear equations using iterative refinement (coefficient matrix already factorized by F03AFF)
F04AJF Solution of real simultaneous linear equations (coefficient matrix already factorized by F03AFF)
F07AHF Refined solution with error bounds of real system of linear equations, multiple right-hand sides
F07AVF Refined solution with error bounds of complex system of linear equations, multiple right-hand sides
F07BDF LU factorization of real m by n band matrix
F07BEF Solution of real band system of linear equations, multiple right-hand sides, matrix already factorized by F07BDF (DGBTRF)
F07BHF Refined solution with error bounds of real band system of linear equations, multiple right-hand sides
F07BRF LU factorization of complex m by n band matrix
F07BSF Solution of complex band system of linear equations, multiple right-hand sides, matrix already factorized by F07BRF (ZGBTRF)
F07BVF Refined solution with error bounds of complex band system of linear equations, multiple right-hand sides
F07CHF Refined solution with error bounds of real tridiagonal system of linear equations, multiple right-hand sides
F07CVF Refined solution with error bounds of complex tridiagonal system of linear equations, multiple right-hand sides
F07FHF Refined solution with error bounds of real symmetric positive-definite system of linear equations, multiple right-hand sides
F07FVF Refined solution with error bounds of complex Hermitian positive-definite system of linear equations, multiple right-hand sides
F07GEF Solution of real symmetric positive-definite system of linear equations, multiple right-hand sides, matrix already factorized by F07GDF (DPPTRF), packed storage
F07GHF Refined solution with error bounds of real symmetric positive-definite system of linear equations, multiple right-hand sides, packed storage
F07GSF Solution of complex Hermitian positive-definite system of linear equations, multiple right-hand sides, matrix already factorized by F07GRF (ZPPTRF), packed storage
F07GVF Refined solution with error bounds of complex Hermitian positive-definite system of linear equations, multiple right-hand sides, packed storage

F07HEF Solution of real symmetric positive-definite band system of linear equations, multiple right-hand sides, matrix already factorized by F07HDF (DPBTRF)
F07HHF Refined solution with error bounds of real symmetric positive-definite band system of linear equations, multiple right-hand sides
F07HSF Solution of complex Hermitian positive-definite band system of linear equations, multiple right-hand sides, matrix already factorized by F07HRF (ZPBTRF)
F07HVF Refined solution with error bounds of complex Hermitian positive-definite band system of linear equations, multiple right-hand sides
F07JHF Refined solution with error bounds of real symmetric positive-definite tridiagonal system of linear equations, multiple right-hand sides
F07JVF Refined solution with error bounds of complex Hermitian positive-definite tridiagonal system of linear equations, multiple right-hand sides
F07MHF Refined solution with error bounds of real symmetric indefinite system of linear equations, multiple right-hand sides
F07MVF Refined solution with error bounds of complex Hermitian indefinite system of linear equations, multiple right-hand sides
F07NVF Refined solution with error bounds of complex symmetric system of linear equations, multiple right-hand sides
F07PHF Refined solution with error bounds of real symmetric indefinite system of linear equations, multiple right-hand sides, packed storage
F07PVF Refined solution with error bounds of complex Hermitian indefinite system of linear equations, multiple right-hand sides, packed storage
F07QVF Refined solution with error bounds of complex symmetric system of linear equations, multiple right-hand sides, packed storage
F07THF Error bounds for solution of real triangular system of linear equations, multiple right-hand sides
F07TVF Error bounds for solution of complex triangular system of linear equations, multiple right-hand sides
F07UEF Solution of real triangular system of linear equations, multiple right-hand sides, packed storage
F07UHF Error bounds for solution of real triangular system of linear equations, multiple right-hand sides, packed storage
F07USF Solution of complex triangular system of linear equations, multiple right-hand sides, packed storage
F07UVF Error bounds for solution of complex triangular system of linear equations, multiple right-hand sides, packed storage
F07VEF Solution of real band triangular system of linear equations, multiple right-hand sides
F07VHF Error bounds for solution of real band triangular system of linear equations, multiple right-hand sides
F07VSF Solution of complex band triangular system of linear equations, multiple right-hand sides
F07VVF Error bounds for solution of complex band triangular system of linear equations, multiple right-hand sides
F08HEF Orthogonal reduction of real symmetric band matrix to symmetric tridiagonal form
F08HSF Unitary reduction of complex Hermitian band matrix to real symmetric tridiagonal form
F08JJF Selected eigenvalues of real symmetric tridiagonal matrix by bisection
F08JKF Selected eigenvectors of real symmetric tridiagonal matrix by inverse iteration, storing eigenvectors in real array
F08JXF Selected eigenvectors of real symmetric tridiagonal matrix by inverse iteration, storing eigenvectors in complex array
F08PEF Eigenvalues and Schur factorization of real upper Hessenberg matrix reduced from real general matrix
F08PKF Selected right and/or left eigenvectors of real upper Hessenberg matrix by inverse iteration
F08PSF Eigenvalues and Schur factorization of complex upper Hessenberg matrix reduced from complex general matrix
F08PXF Selected right and/or left eigenvectors of complex upper Hessenberg matrix by inverse iteration
F08TAF Computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, packed storage
F08TBF Computes selected eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, packed storage

F08TCF Computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, packed storage (divide-and-conquer)
F08TNF Computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, packed storage
F08TPF Computes selected eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, packed storage
F08TQF Computes selected eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, packed storage (divide-and-conquer)
F11BSF Complex sparse non-Hermitian linear systems, preconditioned RGMRES, CGS, Bi-CGSTAB or TFQMR method
F11GSF Complex sparse Hermitian linear systems, preconditioned conjugate gradient or Lanczos
F11MEF *LU* factorization of real sparse matrix
F11MFF Solution of real sparse simultaneous linear equations (coefficient matrix already factorized)
F11MHF Refined solution with error bounds of real system of linear equations, multiple right-hand sides
F11MKF Real sparse nonsymmetric matrix matrix multiply, compressed column storage
F11XNF Complex sparse non-Hermitian matrix vector multiply
F11XSF Complex sparse Hermitian matrix vector multiply
F12ABF Implements a reverse communication interface for the Implicitly Restarted Arnoldi iteration for computing selected eigenvalues and, optionally, eigenvectors of a real nonsymmetric sparse (standard or generalized) eigenproblem
F12AGF Computes approximations to selected eigenvalues of a real nonsymmetric banded (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace

3 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 159 newly enhanced routines at this mark; these include the areas of zeros of polynomials, PDEs, optimization, dense and sparse linear algebra, and multivariate statistics.

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
D03FAF Elliptic PDE, Helmholtz equation, three-dimensional Cartesian co-ordinates
D03NCF Finite difference solution of the Black–Scholes equations
E02RAF Padé approximants
E04USF Minimum of a sum of squares, nonlinear constraints, sequential QP method, using function values and optionally first derivatives (comprehensive)
E04YCF Covariance matrix for nonlinear least-squares problem (unconstrained)
F02ECF Selected eigenvalues and eigenvectors of real nonsymmetric matrix (Black Box)
F02WDF *QR* factorization, possibly followed by SVD
F02WUF SVD of real upper triangular matrix (Black Box)
F02XUF SVD of complex upper triangular matrix (Black Box)
F03ADF Determinant of complex matrix (Black Box)
F03AFF *LU* factorization and determinant of real matrix
F04AEF Solution of real simultaneous linear equations with multiple right-hand sides using iterative refinement (Black Box)
F04ATF Solution of real simultaneous linear equations, one right-hand side using iterative refinement (Black Box)
F04BAF Computes the solution and error-bound to a real system of linear equations
F04BBF Computes the solution and error-bound to a real banded system of linear equations
F04BDF Computes the solution and error-bound to a real symmetric positive-definite system of linear equations
F04BEF Computes the solution and error-bound to a real symmetric positive-definite system of linear equations, packed storage
F04BFF Computes the solution and error-bound to a real symmetric positive-definite banded system of linear equations

F04CAF Computes the solution and error-bound to a complex system of linear equations
F04CBF Computes the solution and error-bound to a complex banded system of linear equations
F04CDF Computes the solution and error-bound to a complex Hermitian positive-definite system of linear equations
F04CEF Computes the solution and error-bound to a complex Hermitian positive-definite system of linear equations, packed storage
F04CFF Computes the solution and error-bound to a complex Hermitian positive-definite banded system of linear equations
F04JGF Least-squares (if rank $= n$) or minimal least-squares (if rank $< n$) solution of m real equations in n unknowns, rank $\leq n$, $m \geq n$
F07AAF Computes the solution to a real system of linear equations
F07ABF Uses the LU factorization to compute the solution, error-bound and condition estimate for a real system of linear equations
F07ANF Computes the solution to a complex system of linear equations
F07APF Uses the LU factorization to compute the solution, error-bound and condition estimate for a complex system of linear equations
F07BAF Computes the solution to a real banded system of linear equations
F07BBF Uses the LU factorization to compute the solution, error-bound and condition estimate for a real banded system of linear equations
F07BNF Computes the solution to a complex banded system of linear equations
F07BPF Uses the LU factorization to compute the solution, error-bound and condition estimate for a complex banded system of linear equations
F07CBF Uses the LU factorization to compute the solution, error-bound and condition estimate for a real tridiagonal system of linear equations
F07CPF Uses the LU factorization to compute the solution, error-bound and condition estimate for a complex tridiagonal system of linear equations
F07FAF Computes the solution to a real symmetric positive-definite system of linear equations
F07FBF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a real symmetric positive-definite system of linear equations
F07FNF Computes the solution to a complex Hermitian positive-definite system of linear equations
F07FPF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a complex Hermitian positive-definite system of linear equations
F07GAF Computes the solution to a real symmetric positive-definite system of linear equations, packed storage
F07GBF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a real symmetric positive-definite system of linear equations, packed storage
F07GNF Computes the solution to a complex Hermitian positive-definite system of linear equations, packed storage
F07GPF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a complex Hermitian positive-definite system of linear equations, packed storage
F07HAF Computes the solution to a real symmetric positive-definite banded system of linear equations
F07HBF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a real symmetric positive-definite banded system of linear equations
F07HNF Computes the solution to a complex Hermitian positive-definite banded system of linear equations
F07HPF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a complex Hermitian positive-definite banded system of linear equations
F07JBF Uses the modified Cholesky factorization to compute the solution, error-bound and condition estimate for a real symmetric positive-definite tridiagonal system of linear equations
F07JPF Uses the modified Cholesky factorization to compute the solution, error-bound and condition estimate for a complex Hermitian positive-definite tridiagonal system of linear equations
F07MBF Uses the diagonal pivoting factorization to compute the solution to a real symmetric system of linear equations
F07MPF Uses the diagonal pivoting factorization to compute the solution to a complex Hermitian system of linear equations
F07NPF Uses the diagonal pivoting factorization to compute the solution to a complex symmetric system of linear equations
F07PBF Uses the diagonal pivoting factorization to compute the solution to a real symmetric system of linear equations, packed storage

F07PPF	Uses the diagonal pivoting factorization to compute the solution to a complex Hermitian system of linear equations, packed storage
F07QPF	Uses the diagonal pivoting factorization to compute the solution to a complex symmetric system of linear equations, packed storage
F08AAF	Solves an overdetermined or underdetermined real linear system
F08ANF	Solves an overdetermined or underdetermined complex linear system
F08BAF	Computes the minimum-norm solution to a real linear least-squares problem
F08BFF	*QR* factorization of real general rectangular matrix with column pivoting, using BLAS-3
F08BNF	Computes the minimum-norm solution to a complex linear least-squares problem
F08BTF	*QR* factorization of complex general rectangular matrix with column pivoting, using BLAS-3
F08FAF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix
F08FBF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix
F08FDF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix (Relatively Robust Representations)
F08FNF	Computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix
F08FPF	Computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix
F08FRF	Computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix (Relatively Robust Representations)
F08GAF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix, packed storage
F08GBF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix, packed storage
F08GNF	Computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix, packed storage
F08GPF	Computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix, packed storage
F08HAF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric band matrix
F08HBF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric band matrix
F08HNF	Computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix
F08HPF	Computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix
F08JAF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix
F08JBF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix
F08JDF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix (Relatively Robust Representations)
F08JHF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix or a matrix reduced to this form (divide-and-conquer)
F08JLF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix or a symmetric matrix reduced to this form (Relatively Robust Representations)
F08JVF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix or a complex Hermitian matrix reduced to this form (divide-and-conquer)
F08JYF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix or a complex Hermitian matrix reduced to this form (Relatively Robust Representations)
F08KAF	Computes the minimum-norm solution to a real linear least-squares problem using singular value decomposition
F08KBF	Computes the singular value decomposition of a real matrix, optionally computing the left and/or right singular vectors
F08KCF	Computes the minimum-norm solution to a real linear least-squares problem using singular value decomposition (divide-and-conquer)
F08KDF	Computes the singular value decomposition of a real matrix, optionally computing the left and/or right singular vectors (divide-and-conquer)
F08KNF	Computes the minimum-norm solution to a complex linear least-squares problem using singular value decomposition
F08KPF	Computes the singular value decomposition of a complex matrix, optionally computing the left and/or right singular vectors
F08KQF	Computes the minimum-norm solution to a complex linear least-squares problem using singular value decomposition (divide-and-conquer)

F08KRF Computes the singular value decomposition of a complex matrix, optionally computing the left and/or right singular vectors (divide-and-conquer)
F08MDF Computes the singular value decomposition of a real bidiagonal matrix, optionally computing the singular vectors (divide-and-conquer)
F08NAF Computes all eigenvalues and, optionally, left and/or right eigenvectors of a real nonsymmetric matrix
F08NBF Computes all eigenvalues and, optionally, left and/or right eigenvectors of a real nonsymmetric matrix; also, optionally, the balancing transformation, the reciprocal condition numbers for the eigenvalues and for the right eigenvectors
F08NNF Computes all eigenvalues and, optionally, left and/or right eigenvectors of a complex nonsymmetric matrix
F08NPF Computes all eigenvalues and, optionally, left and/or right eigenvectors of a complex nonsymmetric matrix; also, optionally, the balancing transformation, the reciprocal condition numbers for the eigenvalues and for the right eigenvectors
F08PAF Computes for real square nonsymmetric matrix, the eigenvalues, the real Schur form, and, optionally, the matrix of Schur vectors
F08PBF Computes for real square nonsymmetric matrix, the eigenvalues, the real Schur form, and, optionally, the matrix of Schur vectors; also, optionally, computes reciprocal condition numbers for selected eigenvalues
F08PNF Computes for complex square nonsymmetric matrix, the eigenvalues, the Schur form, and, optionally, the matrix of Schur vectors
F08PPF Computes for real square nonsymmetric matrix, the eigenvalues, the Schur form, and, optionally, the matrix of Schur vectors; also, optionally, computes reciprocal condition numbers for selected eigenvalues
F08SAF Computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
F08SBF Computes selected eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
F08SCF Computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem (divide-and-conquer)
F08SNF Computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
F08SPF Computes selected eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
F08SQF Computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem (divide-and-conquer)
F08UAF Computes all the eigenvalues, and optionally, the eigenvectors of a real banded generalized symmetric-definite eigenproblem
F08UBF Computes selected eigenvalues, and optionally, the eigenvectors of a real banded generalized symmetric-definite eigenproblem
F08UCF Computes all the eigenvalues, and optionally, the eigenvectors of a real banded generalized symmetric-definite eigenproblem (divide-and-conquer)
F08UNF Computes all the eigenvalues, and optionally, the eigenvectors of a complex banded generalized Hermitian-definite eigenproblem
F08UPF Computes selected eigenvalues, and optionally, the eigenvectors of a complex banded generalized Hermitian-definite eigenproblem
F08UQF Computes all the eigenvalues, and optionally, the eigenvectors of a complex banded generalized Hermitian-definite eigenproblem (divide-and-conquer)
F08WAF Computes, for a real nonsymmetric matrix pair, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
F08WBF Computes, for a real nonsymmetric matrix pair, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors; also, optionally, the balancing transformation, the reciprocal condition numbers for the eigenvalues and for the right eigenvectors
F08WNF Computes, for a complex nonsymmetric matrix pair, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
F08WPF Computes, for a complex nonsymmetric matrix pair, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors; also, optionally, the balancing transformation, the reciprocal condition numbers for the eigenvalues and for the right eigenvectors

F08XAF	Computes, for a real nonsymmetric matrix pair, the generalized eigenvalues, the generalized real Schur form and, optionally, the left and/or right matrices of Schur vectors
F08XBF	Computes, for a real nonsymmetric matrix pair, the generalized eigenvalues, the generalized real Schur form and, optionally, the left and/or right matrices of Schur vectors; also, optionally, computes reciprocal condition numbers for selected eigenvalues
F08XNF	Computes, for a complex nonsymmetric matrix pair, the generalized eigenvalues, the generalized complex Schur form and, optionally, the left and/or right matrices of Schur vectors
F08XPF	Computes, for a complex nonsymmetric matrix pair, the generalized eigenvalues, the generalized complex Schur form and, optionally, the left and/or right matrices of Schur vectors; also, optionally, computes reciprocal condition numbers for selected eigenvalues
F08ZAF	Solves the real linear equality-constrained least-squares (LSE) problem
F08ZBF	Solves a real general Gauss–Markov linear model (GLM) problem
F08ZEF	Computes a generalized *QR* factorization of a real matrix pair
F08ZFF	Computes a generalized *RQ* factorization of a real matrix pair
F08ZNF	Solves the complex linear equality-constrained least-squares (LSE) problem
F08ZPF	Solves a complex general Gauss–Markov linear model (GLM) problem
F08ZSF	Computes a generalized *QR* factorization of a complex matrix pair
F08ZTF	Computes a generalized *RQ* factorization of a complex matrix pair
F11DCF	Solution of real sparse nonsymmetric linear system, RGMRES, CGS, Bi-CGSTAB or TFQMR method, preconditioner computed by F11DAF
F11DEF	Solution of real sparse nonsymmetric linear system, RGMRES, CGS, Bi-CGSTAB, or TFQMR method, Jacobi or SSOR preconditioner (Black Box)
F11DKF	Real sparse nonsymmetric linear systems, line Jacobi preconditioner
F11DQF	Solution of complex sparse non-Hermitian linear system, RGMRES, CGS, Bi-CGSTAB or TFQMR method, preconditioner computed by F11DNF (Black Box)
F11DSF	Solution of complex sparse non-Hermitian linear system, RGMRES, CGS, Bi-CGSTAB or TFQMR method, Jacobi or SSOR preconditioner Black Box
F11DXF	Complex sparse nonsymmetric linear systems, line Jacobi preconditioner
F11JCF	Solution of real sparse symmetric linear system, conjugate gradient/Lanczos method, preconditioner computed by F11JAF (Black Box)
F11JEF	Solution of real sparse symmetric linear system, conjugate gradient/Lanczos method, Jacobi or SSOR preconditioner (Black Box)
F11JQF	Solution of complex sparse Hermitian linear system, conjugate gradient/Lanczos method, preconditioner computed by F11JNF (Black Box)
F11JSF	Solution of complex sparse Hermitian linear system, conjugate gradient/Lanczos method, Jacobi or SSOR preconditioner (Black Box)
F12FCF	Returns the converged approximations (as determined by F12ABF) to eigenvalues of a real symmetric sparse (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace
F12FGF	Computes approximations to selected eigenvalues of a real symmetric banded (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace
G01HBF	Computes probabilities for the multivariate Normal distribution
G02BYF	Computes partial correlation/variance-covariance matrix from correlation/variance-covariance matrix computed by G02BXF
G02DDF	Estimates of linear parameters and general linear regression model from updated model
G02DKF	Estimates and standard errors of parameters of a general linear regression model for given constraints
G02GKF	Estimates and standard errors of parameters of a general linear model for given constraints
G02HDF	Robust regression, compute regression with user-supplied functions and weights
G02JAF	Linear mixed effects regression using Restricted Maximum Likelihood (REML)
G03FAF	Performs principal co-ordinate analysis, classical metric scaling
G05PCF	Generates a realisation of a multivariate time series from a VARMA model
G11CAF	Returns parameter estimates for the conditional analysis of stratified data
G12BAF	Fits Cox's proportional hazard model
G13ADF	Univariate time series, preliminary estimation, seasonal ARIMA model
G13DXF	Calculates the zeros of a vector autoregressive (or moving average) operator

G13FAF Univariate time series, parameter estimation for either a symmetric GARCH process or a GARCH process with asymmetry of the form $(\epsilon_{t-1}+\gamma)^2$
G13FCF Univariate time series, parameter estimation 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
G13FGF Univariate time series, parameter estimation for an exponential GARCH (EGARCH) process

4 New Routines

The 375 new user-callable routines included in the SMP Library at Mark 21 are as follows.

A00ACF Check availability of a valid licence key
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
E04NPF Initialization routine for E04NQF
E04NQF LP or QP problem (suitable for sparse problems)
E04NRF Supply optional parameter values for E04NQF from external file
E04NSF Set a single option for E04NQF from a character string
E04NTF Set a single option for E04NQF from an INTEGER argument
E04NUF Set a single option for E04NQF from a ***double precision*** argument
E04NXF Get the setting of an INTEGER valued option of E04NQF
E04NYF Get the setting of a ***double precision*** valued option of E04NQF
E04USF Minimum of a sum of squares, nonlinear constraints, sequential QP method, using function values and optionally first derivatives (comprehensive)
E04VGF Initialization routine for E04VHF
E04VHF General sparse nonlinear optimizer
E04VJF Determine the pattern of nonzeros in the Jacobian matrix for E04VHF
E04VKF Supply optional parameter values for E04VHF from external file
E04VLF Set a single option for E04VHF from a character string
E04VMF Set a single option for E04VHF from an INTEGER argument
E04VNF Set a single option for E04VHF from a ***double precision*** argument
E04VRF Get the setting of an INTEGER valued option of E04VHF
E04VSF Get the setting of a ***double precision*** valued option of E04VHF
E04WBF Initialization routine for E04DGA E04MFA E04NCA E04NFA E04UFA E04UGA E04USA
E04WCF Initialization routine for E04WDF
E04WDF Solves the nonlinear programming (NP) problem
E04WEF Supply optional parameter values for E04WDF from external file
E04WFF Set a single option for E04WDF from a character string
E04WGF Set a single option for E04WDF from an INTEGER argument
E04WHF Set a single option for E04WDF from a ***double precision*** argument
E04WJF Determine whether an E04WDF option has been set or not
E04WKF Get the setting of an INTEGER valued option of E04WDF
E04WLF Get the setting of a ***double precision*** valued option of E04WDF

F04BAF	Computes the solution and error-bound to a real system of linear equations
F04BBF	Computes the solution and error-bound to a real banded system of linear equations
F04BCF	Computes the solution and error-bound to a real tridiagonal system of linear equations
F04BDF	Computes the solution and error-bound to a real symmetric positive-definite system of linear equations
F04BEF	Computes the solution and error-bound to a real symmetric positive-definite system of linear equations, packed storage
F04BFF	Computes the solution and error-bound to a real symmetric positive-definite banded system of linear equations
F04BGF	Computes the solution and error-bound to a real symmetric positive-definite tridiagonal system of linear equations
F04BHF	Computes the solution and error-bound to a real symmetric system of linear equations
F04BJF	Computes the solution and error-bound to a real symmetric system of linear equations, packed storage
F04CAF	Computes the solution and error-bound to a complex system of linear equations
F04CBF	Computes the solution and error-bound to a complex banded system of linear equations
F04CCF	Computes the solution and error-bound to a complex tridiagonal system of linear equations
F04CDF	Computes the solution and error-bound to a complex Hermitian positive-definite system of linear equations
F04CEF	Computes the solution and error-bound to a complex Hermitian positive-definite system of linear equations, packed storage
F04CFF	Computes the solution and error-bound to a complex Hermitian positive-definite banded system of linear equations
F04CGF	Computes the solution and error-bound to a complex Hermitian positive-definite tridiagonal system of linear equations
F04CHF	Computes the solution and error-bound to a complex Hermitian system of linear equations
F04CJF	Computes the solution and error-bound to a complex Hermitian system of linear equations, packed storage
F04DHF	Computes the solution and error-bound to a complex symmetric system of linear equations
F04DJF	Computes the solution and error-bound to a complex symmetric system of linear equations, packed storage.
F06FEF	Multiply real vector by reciprocal of scalar
F06KEF	Multiply complex vector by reciprocal of real scalar
F06RNF	1-norm, ∞-norm, Frobenius norm, largest absolute element, real tridiagonal matrix
F06RPF	1-norm, ∞-norm, Frobenius norm, largest absolute element, real symmetric tridiagonal matrix
F06TAF	Matrix-vector product, complex symmetric matrix
F06TBF	Rank-1 update, complex symetric matrix
F06TCF	Matrix-vector product, complex symmetric packed matrix
F06TDF	Rank-1 update, complex symetric packed matrix
F06UNF	1-norm, ∞-norm, Frobenius norm, largest absolute element, complex tridiagonal matrix
F06UPF	1-norm, ∞-norm, Frobenius norm, largest absolute element, complex Hermitian tridiagonal matrix
F07AAF	Computes the solution to a real system of linear equations
F07ABF	Uses the *LU* factorization to compute the solution, error-bound and condition estimate for a real system of linear equations
F07AFF	Computes row and column scalings intended to equilibrate a general real matrix and reduce its condition number
F07ANF	Computes the solution to a complex system of linear equations
F07APF	Uses the *LU* factorization to compute the solution, error-bound and condition estimate for a complex system of linear equations
F07ATF	Computes row and column scalings intended to equilibrate a general complex matrix and reduce its condition number
F07BAF	Computes the solution to a real banded system of linear equations
F07BBF	Uses the *LU* factorization to compute the solution, error-bound and condition estimate for a real banded system of linear equations
F07BFF	Computes row and column scalings intended to equilibrate a real banded matrix and reduce its condition number
F07BNF	Computes the solution to a complex banded system of linear equations

F07BPF Uses the *LU* factorization to compute the solution, error-bound and condition estimate for a complex banded system of linear equations
F07BTF Computes row and column scalings intended to equilibrate a complex banded matrix and reduce its condition number
F07CAF Computes the solution to a real tridiagonal system of linear equations
F07CBF Uses the *LU* factorization to compute the solution, error-bound and condition estimate for a real tridiagonal system of linear equations
F07CDF *LU* factorization of real tridiagonal matrix
F07CEF Solves a real tridiagonal system of linear equations using the *LU* factorization computed by F07CDF (DGTTRF)
F07CGF Estimates the reciprocal of the condition number of a real tridiagonal matrix using the *LU* factorization computed by F07CDF (DGTTRF)
F07CHF Refined solution with error bounds of real tridiagonal system of linear equations, multiple right-hand sides
F07CNF Computes the solution to a complex tridiagonal system of linear equations
F07CPF Uses the *LU* factorization to compute the solution, error-bound and condition estimate for a complex tridiagonal system of linear equations
F07CRF *LU* factorization of complex tridiagonal matrix
F07CSF Solves a complex tridiagonal system of linear equations using the *LU* factorization computed by F07CDF (DGTTRF)
F07CUF Estimates the reciprocal of the condition number of a complex tridiagonal matrix using the *LU* factorization computed by F07CDF (DGTTRF)
F07CVF Refined solution with error bounds of complex tridiagonal system of linear equations, multiple right-hand sides
F07FAF Computes the solution to a real symmetric positive-definite system of linear equations
F07FBF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a real symmetric positive-definite system of linear equations
F07FFF Computes row and column scalings intended to equilibrate a real symmetric positive-definite matrix and reduce its condition number
F07FNF Computes the solution to a complex Hermitian positive-definite system of linear equations
F07FPF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a complex Hermitian positive-definite system of linear equations
F07FTF Computes row and column scalings intended to equilibrate a complex Hermitian positive-definite matrix and reduce its condition number
F07GAF Computes the solution to a real symmetric positive-definite system of linear equations, packed storage
F07GBF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a real symmetric positive-definite system of linear equations, packed storage
F07GFF Computes row and column scalings intended to equilibrate a real symmetric positive-definite matrix and reduce its condition number, packed storage
F07GNF Computes the solution to a complex Hermitian positive-definite system of linear equations, packed storage
F07GPF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a complex Hermitian positive-definite system of linear equations, packed storage
F07GTF Computes row and column scalings intended to equilibrate a complex Hermitian positive-definite matrix and reduce its condition number, packed storage
F07HAF Computes the solution to a real symmetric positive-definite banded system of linear equations
F07HBF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a real symmetric positive-definite banded system of linear equations
F07HFF Computes row and column scalings intended to equilibrate a real symmetric positive-definite banded matrix and reduce its condition number
F07HNF Computes the solution to a complex Hermitian positive-definite banded system of linear equations
F07HPF Uses the Cholesky factorization to compute the solution, error-bound and condition estimate for a complex Hermitian positive-definite banded system of linear equations
F07HTF Computes row and column scalings intended to equilibrate a complex Hermitian positive-definite banded matrix and reduce its condition number
F07JAF Computes the solution to a real symmetric positive-definite tridiagonal system of linear equations

F07JBF	Uses the modified Cholesky factorization to compute the solution, error-bound and condition estimate for a real symmetric positive-definite tridiagonal system of linear equations
F07JDF	Computes the modified Cholesky factorization of a real symmetric positive-definite tridiagonal matrix
F07JEF	Solution of real symmetric tridiagonal linear system, matrix already factorized by F07JDF (DPTTRF)
F07JGF	Computes the reciprocal of the condition number of a real symmetric positive-definite tridiagonal system using the modified Cholesky factorization computed by F07JDF (DPTTRF)
F07JHF	Refined solution with error bounds of real symmetric positive-definite tridiagonal system of linear equations, multiple right-hand sides
F07JNF	Computes the solution to a complex Hermitian positive-definite tridiagonal system of linear equations
F07JPF	Uses the modified Cholesky factorization to compute the solution, error-bound and condition estimate for a complex Hermitian positive-definite tridiagonal system of linear equations
F07JRF	Computes the modified Cholesky factorization of a complex Hermitian positive-definite tridiagonal matrix
F07JSF	Solves a complex Hermitian positive-definite tridiagonal system using the modified Cholesky factorization computed by F07JRF (ZPTTRF)
F07JUF	Computes the reciprocal of the condition number of a complex Hermitian positive-definite tridiagonal system using the modified Cholesky factorization computed by F07JRF (ZPTTRF)
F07JVF	Refined solution with error bounds of complex Hermitian positive-definite tridiagonal system of linear equations, multiple right-hand sides
F07MAF	Computes the solution to a real symmetric system of linear equations
F07MBF	Uses the diagonal pivoting factorization to compute the solution to a real symmetric system of linear equations
F07MNF	Computes the solution to a complex Hermitian system of linear equations
F07MPF	Uses the diagonal pivoting factorization to compute the solution to a complex Hermitian system of linear equations
F07NNF	Computes the solution to a complex symmetric system of linear equations
F07NPF	Uses the diagonal pivoting factorization to compute the solution to a complex symmetric system of linear equations
F07PAF	Computes the solution to a real symmetric system of linear equations, packed storage
F07PBF	Uses the diagonal pivoting factorization to compute the solution to a real symmetric system of linear equations, packed storage
F07PNF	Computes the solution to a complex Hermitian system of linear equations, packed storage
F07PPF	Uses the diagonal pivoting factorization to compute the solution to a complex Hermitian system of linear equations, packed storage
F07QNF	Computes the solution to a complex symmetric system of linear equations, packed storage
F07QPF	Uses the diagonal pivoting factorization to compute the solution to a complex symmetric system of linear equations, packed storage
F08AAF	Solves an overdetermined or underdetermined real linear system
F08ANF	Solves an overdetermined or underdetermined complex linear system
F08BAF	Computes the minimum-norm solution to a real linear least-squares problem
F08BFF	*QR* factorization of real general rectangular matrix with column pivoting, using BLAS-3
F08BHF	Reduces a real upper trapezoidal matrix to upper triangular form
F08BKF	Apply orthogonal transformation determined by F08BHF (DTZRZF)
F08BNF	Computes the minimum-norm solution to a complex linear least-squares problem
F08BTF	*QR* factorization of complex general rectangular matrix with column pivoting, using BLAS-3
F08BVF	Reduces a complex upper trapezoidal matrix to upper triangular form
F08BXF	Apply unitary transformation determined by F08BVF (ZTZRZF)
F08CEF	*QL* factorization of real general rectangular matrix
F08CFF	Form all or part of orthogonal Q from *QL* factorization determined by F08CEF (DGEQLF)
F08CGF	Apply orthogonal transformation determined by F08CEF (DGEQLF)
F08CHF	*RQ* factorization of real general rectangular matrix
F08CJF	Form all or part of orthogonal Q from *RQ* factorization determined by F08CHF (DGERQF)
F08CKF	Apply orthogonal transformation determined by F08CHF (DGERQF)
F08CSF	*QL* factorization of complex general rectangular matrix
F08CTF	Form all or part of orthogonal Q from *QL* factorization determined by F08CSF (ZGEQLF)
F08CUF	Apply unitary transformation determined by F08CSF (ZGEQLF)

F08CVF	*RQ* factorization of complex general rectangular matrix
F08CWF	Form all or part of orthogonal *Q* from *RQ* factorization determined by F08CVF (ZGERQF)
F08CXF	Apply unitary transformation determined by F08CVF (ZGERQF)
F08FAF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix
F08FBF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix
F08FDF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix (Relatively Robust Representations)
F08FLF	Computes the reciprocal condition numbers for the eigenvectors of a real symmetric or complex Hermitian matrix or for the left or right singular vectors of a general matrix
F08FNF	Computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix
F08FPF	Computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix
F08FRF	Computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix (Relatively Robust Representations)
F08GAF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix, packed storage
F08GBF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix, packed storage
F08GNF	Computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix, packed storage
F08GPF	Computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix, packed storage
F08HAF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric band matrix
F08HBF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric band matrix
F08HNF	Computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix
F08HPF	Computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix
F08JAF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix
F08JBF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix
F08JDF	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix (Relatively Robust Representations)
F08JHF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix or a matrix reduced to this form (divide-and-conquer)
F08JLF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix or a symmetric matrix reduced to this form (Relatively Robust Representations)
F08JVF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix or a complex Hermitian matrix reduced to this form (divide-and-conquer)
F08JYF	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix or a complex Hermitian matrix reduced to this form (Relatively Robust Representations)
F08KAF	Computes the minimum-norm solution to a real linear least-squares problem using singular value decomposition
F08KBF	Computes the singular value decomposition of a real matrix, optionally computing the left and/or right singular vectors
F08KCF	Computes the minimum-norm solution to a real linear least-squares problem using singular value decomposition (divide-and-conquer)
F08KDF	Computes the singular value decomposition of a real matrix, optionally computing the left and/or right singular vectors (divide-and-conquer)
F08KNF	Computes the minimum-norm solution to a complex linear least-squares problem using singular value decomposition
F08KPF	Computes the singular value decomposition of a complex matrix, optionally computing the left and/or right singular vectors
F08KQF	Computes the minimum-norm solution to a complex linear least-squares problem using singular value decomposition (divide-and-conquer)
F08KRF	Computes the singular value decomposition of a complex matrix, optionally computing the left and/or right singular vectors (divide-and-conquer)
F08MDF	Computes the singular value decomposition of a real bidiagonal matrix, optionally computing the singular vectors (divide-and-conquer)
F08NAF	Computes all eigenvalues and, optionally, left and/or right eigenvectors of a real nonsymmetric matrix

F08NBF	Computes all eigenvalues and, optionally, left and/or right eigenvectors of a real nonsymmetric matrix; also, optionally, the balancing transformation, the reciprocal condition numbers for the eigenvalues and for the right eigenvectors
F08NNF	Computes all eigenvalues and, optionally, left and/or right eigenvectors of a complex nonsymmetric matrix
F08NPF	Computes all eigenvalues and, optionally, left and/or right eigenvectors of a complex nonsymmetric matrix; also, optionally, the balancing transformation, the reciprocal condition numbers for the eigenvalues and for the right eigenvectors
F08PAF	Computes for real square nonsymmetric matrix, the eigenvalues, the real Schur form, and, optionally, the matrix of Schur vectors
F08PBF	Computes for real square nonsymmetric matrix, the eigenvalues, the real Schur form, and, optionally, the matrix of Schur vectors; also, optionally, computes reciprocal condition numbers for selected eigenvalues
F08PNF	Computes for complex square nonsymmetric matrix, the eigenvalues, the Schur form, and, optionally, the matrix of Schur vectors
F08PPF	Computes for real square nonsymmetric matrix, the eigenvalues, the Schur form, and, optionally, the matrix of Schur vectors; also, optionally, computes reciprocal condition numbers for selected eigenvalues
F08SAF	Computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
F08SBF	Computes selected eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem
F08SCF	Computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem (divide-and-conquer)
F08SNF	Computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
F08SPF	Computes selected eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem
F08SQF	Computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem (divide-and-conquer)
F08TAF	Computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, packed storage
F08TBF	Computes selected eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, packed storage
F08TCF	Computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, packed storage (divide-and-conquer)
F08TNF	Computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, packed storage
F08TPF	Computes selected eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, packed storage
F08TQF	Computes selected eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, packed storage (divide-and-conquer)
F08UAF	Computes all the eigenvalues, and optionally, the eigenvectors of a real banded generalized symmetric-definite eigenproblem
F08UBF	Computes selected eigenvalues, and optionally, the eigenvectors of a real banded generalized symmetric-definite eigenproblem
F08UCF	Computes all the eigenvalues, and optionally, the eigenvectors of a real banded generalized symmetric-definite eigenproblem (divide-and-conquer)
F08UNF	Computes all the eigenvalues, and optionally, the eigenvectors of a complex banded generalized Hermitian-definite eigenproblem
F08UPF	Computes selected eigenvalues, and optionally, the eigenvectors of a complex banded generalized Hermitian-definite eigenproblem
F08UQF	Computes all the eigenvalues, and optionally, the eigenvectors of a complex banded generalized Hermitian-definite eigenproblem (divide-and-conquer)
F08VAF	Computes the generalized singular value decomposition of a real matrix pair
F08VEF	Computes orthogonal matrices as processing steps for computing the generalized singular value decomposition of a real matrix pair
F08VNF	Computes the generalized singular value decomposition of a complex matrix pair

F08VSF	Computes orthogonal matrices as processing steps for computing the generalized singular value decomposition of a complex matrix pair
F08WAF	Computes, for a real nonsymmetric matrix pair, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
F08WBF	Computes, for a real nonsymmetric matrix pair, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors; also, optionally, the balancing transformation, the reciprocal condition numbers for the eigenvalues and for the right eigenvectors
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 (DGGBAL)
F08WNF	Computes, for a complex nonsymmetric matrix pair, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
F08WPF	Computes, for a complex nonsymmetric matrix pair, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors; also, optionally, the balancing transformation, the reciprocal condition numbers for the eigenvalues and for the right eigenvectors
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 (ZGGBAL)
F08XAF	Computes, for a real nonsymmetric matrix pair, the generalized eigenvalues, the generalized real Schur form and, optionally, the left and/or right matrices of Schur vectors
F08XBF	Computes, for a real nonsymmetric matrix pair, the generalized eigenvalues, the generalized real Schur form and, optionally, the left and/or right matrices of Schur vectors; also, optionally, computes reciprocal condition numbers for selected eigenvalues
F08XEF	Eigenvalues and generalized Schur factorization of real generalized upper Hessenberg form reduced from a pair of real general matrices
F08XNF	Computes, for a complex nonsymmetric matrix pair, the generalized eigenvalues, the generalized complex Schur form and, optionally, the left and/or right matrices of Schur vectors
F08XPF	Computes, for a complex nonsymmetric matrix pair, the generalized eigenvalues, the generalized complex Schur form and, optionally, the left and/or right matrices of Schur vectors; also, optionally, computes reciprocal condition numbers for selected eigenvalues
F08XSF	Eigenvalues and generalized Schur factorization of complex generalized upper Hessenberg form reduced from a pair of complex general matrices
F08YEF	Computes the generalized singular value decomposition of a real upper triangular (or trapezoidal) matrix pair
F08YFF	Reorders the generalized real Schur decomposition of a real matrix pair using an orthogonal equivalence transformation
F08YGF	Reorders the generalized real Schur decomposition of a real matrix pair using an orthogonal equivalence transformation, computes the generalized eigenvalues of the reordered pair and, optionally, computes the estimates of reciprocal condition numbers for eigenvalues and eigenspaces
F08YHF	Solves the real-valued generalized Sylvester equation
F08YKF	Left and right eigenvectors of a pair of real upper quasi-triangular matrices
F08YLF	Estimates reciprocal condition numbers for specified eigenvalues and/or eigenvectors of a real matrix pair in generalized real Schur canonical form
F08YSF	Computes the generalized singular value decomposition of a complex upper triangular (or trapezoidal) matrix pair
F08YTF	Reorders the generalized Schur decomposition of a complex matrix pair using an unitary equivalence transformation
F08YUF	Reorders the generalized Schur decomposition of a complex matrix pair using an unitary equivalence transformation, computes the generalized eigenvalues of the reordered pair and, optionally, computes the estimates of reciprocal condition numbers for eigenvalues and eigenspaces
F08YVF	Solves the complex generalized Sylvester equation
F08YXF	Left and right eigenvectors of a pair of complex upper triangular matrices
F08YYF	Estimates reciprocal condition numbers for specified eigenvalues and/or eigenvectors of a complex matrix pair in generalized Schur canonical form

F08ZAF	Solves the real linear equality-constrained least-squares (LSE) problem
F08ZBF	Solves a real general Gauss–Markov linear model (GLM) problem
F08ZEF	Computes a generalized *QR* factorization of a real matrix pair
F08ZFF	Computes a generalized *RQ* factorization of a real matrix pair
F08ZNF	Solves the complex linear equality-constrained least-squares (LSE) problem
F08ZPF	Solves a complex general Gauss–Markov linear model (GLM) problem
F08ZSF	Computes a generalized *QR* factorization of a complex matrix pair
F08ZTF	Computes a generalized *RQ* factorization of a complex matrix pair
F11DXF	Complex sparse nonsymmetric linear systems, line Jacobi preconditioner
F11GRF	Complex sparse Hermitian linear systems, setup for F11GSF
F11GSF	Complex sparse Hermitian linear systems, preconditioned conjugate gradient or Lanczos
F11GTF	Complex sparse Hermitian linear systems, diagnostic for F11GSF
F11MDF	Real sparse nonsymmetric linear systems, setup for F11MEF
F11MEF	*LU* factorization of real sparse matrix
F11MFF	Solution of real sparse simultaneous linear equations (coefficient matrix already factorized)
F11MGF	Estimate condition number of real matrix, matrix already factorized by F11MEF
F11MHF	Refined solution with error bounds of real system of linear equations, multiple right-hand sides
F11MKF	Real sparse nonsymmetric matrix matrix multiply, compressed column storage
F11MLF	1-norm, ∞-norm, largest absolute element, real general matrix
F11MMF	Real sparse nonsymmetric linear systems, diagnostic for F11MEF
F12AAF	Initialization routine for (F12ABF) computing selected eigenvalues and, optionally, eigenvectors of a real nonsymmetric sparse (standard or generalized) eigenproblem
F12ABF	Implements a reverse communication interface for the Implicitly Restarted Arnoldi iteration for computing selected eigenvalues and, optionally, eigenvectors of a real nonsymmetric sparse (standard or generalized) eigenproblem
F12ACF	Returns the converged approximations (as determined by F12ABF) to eigenvalues of a real nonsymmetric sparse (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace
F12ADF	Set a single option from a string (F12ABF/F12ACF/F12AGF)
F12AEF	Provides monitoring information for F12ABF
F12AFF	Initialization routine for (F12AGF) computing selected eigenvalues and, optionally, eigenvectors of a real nonsymmetric banded (standard or generalized) eigenproblem
F12AGF	Computes approximations to selected eigenvalues of a real nonsymmetric banded (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace
F12ANF	Initialization routine for (F12APF) computing selected eigenvalues and, optionally, eigenvectors of a complex sparse (standard or generalized) eigenproblem
F12APF	Implements a reverse communication interface for the Implicitly Restarted Arnoldi iteration for computing selected eigenvalues and, optionally, eigenvectors of a complex sparse (standard or generalized) eigenproblem
F12AQF	Returns the converged approximations (as determined by F12ABF) to eigenvalues of a complex sparse (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace
F12ARF	Set a single option from a string (F12APF/F12AQF)
F12ASF	Provides monitoring information for F12APF
F12FAF	Initialization routine for (F12FBF) computing selected eigenvalues and, optionally, eigenvectors of a real symmetric sparse (standard or generalized) eigenproblem
F12FBF	Implements a reverse communication interface for the Implicitly Restarted Arnoldi iteration for computing selected eigenvalues and, optionally, eigenvectors of a real symmetric sparse (standard or generalized) eigenproblem
F12FCF	Returns the converged approximations (as determined by F12ABF) to eigenvalues of a real symmetric sparse (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace
F12FDF	Set a single option from a string (F12FBF/F12FCF/F12FGF)
F12FEF	Provides monitoring information for F12FBF

F12FFF	Initialization routine for (F12FGF) computing selected eigenvalues and, optionally, eigenvectors of a real symmetric banded (standard or generalized) eigenproblem
F12FGF	Computes approximations to selected eigenvalues of a real symmetric banded (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace
G01ETF	Landau distribution function $\Phi(\lambda)$
G01EUF	Vavilov distribution function $\Phi_V\left(\lambda;\kappa,\beta^2\right)$
G01FTF	Landau inverse function $\Psi(x)$
G01MTF	Landau density function $\phi(\lambda)$
G01MUF	Vavilov density function $\phi_V\left(\lambda;\kappa,\beta^2\right)$
G01PTF	Landau first moment function $\Phi_1(x)$
G01QTF	Landau second moment function $\Phi_2(x)$
G01RTF	Landau derivative function $\phi\prime(\lambda)$
G01ZUF	Initialization routine for G01MUF and G01EUF
G02EFF	Stepwise linear regression
G02JAF	Linear mixed effects regression using Restricted Maximum Likelihood (REML)
G02JBF	Linear mixed effects regression using Maximum Likelihood (ML)
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	Initialize seeds of a given generator for random number generating routines (that pass seeds explicitly) to give a repeatable sequence
G05KCF	Initialize 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
G05LXF	Generates a matrix of random numbers from a multivariate Student's *t*-distribution, seeds and generator passed explicitly
G05LYF	Generates a matrix of random numbers from a multivariate Normal distribution, seeds and generator 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
G05RAF	Generates a matrix of random numbers from a Gaussian Copula, seeds and generator passed explicitly
G05RBF	Generates a matrix of random numbers from a Student's *t*-Copula, seeds and generator passed explicitly
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
G05YCF	Initializes the Faure generator (G05YDF/G05YJF/G05YKF)
G05YDF	Generates a sequence of quasi-random numbers using Faure's method
G05YEF	Initializes the Sobol generator (G05YFF/G05YJF/G05YKF)
G05YFF	Generates a sequence of quasi-random numbers using Sobol's method
G05YGF	Initializes the Neiderreiter generator (G05YHF/G05YJF/G05YKF)
G05YHF	Generates a sequence of quasi-random numbers using Neiderreiter's method
G05YJF	Generates a Normal quasi-random number sequence using Faure's, Sobol's or Neiderreiter's method
G05YKF	Generates a log-Normal quasi-random number sequence using Faure's, Sobol's or Neiderreiter's method
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 $(\lvert\epsilon_{t-1}\rvert + \gamma\epsilon_{t-1})^2$
G13FDF	Univariate time series, forecast function for a GARCH process with asymmetry of the form $(\lvert\epsilon_{t-1}\rvert + \gamma\epsilon_{t-1})^2$
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, parameter estimation 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
S14AGF	Logarithm of the Gamma function $\ln\Gamma(z)$
S17ALF	Zeros of Bessel functions $J_\alpha(x)$, $J_\alpha\prime(x)$, $Y_\alpha(x)$ or $Y_\alpha\prime(x)$
S18GKF	Bessel function of the 1st kind $J_{\alpha+n}(z)$
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 $F(z,k\prime,a,b)$ of complex argument
S22AAF	Legendre functions of 1st kind $P_n^m(x)$ or $\overline{P_n^m}(x)$

5 Withdrawn SMP Functionality

The random number generator routines parallelized in Release 2 have now been scheduled for withdrawal at Mark 22, as the interfaces used were not thread-safe due to the internal use of COMMON blocks. Therefore, the SMP functionality has not been included in this release, to encourage users to switch to the new thread-safe replacement routines. Users can easily take advantage of the new thread-safe replacement routines on multiple processors by calling the routines within their own OpenMP parallel region, using a different generator number and seed array for each thread. As there are 273 separate Wichmann–Hill generators available, statistically independent sequences of random numbers can be generated on up to 273 processors simultaneously.

Routines Scheduled for Withdrawal	**Replacement Routine(s)**
G05FAF	G05LGF
G05FBF	G05LJF
G05FDF	G05LAF
G05FEF	G05LEF
G05FFF	G05LFF
G05FSF	G05LPF
G05GAF	G05QAF
G05GBF	G05QBF
G05HDF	G05PCF

6 Withdrawn Routines

The following routines have been withdrawn from the NAG SMP Library at Mark 21. Warning of their withdrawal was included in the NAG Fortran Library Manual at Mark 20, 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
F11BAF	F11BDF
F11BBF	F11BEF
F11BCF	F11BFF

7 Routines Scheduled for Withdrawal

The routines listed below are scheduled for withdrawal from the SMP 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 22.

Routine Scheduled for Withdrawal	**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
G05ZAF	No replacement document required

The following routines have been superseded, but will not be withdrawn from the Library until Mark 23 at the earliest.

Superseded Routine	Replacement Routine(s)
E04NKF/E04NKA	E04NQF
E04NLF/E04NLA	E04NRF
E04UCF/E04UCA	E04WDF
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	G05YCF, G05YDF, G05YEF, G05YFF, G05YGF, G05YHF, G05YJF and G05YKF
G05YBF	G05YCF, G05YDF, G05YEF, G05YFF, G05YGF, G05YHF, G05YJF and G05YKF