

Mark 19 News

1 Introduction

At Mark 19 of the Fortran Library new functionality has been introduced in addition to improvements in existing areas. The Library now contains 1155 documented routines, of which 62 are new at this Mark. These extend the areas of fast Fourier transforms (FFTs), optimization, eigenvalue problems (LAPACK), sparse linear algebra, statistics, operations research (OR) and sorting as summarized below.

The most significant additions to the FFT chapter (Chapter C06) are as follows:

- new routines for complex Fourier transforms using complex data type arrays;
- new routines for sine and cosine transforms.

Coverage in the optimization chapter (Chapter E04) has been extended with the addition of a routine to solve sparse nonlinear programming problems.

New routines for solving eigenproblems (Chapter F08) are included for:

- computing all the eigenvalues (and optionally all the eigenvectors) of real symmetric and complex Hermitian matrices;
- reducing real and complex rectangular band matrices to upper bidiagonal form;
- computing a split Cholesky factorization of real symmetric positive-definite and complex Hermitian positive-definite band matrices;
- reducing real symmetric-definite and complex Hermitian-definite banded generalized eigenproblems to standard form.

Coverage in the sparse linear algebra chapter (Chapter F11) has been extended to provide iterative methods and preconditioners for complex symmetric and non-Hermitian linear systems of equations.

Two of the new routines are in the statistics chapters (Chapter G01 to Chapter G13). They include facilities (in the stated chapters) for:

- conditional logistic analysis for case-control studies and survival analysis (G11);
- computing the risk sets in the analysis of survival data (G12).

Coverage in the OR chapter (Chapter H) has been extended to provide solvers for dense and sparse integer quadratic programming problems.

A new routine for sorting a vector of complex numbers into the order specified by a vector of ranks is included in Chapter M01.

2 New Routines

The 62 new user-callable routines included in the NAG Fortran Library at Mark 19 are as follows.

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
C06PFF	One-dimensional complex discrete Fourier transform of multi-dimensional data (using complex data type)
C06PJF	Multi-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)
E04UGF	NLP problem (sparse)
E04UHF	Read optional parameter values for E04UGF from external file
E04UJF	Supply optional parameter values to E04UGF
F08FCF	(SSYEVD/DSYEVD) All eigenvalues and optionally all eigenvectors of real symmetric matrix, using divide and conquer
F08FQF	(CHEEVD/ZHEEVD) All eigenvalues and optionally all eigenvectors of complex Hermitian matrix, using divide and conquer
F08GCF	(SPEVD/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	(SBEVD/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
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
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
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
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
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)
H02CFE	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

3 Withdrawn Routines

The following routines have been withdrawn from the NAG Fortran Library at Mark 19. Warning of their withdrawal was included in the Mark 18 Library Manual, together with advice on which routines to use instead. See the document ‘Advice on Replacement Calls for Superseded/Withdrawn Routines’ for more detailed guidance.

Withdrawn Routine	Recommended Replacement
E04FDF	E04FYF
E04GCF	E04GYF
E04GEF	E04GZF
E04HFF	E04HYF
E04JAF	E04JYF
E04KAF	E04KYF
E04KCF	E04KZF
E04LAF	E04LYF
E04UPF	E04UNF
F01MAF	F11JAF
F02BBF	F02FCF
F02BCF	F02ECF
F02BDF	F02GCF
F04MAF	F11JCF
F04MBF	F11GAF, F11GBF and F11GCF (or F11JCF or F11JEF)

4 Routines Scheduled for Withdrawal

The routines listed below are scheduled for withdrawal from the NAG Fortran Library, because improved routines have now been included in the Library. Users are advised to stop using routines which are scheduled for withdrawal immediately and to use recommended replacement routines instead. See the document ‘Advice on Replacement Calls for 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 Mark 20.

Routine Scheduled for Withdrawal	Recommended Replacement
E01SEF	E01SGF
E01SFF	E01SHF

The following routines have been superseded, but will not be withdrawn from the Library until Mark 21 at the earliest.

Superseded routine	Recommended Replacement
F11BAF	F11BDF
F11BBF	F11BEF
F11BCF	F11BFF
