

Mark 18 News

1 New Features of Mark 18

At Mark 18 of the Fortran Library a variety of new facilities have been introduced and improvements made in existing areas. The Library now contains a total of 1108 documented routines, of which 35 are new at this Mark. These extend the areas of ordinary differential equations (ODEs), partial differential equations (PDEs), interpolation, optimization, sparse linear algebra and operations research (OR).

Coverage in the differential equations chapters (Chapter D02 and Chapter D03) has been extended as follows:

- simple driver interface for the integration of a system of first order ODEs using a fixed order Runge–Kutta method until a user-specified function is zero (Chapter D02)
- new approximate and exact Riemann solvers for 1-D Euler equations (Chapter D03)
- solution of time dependent second order PDEs in 2-D using adaptive mesh refinement (Chapter D03)

New routines for generating and evaluating interpolants to 2-D and 3-D scattered data sets (using a modified Shepard interpolant) are included in the interpolation chapter (Chapter E01).

The most significant additions to the optimization chapter (Chapter E04) are as follows:

- new routines to solve sparse LP and QP problems (including MPSX data-handling capabilities)
- new routines for unconstrained minimization with an extended parameter list to replace existing routines with reserved names
- a new reverse communication routine for constrained minimization using a sequential quadratic programming method

Coverage in the sparse linear algebra chapter (Chapter F11) has been extended to provide iterative methods and preconditioners for real nonsymmetric linear systems of equations.

A new routine for finding the shortest path through a network is included in the operations research chapter (Chapter H).

2 New Routines

For details, please refer to the relevant chapter introductions and routine documents. A concise summary of the purpose of all documented routines in the Library (with the exception of routines which have been superseded) is given in the document ‘Library Contents, Mark 18’.

The following 35 new user-callable routines are included in the NAG Fortran Library at Mark 18:

D02BJF	D03PWF	D03PXF	D03RAF	D03RBF	D03RYF
D03RZF	E01SGF	E01SHF	E01TGF	E01THF	E04FYF
E04GYF	E04GZF	E04HYF	E04JYF	E04KYF	E04KZF
E04LYF	E04MZF	E04NKF	E04NLF	E04NMF	E04UFF
F11BAF	F11BBF	F11BCF	F11DAF	F11DBF	F11DCF
F11DDF	F11DEF	F11XAF	F11ZAF	H03ADF	

3 Withdrawn Routines

The following routines have been withdrawn from the NAG Fortran Library at Mark 18. Warning of their withdrawal was included in the Mark 17 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
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
E04MBF	E04MFF
E04NAF	E04NFF
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)
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)
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)
G01CEF	G01FAF

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 detailed advice on how to change a call to the old routine into a call to the new routine.

The following routines will be withdrawn at Mark 19:

Routine Scheduled for Withdrawal	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)

The following routines have been superseded, but will not be withdrawn from the Library until Mark 20 at the earliest. They are being retained at Marks 18 and 19 because of their length of life in the Library, and to give users a longer time to make the transition to the new routines.

Superseded routine	Recommended Replacement
E01SEF	E01SGF
E01SFF	E01SHF