# NAG Fortran Library

# Advice on Replacement Calls for Withdrawn/Superseded Routines

The following list gives the names of replacement routines for those routines that have been withdrawn or superseded. For routines that have been withdrawn or superseded since Mark 13 replacement calls are also given. The list indicates the minimum change necessary, but many of the replacement routines have additional flexibility and users may wish to take advantage of new features. It is strongly recommended that users consult the routine documents.

Files containing the replacement call information are provided as part of the distribution materials and can be found in the directory examples/replaced.

## C02 – Zeros of Polynomials

## C02ADF

Withdrawn at Mark 15 Replaced by C02AFF

Old: CALL CO2ADF(AR,AC,N,REZ,IMZ,TOL,IFAIL)
New: CALL CO2AFF(A,N-1,SCALE,Z,W,IFAIL)

The coefficients are stored in the *double precision* array A of dimension (2, N + 1) rather than in the arrays AR and AC, the zeros are returned in the *double precision* array Z of dimension (2, N) rather than in the arrays REZ and IMZ, and W is a *double precision* work array of dimension  $(4 \times (N + 1))$ .

## C02AEF

Withdrawn at Mark 16 Replaced by C02AGF

> Old: CALL CO2AEF(A,N,REZ,IMZ,TOL,IFAIL) New: CALL CO2AGF(A,N-1,SCALE,Z,W,IFAIL)

The zeros are returned in the *double precision* array Z of dimension (2, N) rather than in the arrays REZ and IMZ, and W is a *double precision* work array of dimension  $(2 \times (N + 1))$ .

## C05 – Roots of One or More Transcendental Equations

**C05AAF** Withdrawn at Mark 9 Replaced by C05ADF

## C05ABF

Withdrawn at Mark 9 Replaced by C05ADF

## C05ACF

Withdrawn at Mark 9 Replaced by C05ADF

## C05NAF

Withdrawn at Mark 10 Replaced by C05NBF or C05NCF

## C05PAF

Withdrawn at Mark 8 Replaced by C05PBF or C05PCF

## C06 – Summation of Series

## C06AAF

Withdrawn at Mark 9 Replaced by C06ECF or C06FRF

## C06ABF

Withdrawn at Mark 9 Replaced by C06EAF or C06FPF

## C06ACF

Withdrawn at Mark 12 Replaced by C06EKF or C06FKF

## C06ADF

Withdrawn at Mark 12 Replaced by C06FFF

## **D01 – Quadrature**

## D01AAF

Withdrawn at Mark 8 Replaced by D01AJF

## D01ABF

Withdrawn at Mark 8 Replaced by D01AJF

## D01ACF

Withdrawn at Mark 9 Replaced by D01BDF

## D01ADF

Withdrawn at Mark 8 Replaced by D01BAF or D01BBF

## D01AEF

Withdrawn at Mark 8 Replaced by D01BAF or D01BBF

## D01AFF

Withdrawn at Mark 8 Replaced by D01BAF or D01BBF

## D01AGF

Withdrawn at Mark 9 Replaced by D01AJF

## D01FAF

Withdrawn at Mark 11 Replaced by D01GBF

## **D02** – Ordinary Differential Equations

## D02AAF

Withdrawn at Mark 8 Replaced by D02PDF and related routines

## D02ABF

Withdrawn at Mark 8 Replaced by D02PCF and related routines

## D02ADF

Withdrawn at Mark 9 Replaced by D02GAF or D02HAF

## D02AFF

Withdrawn at Mark 9 Replaced by D02TGF

#### D02AHF

Withdrawn at Mark 8 Replaced by D02CJF or D02QFF

## D02AJF

Withdrawn at Mark 8 Replaced by D02EJF and D02NBF and related routines

#### D02BAF

```
Withdrawn at Mark 18
Replaced by D02PCF and associated D02P routines
```

```
Old: CALL D02BAF(X,XEND,N,Y,TOL,FCN,W,IFAIL)
New: D0 10 L = 1,N
        THRES(L) = TOL
10 CONTINUE
        CALL D02PVF(N,X,Y,XEND,TOL,THRES,2,'usualtask',.FALSE.,
        + 0.0D0,W,20*N,IFAIL)
        CALL D02PCF(FCN,XEND,X,Y,YP,YMAX,W,IFAIL)
```

THRES, YP and YMAX are *double precision* arrays of length N and the length of array W needs extending to length  $20 \times N$ .

## D02BBF

Withdrawn at Mark 18 Replaced by D02PCF and associated D02P routines

THRES, YP and YMAX are *double precision* arrays of length N and the length of array W needs extending to length  $20 \times N$ .

#### D02BDF

Withdrawn at Mark 18 Replaced by D02PCF and associated D02P routines

THRES, YP, YMAX and RMSERR are *double precision* arrays of length N and W is now a *double precision* one-dimensional array of length  $32 \times N$ .

#### D02CAF

Withdrawn at Mark 18 Replaced by D02CJF

> Old: CALL D02CAF(X,XEND,N,Y,TOL,FCN,W,IFAIL) New: CALL D02CJF(X,XEND,N,Y,FCN,TOL,'M',D02CJX,D02CJW,W,IFAIL)

D02CJX is a subroutine provided in the NAG Fortran Library and D02CJW is a *double precision* function also provided. Both must be declared as EXTERNAL. The array W needs to be 5 elements greater in length.

#### D02CBF

Withdrawn at Mark 18 Replaced by D02CJF

> Old: CALL D02CBF(X,XEND,N,Y,TOL,IRELAB,FCN,OUTPUT,W,IFAIL) New: CALL D02CJF(X,XEND,N,Y,FCN,TOL,RELABS,OUTPUT,D02CJW,W,IFAIL)

D02CJW is a *double precision* function provided in the NAG Fortran Library and must be declared as EXTERNAL. The array W needs to be 5 elements greater in length. The integer parameter IRELAB (which can take values 0, 1 or 2) is catered for by the new CHARACTER\*1 argument RELABS (whose corresponding values are 'M', 'A' and 'R').

#### D02CGF

D02CJX is a subroutine provided in the NAG Fortran Library and should be declared as EXTERNAL. Note the functionality of HMAX is no longer available directly. Checking the value of Y(M) - VAL at intervals of length HMAX can be effected by a user-supplied procedure OUTPUT in place of D02CJX in the call described above. See the routine document for D02CJF for more details.

#### D02CHF

Withdrawn at Mark 18 Replaced by D02CJF

> Old: CALL D02CHF(X,XEND,N,Y,TOL,IRELAB,HMAX,FCN,G,W,IFAIL) New: CALL D02CJF(X,XEND,N,Y,FCN,TOL,RELABS,D02CJX,G,W,IFAIL)

D02CJX is a subroutine provided by the NAG Fortran Library and should be declared as EXTERNAL. The functionality of HMAX can be provided as described under the replacement call for D02CGF above. The relationship between the parameters IRELAB and RELABS is described under the replacement call for D02CBF.

#### **D02EAF**

Withdrawn at Mark 18 Replaced by D02EJF

D02EJY and D02EJX are subroutines provided in the NAG Fortran Library and D02EJW is a *double precision* function also provided. All must be declared as EXTERNAL.

#### D02EBF

Withdrawn at Mark 18 Replaced by D02EJF

D02EJW is a *double precision* function provided in the NAG Fortran Library and must be declared as EXTERNAL. The integer parameter IRELAB (which can take values 0, 1 or 2) is catered for by the new CHARACTER\*1 argument RELABS (whose corresponding values are 'M', 'A' and 'R'). If MPED = 0 in the call of D02EBF then PEDERV must be the routine D02EJY, which is supplied in the Library and should be declared as EXTERNAL.

#### **D02EGF**

Withdrawn at Mark 18 Replaced by D02EJF

D02EJY and D02EJX are subroutines provided in the NAG Fortran Library and should be declared as EXTERNAL. Note that the functionality of HMAX is no longer available directly. Checking the value of Y(M) - VAL at intervals of length HMAX can be effected by a user-supplied procedure OUTPUT in place of D02EJX in the call described above. See the routine document for D02EJF for more details.

#### D02EHF

```
Withdrawn at Mark 18
Replaced by D02EJF
Old: CALL D02EHF(X,XEND,N,Y,TOL,IRELAB,HMAX,MPED,PEDERV,FCN,G,W,IFAIL)
New: CALL D02EJF(X,XEND,N,Y,FCN,PEDERV,TOL,RELABS,D02EJX,G,W,IFAIL)
```

D02EJX is a subroutine provided by the NAG Fortran Library and should be declared as EXTERNAL. The functionality of HMAX can be provided as described under the replacement call for D02EGF above.

The relationship between the parameters IRELAB and RELABS is described under the replacement call for D02EBF. If MPED = 0 in the call of D02EHF then PEDERV must be the routine D02EJY, which is supplied in the Library and should be declared as EXTERNAL.

### D02PAF

Withdrawn at Mark 18 Replaced by D02PDF and associated D02P routines

Existing programs should be modified to call D02PVF and D02PDF. The interfaces are significantly different and therefore precise details of a replacement call cannot be given. Please consult the appropriate routine documents.

## D02QAF

Withdrawn at Mark 14 Replaced by D02QFF, D02QWF and D02QXF

Existing programs should be modified to call D02QWF and D02QFF. The interfaces are significantly different and therefore precise details of a replacement call cannot be given. Please consult the appropriate routine documents.

#### D02QBF

Withdrawn at Mark 13 Replaced by D02NBF and related routines

Existing programs should be modified to call D02NSF, D02NVF and D02NBF. The interfaces are significantly different and therefore precise details of a replacement call cannot be given. Please consult the appropriate routine documents.

## D02QDF

Withdrawn at Mark 17 Replaced by D02NBF or D02NCF

Existing programs should be modified to call D02NSF, D02NVF and D02NBF, or D02NTF, D02NVF and D02NCF. The interfaces are significantly different and therefore precise details of a replacement call cannot be given. Please consult the appropriate routine documents.

## D02QQF

Withdrawn at Mark 17 not needed except with D02QDF

Not needed except with D02QDF.

#### D02XAF

Withdrawn at Mark 18 Replaced by D02PXF and associated D02P routines

Not needed except with D02PAF. The equivalent routine is D02PXF.

## D02XBF

Withdrawn at Mark 18 Replaced by D02PXF and associated D02P routines

Not needed except with D02PAF.

#### D02XGF

Withdrawn at Mark 14 Replaced by D02QZF

Not needed except with D02QAF. The equivalent routine is D02QZF.

## D02XHF

Withdrawn at Mark 14 Replaced by D02QZF

Not needed except with D02QAF. The equivalent routine is D02QZF.

#### D02YAF

Withdrawn at Mark 18 Replaced by D02PDF and associated D02P routines

There is no precise equivalent to this routine. The closest alternative routine is D02PDF.

## **D03 – Partial Differential Equations**

#### D03PAF

Withdrawn at Mark 17 Replaced by D03PCF/D03PCA

Existing programs should be modified to call D03PCF/D03PCA. The replacement routine is designed to solve a broader class of problems. Therefore it is not possible to give precise details of a replacement call. Please consult the appropriate routine documents.

#### **D03PBF**

Withdrawn at Mark 17 Replaced by D03PCF/D03PCA

Existing programs should be modified to call D03PCF/D03PCA. The replacement routine is designed to solve a broader class of problems. Therefore it is not possible to give precise details of a replacement call. Please consult the appropriate routine documents.

#### D03PGF

Withdrawn at Mark 17 Replaced by D03PCF/D03PCA

Existing programs should be modified to call D03PCF/D03PCA. The replacement routine is designed to solve a broader class of problems. Therefore it is not possible to give precise details of a replacement call. Please consult the appropriate routine documents.

## **E01** – Interpolation

## E01ACF

Withdrawn at Mark 15 Replaced by E01DAF and E02DEF Old: CALL E01ACF(A,B,X,Y,F,VAL,VALL,IFAIL,XX,WORK,AM,D,IG1,M1,N1) New: CALL E01DAF(N1,M1,X,Y,F,PX,PY,LAMDA,MU,C,WRK,IFAIL) A1(1) = A B1(1) = B M = 1 CALL E02DEF(M,PX,PY,A1,B1,LAMDA,MU,C,FF,WRK,IWRK,IFAIL) VAL = FF(1) VALL = VAL

where PX, PY and M are INTEGER variables, LAMDA is a *double precision* array of dimension (N1 + 4), MU is a *double precision* array of dimension (M1 + 4), C is a *double precision* array of dimension  $(N1 \times M1)$ , WRK is a *double precision* array of dimension  $((N1 + 6) \times (M1 + 6))$ , A1, B1 and FF are *double precision* arrays of dimension (1), and IWRK is an INTEGER array of dimension (M1).

The above new calls duplicate almost exactly the effect of the old call, except that the new routines produce a single interpolated value for each point, rather than the two alternative values VAL and VALL produced by the old routine. By attempting this duplication, however, efficiency is probably being sacrificed. In general it is preferable to evaluate the interpolating function provided by E01DAF at a set of

M points, supplied in arrays A1 and B1, rather than at a single point. In this case, A1, B1 and FF must be dimensioned of length M.

Note also that E01ACF uses natural splines, i.e., splines having zero second derivatives at the ends of the ranges. This is likely to be slightly unsatisfactory, and E01DAF does not have this problem. It does mean however that results produced by E01DAF may not be exactly the same as those produced by E01ACF.

### E01ADF

Withdrawn at Mark 9 Replaced by E01BAF

### E01SEF

Withdrawn at Mark 20 Replaced by E01SGF

Old: CALL E01SEF(M,X,Y,F,RNW,RNQ,NW,NQ,FNODES,MINNQ,WRK,IFAIL)
New: CALL E01SGF(M,X,Y,F,NW,NQ,IQ,LIQ,RQ,LRQ,IFAIL)

E01SEF has been superseded by E01SGF which gives improved accuracy, facilities for obtaining gradient values and a consistent interface with E01TGF for interpolation of scattered data in three dimensions.

The interpolant generated by the two routines will not be identical, but similar results may be obtained by using the same values of NW and NQ. Details of the interpolant are passed to the evaluator through the arrays IQ and RQ rather than FNODES and RNW.

## E01SFF

Withdrawn at Mark 20 Replaced by E01SHF

> Old: CALL E01SFF(M,X,Y,F,RNW,FNODES,PX,PY,PF,IFAIL) New: CALL E01SHF(M,X,Y,F,IQ,LIQ,RQ,LRQ,1,PX,PY,PF,QX,QY,IFAIL)

The two calls will not produce identical results due to differences in the generation routines E01SEF and E01SGF. Details of the interpolant are passed from E01SGF through the arrays IQ and RQ rather than FNODES and RNW.

E01SHF also returns gradient values in QX and QY and allows evaluation at arrays of points rather than just single points.

## E02 – Curve and Surface Fitting

#### E02DBF

Withdrawn at Mark 16 Replaced by E02DEF

> Old: CALL E02DBF(M,PX,PY,X,Y,FF,LAMDA,MV,POINT,NPOINT,C,NC,IFAIL) New: CALL E02DEF(M,PX,PY,X,Y,LAMDA,MU,C,FF,WRK,IWRK,IFAIL)

where WRK is a *double precision* array of dimension (PY - 4), and IWRK is an INTEGER array of dimension (PY - 4).

## E04 – Minimizing or Maximizing a Function

### E04AAF

Withdrawn at Mark 7 Replaced by E04ABF/E04ABA

## E04BAF

Withdrawn at Mark 7 Replaced by E04BBF/E04BBA Withdrawn at Mark 7 Replaced by E04UCF/E04UCA

### E04CEF

Withdrawn at Mark 7 Replaced by E04JAF

## E04CFF

Withdrawn at Mark 8 Replaced by E04UCF/E04UCA

## E04CGF

Withdrawn at Mark 13 Replaced by E04JAF

```
Old: CALL E04CGF(N,X,F,IW,LIW,W,LW,IFAIL)
New: CALL E04JAF(N,1,W,W(N+1),X,F,IW,LIW,W(2*N+1),LW-2*N,IFAIL)
```

## E04DBF

С

Withdrawn at Mark 13 Replaced by E04DGF/E04DGA

```
Old: CALL E04DBF(N,X,F,G,XTOL,FEST,DUM,W,FUNCT,MONIT,MAXCAL,IFAIL)
New: CALL E04DGF(N,OBJFUN,ITER,F,G,X,IWORK,WORK,IUSER,USER,IFAIL)
```

The subroutine providing function and gradient values to E04DGF/E04DGA is OBJFUN; it has a different parameter list to FUNCT, but can be constructed simply as

```
SUBROUTINE OBJFUN(MODE,N,XC,FC,GC,NSTATE,IUSER,USER)
INTEGER MODE, N, NSTATE, IUSER(*)
double precision XC(N), FC, GC(N), USER(*)
CALL FUNCT(N,XC,FC,GC)
RETURN
END
```

The parameters IWORK and WORK are workspace parameters for E04DGF/E04DGA and must have lengths at least (N + 1) and  $(12 \times N)$  respectively. IUSER and USER must be declared as arrays each of length at least (1).

There is no parameter MONIT to E04DGF/E04DGA, but monitoring output may be obtained by calling an option setting routine. Similarly, values for FEST and MAXCAL may be supplied by calling an option setting routine. See the routine document for further information.

#### E04DCF

Withdrawn at Mark 7 Replaced by E04KDF or E04UCF/E04UCA

## E04DDF

Withdrawn at Mark 8 Replaced by E04KDF or E04UCF/E04UCA

## E04DEF

Withdrawn at Mark 13 Replaced by E04KAF

```
Old: CALL E04DEF(N,X,F,G,IW,LIW,W,LW,IFAIL)
New: CALL E04KAF(N,1,W,W(N+1),X,F,G,IW,LIW,W(2*N+1),LW-2*N,IFAIL)
```

## E04DFF

```
Withdrawn at Mark 13
Replaced by E04KCF
```

```
Old: CALL E04DFF(N,X,F,G,IW,LIW,W,LW,IFAIL)
New: CALL E04KCF(N,1,W,W(N+1),X,F,G,IW,LIW,W(2*N+1),LW-2*N,IFAIL)
```

#### E04EAF

Withdrawn at Mark 8 Replaced by E04LBF

#### E04EBF

Withdrawn at Mark 13 Replaced by E04LAF

```
Old: CALL EO4EBF(N,X,F,G,IW,LIW,W,LW,IFAIL)
New: CALL EO4LYF(N,1,FUNCT,HESS,W,W(N+1),X,F,G,IW,LIW,W(2*N+1),LW-2*N,
+ IUSER,USER,IFAIL)
```

FUNCT and HESS appear in the parameter list instead of the fixed-name subroutines FUNCT2 and HESS2 of E04LAF. FUNCT and HESS must both be declared as EXTERNAL in the calling (sub)program. In addition they have an extra two parameters, IUSER and USER, over and above those of FUNCT2 and HESS2. They may be derived from FUNCT2 and HESS2 as follows:

```
SUBROUTINE FUNCT(N,XC,FC,GC,IUSER,USER)
                  N, IUSER(*)
      INTEGER
      double precision XC(N), FC, GC(N), USER(*)
С
      CALL FUNCT2(N,XC,FC,GC)
С
      RETURN
      END
      SUBROUTINE HESS(N,XC,HESLC,LH,HESDC,IUSER,USER)
               N, LH, IUSER(*)
      INTEGER
      double precision XC(N), HESLC(LH), HESDC(N), USER(*)
С
      CALL HESS2(N,XC,HESLC,LH,HESDC)
С
      RETURN
      END
```

In general, the extra parameters, IUSER and USER, should be declared in the calling program as IUSER(1) and USER(1), but will not need initialising.

#### E04FAF

Withdrawn at Mark 8 Replaced by E04FCF or E04FDF

#### E04FBF

Withdrawn at Mark 7 Replaced by E04FCF or E04FDF

## E04FDF

Withdrawn at Mark 19 Replaced by E04FYF

Old: CALL E04FDF(M,N,X,FSUMSQ,IW,LIW,W,LW,IFAIL)
New: CALL E04FYF(M,N,LSFUN,X,FSUMSQ,W,LW,IUSER,USER,IFAIL)

С

С

LSFUN appears in the parameter list instead of the fixed-name subroutine LSFUN1 of E04FDF. LSFUN must be declared as EXTERNAL in the calling (sub)program. In addition it has an extra two parameters, IUSER and USER, over and above those of LSFUN1. It may be derived from LSFUN1 as follows:

```
SUBROUTINE LSFUN(M,N,XC,FVECC,IUSER,USER)
INTEGER M, N, IUSER(*)
double precision XC(N), FVECC(M), USER(*)
CALL LSFUN1(M,N,XC,FVECC)
RETURN
END
```

In general the extra parameters, IUSER and USER, should be declared in the calling program as IUSER(1) and USER(1), but will not need initialising.

#### E04GAF

Withdrawn at Mark 8 Replaced by E04GBF, E04GCF, E04GDF or E04GEF

#### E04GCF

Withdrawn at Mark 19 Replaced by E04GYF

> Old: CALL E04GCF(M,N,X,FSUMSQ,IW,LIW,W,LW,IFAIL) New: CALL E04GYF(M,N,LSFUN,X,FSUMSQ,W,LW,IUSER,USER,IFAIL)

LSFUN appears in the parameter list instead of the fixed-name subroutine LSFUN2 of E04GCF. LSFUN must be declared as EXTERNAL in the calling (sub)program. In addition it has an extra two parameters, IUSER and USER, over and above those of LSFUN2. It may be derived from LSFUN2 as follows:

```
SUBROUTINE LSFUN(M,N,XC,FVECC,FJACC,LJC,IUSER,USER)
INTEGER M, N, LJC, IUSER(*)
double precision XC(N), FVECC(M), FJACC(LJC,N), USER(*)
C
CALL LSFUN2(M,N,XC,FVECC,FJACC,LJC)
C
RETURN
END
```

In general the extra parameters, IUSER and USER, should be declared in the calling program as IUSER(1) and USER(1), but will not need initialising. If however, the array IW was used to pass information through E04GCF into LSFUN2, or get information from LSFUN2, then the array IUSER should be declared appropriately and used for this purpose.

#### E04GEF

Withdrawn at Mark 19 Replaced by E04GZF

Old: CALL E04GEF(M,N,X,FSUMSQ,IW,LIW,W,LW,IFAIL)
New: CALL E04GZF(M,N,LSFUN,X,FSUMSQ,W,LW,IUSER,USER,IFAIL)

LSFUN appears in the parameter list instead of the fixed-name subroutine LSFUN2 of E04GEF. LSFUN must be declared as EXTERNAL in the calling (sub)program. In addition it has an extra two parameters, IUSER and USER, over and above those of LSFUN2. It may be derived from LSFUN2 as follows:

```
SUBROUTINE LSFUN(M,N,X,FVECC,FJACC,LJC,IUSER,USER)
INTEGER M, N, LJC, IUSER(*)
double precision XC(N), FVECC(M), FJACC(LJC,N), USER(*)
C
CALL LSFUN2(M,N,XC,FVECC,FJACC,LJC)
C
RETURN
END
```

In general the extra parameters, IUSER and USER, should be declared in the calling program as IUSER(1) and USER(1), but will not need initialising. If however, the array IW was used to pass information

through E04GEF into LSFUN2, or get information from LSFUN2, then the array IUSER should be declared appropriately and used for this purpose.

## E04HAF

Withdrawn at Mark 7 Replaced by E04UCF/E04UCA

#### E04HBF

Withdrawn at Mark 16 no longer required

## E04HFF

Withdrawn at Mark 19 Replaced by E04HYF

```
Old: CALL E04HFF(M,N,X,FSUMSQ,IW,LIW,W,LW,IFAIL)
New: CALL E04HYF(M,N,LSFUN,LSHES,X,FSUMSQ,W,LW,IUSER,USER,IFAIL)
```

LSFUN and LSHES appear in the parameter list instead of the fixed-name subroutines LSFUN2 and LSHES2 of E04HFF. LSFUN and LSHES must both be declared as EXTERNAL in the calling (sub)program. In addition they have an extra two parameters, IUSER and USER, over and above those of LSFUN2 and LSHES2. They may be derived from LSFUN2 and LSHES2 as follows:

```
SUBROUTINE LSFUN(M,N,XC,FVECC,FJACC,LJC,IUSER,USER)
      INTEGER
                  M, N, LJC, IUSER(*)
      double precision XC(N), FVECC(M), FJACC(LJC,N), USER(*)
С
      CALL LSFUN2(M,N,XC,FVECC,FJACC,LJC)
С
      RETURN
      END
С
      SUBROUTINE LSHES(M,N,FVECC,XC,B,LB,IUSER,USER)
      INTEGER
                  M, N, LB, IUSER(*)
      double precision FVECC(M), XC(N), B(LB), USER(*)
С
      CALL LSHES2(M,N,FVECC,XC,B,LB)
С
      RETURN
      END
```

In general, the extra parameters, IUSER and USER, should be declared in the calling program as IUSER(1) and USER(1), but will not need initialising. If, however, the array IW was used to pass information through E04HFF into LSFUN2 or LSHES2, or to get information from LSFUN2, then the array IUSER should be declared appropriately and used for this purpose.

#### E04JAF

Withdrawn at Mark 19 Replaced by E04JYF

Old: CALL E04JAF(N,IBOUND,BL,BU,X,F,IW,LIW,LW,IFAIL)
New: CALL E04JYF(N,IBOUND,FUNCT,BL,BU,X,F,IW,LIW,W,LW,IUSER,USER,IFAIL)

FUNCT appears in the parameter list instead of the fixed-name subroutine FUNCT1 of E04JAF. FUNCT must be declared as EXTERNAL in the calling (sub)program. In addition it has an extra two parameters, IUSER and USER, over and above those of FUNCT1. It may be derived from FUNCT1 as follows:

```
SUBROUTINE FUNCT(N,XC,FC,IUSER,USER)
INTEGER N, IUSER(*)
double precision XC(N), FC, USER(*)
C
CALL FUNCT1(N,XC,FC)
C
RETURN
END
```

The extra parameters, IUSER and USER, should be declared in the calling program as IUSER(1) and USER(1), but will not need initialising.

### E04JBF

С

Withdrawn at Mark 16 Replaced by E04UCF/E04UCA

No comparative calls are given between E04JBF and E04UCF/E04UCA since both routines have considerable flexibility and can be called with many different options. E04UCF/E04UCA allows some values to be passed to it, not through the parameter list, but as 'optional parameters', supplied through calls to E04UDF/E04UDA or E04UEF/E04UEA. Names of optional parameters are given here in **bold** type.

E04UCF/E04UCA is a more powerful routine than E04JBF, in that it allows for general linear and nonlinear constraints, and for some or all of the first derivatives to be supplied; however when replacing E04JBF, only the simple bound constraints are relevant, and only function values are assumed to be available.

Therefore E04UCF/E04UCA must be called with NCLIN = NCNLN = 0, with dummy arrays of size (1) supplied as the arguments A, C and CJAC, and with the name of the auxiliary routine E04UDM (UDME04 in some implementations) as the argument CONFUN. The optional parameter **Derivative** Level must be set to 0.

The subroutine providing function values to E04UCF/E04UCA is OBJFUN. It has a different parameter list to FUNCT, but can be constructed as follows:

```
SUBROUTINE OBJFUN(MODE,N,X,OBJF,OBJGRD,NSTATE,IUSER,USER)
INTEGER MODE, N, NSTATE, IUSER(*)
double precision X(N), OBJF, OBJGRD(N), USER(*)
INTEGER IFLAG,IW(1)
double precision W(1)
IFLAG = 0
CALL FUNCT(IFLAG,N,X,OBJF,OBJGRD,IW,1,W,1)
IF (IFLAG.LT.0) MODE = IFLAG
RETURN
END
```

(This assumes that the arrays IW and W are not used to communicate between FUNCT and the calling program; E04UCF/E04UCA supplies the arrays IUSER and USER specifically for this purpose.)

The functions of the parameters BL and BU are similar, but E04UCF/E04UCA has no parameter corresponding to IBOUND; all elements of BL and BU must be set (as when IBOUND = 0 in the call to E04JBF). The optional parameter **Infinite bound size** must be set to 1.0D+6 if there are any infinite bounds. The function of the parameter ISTATE is similar but the specification is slightly different. The parameters F and G are equivalent to OBJF and OBJGRD of E04UCF/E04UCA. It should also be noted that E04UCF/E04UCA does not allow a user-supplied routine MONIT, but intermediate output is provided by the routine, under the control of the optional parameters **Major print level** and **Minor print level**.

Most of the 'tuning' parameters in E04JBF have their counterparts as 'optional parameters' to E04UCF/E04UCA, as indicated in the following list, but the correspondence is not exact and the specifications must be read carefully.

IPRINT	Minor print level
INTYPE	Cold start/Warm start
MAXCAL	Minor iteration limit (note that this counts iterations rather than function calls)
ETA	Line search tolerance
XTOL	<b>Optimality tolerance</b> (note that this specifies the accuracy in F rather than the accuracy in X)
STEPMX	Step limit
DELTA	Difference interval

## E04KAF

Withdrawn at Mark 19 Replaced by E04KYF

Old: CALL E04KAF(N,IBOUND,BL,BU,X,F,G,IW,LIW,W,LW,IFAIL)
New: CALL E04KYF(N,IBOUND,FUNCT,BL,BU,X,F,G,IW,LIW,W,LW,IUSER,USER,IFAIL)

FUNCT appears in the parameter list instead of the fixed-name subroutine FUNCT2 of E04KAF. FUNCT must be declared as EXTERNAL in the calling (sub)program. In addition it has an extra two parameters, IUSER and USER, over and above those of FUNCT2. It may be derived from FUNCT2 as follows:

```
SUBROUTINE FUNCT(N,XC,FC,GC,IUSER,USER)
INTEGER N, IUSER(*)
double precision XC(N), FC, GC(N), USER(*)
C
CALL FUNCT2(N,XC,FC,GC)
C
RETURN
END
```

The extra parameters, IUSER and USER, should be declared in the calling program as IUSER(1) and USER(1), but will not need initialising.

## E04KBF

Withdrawn at Mark 16 Replaced by E04UCF/E04UCA

No comparative calls are given between E04KBF and E04UCF/E04UCA since both routines have considerable flexibility and can be called with many different options. Most of the advice given for replacing E04JBF (see above) applies also to E04KBF, and only the differences are given here.

The optional parameter **Derivative Level** must be set to 1.

The subroutine providing both function and gradient values to E04UCF/E04UCA is OBJFUN. It has a different parameter list to FUNCT, but can be constructed as follows:

```
SUBROUTINE OBJFUN(MODE,N,X,OBJF,OBJGRD,NSTATE,IUSER,USER)
INTEGER MODE, N, NSTATE, IUSER(*)
double precision X(N), OBJF, OBJGRD(N), USER(*)
INTEGER IW(1)
double precision W(1)
CALL FUNCT(MODE,N,X,OBJF,OBJGRD,IW,1,W,1)
RETURN
END
```

#### E04KCF

С

Withdrawn at Mark 19 Replaced by E04KZF

Old: CALL E04KCF(N,IBOUND,BL,BU,X,F,G,IW,LIW,W,LW,IFAIL)
New: CALL E04KZF(N,IBOUND,FUNCT,BL,BU,X,F,G,IW,LIW,W,LW,IUSER,USER,IFAIL)

FUNCT appears in the parameter list instead of the fixed-name subroutine FUNCT2 of E04KCF. FUNCT must be declared as EXTERNAL in the calling (sub)program. In addition it has an extra two parameters, IUSER and USER, over and above those of FUNCT2. It may be derived from FUNCT2 as follows:

```
SUBROUTINE FUNCT(N,XC,FC,GC,IUSER,USER)
INTEGER N, IUSER(*)
double precision XC(N), FC, GC(N), USER(*)
C
CALL FUNCT2(N,XC,FC,GC)
C
RETURN
END
```

The extra parameters, IUSER and USER, should be declared in the calling program as IUSER(1) and USER(1), but will not need initialising.

E04LAF Withdrawn at Mark 19 Replaced by E04LYF Old: CALL E04LAF(N, IBOUND, BL, H

FUNCT and HESS appear in the parameter list instead of the fixed-name subroutines FUNCT2 and HESS2 of E04LAF. FUNCT and HESS must both be declared as EXTERNAL in the calling (sub)program. In addition they have an extra two parameters, IUSER and USER, over and above those of FUNCT2 and HESS2. They may be derived from FUNCT2 and HESS2 as follows:

```
FUNCT(N,XC,FC,GC,IUSER,USER)
      SUBROUTINE
      INTEGER
                   N, IUSER(*)
      double precision XC(N), FC, GC(N), USER(*)
С
      CALL FUNCT2(N,XC,FC,GC)
С
      RETURN
      END
      SUBROUTINE HESS (N, XC, HESLC, LH, HESDC, IUSER, USER)
                   N, LH, IUSER(*)
      INTEGER
      double precision XC(N), HESLC(LH), HESDC(N), USER(*)
С
      CALL HESS2(N,XC,HESLC,LH,HESDC)
С
      RETURN
      END
```

In general, the extra parameters, IUSER and USER, should be declared in the calling program as IUSER(1) and USER(1), but will not need initialising.

#### E04MBF

Withdrawn at Mark 18 Replaced by E04MFF/E04MFA

```
Old: CALL EO4MBF(ITMAX,MSGLVL,N,NCLIN,NCTOTL,NROWA,A,BL,BU,CVEC,
+ LINOBJ,X,ISTATE,OBJLP,CLAMDA,IWORK,LIWORK,WORK,
+ LWORK,IFAIL)
New: CALL EO4MFF(N,NCLIN,A,NROWA,BL,BU,CVEC,ISTATE,X,ITER,OBJLP,
+ AX,CLAMDA,IWORK,LIWORK,UWORK,IFAIL)
```

The parameter NCTOTL is no longer required. Values for ITMAX, MSGLVL and LINOBJ may be supplied by calling an option setting routine.

E04MFF/E04MFA contains two additional parameters as follows:

ITER - INTEGER.

AX(\*) – *double precision* array of dimension at least max(1, NCLIN).

The minimum value of the parameter LIWORK must be increased from  $2 \times N$  to  $2 \times N + 3$ . The minimum value of the parameter LWORK may also need to be changed. See the routine documents for further information.

#### E04NAF

The specification of the subroutine QPHESS must also be changed as follows:

Old:	SUBROUTINE	QPHESS(N,NROWH,NCOLH,JTHCOL,HESS,X,HX)		
	INTEGER	N, NROWH, NCOLH, JTHCOL		
	double precision	HESS(NROWH, NCOLH), X(N), HX(N)		
New:	SUBROUTINE	QPHESS(N,JTHCOL,HESS,NROWH,X,HX)		
	INTEGER	N, JTHCOL, NROWH		
	double precision	$HESS(NROWH, \star)$ , $X(N)$ , $HX(N)$		

The parameters NCTOTL, NCOLH and ORTHOG are no longer required. Values for ITMAX, MSGLVL, BIGBND, FEATOL, COLD and LP may be supplied by calling an option setting routine.

E04NFF/E04NFA contains one additional parameter as follows:

AX(\*) – *double precision* array of dimension at least max(1, NCLIN).

The minimum value of the parameter LIWORK must be increased from  $2 \times N$  to  $2 \times N + 3$ . The minimum value of the parameter LWORK may also need to be changed. See the routine documents for further information.

## E04NKF

Scheduled for withdrawal at Mark 23 Replaced by E04NQF

Old: CALL	EO4NKF(N,M,NNZ,IOBJ,NCOLH,QPHX,A,HA,KA,BL,BU,START,
+	NAMES,NNAME,CRNAME,NS,XS,ISTATE,MINIZ,MINZ,NINF,
+	SINF,OBJ,CLAMDA,IZ,LENIZ,Z,LENZ,IFAIL)
New: CALL	E04NQF(START,QPHX,M,N,NE,NNAME,LENC,NCOLH,IOBJ,OBJADD,
+	PROB,ACOL,INDA,LOCA,BL,BU,C,NAMES,HELAST,HS,X,PI,RC,NS,
+	NINF,SINF,OBJ,CW,LENCW,IW,LENIW,RW,LENRW,
+	CUSER,IUSER,RUSER,IFAIL)

where:

START has the same meaning in both calls

QPHX is a user-provided function supplying the matrix product Hx in both calls:

Old: SUBROUTINE QPHX(NSTATE, NCOLH, X, HX) New: SUBROUTINE QPHX(NCOLH,X,HX,NSTATE,CUSER,IUSER,RUSER)

Here parameters with the same name have the same roles. The extra parameters CUSER, USER, USER are user workspace that may be used instead of COMMON to pass information into QPHX.

M has the same meaning, the number of linear constraints.

N has the same meaning, the number of variables.

NE has the same meaning as NNZ in E04NKF.

NNAME has the same meaning in both calls.

LENC is unique to E04NQF.

- NCOLH has the same meaning in both calls.
- IOBJ has the same meaning in both calls.

OBJADD is unique to E04NQF.

PROB is unique to E04NQF, but see NAME(1) of E04NKF.

ACOL is A in the call to E04NKF.

INDA is HA in the call to E04NKF.

LOCA is KA in the call to E04NKF.

BL has the same meaning in both calls.

BU has the same meaning in both calls.

C is unique to E04NQF.

NAMES corresponds to CRNAME of E04NKF - NOT to NAMES of E04NKF. HELAST is unique to E04NQF. HS corresponds to ISTATE in E04NQF. Х is XS in the call to E04NKF. ΡI is unique to E04NQF. RC is CLAMDA in the call to E04NKF. NS has the same meaning in both calls. NINF has the same meaning in both calls. SINF has the same meaning in both calls. OBJ has the same meaning in both calls. CW is unique to E04NQF. LENCW is unique to E04NQF. IW corresponds (roughly) to IZ in the call to E04NKF. corresponds to LENIZ in the call to E04NKF. LENIW RW corresponds (roughly) to Z in the call to E04NKF. corresponds to LENZ in the call to E04NKF. LENRW CUSER is unique to E04NQF. **IUSER** is unique to E04NOF. RUSER is unique to E04NQF. IFAIL has the same meaning in both calls. E04NLF Scheduled for withdrawal at Mark 23 Replaced by E04NRF Old: CALL E04NLF(IOPTNS, INFORM) New: CALL E04NPF(CW,LENCW,IW,LENIW,RW,LENRW,IFAIL) !initialisation IF (IFAIL.EQ.O) THEN INFORM=1 CALL E04NRF(IOPTNS,CW,IW,RW,INFORM) !set options etc ... E04NMF Scheduled for withdrawal at Mark 23 Replaced by E04NSF, E04NTF and E04NUF Old: CALL EO4NMF(string)

New: CALL E04NPF(CW,LENCW,IW,LENIW,RW,LENRW,IFAIL) !initialisation
IF (IFAIL.EQ.0) THEN
INFORM=0
CALL E04NSF(string,CW,IW,RW,INFORM) !set options
etc ...

Or to set an integer value:

Old: CALL E04NMF('option = n')
New: CALL E04NPF(CW,LENCW,IW,LENIW,RW,LENRW,IFAIL) !initialisation
IF (IFAIL.EQ.0) THEN
INFORM=0
CALL E04NTF('option',n,CW,IW,RW,INFORM) !set options
etc ...

Or to set a double precision value:

```
Old: CALL E04NMF('option = v')
New: CALL E04NPF(CW,LENCW,IW,LENIW,RW,LENRW,IFAIL) !initialisation
IF (IFAIL.EQ.0) THEN
INFORM=0
CALL E04NUF('option',v,CW,IW,RW,INFORM) !set options
etc ...
```

#### E04UAF

Withdrawn at Mark 13 Replaced by E04UCF/E04UCA

No comparative calls are given between E04UAF and E04UCF/E04UCA since both routines have considerable flexibility and can be called with many different options. However users of E04UAF should have no difficulty in making the transition. Most of the 'tuning' parameters in E04UAF have their counterparts as optional parameters to E04UCF/E04UCA, and these may be provided by calling an option setting routine prior to the call to E04UCF/E04UCA. The subroutines providing function and constraint values to E04UCF/E04UCA are OBJFUN and CONFUN respectively; they have different parameter lists to FUNCT1 and CON1, but can be constructed simply as

```
SUBROUTINE OBJFUN(MODE, N, X, OBJF, OBJGRD, NSTATE, IUSER, USER)
                   MODE, N, NSTATE, IUSER(*)
      INTEGER
      double precision X(N), OBJF, OBJGRD(N), USER(*)
С
      CALL FUNCT1(MODE, N, X, OBJF)
      RETURN
      END
      SUBROUTINE CONFUN(MODE,NCNLN,N,NROWJ,NEEDC,X,C,CJAC.NSTATE,
                   IUSER, USER)
                   MODE, NCNLN, N, NROWJ, NEEDC(*), NSTATE, IUSER(*)
      TNTEGER
      double precision X(X), C(*), CJAC(NROWJ,*), USER(*)
С
      CALL CON1(MODE, N, NCNLN, X, C)
      RETURN
      END
```

The parameters OBJGRD, NEEDC, CJAC, IUSER and USER are the same as those for E04UCF/E04UCA itself. It is important to note that, unlike FUNCT1 and CON1, a call to CONFUN is not preceded by a call to OBJFUN with the same values in X, so that FUNCT1 and CON1 will need to be modified if this property was being utilized. It should also be noted that E04UCF/E04UCA allows general linear constraints to be supplied separately from nonlinear constraints, and indeed this is to be encouraged, but the above call to CON1 assumes that linear constraints are being regarded as nonlinear.

#### E04UCF

Scheduled for withdrawal at Mark 23 Replaced by E04WDF

```
Old: CALL EO4UCF(N,NCLIN,NCNLN,LDA,LDCJ,LDR,A,BL,BU,CONFUN,

+ OBJFUN,ITER,ISTATE,C,CJAC,CLAMDA,OBJF,OBJGRD,

+ R,X,IWORK,LIWORK,WORK,LWORK,IUSER,USER,IFAIL)

New: CALL EO4WDF(N,NCLIN,NCNLN,LDA,LDCJ,LDH,A,BL,BU,CONFUN,OBJFUN,

+ MAJITS,ISTATE,CCON,CJAC,CLAMDA,OBJF,GRAD,HESS,X,IW,

+ LENIW,RW,LENRW,IUSER,RUSER,IFAIL)
```

where

N, NCLIN, NCNLN, LDA, LDCJ have the same meaning in both calls.

LDH corresponds to LDR.

A, BL, BU have the same meaning in both calls.

CONFUN has the same parameter list and definitions in both calls. Note however that the MODE parameter of CONFUN in E04WDF has an extended definition to allow you set MODE = -1. This requests E04WDF to evaluate the functions closer to the last acceptable point.

OBJFUN has the same parameter list and definitions in both calls. Note however that the MODE parameter of OBJFUN in E04WDF has an extended definition to allow you set MODE = -1. This requests E04WDF to evaluate the functions closer to the last acceptable point.

MAJITS corresponds to ITER of E04UCF/E04UCA.

ISTATE is similar in both calls. However the negative values allowed in E04UCF/E04UCA are not permitted in E04WDF.

CCON corresponds to C in E04UCF/E04UCA.

CJAC, CLAMDA, OBJ have the same meaning in both calls.

GRAD corresponds to OBJGRD in E04UCF/E04UCA.

HESS roughly corresponds to R in E04UCF/E04UCA:

- (i) There is exact correspondence if a 'Cold Start' option is used.
- (ii) For a 'Warm Start' HESS must contain an approximation to the Hessian of the Lagrangian, whereas R in E04UCF/E04UCA contained a triangular factor of a Cholesky decomposition of this matrix.

X has the same meaning in both calls.

IW, LENIW, RW, LENRW are unique to E04WDF.

IUSER has the same meaning in both calls.

RUSER corresponds USER in E04UCF/E04UCA.

IFAIL has the same meaning in both calls.

## E04UDF

Scheduled for withdrawal at Mark 23 Replaced by E04WEF

CALL E04UDF(IOPTNS,INFORM) CALL E04WCF(IW,LENIW,RW,LENRW,IFAIL) IF (IFAIL.E0.0) THEN	! Initialisation
INFORM=1 CALL E04WEF(IOPTS,IW,RW,INFORM) etc	! Set options

#### E04UEF

Scheduled for withdrawal at Mark 23 Replaced by E04WFF, E04WGF and E04WHF

Old:	CALL EO4UEF(string)	
New:	CALL E04WCF(IW,LENIW,RW,LENRW,IFAIL)	!initialisation
	IF (IFAIL.EQ.O) THEN	
	INFORM=0	
	CALL EO4WFF(string,IW,RW,INFORM)	!set options
	etc	_

Or to set an integer value:

Old: CALL E04UEF('option = n')	
New: CALL EO4WCF(IW,LENIW,RW,LENRW,IFAIL)	!initialisation
IF (IFAIL.EQ.O) THEN	
INFORM=0	
CALL EO4WGF('option',n,IW,RW,INFORM)	!set options
etc	

Or to set a double precision value:

Old: CALL E04UEF('option = v')
New: CALL E04WCF(IW,LENIW,RW,LENRW,IFAIL) !initialisation
IF (IFAIL.EQ.0) THEN
INFORM=0
CALL E04WGF('option',v,IW,RW,INFORM) !set options
etc ...

#### E04UHF

Scheduled for withdrawal at Mark 23 Replaced by E04VKF

```
Old: CALL E04UHF(IOPTNS,INFORM)
New: CALL E04VGF(CW,LENCW,IW,LENIW,RW,LENRW,IFAIL) ! Initialisation
IF (IFAIL.EQ.0) THEN
INFORM=1
CALL E04VKF(IOPTS,CW,IW,RW,INFORM) ! Set options
etc ...
```

#### E04UJF

Scheduled for withdrawal at Mark 23 Replaced by E04VLF, E04VMF and E04VNF

Old: CALL E04UJF(string)
New: CALL E04VGF(CW,LENCW,IW,LENIW,RW,LENRW,IFAIL) ! Initialisation
IF (IFAIL.EQ.0) THEN
INFORM=0
CALL E04VLF(string,CW,IW,RW,INFORM) !set options
etc ...

Or to set an integer value:

```
Old: CALL E04UJF('option = n')
New: CALL E04VGF(CW,LENCW,IW,LENIW,RW,LENRW,IFAIL) ! Initialisation
IF (IFAIL.EQ.0) THEN
INFORM=0
CALL E04VMF('option',n,CW,IW,RW,INFORM) !set options
etc ...
```

Or to set a double precision value:

```
Old: CALL E04UJF('option = v')
New: CALL E04VGF(CW,LENCW,IW,LENIW,RW,LENRW,IFAIL) ! Initialisation
IF (IFAIL.EQ.0) THEN
INFORM=0
CALL E04VNF('option',v,CW,IW,RW,INFORM) !set options
etc ...
```

#### E04UNF

Scheduled for withdrawal at Mark 22 Replaced by E04USF/E04USA

```
Old: CALL E04UNF(M,N,NCLIN,NCNLN,LDA,LDCJ,LDFJ,
                  LDR, A, BL, BU, Y, CONFUN, OBJFUN, ITER,
    +
                  ISTATE, C, CJAC, F, FJAC, CLAMDA, OBJF,
    +
                  R,X,IWORK,LIWORK,WORK,LWORK,IUSER,
                  USER, IFAIL)
New: CALL EO4USF(M,N,NCLIN,NCNLN,LDA,LDCJ,LDFJ,
                  LDR, A, BL, BU, Y, CONFUN, OBJFUN, ITER,
    +
                  ISTATE, C, CJAC, F, FJAC, CLAMDA, OBJF,
    +
    +
                  R,X,IWORK,LIWORK,WORK,LWORK,IUSER,
    +
                  USER, IFAIL)
```

The specification of the subroutine OBJFUN must also be changed as follows:

Old: SUBROUTINE OBJFUN(MODE,M,N,LDFJ,X,F,FJAC,NSTATE,IUSER,USER)
INTEGER MODE,M,N,LDFJ,NSTATE,IUSER(\*)
double precision X(N),F(\*),FJAC(LDFJ,\*),USER(\*)
New: SUBROUTINE OBJFUN(MODE,M,N,LDFJ,NEEDFI,X,F,FJAC,NSTATE,
+ IUSER,USER)
INTEGER MODE,M,N,NEEFI,NSTATE,IUSER(\*)
double precision X(N),F(\*),FJAC(LDFJ,\*),USER(\*)

See the routine documents for further information.

```
E04UPF
Withdrawn at Mark 19
Replaced by E04UNF
     Old: CALL EO4UPF(M,N,NCLIN,NCNLN,LDA,LDCJ,LDFJ,LDR,A,BL,BU,
                        CONFUN, OBJFUN, ITER, ISTATE, C, CJAC, F, FJAC,
          +
                        CLAMDA, OBJF, R, X, IWORK, LIWORK, WORK, LWORK,
          +
                        IUSER, USER, IFAIL)
     New: CALL EO4USF(M,N,NCLIN,NCNLN,LDA,LDCJ,LDFJ,
                        LDR, A, BL, BU, Y, CONFUN, OBJFUN, ITER,
          +
                        ISTATE, C, CJAC, F, FJAC, CLAMDA, OBJF,
          +
          +
                        R,X,IWORK,LIWORK,WORK,LWORK,IUSER,
                        USER, IFAIL)
          +
```

E04USF/E04USA contains one additional parameter as follows:

Y(M) - double precision array.

Note that a call to E04UPF is the same as a call to E04USF/E04USA with Y(i) = 0.0, for i = 1, 2, ..., M.

The specification of the subroutine OBJFUN must also be changed as follows:

Old: SUBROUTINE OBJFUN(MODE,M,N,LDFJ,X,F,FJAC,NSTATE,IUSER,USER)
INTEGER MODE,M,N,LDFJ,NSTATE,IUSER(\*)
double precision X(N),F(\*),FJAC(LDFJ,\*),USER(\*)

New: SUBROUTINE OBJFUN(MODE,M,N,LDFJ,NEEDFI,X,F,FJAC,NSTATE, + IUSER,USER) INTEGER MODE,M,N,NEEFI,NSTATE,IUSER(\*) double precision X(N),F(\*),FJAC(LDFJ,\*),USER(\*)

See the routine documents for further information.

#### E04VAF

Withdrawn at Mark 12 Replaced by E04UCF/E04UCA

#### E04VBF

Withdrawn at Mark 12 Replaced by E04UCF/E04UCA

#### E04VCF

Withdrawn at Mark 17 Replaced by E04UCF/E04UCA

```
Old: CALL E04VCF(ITMAX,MSGLVL,N,NCLIN,NCNLN,NCTOTL,NROWA,NROWJ,
+ NROWR,BIGBND,EPSAF,ETA,FTOL,A,BL,BU,FEATOL,
+ CONFUN,OBJFUN,COLD,FEALIN,ORTHOG,X,ISTATE,R,ITER,
+ C,CJAC,OBJF,OBJGRD,CLAMDA,IWORK,LIWORK,WORK,LWORK,
+ IFAIL)
New: CALL E04UCF(N,NCLIN,NCNLN,NROWA,NROWJ,NROWR,A,BL,BU,CONFUN,
+ OBJFUN,ITER,ISTATE,C,CJAC,CLAMDA,OBJF,OBJGRD,R,X,
+ IWORK,LIWORK,WORK,LWORK,IUSER,USER,IFAIL)
```

The specification of the subroutine OBJFUN must also be changed as follows:

Old: SUBROUTINE OBJFUN(MODE,N,X,OBJF,OBJGRD,NSTATE)
INTEGER MODE, N, NSTATE
double precision X(N), OBJF, OBJGRD(N)
New: SUBROUTINE OBJFUN(MODE,N,X,OBJF,OBJGRD,NSTATE,IUSER,USER)
INTEGER MODE, N, NSTATE, IUSER(\*)
double precision X(N), OBJF, OBJGRD(N), USER(\*)

If NCNLN > 0, the specification of the subroutine CONFUN must also be changed as follows:

Old: SUBROUTINE CONFUN(MODE,NCNLN,N,NROWJ,X,C,CJAC,NSTATE) INTEGER MODE, NCNLN, N, NROWJ, NSTATE double precision X(N), C(NROWJ), CJAC(NROWJ,N) New: SUBROUTINE CONFUN(MODE,NCNLN,N,NROWJ,NEEDC,X,C,CJAC,NSTATE, + IUSER,USER) INTEGER MODE, NCNLN, N, NROWJ, NEEDC(NCNLN), NSTATE, IUSER(\*) double precision X(N), C(NCNLN), CJAC(NROWJ,N), USER(\*)

If NCNLN = 0, then the name of the dummy routine E04VDM (VDME04 in some implementations) may need to be changed to E04UDM (UDME04 in some implementations) in the calling program.

The parameters NCTOTL, EPSAF, FEALIN and ORTHOG are no longer required. Values for ITMAX, MSGLVL, BIGBND, ETA, FTOL, COLD and FEATOL may be supplied by calling an option setting routine.

E04UCF/E04UCA contains two additional parameters as follows:

IUSER(\*) – INTEGER array of dimension at least 1.

USERR(\*) - double precision array of dimension at least 1.

The minimum value of the parameter LIWORK must be increased from  $3 \times N + NCLIN + NCNLN$  to  $3 \times N + NCLIN + 2 \times NCNLN$ . The minimum value of the parameter LWORK may also need to be changed. See the routine documents for further information.

#### E04VDF

Withdrawn at Mark 17 Replaced by E04UCF/E04UCA

```
Old: IFAIL = 110
CALL E04VDF(ITMAX,MSGLVL,N,NCLIN,NCNLN,NCTOTL,NROWA,NROWJ,
+ CTOL,FTOL,A,BL,BU,CONFUN,OBJFUN,X,ISTATE,C,CJAC,
+ CJAC,OBJF,OBJGRD,CLAMDA,IWORK,LIWORK,WORK,LWORK,
+ IFAIL)
New: IFAIL = -1
CALL E04UCF(N,NCLIN,NCNLN,NROWA,NROWJ,N,A,BL,BU,CONFUN,OBJFUN,
+ ITER,ISTATE,C,CJAC,CLAMDA,OBJF,OBJGRD,R,X,IWORK,
+ LIWORK,WORK,LWORK,IUSER,USER,IFAIL)
```

The specification of the subroutine OBJFUN must also be changed as follows:

```
Old: SUBROUTINE OBJFUN(MODE,N,X,OBJF,OBJGRD,NSTATE)
INTEGER MODE, N, NSTATE
double precision X(N), OBJF, OBJGRD(N)
New: SUBROUTINE OBJFUN(MODE,N,X,OBJF,OBJGRD,NSTATE,IUSER,USER)
INTEGER MODE, N, NSTATE, IUSER(*)
double precision X(N), OBJF, OBJGRD(N), USER(*)
```

If NCNLN > 0, the specification of the subroutine CONFUN must also be changed as follows:

Old: SUBROUTINE CONFUN(MODE,NCNLN,N,NROWJ,X,C,CJAC,NSTATE)
INTEGER MODE, NCNLN, N, NROWJ, NSTATE
double precision X(N), C(NROWJ), CJAC(NROWJ,N)
New: SUBROUTINE CONFUN(MODE,NCNLN,N,NROWJ,NEEDC,X,C,CJAC,NSTATE,
+ IUSER,USER)
INTEGER MODE, NCNLN, N, NROWJ, NEEDC(NCNLN), NSTATE, IUSER(\*)
double precision X(N), C(NCNLN), CJAC(NROWJ,N), USER(\*)

If NCNLN = 0, then the name of the dummy routine E04VDM (VDME04 in some implementations) may need to be changed to E04UDM (UDME04 in some implementations) in the calling program.

The parameter NCTOTL is no longer required. Values for ITMAX, MSGLVL, CTOL and FTOL may be supplied by calling an option setting routine.

E04UCF/E04UCA contains four additional parameters as follows:

ITER – INTEGER.

R(NN) – *double precision* array.

IUSER(\*) – INTEGER array of dimension at least 1.

USER(\*) - double precision array of dimension at least 1.

The minimum value of the parameter LIWORK must be increased from  $3 \times N + NCLIN + NCNLN$  to  $3 \times N + NCLIN + 2 \times NCNLN$ . The minimum value of the parameter LWORK may also need to be changed. See the routine documents for further information.

## E04WAF

Withdrawn at Mark 12 Replaced by E04UCF/E04UCA

## E04ZAF

Withdrawn at Mark 12 Replaced by E04ZCF/E04ZCA

## E04ZBF

Withdrawn at Mark 12 no longer required

## **F01 – Matrix Factorizations**

## F01AAF

Withdrawn at Mark 17 Replaced by F07ADF (DGETRF) and F07AJF (DGETRI)

Old: CALL F01AAF(A,IA,N,X,IX,WKSPCE,IFAIL)
New: CALL sgetrf(N,N,A,IA,IPIV,IFAIL)
CALL F06QFF('General',N,N,A,IA,X,IX)
CALL sgetri(N,X,IX,IPIV,WKSPCE,LWORK,IFAIL)

where IPIV is an INTEGER vector of length N, and the INTEGER LWORK is the length of array WKSPCE, which must be at least max(1, N). In the replacement calls, F07ADF (DGETRF) computes the *LU* factorization of the matrix *A*, F06QFF copies the factorization from A to X, and F07AJF (DGETRI) overwrites X by the inverse of *A*. If the original matrix *A* is no longer required, the call to F06QFF is not necessary, and references to X and IX in the call of F07AJF (DGETRI) may be replaced by references to A and IA, in which case A will be overwritten by the inverse.

## F01ACF

Withdrawn at Mark 16 Replaced by F01ABF

> Old: CALL FO1ACF(N,EPS,A,IA,B,IB,Z,L,IFAIL) New: CALL FO1ABF(A,IA,N,B,IB,Z,IFAIL)

The number of iterative refinement corrections returned by F01ACF in L is no longer available. The parameter EPS is no longer required.

## F01AEF

Withdrawn at Mark 18 Replaced by F06EGF (DSWAP), F07FDF (DPOTRF) and F08SEF (DSYGST)

IFAIL is set to 1 if the matrix B is not positive-definite. It is essential to test IFAIL.

## F01AFF

```
Withdrawn at Mark 18
Replaced by F06EGF (DSWAP) and F06YJF (DTRSM)
Old: CALL F01AFF(N,M1,M2,B,IB,DL,Z,IZ)
New: CALL sswap(N,DL,1,B,IB+1)
CALL strsm('L','L','T','N',N,M2-M1+1,1.0D0,B,IB,Z(1,M1),IZ)
```

CALL sswap(N,DL,1,B,IB+1)

#### F01AGF

```
Withdrawn at Mark 18
Replaced by F08FEF (DSYTRD)
```

```
Old: CALL F01AGF(N,TOL,A,IA,D,E,E2)
New: CALL ssytrd('L',N,A,IA,D,E(2),TAU,WORK,LWORK,INFO)
    E(1) = 0.0D0
    D0 10 I = 1, N
        E2(I) = E(I)*E(I)
    10 CONTINUE
```

where TAU is a *double precision* array of length at least (N - 1), WORK is a *real* array of length at least (1) and LWORK is its actual length.

Note that the tridiagonal matrix computed by F08FEF (DSYTRD) is different from that computed by F01AGF, but it has the same eigenvalues.

#### F01AHF

Withdrawn at Mark 18 Replaced by F08FGF (DORMTR)

The following replacement is valid only if the previous call to F01AGF has been replaced by a call to F08FEF (DSYTRD) as shown above.

```
Old: CALL FO1AHF(N,M1,M2,A,IA,E,Z,IZ)
New: CALL sormtr('L','L','N',N,M2-M1+1,A,IA,TAU,Z(1,M1),IZ,WORK,
+ LWORK,INFO)
```

where WORK is a *double precision* array of length at least (M2 - M1 + 1), and LWORK is its actual length.

### F01AJF

Withdrawn at Mark 18 Replaced by F08FEF (DSYTRD) and F08FFF (DORGTR)

```
Old: CALL F01AJF(N,TOL,A,IA,D,E,Z,IZ)
New: CALL ssytrd('L',N,A,IA,D,E(2),TAU,WORK,LWORK,INFO)
    E(1) = 0.0D0
    CALL F06QFF('L',N,N,A,IA,Z,IZ)
    CALL sorgtr('L',N,Z,IZ,TAU,WORK,LWORK,INFO)
```

where TAU is a *double precision* array of length at least (N - 1), WORK is a *real* array of length at least (N - 1) and LWORK is its actual length.

Note that the tridiagonal matrix T and the orthogonal matrix Q computed by F08FEF (DSYTRD) and F08FFF (DORGTR) are different from those computed by F01AJF, but they satisfy the same relation  $Q^{T}AQ = T$ .

#### F01AKF

Withdrawn at Mark 18 Replaced by F08NEF (DGEHRD)

> Old: CALL FO1AKF(N,K,L,A,IA,INTGER) New: CALL *sgehrd*(N,K,L,A,IA,TAU,WORK,LWORK,INFO)

where TAU is a *double precision* array of length at least (N - 1), WORK is a *real* array of length at least (N) and LWORK is its actual length.

Note that the Hessenberg matrix computed by F08NEF (DGEHRD) is different from that computed by F01AKF, because F08NEF (DGEHRD) uses orthogonal transformations, whereas F01AKF uses stabilized elementary transformations.

#### F01ALF

Withdrawn at Mark 18 Replaced by F08NGF (DORMHR)

The following replacement is valid only if the previous call to F01AKF has been replaced by a call to F08NEF (DGEHRD) as indicated above.

Old: CALL F01ALF(K,L,IR,A,IA,INTGER,Z,IZ,N) New: CALL *sormhr*('L','N',N,IR,K,L,A,IA,TAU,Z,IZ,WORK,LWORK,INFO)

where WORK is a *double precision* array of length at least (IR) and LWORK is its actual length.

#### F01AMF

Withdrawn at Mark 18 Replaced by F08NSF (ZGEHRD)

where A is a *complex\*16* array of dimension (IA, N), TAU is a *complex\*16* array of length at least (N - 1), WORK is a *complex\*16* array of length at least (N) and LWORK is its actual length.

Note that the Hessenberg matrix computed by F08NSF (ZGEHRD) is different from that computed by F01AMF, because F08NSF (ZGEHRD) uses orthogonal transformations, whereas F01AMF uses stabilized elementary transformations.

### F01ANF

Withdrawn at Mark 18 Replaced by F08NTF (ZUNGHR)

The following replacement is valid only if the previous call to F01AMF has been replaced by a call to F08NSF (ZGEHRD) as indicated above.

```
Old: CALL F01ANF(K,L,IR,AR,IAR,AI,IAI,INTGER,ZR,IZR,ZI,IZI,N)
New: CALL cunhmr('L','N',N,IR,K,L,A,IA,TAU,Z,IZ,WORK,LWORK,INFO)
D0 20 J = 1, IR
D0 10 I = 1, N
ZR(I,J) = real(Z(I,J))
ZI(I,J) = imag(Z(I,J))
10 CONTINUE
20 CONTINUE
```

where A is a *complex\*16* array of dimension (IA, N), TAU is a *complex\*16* array of length at least (N-1), Z is a *complex\*16* array of dimension (IZ, IR), WORK is a *complex\*16* array of length at least (IR) and LWORK is its actual length.

## F01APF

Withdrawn at Mark 18 Replaced by F06QFF and F08NFF (DORGHR)

The following replacement is valid only if the previous call to F01AKF has been replaced by a call to F08NEF (DGEHRD) as indicated above.

Old: CALL FO1APF(N,K,L,INTGER,H,IH,V,IV) New: CALL FO6QFF('L',N,N,H,IH,V,IV) CALL *sorghr*(N,K,L,V,IV,TAU,WORK,LWORK,INFO)

where WORK is a *double precision* array of length at least (N), and LWORK is its actual length.

Note that the orthogonal matrix formed by F08NFF (DORGHR) is not the same as the non-orthogonal matrix formed by F01APF. See F01AKF above.

### F01ATF

Withdrawn at Mark 18 Replaced by F08NHF (DGEBAL)

> Old: CALL FO1ATF(N,IB,A,IA,K,L,D) New: CALL *sgebal*('B',N,A,IA,K,L,D,INFO)

Note that the balanced matrix returned by F08NHF (DGEBAL) may be different from that returned by F01ATF.

## F01AUF

Withdrawn at Mark 18 Replaced by F08NJF (DGEBAK)

> Old: CALL F01AUF(N,K,L,M,D,Z,IZ) New: CALL *sgebak*('B','R',N,K,L,D,M,Z,IZ,INFO)

#### F01AVF

```
Withdrawn at Mark 18
Replaced by F08NVF (ZGEBAL)
```

where A is a *complex\*16* array of dimension (IA, N).

Note that the balanced matrix returned by F08NVF (ZGEBAL) may be different from that returned by F01AVF.

## F01AWF

```
Withdrawn at Mark 18
Replaced by F08NWF (ZGEBAK)
     Old: CALL FO1AWF(N,K,L,M,D,ZR,IZR,ZI,IZI)
     New: DO 20 J = 1, M
             DO 10 I = 1, N
                Z(I,J) = cmplx(ZR(I,J),ZI(I,J))
       10
             CONTINUE
       20 CONTINUE
          CALL cgebak('B','R',N,K,L,D,M,Z,IZ,INFO)
          DO 40 J = 1, M
             DO 30 I = 1, N
                 ZR(I,J) = real(Z(I,J))
                 ZI(I,J) = imag(Z(I,J))
      30
             CONTINUE
      40
         CONTINUE
```

where Z is a *complex\*16* array of dimension (IZ, M).

**F01AXF** Withdrawn at Mark 18 Replaced by F08BEF (DGEQPF) and F06EFF (DCOPY)

Old: CALL F01AXF(M,N,QR,IQR,ALPHA,IPIV,Y,E,IFAIL)
New: CALL sgeqpf(M,N,QR,IQR,IPIV,Y,WORK,INFO)
CALL scopy(N,QR,IQR+1,ALPHA,1)

where WORK is a *double precision* array of length at least  $(3 \times N)$ .

Note that the details of the Householder matrices returned by F08BEF (DGEQPF) are different from those returned by F01AXF, but they determine the same orthogonal matrix Q.

## F01AYF

```
Withdrawn at Mark 18
Replaced by F08GEF (DSPTRD)
```

```
Old: CALL F01AYF(N,TOL,A,IA,D,E,E2)
New: CALL ssptrd('U',N,A,D,E(2),TAU,INFO)
        E(1) = 0.0D0
        DO 10 I = 1, N
        E2(I) = E(I)*E(I)
        10 CONTINUE
```

where TAU is a *double precision* array of length at least (N - 1).

## F01AZF

Withdrawn at Mark 18 Replaced by F08GGF (DOPMTR)

The following replacement is valid only if the previous call to F01AYF has been replaced by a call to F08GEF (DSPTRD) as shown above.

Old: CALL F01AZF(N,M1,M2,A,IA,Z,IZ) New: CALL *sopmtr*('L','U','N',N,M2-M1+1,A,TAU,Z(1,M1),IZ,WORK,INFO)

where WORK is a *double precision* array of length at least (M2 - M1 + 1).

#### F01BCF

Withdrawn at Mark 18 Replaced by F08FSF (ZHETRD) and F08FTF (ZUNGTR)

```
Old: CALL FO1BCF(N,TOL,AR,IAR,AI,IAI,D,E,WK1,WK2)
New: DO 20 J = 1, N
        DO 10 I = 1, N
           A(I,J) = cmplx(AR(I,J),AI(I,J))
  10
        CONTINUE
  20 CONTINUE
     CALL chetrd('L', N, A, IA, D, E(2), TAU, WORK, LWORK, INFO)
     E(1) = 0.0D0
     CALL cungtr('L', N, A, IA, TAU, WORK, LWORK, INFO)
     DO 40 J = 1, N
        DO 30 I = 1, N
           AR(I,J) = real(A(I,J))
           AI(I,J) = imag(A(I,J))
 30
        CONTINUE
 40 CONTINUE
```

where A is a *complex\*16* array of dimension (IA, N), TAU is a *complex\*16* array of length at least (N-1), WORK is a *complex\*16* array of length at least (N-1), and LWORK is actual length.

Note that the tridiagonal matrix T and the unitary matrix Q computed by F08FSF (ZHETRD) and F08FTF (ZUNGTR) are different from those computed by F01BCF, but they satisfy the same relation  $Q^{\rm H}AQ = T$ .

## F01BDF

```
Withdrawn at Mark 18
Replaced by F06EGF (DSWAP), F07FDF (DPOTRF) and F08SEF (DSYGST)
     Old: CALL F01BDF(N,A,IA,B,IB,DL,IFAIL)
     New: DO 20 J = 1, N
             DO 10 I = J, N
                A(I,J) = A(J,I)
                 B(I,J) = B(J,I)
       10
             CONTINUE
             DL(J) = B(J,J)
       20 CONTINUE
          CALL spotrf('L', N, B, IB, INFO)
          IF (INFO.EQ.O) THEN
             CALL ssygst(2,'L',N,A,IA,B,IB,INFO)
          ELSE
             IFAIL = 1
          END IF
          CALL sswap(N, DL, 1, B, IB+1)
```

IFAIL is set to 1 if the matrix B is not positive-definite. It is essential to test IFAIL.

#### F01BEF

Withdrawn at Mark 18 Replaced by F06YFF (DTRMM)

#### F01BFF

Withdrawn at Mark 8 Replaced by F07GDF (DPPTRF) or F07PDF (DSPTRF)

## F01BHF

Withdrawn at Mark 9 Replaced by F02WEF

## F01BJF

Withdrawn at Mark 9 Replaced by F08HEF (DSBTRD)

## F01BKF

Withdrawn at Mark 9 Replaced by F02WDF

## F01BMF

Withdrawn at Mark 9 Replaced by F07BDF (DGBTRF)

#### F01BNF

Withdrawn at Mark 17 Replaced by F07FRF (ZPOTRF)

> Old: CALL FO1BNF(N,A,IA,P,IFAIL) New: CALL *cpotrf*('Upper',N,A,IA,IFAIL)

where, before the call, array A contains the upper triangle of the matrix to be factorized rather than the lower triangle (note that the elements of the upper triangle are the complex conjugates of the elements of the lower triangle). The *double precision* array P is no longer required; the upper triangle of A is overwritten by the upper triangular factor U, including the diagonal elements (which are not reciprocated).

**F01BPF** Withdrawn at Mark 17 Replaced by F07FRF (ZPOTRF) and F07FWF (ZPOTRI)

Old: CALL F01BPF(N,A,IA,V,IFAIL)
New: CALL cpotrf('Upper',N,A,IA,IFAIL)
CALL cpotri('Upper',N,A,IA,IFAIL)

where, before the calls, the upper triangle of the matrix to be inverted must be contained in rows 1 to N of A, rather than the lower triangle being in rows 2 to N + 1 (note that the elements of the upper triangle are the complex conjugates of the elements of the lower triangle). The workspace vector V is no longer required.

#### F01BQF

Withdrawn at Mark 16 Replaced by F07GDF (DPPTRF) or F07PDF (DSPTRF)

The replacement routines do not have exactly the same functionality as F01BQF; if this functionality is genuinely required, please contact NAG.

(a) where the symmetric matrix is known to be positive-definite (if the matrix is in fact not positive-definite, the replacement routine will return a positive value in IFAIL)

```
Old: CALL F01BQF(N,EPS,RL,IRL,D,IFAIL)
New: CALL spptrf('Lower',N,RL,IFAIL)
```

(b) where the matrix is not positive-definite (the replacement routine forms an  $LDL^{T}$  factorization where D is block diagonal, rather than a Cholesky factorization)

```
Old: CALL F01BQF(N,EPS,RL,IRL,D,IFAIL)
New: CALL ssptrf('Lower',N,RL,IPIV,IFAIL)
```

For the replacement calls in both (a) and (b), the array RL must now hold the complete lower triangle of the symmetric matrix, including the diagonal elements, which are no longer required to be stored in the redundant array D. The declared dimension of RL must be increased from at least N(N - 1)/2 to at least N(N + 1)/2. It is important to note that for the calls of F07GDF (DPPTRF) and F07PDF (DSPTRF), the lower triangle of the matrix must be stored packed by column instead of by row. The dimension parameter IRL is no longer required. For the call of F07PDF (DSPTRF), the INTEGER array IPIV of length N must be supplied.

### F01BTF

Withdrawn at Mark 18 Replaced by F07ADF (DGETRF)

Old: CALL F01BTF(N,A,IA,P,DP,IFAIL)
New: CALL sgetrf(N,N,A,IA,IPIV,IFAIL)

where IPIV is an INTEGER array of length N which holds the indices of the pivot elements, and the array P is no longer required. It may be important to note that after a call of F07ADF (DGETRF), A is overwritten by the upper triangular factor U and the off-diagonal elements of the unit lower triangular factor L, whereas the factorization returned by F01BTF gives U the unit diagonal. The permutation determinant DP returned by F01BTF is not computed by F07ADF (DGETRF). If this value is required, it may be calculated after a call of F07ADF (DGETRF) by code similar to the following:

```
DP = 1.0D0
DO 10 I = 1, N
IF (I.NE.IPIV(I)) DP = -DP
10 CONTINUE
```

#### F01BWF

Withdrawn at Mark 18 Replaced by F08HEF (DSBTRD)

where Q is a dummy *double precision* array of length (1) (not used in this call), and WORK is a *double precision* array of length at least (N).

Note that the tridiagonal matrix computed by F08HEF (DSBTRD) is different from that computed by F01BWF, but it has the same eigenvalues.

#### F01BXF

Withdrawn at Mark 17 Replaced by F07FDF (DPOTRF)

Old: CALL F01BXF(N,A,IA,P,IFAIL)
New: CALL spotrf('Upper',N,A,IA,IFAIL)

where, before the call, array A contains the upper triangle of the matrix to be factorized rather than the lower triangle. The array P is no longer required; the upper triangle of A is overwritten by the upper triangular factor U, including the diagonal elements (which are not reciprocated).

## F01CAF

Withdrawn at Mark 14 Replaced by F06QHF

> Old: CALL F01CAF(A,M,N,IFAIL) New: CALL F06QHF('General',M,N,0.0D0,0.0D0,A,M)

#### F01CBF

Withdrawn at Mark 14 Replaced by F06QHF

> Old: CALL F01CBF(A,M,N,IFAIL) New: CALL F06QHF('General',M,N,0.0D0,1.0D0,A,M)

## F01CCF

Withdrawn at Mark 7 Replaced by F06QFF

#### F01CDF

Withdrawn at Mark 15 Replaced by F01CTF

Old: CALL F01CDF(A,B,C,M,N,IFAIL)
New: CALL F01CTF('N','N',M,N,1.0D0,B,M,1.0D0,C,M,A,M,IFAIL)

#### F01CEF

Withdrawn at Mark 15 Replaced by F01CTF

Old: CALL F01CEF(A,B,C,M,N,IFAIL)
New: CALL F01CTF('N','N',M,N,1.0D0,B,M,-1.0D0,C,M,A,M,IFAIL)

#### F01CFF

Withdrawn at Mark 14 Replaced by F06QFF

> Old: CALL F01CFF(A,MA,NA,P,Q,B,MB,NB,M1,M2,N1,N2,IFAIL) New: CALL F06QFF('General',M2-M1+1,N2-N1+1,B(M1,N1),MB,A(P,Q),MA)

## F01CGF

Withdrawn at Mark 15 Replaced by F01CTF

> Old: CALL FO1CGF(A,MA,NA,P,Q,B,MB,NB,M1,M2,N1,N2,IFAIL) New: CALL FO1CTF('N','N',M2-M1+1,N2-N1+1,1.0D0,A(P,Q),MA,1.0D0, + B(M1,N1),MB,A(P,Q),MA,IFAIL)

## F01CHF

Withdrawn at Mark 15 Replaced by F01CTF

```
Old: CALL F01CHF(A,MA,NA,P,Q,B,MB,NB,M1,M2,N1,N2,IFAIL)
New: CALL F01CTF('N','N',M2-M1+1,N2-N1+1,1.0D0,A(P,Q),MA,-1.0D0,
+ B(M1,N1),MB,A(P,Q),MA,IFAIL)
```

#### F01CJF

Withdrawn at Mark 8 Replaced by F01CRF

### F01CLF

Withdrawn at Mark 16 Replaced by F06YAF (DGEMM)

> Old: CALL FO1CLF(A,B,C,N,P,M,IFAIL) New: CALL sgemm('N','T',N,P,M,1.0D0,B,N,C,P,0.0D0,A,N)

#### F01CMF

Withdrawn at Mark 14 Replaced by F06QFF

Old: CALL F01CMF(A,LA,B,LB,M,N)
New: CALL F06QFF('General',M,N,A,LA,B,LB)

## F01CNF

Withdrawn at Mark 13 Replaced by F06EFF (DCOPY)

Old: CALL FO1CNF(V,M,A,LA,I)
New: CALL scopy(M,V,1,A(I,1),LA)

#### F01CPF

Withdrawn at Mark 13 Replaced by F06EFF (DCOPY)

> Old: CALL FO1CPF(A,B,N) New: CALL *scopy*(N,A,1,B,1)

#### F01CQF

Withdrawn at Mark 13 Replaced by F06FBF

> Old: CALL FO1CQF(A,N) New: CALL F06FBF(N,0.0D0,A,1)

#### F01CSF

Withdrawn at Mark 13 Replaced by F06PEF (DSPMV)

> Old: CALL F01CSF(A,LA,B,N,C) New: CALL *sspmv*('U',N,1.0D0,A,B,1,0.0D0,C,1)

### F01DAF

Withdrawn at Mark 13 Replaced by F06EAF (DDOT)

Old: F01DAF(L,M,C1,IRA,ICB,A,IA,B,IB,N)
New: C1 + sdot(M-L+1,A(IRA,L)IA,B(L,ICB),1)

### F01DBF

Withdrawn at Mark 13 Replaced by X03AAF

(here D2 is a new *double precision* variable whose value is not used).

## F01DCF

Withdrawn at Mark 13 Replaced by F06GAF (ZDOTU)

```
Old: CALL F01DCF(L,M,CX,IRA,ICB,A,IA,B,IB,N,CR,CI)
New: DX = CX - cdotu(M-L+1,A(IRA,L),IA,B(L,ICB),1)
        CR = real(DX)
        CI = imag(DX)
```

(here DX is a new *complex* variable).

#### F01DDF

Withdrawn at Mark 13 Replaced by X03ABF

(here DX is a new *complex* variable).

## F01DEF

Withdrawn at Mark 14 Replaced by F06EAF (DDOT)

> Old: FO1DEF(A,B,N) New: *sdot*(N,A,1,B,1)

#### F01LBF

Withdrawn at Mark 18 Replaced by F07BDF (DGBTRF)

```
Old: CALL FO1LBF(N,M1,M2,A,IA,AL,IL,IN,IV,IFAIL)
New: CALL sgbtrf(N,N,M1,M2,A,IA,IN,IFAIL)
```

where the size of array A must now have a leading dimension IA of at least  $2 \times M1 + M2 + 1$ . The array AL, its associated dimension parameter IL, and the parameter IV are not required for F07BDF (DGBTRF) because this routine overwrites A by both the *L* and *U* factors. The scheme by which the matrix is packed into the array is completely different from that used by F01LBF; the relevant routine document should be consulted for details.

#### F01LZF

```
ELSE IF (WANTZ) THEN
CALL sormbr('P','L','T',N,NCZ,N,A,NRA,TAUP,Z,NRZ,WORK1,LWORK,
+ INFO)
END IF
```

where TAUQ and TAUP are real arrays of length at least (N) and LWORK is the actual length of WORK1. The parameter WORK2 is no longer required.

#### F01MAF

Withdrawn at Mark 19 Replaced by F11JAF

Existing programs should be modified to call F11JAF. The interfaces are significantly different and therefore precise details of a replacement call cannot be given. Please consult the appropriate routine document.

#### F01NAF

Withdrawn at Mark 17 Replaced by F07BRF (ZGBTRF)

Old: CALL F01NAF(N,ML,MU,A,NRA,TOL,IN,SCALE,IFAIL)
New: CALL cgbtrf(N,N,ML,MU,A,NRA,IN,IFAIL)

where the parameter TOL and array SCALE are no longer required. The input matrix must be stored using the same scheme as for F01NAF, except in rows ML + 1 to  $2 \times ML + MU + 1$  of A instead of rows 1 to ML + MU + 1. In F07BRF (ZGBTRF), the value returned in IN(N) has no significance as an indicator of near-singularity of the matrix.

#### F01QAF

Withdrawn at Mark 15 Replaced by F08AEF (DGEQRF)

Old: CALL F01QAF(M,N,A,NRA,C,NRC,Z,IFAIL)
New: CALL sgeqrf(M,N,A,NRA,Z,WORK,LWORK,INFO)

where WORK is a real array of length at least (LWORK). The parameters C and NRC are no longer required.

Note that the representation of the matrix Q is not identical, but subsequent calls to routines F08AFF (DORGQR) and F08AGF (DORMQR) may be used to obtain Q explicitly and to transform by Q or  $Q^{T}$  respectively.

#### F01QBF

Withdrawn at Mark 15 Replaced by F01QJF Old: CALL F01QBF(M,N,A,NRA,C,NRC,WORK,IFAIL) New: CALL F06QFF('General',M,N,A,NRA,C,NRC) CALL F01QJF(M,N,C,NRC,WORK,IFAIL)

The call to F06QFF simply copies the leading M by N part of A to C. This may be omitted if it is desired to use the same arrays for A and C. Note that the representation of the orthogonal matrix Q is not identical, but following F01QJF routine F01QKF may be used to form Q.

#### F01QCF

Withdrawn at Mark 18 Replaced by F08AEF (DGEQRF) Old: CALL F01QCF(M,N,A,LDA,ZETA,IFAIL) New: CALL sgeqrf(M,N,A,LDA,ZETA,WORK,LWORK,INFO)

where WORK is a *double precision* array of length at least (N), and LWORK is its actual length.

The subdiagonal elements of A and the elements of ZETA returned by F08AEF (DGEQRF) are not the same as those returned by F01QCF. Subsequent calls to F01QDF or F01QEF must also be replaced by calls to F08AGF (DORMQR) or F08AFF (DORGQR) as shown below.

#### F01QDF

Withdrawn at Mark 18 Replaced by F08AGF (DORMQR)

The following replacement is valid only if the previous call to F01QCF has been replaced by a call to F08AEF (DGEQRF) as shown above. It also assumes that the second argument of F01QDF (WHERET) is 'S', which is appropriate if the contents of A and ZETA have not been changed after the call of F01QCF.

Old: CALL F01QDF(TRANS,'S',M,N,A,LDA,ZETA,NCOLB,B,LDB,WORK,IFAIL) New: CALL *sormqr*('L',TRANS,M,NCOLB,N,A,LDA,ZETA,B,LDB,WORK,LWORK,INFO)

where LWORK is the actual length of WORK.

## F01QEF

Withdrawn at Mark 18 Replaced by F08AFF (DORGQR)

The following replacement is valid only if the previous call to F01QCF has been replaced by a call to F08AEF (DGEQRF) as shown above. It also assumes that the first argument of F01QEF (WHERET) is 'S', which is appropriate if the contents of A and ZETA have not been changed after the call of F01QCF.

Old: CALL F01QEF('S',M,N,NCOLQ,A,LDA,ZETA,WORK,IFAIL) New: CALL *sorgqr*(M,NCOLQ,N,A,LDA,ZETA,WORK,LWORK,INFO)

where LWORK is the actual length of WORK.

#### F01QFF

Withdrawn at Mark 18 Replaced by F08BEF (DGEQPF)

The following replacement assumes that the 1st argument of F01QFF (PIVOT) is 'C'. There is no direct replacement if PIVOT = 'S'.

where WORK is a *double precision* array of length at least  $(3 \times N)$  (F01QFF only requires WORK to be of length  $(2 \times N)$ ).

The subdiagonal elements of A and the elements of ZETA returned by F08BEF (DGEQPF) are not the same as those returned by F01QFF. Subsequent calls to F01QDF or F01QEF must also be replaced by calls to F08AGF (DORMQR) or F08AFF (DORGQR) as shown above. Note also that the array PERM returned by F08BEF (DGEQPF) holds details of the interchanges in a different form than that returned by F01QFF.

#### F01RCF

Withdrawn at Mark 18 Replaced by F08ASF (ZGEQRF)

> Old: CALL F01RCF(M,N,A,LDA,THETA,IFAIL) New: CALL *cgeqrf*(M,N,A,LDA,THETA,WORK,LWORK,INFO)

where WORK is a *complex\*16* array of length at least (N), and LWORK is its actual length.

The subdiagonal elements of A and the elements of THETA returned by F08ASF (ZGEQRF) are not the same as those returned by F01RCF. Subsequent calls to F01RDF or F01REF must also be replaced by calls to F08AUF (ZUNMQR) or F08ATF (ZUNGQR) as shown below.

## F01RDF

Withdrawn at Mark 18 Replaced by F08AUF (ZUNMQR)

The following replacement is valid only if the previous call to F01RCF has been replaced by a call to F08ASF (ZGEQRF) as shown above. It also assumes that the second argument of F01RDF (WHERET) is 'S', which is appropriate if the contents of A and THETA have not been changed after the call of F01RCF.

where LWORK is the actual length of WORK.

#### F01REF

Withdrawn at Mark 18 Replaced by F08ATF (ZUNGQR)

The following replacement is valid only if the previous call to F01RCF has been replaced by a call to F08ASF (ZGEQRF) as shown above. It also assumes that the first argument of F01REF (WHERET) is 'S', which is appropriate if the contents of A and THETA have not been changed after the call of F01RCF.

Old: CALL F01REF('S',M,N,NCOLQ,A,LDA,THETA,WORK,IFAIL) New: CALL *cungqr*(M,NCOLQ,N,A,LDA,THETA,WORK,LWORK,INFO)

where LWORK is the actual length of WORK.

#### F01RFF

Withdrawn at Mark 18 Replaced by F08BSF (ZGEQPF)

The following replacement assumes that the first argument of F01RFF (PIVOT) is 'C'. There is no direct replacement if PIVOT = 'S'.

where CWORK is a *complex\*16* array of length at least (N).

The subdiagonal elements of A and the elements of THETA returned by F08BSF (ZGEQPF) are not the same as those returned by F01RFF. Subsequent calls to F01RDF or F01REF must also be replaced by calls to F08AUF (ZUNMQR) or F08ATF (ZUNGQR) as shown above. Note also that the array PERM returned by F08BSF (ZGEQPF) holds details of the interchanges in a different form than that returned by F01RFF.

## F02 – Eigenvalues and Eigenvectors

## F02AAF

Withdrawn at Mark 18 Replaced by F02FAF

Old: CALL F02AAF(A,IA,N,R,E,IFAIL)
New: CALL F02FAF('N','L',N,A,IA,R,WORK,LWORK,IFAIL)

where WORK is a *double precision* array of length at least  $(3 \times N)$  and LWORK is its actual length.

#### F02ABF

Withdrawn at Mark 18 Replaced by F02FAF

> Old: CALL F02ABF(A,IA,N,R,V,IV,E,IFAIL) New: CALL F06QFF('L',N,N,A,IA,V,IV) CALL F02FAF('V','L',N,V,IV,R,WORK,LWORK,IFAIL)

where WORK is a *double precision* array of length at least  $(3 \times N)$  and LWORK is its actual length. If F02ABF was called with the same array supplied for V and A, then the call to F06QFF may be omitted.

#### F02ADF

Withdrawn at Mark 18 Replaced by F02FDF Old: CALL F02ADF(A,IA,B,IB,N,R,DE,IFAIL) New: CALL F02FDF(1,'N','U',N,A,IA,B,IB,R,WORK,LWORK,IFAIL)

where WORK is a *double precision* array of length at least  $(3 \times N)$  and LWORK is its actual length.

Note that the call to F02FDF will overwrite the upper triangles of the arrays A and B and leave the subdiagonal elements unchanged, whereas the call to F02ADF overwrites the lower triangle and leaves the elements above the diagonal unchanged.

#### F02AEF

```
Withdrawn at Mark 18
Replaced by F02FDF
```

where WORK is a *double precision* array of length at least  $(3 \times N)$  and LWORK is its actual length.

Note that the call to F02FDF will overwrite the upper triangle of the array B and leave the subdiagonal elements unchanged, whereas the call to F02ADF overwrites the lower triangle and leaves the elements above the diagonal unchanged. The call to F06QFF copies A to V, so A is left unchanged. If F02AEF was called with the same array supplied for V and A, then the call to F06QFF may be omitted.

#### F02AFF

Withdrawn at Mark 18 Replaced by F02EBF Old: CALL F02AFF(A,IA,N,RR,RI,INTGER,IFAIL) New: CALL F02EBF('N',N,A,IA,RR,RI,VR,1,VI,1,WORK,LWORK,IFAIL)

where VR and VI are dummy arrays of length (1) (not used in this call), WORK is a *double precision* array of length at least  $(4 \times N)$  and LWORK is its actual length; the iteration counts (returned by F02AFF in the array INTGER) are not available from F02EBF.

#### F02AGF

Withdrawn at Mark 18 Replaced by F02EBF

> Old: CALL F02AGF(A,IA,N,RR,RI,VR,IVR,VI,IVI,INTGER,IFAIL) New: CALL F02EBF('V',N,A,IA,RR,RI,VR,IVR,VI,IVI,WORK,LWORK,IFAIL)

where WORK is a *double precision* array of length at least  $(4 \times N)$  and LWORK is its actual length; the iteration counts (returned by F02AGF in the array INTGER) are not available from F02EBF.

#### F02AHF

Withdrawn at Mark 8 Replaced by F02ECF

#### F02AJF

```
Withdrawn at Mark 18

Replaced by F02GBF

Old: CALL F02AJF(AR,IAR,AI,IAI,N,RR,RI,INTGER,IFAIL)

New: D0 20 J = 1, N

D0 10 I = 1, N

A(I,J) = cmplx(AR(I,J),AI(I,J))

10 CONTINUE
```

```
20 CONTINUE
CALL F02GBF('N',N,A,IA,R,V,1,RWORK,WORK,LWORK,IFAIL)
D0 30 I = 1, N
RR(I) = real(R(I))
RI(I) = imag(R(I))
30 CONTINUE
```

where A is a *complex\*16* array of dimension (IA, N), R is a *complex\*16* array of dimension (N), V is a dummy *complex\*16* array of length (1) (not used in this call), RWORK is a *double precision* array of length at least  $(2 \times N)$ , WORK is a *complex\*16* array of length at least  $(2 \times N)$  and LWORK is its actual length.

### F02AKF

Withdrawn at Mark 18 Replaced by F02GBF

```
Old: CALL F02AKF(AR, IAR, AI, IAI, N, RR, RI, VR, IVR, VI, IVI, INTGER, IFAIL)
New: DO 20 J = 1, N
        DO 10 I = 1, N
           A(I,J) = cmplx(AR(I,J),AI(I,J))
  10
        CONTINUE
  20 CONTINUE
     CALL F02GBF('V',N,A,IA,R,V,IV,RWORK,WORK,LWORK,IFAIL)
     DO 40 J = 1, N
        RR(J) = real(R(J))
        RI(J) = imag(R(J))
        DO 30 I = 1, N
            VR(I,J) = real(V(I,J))
           VI(I,J) = imag(V(I,J))
  30
        CONTINUE
  40 CONTINUE
```

where A is a *complex\*16* array of dimension (IA, N), R is a *complex\*16* array of length (N), V is a *complex\*16* array of dimension (IV, N), RWORK is a *double precision* array of length at least  $(2 \times N)$ , WORK is a *complex\*16* array of length at least  $(2 \times N)$  and LWORK is is actual length.

#### F02ALF

Withdrawn at Mark 8 Replaced by F02GCF

#### F02AMF

Withdrawn at Mark 18 Replaced by F08JEF (DSTEQR)

Old: CALL F02AMF(N,EPS,D,E,V,IV,IFAIL)
New: CALL ssteqr('V',N,D,E(2),V,IV,WORK,INFO)

where WORK is a *double precision* array of length at least (2(N-1)).

### F02ANF

Withdrawn at Mark 18 Replaced by F08PSF (ZHSEQR)

where H is a *complex\*16* array of dimension (IH, N), R is a *complex\*16* array of length (N), Z is a dummy *complex\*16* array of length (1) (not used in this call), and WORK is a *complex\*16* array of length at least (N).

## F02APF

Withdrawn at Mark 18 Replaced by F08PEF (DHSEQR)

> Old: CALL F02APF(N,EPS,H,IH,RR,RI,ICNT,IFAIL) New: CALL *shseqr*('E','N',N,1,N,H,IH,RR,RI,Z,1,WORK,1,INFO)

where Z is a dummy *double precision* array of length (1) (not used in this call), and WORK is a *double precision* array of length at least  $(3 \times N)$ ; the iteration counts (returned by F02APF in the array ICNT) are not available from F08PEF (DHSEQR).

## F02AQF

Withdrawn at Mark 18 Replaced by F08PEF (DHSEQR) and F08QKF (DTREVC)

Old: CALL F02AQF(N,K,L,EPS,H,IH,V,IV,RR,RI,INTGER,IFAIL)
New: CALL shseqr('S','V',N,K,L,H,IH,RR,RI,V,IV,WORK,1,INFO)
CALL strevc('R','O',SELECT,N,H,IH,V,IV,V,IV,N,M,WORK,INFO)

where SELECT is a dummy logical array of length (1) (not used in this call), and WORK is a *double precision* array of length at least  $(3 \times N)$ ; the iteration counts (returned by F02AQF in the array INTGER) are not available from F08PEF (DHSEQR); M is an integer which is set to N by F08QKF (DTREVC).

## F02ARF

Withdrawn at Mark 18 Replaced by F08PSF (ZHSEQR) and F08QXF (ZTREVC)

```
Old: CALL F02ARF(N,K,L,EPS,INTGER,HR,IHR,HI,IHI,RR,RI,VR,IVR,VI,
                 IVI, IFAIL)
New: DO 20 J = 1, N
        DO 10 I = 1, N
           H(I,J) = cmplx(HR(I,J),HI(I,J))
  10
        CONTINUE
  20 CONTINUE
     CALL chseqr('S','V',N,K,L,H,IH,R,V,IV,WORK,1,INFO)
     CALL ctrevc('R','O',SELECT,N,H,IH,V,IV,V,IV,N,M,WORK,INFO)
     DO 40 J = 1, N
        RR(J) = real(R(J))
        RI(J) = imag(R(J))
        DO 30 I = 1, N
           VR(I,J) = real(V(I,J))
           VI(I,J) = imag(V(I,J))
 30
        CONTINUE
40
    CONTINUE
```

where H is a *complex\*16* array of dimension (IH, N), R is a *complex\*16* array of length (N), V is a *complex\*16* array of dimension (IV, N), WORK is a *complex\*16* array of length at least  $(2 \times N)$  and RWORK is a *double precision* array of length at least (N); M is an integer which is set to N by F08QXF (ZTREVC).

If F02ARF was preceded by a call to F01AMF to reduce a full complex matrix to Hessenberg form, then the call to F01AMF must also be replaced by calls to F08NSF (ZGEHRD) and F08NTF (ZUNGHR).

## F02ATF

Withdrawn at Mark 8 Replaced by F08PKF (DHSEIN)

## F02AUF

Withdrawn at Mark 8 Replaced by F08PXF (ZHSEIN)

#### **F02AVF** Withdrawn at Mark 18

Replaced by F08JFF (DSTERF)

```
Old: CALL F02AVF(N,EPS,D,E,IFAIL)
New: CALL ssterf(N,D,E(2),INFO)
```

## F02AWF

Withdrawn at Mark 18 Replaced by F02HAF

where A is a *complex\*16* array of dimension (IA, N), RWORK is a *double precision* array of length at least  $(3 \times N)$ , WORK is a *complex\*16* array of length at least  $(2 \times N)$  and LWORK is its actual length.

## F02AXF

```
Withdrawn at Mark 18
Replaced by F02HAF
```

where A is a *complex\*16* array of dimension (IA, N), V is a *complex\*16* array of dimension (IV, N), RWORK is a *double precision* array of length at least  $(3 \times N)$ , WORK is a *complex\*16* array of length at least  $(2 \times N)$  and LWORK is its actual length. If F02AXF was called with the same arrays supplied for VR and AR and for VI and AI, then the call to F06TFF may be omitted.

### F02AYF Withdrawn at Mark 18 Replaced by F08JSF (ZSTEQR) Old: CALL F02AYF(N,EPS,D,E,VR,IVR,VI,IVI,IFAIL) New: CALL csteqr('V',N,D,E(2),V,IV,WORK,INFO) DO 40 J = 1, N DO 30 I = 1, N VR(I,J) = reat(V(I,J)) VI(I,J) = imag(V(I,J)) 30 CONTINUE 40 CONTINUE

where V is a *complex\*16* array of dimension (IV, N), and WORK is a *real* array of length at least (2(N-1)).

### F02BBF

Withdrawn at Mark 19 Replaced by F02FCF

where R must have dimension (N), WORK is a *real* array of length at least  $(8 \times N)$ , LWORK is its actual length, and IWORK is an integer array of length at least  $(5 \times N)$ . Note that in the call to F02BBF R needs only to be of dimension (M).

## F02BCF

Withdrawn at Mark 19 Replaced by F02ECF

```
Old: CALL F02BCF(A,IA,N,ALB,UB,M,MM,RR,RI,VR,IVR,VI,IVI,

+ INTGER,ICNT,C,B,IB,U,V,IFAIL)

New: CALL F02ECF('Moduli',N,A,IA,ALB,UB,M,MM,RR,RI,VR,IVR,

+ VI,IVI,WORK,LWORK,ICNT,C,IFAIL)
```

where WORK is a *real* array of length at least (N\*(N+4)) and LWORK is its actual length.

## F02BDF

Withdrawn at Mark 19 Replaced by F02GCF

```
Old: CALL F02BDF(AR, IAR, AI, IAI, N, ALB, UB, M, MM, RR, RI, VR, IVR,
                  VI, IVI, INTGER, C, BR, IBR, BI, IBI, U, V, IFAIL)
New: DO 20 J = 1, N
        DO 10 I = 1, N
           A(I,J) = cmplx(AR(I,J),AI(I,J))
  10
        CONTINUE
  20 CONTINUE
    CALL F02GCF('Moduli',N,A,IA,ALB,UB,M,MM,R,V,IV,WORK,
                 LWORK, RWORK, INTGER, C, IFAIL)
    +
     DO 30 I = 1, N
        RR(I) = real(R(I))
        RI(I) = imag(R(I))
  30 CONTINUE
     DO 50 J = 1, MM
        DO 40 I = 1, N
            VR(I,J) = real(V(I,J))
           VI(I,J) = imag(V(I,J))
  40
        CONTINUE
  50 CONTINUE
```

where A is a *complex\*16* array of dimension (IA, N), R is a *complex\*16* array of dimension (N), V is a *complex\*16* array of dimension (IV, M), WORK is a *complex\*16* array of length at least  $(N \times (N + 2))$ , LWORK is its actual length, and RWORK is a *real* array of length at least  $(2 \times N)$ .

### F02BEF

Withdrawn at Mark 18 Replaced by F08JJF (DSTEBZ) and F08JKF (DSTEIN)

where NSPLIT is an integer variable, IBLOCK, ISPLIT and IFAILV are integer arrays of length at least (N), and IWORK is an integer array of length at least  $(3 \times N)$ .

## F02BFF

Withdrawn at Mark 18 Replaced by F08JJF (DSTEBZ)

```
Old: CALL F02BFF(D,E,E2,N,M1,M2,MM12,EPS1,EPS,EPS2,IZ,R,WU)
New: CALL sstebz('I','E',N,O.ODO,O.ODO,M1,M2,EPS1,D,E(2),M,
                 NSPLIT, R, IBLOCK, ISPLIT, WORK, IWORK, INFO)
```

where M and NSPLIT are integer variables, IBLOCK and ISPLIT are integer arrays of length at least (N), WORK is a *double precision* array of length at least  $(4 \times N)$ , and IWORK is an integer array of length at least  $(3 \times N)$ .

#### F02BJF

Scheduled for withdrawal at Mark 23 Replaced by F08WAF (DGGEV)

```
Old: CALL F02BJF(N,A,IA,B,IB,EPS1,ALFR,ALFI,BETA,MATV,V,IV,ITER,IFAIL)
New: IF (MATV) THEN
      JOBVR = 'V'
     ELSE
       JOBVR = 'N'
     ENDIF
     CALL FO8WAF('N', JOBVR, N, A. IA, B, IB, ALFR, ALFI, BETA, VL, LDVL,
                VR,LDVL,WORK,LWORK,INFO)
     IF (INFO.NE.O) THEN
       . . .
```

## F02BKF

Withdrawn at Mark 18 Replaced by F08PKF (DHSEIN)

```
Old: CALL F02BKF(N,M,H,IH,RI,C,RR,V,IV,B,IB,U,W,IFAIL)
New: CALL shsein ('R','Q','N',C,N,H,IH,RR,RI,V,IV,V,IV,M,M2,B,IFAILR,
                 IFAILR, INFO)
```

where M2 is an integer variable, and IFAILR is an integer array of length at least (N).

Note that the array C may be modified by F08PKF (DHSEIN) if there are complex conjugate pairs of eigenvalues.

## F02BLF

```
Withdrawn at Mark 18
Replaced by F08PXF (ZHSEIN)
     Old: CALL F02BLF(N,M,HR,IHR,HI,IHI,RI,C,RR,VR,IVR,VI,IVI,BR,IBR,BI,
         +
                       IBI,U,W,IFAIL)
     New: DO 20 J = 1, N
              R(J) = cmplx(RR(J), RI(J))
              DO 10 I = 1, N
                H(I,J) = cmplx(HR(I,J),HI(I,J))
             CONTINUE
       10
       20 CONTINUE
          CALL chsein ('R', 'Q', 'N', C, N, H, IH, R, V, IV, V, IV, M, M2, WORK, RWORK,
                       IFAILR, IFAILR, INFO)
          DO 30 I = 1, N
              RR(I) = real(R(I))
       30 CONTINUE
          DO 50 J = 1, M
              DO 40 I = 1, N
                 VR(I,J) = real(V(I,J))
                 VI(I,J) = imag(V(I,J))
       40
              CONTINUE
       50 CONTINUE
```

where H is a *complex\*16* array of dimension (IH, N), R is a *complex\*16* array of length (N), V is a complex\*16, array of dimension (IV, M), M2 is an integer variable, WORK is a complex\*16 array of length at least  $(N \times N)$ , RWORK is a *double precision* array of length at least (N), and IFAILR is an integer array of length at least (N).

[NP3657/21]

# F02BMF

Withdrawn at Mark 9 Replaced by F08HEF (DSBTRD) and F08JJF (DSTEBZ)

### F02EAF

Scheduled for withdrawal at Mark 23 Replaced by F08PAF (DGEES)

```
Old: CALL F02EAF(JOB,N,A,LDA,WR,WI,Z,LDZ,WORK,LWORK,IFAIL)
New: LOGICAL SELECT
    EXTERNAL SELECT
    ...
    IF (JOB.EQ.'N') THEN
        JOBVS = 'N'
    ELSE
        JOBVS = 'V'
    END IF
        CALL F08PAF(JOBVS,'N',SELECT,N,A,LDA,0,WR,WI,Z,LDZ,WORK,
        + LWORK,BWORK,INFO)
    IF (INFO.NE.0) THEN
    ....
```

LOGICAL FUNCTION SELECT(AR,AI) DOUBLE PRECISION AR, AI SELECT = .TRUE. RETURN ENDK

## F02EBF

```
CALL F08NAF('N', JOBVR, N, A, LDA, WR, WI, VL, LDVL, VR1, LDVR1,
+ WORK, LWORK, INFO)
IF (INFO.EQ.O) THEN
C Eigenvector infomation is stored differently in VR1
C VR(j)=VR1(j) if W(j) = 0.0
C VR(j)=VR1(j) and VI(j)=VR1(j+1) and
C VR(j+1)=VR1(j) and VI(j+1) = - VR1(j+1) if w(j)/= (not equals) 0 and
C W(j) = -w(j+1)
```

## F02FAF

Scheduled for withdrawal at Mark 23 Replaced by F08FAF (DSYEV)

```
Old: CALL F02FAF(JOB,UPLO,N,A,LDA,W,WORK,LWORK,IFAIL)
New: CALL F08FAF(JOB,UPLO,N,A,LDA,W,WORK,LWORK,INFO)
IF (INFO.NE.0) THEN
...
C the workspace requirements are slightly different.
```

### F02FCF

Scheduled for withdrawal at Mark 23 Replaced by F08FBF (DSYEVX)

С

+ W,Z,LDZ,WORK,LWORK,IWORK,IFAIL1,INFO)
IF (INFO.NE.0) THEN
...
the workspace requirements are slightly different.

### F02FDF

Scheduled for withdrawal at Mark 23 Replaced by F08SAF (DSYGV)

Old: CALL F02FDF(ITYPE,JOB,UPLO,N,A,LDA,B,LDB,W,WORK,LWORK,IFAIL)
New: CALL F08SAF(ITYPE,JOB,UPLO,N,A,LDA,B,LDB,W,WORK,LWORK,INFO)
IF (INFO.NE.0) THEN
...

C the workspace requirements are slightly different.

### F02FHF

Scheduled for withdrawal at Mark 23 Replaced by F08UAF (DSBGV)

#### F02GAF

Scheduled for withdrawal at Mark 23 Replaced by F08PNF (ZGEES)

```
Old: CALL F02GAF(JOB,N,A,LDA,W,Z,LDZ,RWORK,WORK,LWORK,IFAIL)
New: LOGICAL SELECT
     EXTERNAL SELECT
     IF (JOB.EQ.'N') THEN
       JOBVS = 'N'
     ELSE
       JOBVS = 'V'
     END TF
     CALL FO8UAF(JOBVS, 'N', SELECT, N, A, LDA, O, W, Z, LDZ,
    +
                  WORK, LWORK, BWORK, INFO)
     IF (INFO.NE.O) THEN
       . . .
     Note also the different workspace requirements
С
     LOGICAL FUNCTION SELECT(C)
     COMPLEX*16 C
     SELECT = .TRUE.
     RETURN
     END
```

#### F02GBF

Scheduled for withdrawal at Mark 23 Replaced by F08NNF (ZGEEV)

#### F02GJF

Scheduled for withdrawal at Mark 23 Replaced by F08WNF (ZGGEV)

> Old: CALL F02GJF(N,AR,IAR,AI,IAI,BR,IBR,BI,IBI,EPS1,ALFR,ALFI, + BETA,MATV,VR,IVR,VI,IVI,ITER,IFAIL)

```
New: IF (MATV) THEN
	JOBVR = 'V'
	ELSE
	JOBVR = 'N'
	END IF
C
C Set A=AR + iAI and B = BR+iBI
C
	CALL F08WNF('N',JOBVR,N,A,LDA,B,LDB,ALPHA,BETA1,VL,LDVL,
	+ 	V,LDV,WORK,LWORK,RWORK,INFO)C
C Note results returned in COMPLEX*16 types, unlike F02GJF.
	IF (INFO.NE.0) THEN
	...
```

### F02HAF

Scheduled for withdrawal at Mark 23 Replaced by F08FNF (ZHEEV)

```
Old: CALL F02HAF(JOB,UPLO,N,A,LDA,W,RWORK,WORK,LWORK,IFAIL)
New: CALL F08FNF(JOB,UPLO,N,A,LDA,W,WORK,LWORK,RWORK,INFO)
C Note slightly different workspace requirements.
IF (INFO.NE.O) THEN
...
```

#### F02HCF

Scheduled for withdrawal at Mark 23 Replaced by F08FPF (ZHEEVX)

### F02HDF

Scheduled for withdrawal at Mark 23 Replaced by F08SNF (ZHEGV)

### F02SWF

Withdrawn at Mark 18 Replaced by F08KEF (DGEBRD)

The following replacement ignores the triangular structure of A, and therefore references the subdiagonal elements of A; however on many machines the replacement code will be more efficient.

```
Old: CALL F02SWF(N,A,LDA,D,E,NCOLY,Y,LDY,WANTQ,Q,LDQ,IFAIL)
New: D0 20 J = 1, N
        D0 10 I = J+1, N
        A(I,J) = 0.0D0
10 CONTINUE
20 CONTINUE
CALL sgebrd(N,N,A,LDA,D,E,TAUQ,TAUP,WORK,LWORK,INFO)
IF (WANTQ) THEN
        CALL F06QFF('L',N,N,A,LDA,Q,LDQ)
        CALL sorgbr('Q',N,N,N,Q,LDQ,TAUQ,WORK,LWORK,INFO)
END IF
IF (NCOLY.GT.0) THEN
        CALL sormbr('Q','L','T',N,NCOLY,N,A,LDA,TAUQ,Y,LDY,
```

+ END IF WORK,LWORK,INFO)

where TAUQ, TAUP and WORK are *double precision* arrays of length at least (N), and LWORK is the actual length of WORK.

## F02SXF

Withdrawn at Mark 18 Replaced by F08KFF (DORGBR) and F08KGF (DORMBR)

The following replacement is valid only if the previous call to F02SWF has been replaced by a call to F08KEF (DGEBRD) as shown above.

### F02SYF

Withdrawn at Mark 18 Replaced by F08MEF (DBDSQR)

where WORK is a *double precision* array of length at least (4(N-1)) unless NCOLB = NROWY = NCOLZ = 0.

### F02SZF

Withdrawn at Mark 15 Replaced by F08MEF (DBDSQR)

```
Old: CALL F02SZF(N,D,E,SV,WANTB,B,WANTY,Y,NRY,LY,WANTZ,Z,NRZ,NCZ,
                  WORK1, WORK2, WORK3, IFAIL)
New: IF (WANTB) THEN
        NCC = 1
     ELSE
        NCC = 0
     END IF
     IF (WANTY) THEN
        NRU = LY
     ELSE
        NRU = 0
     END IF
     IF (WANTZ) THEN
        NCVT = NCZ
     ELSE
        NCVT = 0
     END IF
     CALL sbdsqr('U', N, NCVT, NRU, NCC, D, E(2), Z, NRZ, Y, NRY, B, N, WORK, INFO)
```

WORK must be a one-dimensional *double precision* array of length at least *lwork* given by:

lwork = 1 when WANTB, WANTY and WANTZ are all false;

 $lwork = max(4 \times (N - 1), 1)$  otherwise.

The parameters WORK1, WORK2 and WORK3 are no longer required.

### F02UWF

Withdrawn at Mark 18 Replaced by F08KSF (ZGEBRD) The following replacement ignores the triangular structure of A, and therefore references the subdiagonal elements of A; however on many machines the replacement code will be more efficient.

```
old: CALL F02UWF(N,A,LDA,D,E,NCOLY,Y,LDY,WANTO,O,LDO,WORK,IFAIL)
New: DO 20 J = 1, N
        DO 10 I = J+1,
                        N
           A(I,J) = 0.0D0
  10
        CONTINUE
  20 CONTINUE
     CALL cgebrd (N, N, A, LDA, D, E, TAUQ, TAUP, WORK, LWORK, INFO)
     IF (WANTO) THEN
        CALL FO6TFF('L',N,N,A,LDA,Q,LDQ)
        CALL cungbr('Q', N, N, N, Q, LDQ, TAUQ, WORK, LWORK, INFO)
     END IF
     IF (NCOLY.GT.O) THEN
        CALL cunmbr('Q','L','C',N,NCOLY,N,A,LDA,TAUQ,Y,LDY,
    +
                    WORK, LWORK, INFO)
     END IF
```

where TAUQ and TAUP are *complex\*16* arrays of length at least (N), and LWORK is the actual length of WORK.

### F02UXF

Withdrawn at Mark 18 Replaced by F08KTF (ZUNGBR) or F08KUF (ZUNMBR)

The following replacement is valid only if the previous call to F02UWF has been replaced by a call to F08KSF (ZGEBRD) as shown above.

```
Old: CALL F02UXF(N,A,LDA,NCOLY,Y,LDY,RWORK,CWORK,IFAIL)
New: IF (NCOLY.EQ.0) THEN
        CALL cungbr('P',N,N,N,A,LDA,TAUP,CWORK,LWORK,INFO)
        ELSE
        CALL cunmbr('P','L','C',N,NCOLY,N,A,LDA,TAUP,Y,LDY,CWORK,
        + LWORK,INFO)
        END IF
```

where LWORK is the actual length of CWORK.

#### F02UYF

Withdrawn at Mark 18 Replaced by F08MSF (ZBDSQR)

where WORK is a *double precision* array of length at least (4(N-1)) unless NCOLB = NROWY = NCOLZ = 0.

## F02WAF

RWORK must be a one-dimensional *double precision* array of length at least *lwork* given by:

 $lwork = max(3 \times (N - 1), 1)$  when WANTB is false;

 $lwork = max(5 \times (N - 1), 2)$  when WANTB is true.

If, in the call to F02WAF, LWORK satisfies these conditions then F02WEF may be called with RWORK as WORK.

### F02WBF

RWORK must be a one-dimensional *double precision* array of length at least *lwork* given by:

 $lwork = max(3 \times (M - 1), 1)$  when M = N and WANTB is false;  $lwork = max(5 \times (M - 1), 1)$  when M = N and WANTB is true;  $lwork = M2 + 3 \times (M - 1)$  when M < N and WANTB is false;  $lwork = M2 + 5 \times (M - 1)$  when M < N and WANTB is true.

In the cases where WANTB is false F02WEF may be called with RWORK as WORK, but when WANTB is true the user should check that, in the call to F02WBF, LWORK satisfies the above conditions before replacing RWORK with WORK.

### F02WCF

RWORK must be a one-dimensional *double precision* array of length at least *lwork* given by:

 $lwork = N2 + 5 \times (N - 1)$  when  $M \ge N$ ;

 $lwork = M2 + 5 \times (M - 1)$  when M < N.

If, in the call to F02WCF, LWORK satisfies these conditions then F02WEF may be called with RWORK as WORK.

#### F02WEF

Scheduled for withdrawal at Mark 23 Replaced by F08KBF (DGESVD)

```
JOBVT = 'N'
END IF
C Please note that the facility to return Q(t)B is not provided.
CALL F08KBF(JOBU,JOBVT,M,N,A,LDA,SV,Q,LDQ,PT,LDPT,WORK,
+ LWORK,INFO)
C Note slightly different workspace requirements.
IF (INFO.NE.0) THEN
...
```

#### F02XEF

Scheduled for withdrawal at Mark 23 Replaced by F08KPF (ZGESVD)

```
Old: CALL F02XEF(M,N,A,LDA,NCOLB,B,LDB,WANTO,O,LDO,SV,WANTP,
                  PH,LDPH,RWORK,CWORK,IFAIL)
New: IF (WANTQ) THEN
        JOBU = 'A'
     ELSE
        JOBU = 'N'
     END IF
     IF (WANTP) THEN
        JOBVT = 'A'
     ELSE
        JOBVT = 'N'
     END IF
     Please note that the facility to return Q(h)B is not provided.
С
     CALL F08KPF(JOBU, JOBVT, M, N, A, LDA, SV, Q, LDQ, PH, LDPH, CWORK,
                 LWORK, RWORK, INFO)
     Note slightly different workspace requirements.
С
     IF (INFO.NE.O) THEN
        . . .
```

## F03 – Determinants

F03AGF Withdrawn at Mark 17 Replaced by F07HDF (DPBTRF)

```
Old: CALL F03AGF(N,M,A,IA,RL,IL,M1,D1,ID,IFAIL)
New: CALL spbtrf('Lower',N,M,A,IA,IFAIL)
```

where the array RL and its associated dimension parameter IL, and the parameters M1, D1 and ID are no longer required. In F07HDF (DPBTRF), the array A holds the matrix packed using a different scheme to that used by F03AGF; see the routine document for details. F07HDF (DPBTRF) overwrites A with the Cholesky factor L (without reciprocating diagonal elements) rather than returning L in the array RL. F07HDF (DPBTRF) does not compute the determinant of the input matrix, returned as D1 × 2.0ID by F03AGF. If this is required, it may be calculated after the call of F07HDF (DPBTRF) by code similar to the following. The code computes the determinant by multiplying the diagonal elements of the factor L, taking care to avoid possible overflow or underflow.

```
D1 = 1.0D0
   ID = 0
   DO 30 I = 1, N
      D1 = D1 * A(1, I) * * 2
      IF (D1.GE.1.0D0) THEN
10
         D1 = D1 * 0.0625 e0
         ID = ID + 4
         GO TO 10
      END IF
20
      IF (D1.LT.0.0625e0) THEN
         D1 = D1 * 16.0D0
         ID = ID - 4
         GO TO 20
      END IF
30 CONTINUE
```

# F03AHF

Withdrawn at Mark 17 Replaced by F07ARF (ZGETRF)

> Old: CALL F03AHF(N,A,IA,DETR,DETI,ID,RINT,IFAIL) New: CALL *cgetrf*(N,N,A,IA,IPIV,IFAIL)

where IPIV is an INTEGER array of length N which holds the indices of the pivot elements, and the array RINT is no longer required. It may be important to note that after a call of F07ARF (ZGETRF), A is overwritten by the upper triangular factor U and the off-diagonal elements of the unit lower triangular factor L, whereas the factorization returned by F03AHF gives U the unit diagonal. F07ARF (ZGETRF) does not compute the determinant of the input matrix, returned as *cmplx*(DETR,DETI)×2.0ID by F03AHF. If this is required, it may be calculated after a call of F07ARF (ZGETRF) by code similar to the following, where DET is a *complex* variable. The code computes the determinant by multiplying the diagonal elements of the factor U, taking care to avoid possible overflow or underflow.

```
DET = cmplx(1.0D0, 0.0D0)
   ID = 0
   DO 30 I = 1, N
      IF (IPIV(I).NE.I) DET = -DET
      DET = DET * A(I,I)
10
      IF (MAX(ABS(real(DET)), ABS(imag(DET))).GE.1.0D0) THEN
         DET = DET * 0.0625e0
         ID = ID + 4
         GO TO 10
      END IF
20
      IF (MAX(ABS(real(DET)),ABS(imag(DET))).LT.0.0625e0) THEN
         DET = DET * 16.0D0
         ID = ID - 4
         GO TO 20
      END IF
30 CONTINUE
   DETR = real(DET)
   DETI = imag(DET)
```

### F03AJF

Withdrawn at Mark 8 Replaced by F01BRF

## F03AKF

Withdrawn at Mark 8 Replaced by F01BSF

### F03ALF

Withdrawn at Mark 9 Replaced by F07BDF (DGBTRF)

### F03AMF

Withdrawn at Mark 17 No replacement; see Chapter

```
Old: CALL FO1BNF(N,A,IA,P,IFAIL)
     CALL F03AMF(N,TEN,P,D1,D2)
New: CALL cpotrf('Upper',N,A,IA,IFAIL)
     D1 = 1.0D0
     D2 = 0.0D0
     DO 30 I = 1, N
        D1 = D1 * real(A(I,I)) * *2
   10
        IF (D1.GE.1.0D0) THEN
           D1 = D1 * 0.0625 e0
           D2 = D2 + 4
           GO TO 10
        END IF
   20
        IF (D1.LT.0.0625e0) THEN
           D1 = D1 * 16.0D0
```

```
D2 = D2 - 4
GO TO 20
END IF
30 CONTINUE
IF (TEN) THEN
I = D2
D2 = D2*LOG10(2.0D0)
D1 = D1*2.0D0**(I-D2/LOG10(2.0D0))
END IF
```

F03AMF computes the determinant of a Hermitian positive-definite matrix after factorization by F01BNF, and has no replacement routine. F01BNF has been superseded by F07FRF (ZPOTRF). To compute the determinant of such a matrix, in the same form as that returned by F03AMF, code similar to the above may be used. The code computes the determinant by multiplying the (real) diagonal elements of the factor U, taking care to avoid possible overflow or underflow.

Note that before the call of F07FRF (ZPOTRF), array A contains the upper triangle of the matrix rather than the lower triangle.

# F04 – Simultaneous Linear Equations

### F04AAF

Scheduled for withdrawal at Mark 23 Replaced by F07AAF (DGESV)

## F04ACF

Scheduled for withdrawal at Mark 23 Replaced by F07HAF (DPBSV)

#### F04ADF

Scheduled for withdrawal at Mark 23 Replaced by F07ANF (ZGESV)

#### F04AKF

Withdrawn at Mark 17 Replaced by F07ASF (ZGETRS)

Old: CALL F04AKF(N,IR,A,IA,P,B,IB)
New: CALL cgetrs('No Transpose',N,IR,A,IA,IPIV,B,IB,INFO)

It is assumed that the matrix has been factorized by a call of F07ARF (ZGETRF) rather than F03AHF; see F03 Chapter Introduction for details. IPIV is an INTEGER array of length N, as returned by F07ARF (ZGETRF), and the array P is no longer required. INFO is an INTEGER diagnostic parameter; see the F07ASF (ZGETRS) routine document for details.

# F04ALF

Withdrawn at Mark 17 Replaced by F07HEF (DPBTRS)

```
Old: CALL F04ALF(N,M,IR,RL,IRL,M1,B,IB,X,IX)
New: CALL F06QFF('General',N,IR,B,IB,X,IX)
CALL sphtrs('Lower',N,M,IR,A,IA,X,IX,INFO)
```

It is assumed that the matrix has been factorized by a call of F07HDF (DPBTRF) rather than F03AGF; see F03 Chapter Introduction for details. A is the factorized matrix as returned by F07HDF (DPBTRF). The array RL, its associated dimension parameter IRL, and the parameter M1 are no longer required. INFO is an INTEGER diagnostic parameter; see the F07HEF (DPBTRS) routine document for details. If the original right-hand side matrix B is no longer required, the call to F06QFF is not necessary, and references to X and IX in the call of F07HEF (DPBTRS) may be replaced by references to B and IB, in which case B will be overwritten by the solution.

## F04ANF

```
Withdrawn at Mark 18
Replaced by F06EFF (DCOPY), F06PJF (DTRSV) and F08AGF (DORMQR)
Old: CALL F04ANF(M,N,QR,IQR,ALPHA,IPIV,B,X,Z)
New: CALL scopy(N,ALPHA,1,QR,IQR+1)
CALL sormqr('L','T',M,1,N,QR,IQR,Y,B,M,Z,N,INFO)
CALL strsv('U','N','N',N,QR,IQR,B,1)
D0 10 I = 1, N
```

```
X(IPIV(I)) = B(I)
10 CONTINUE
```

where Y must be the same *double precision* array as was used as the seventh argument in the previous call of F01AXF.

This replacement is valid only if the previous call to F01AXF has been replaced by a call to F08BEF (DGEQPF) as shown above.

### F04APF

Withdrawn at Mark 8 Replaced by F04AXF

## F04AQF

Withdrawn at Mark 16 Replaced by F07GEF (DPPTRS) and F07PEF (DSPTRS)

May be replaced by calls to F06EFF (DCOPY), and F07GEF (DPPTRS) or F07PEF (DSPTRS), depending on whether the symmetric matrix has previously been factorized by F07GDF (DPPTRF) or F07PDF (DSPTRF) (see the description above of how to replace calls to F01BQF.

(a) where the symmetric matrix has been factorized by F07GDF (DPPTRF)

(b) where the symmetric matrix has been factorized by F07PDF (DSPTRF)

In both (a) and (b), the array RL must be as returned by the relevant factorization routine. The INTEGER parameter INFO is a diagnostic parameter. The INTEGER array IPIV in (b) must be as returned by F07PDF (DSPTRF). The dimension parameter M, and the array D, are no longer required. If the right-hand-side array B is not needed after solution of the equations, the call to F06EFF (DCOPY), which simply copies array B to X, is not necessary. References to X in the calls of F07GEF (DPPTRS) and F07PEF (DSPTRS) may then be replaced by references to B, in which case B will be overwritten by the solution vector.

### F04ARF

Scheduled for withdrawal at Mark 23 Replaced by F07AAF (DGESV)

> Old: CALL F04ARF(A,IA,B,N,C,WKSPCE,IFAIL) New: CALL F07AAF(N,1,A,IA,IPIV,B,1,INFO) IF (INFO.NE.O) THEN c Answer now in B

### F04AUF

Withdrawn at Mark 9 Replaced by F04JGF

## F04AVF

Withdrawn at Mark 9 Replaced by F07BEF (DGBTRS)

### F04AWF

Withdrawn at Mark 17 Replaced by F07FSF (ZPOTRS)

Old: CALL F04AWF(N,IR,A,IA,P,B,IB,X,IX)
New: CALL F06TFF('General',N,IR,B,IB,X,IX)
CALL cpotrs('Upper',N,IR,A,IA,X,IX,INFO)

It is assumed that the matrix has been factorized by a call of F07FRF (ZPOTRF) rather than F01BNF; see the F01 Chapter Introduction for details. A is the factorized matrix as returned by F07FRF (ZPOTRF). The array P is no longer required. INFO is an INTEGER diagnostic parameter; see the F07FSF (ZPOTRS) routine document for details. If the original right-hand side array B is no longer required, the call to F06TFF is not necessary, and references to X and IX in the call of F07FSF (ZPOTRS) may be replaced by references to B and IB, in which case B will be overwritten by the solution.

## F04AYF

Withdrawn at Mark 18 Replaced by F07AEF (DGETRS)

Old: CALL F04AYF(N,IR,A,IA,P,B,IB,IFAIL)
New: CALL sgetrs('No Transpose',N,IR,A,IA,IPIV,B,IB,IFAIL)

It is assumed that the matrix has been factorized by a call of F07ADF (DGETRF) rather than F01BTF. IPIV is an INTEGER array of length N, and the array P is no longer required.

## F04AZF

Withdrawn at Mark 17 Replaced by F07FEF (DPOTRS)

> Old: CALL F04AZF(N,IR,A,IA,P,B,IB,IFAIL) New: CALL *spotrs*('Upper',N,IR,A,IA,B,IB,IFAIL)

It is assumed that the matrix has been factorized by a call of F07FDF (DPOTRF) rather than F01BXF. The array P is no longer required.

### F04EAF

Scheduled for withdrawal at Mark 23 Replaced by F07CAF (DGTSV)

## F04FAF

Scheduled for withdrawal at Mark 23 Replaced by F07JAF (DPTSV)

#### F04JAF

Scheduled for withdrawal at Mark 23 Replaced by F08KAF (DGELSS)

```
Old: CALL F04JAF(M,N,A,NRA,B,TOL,SIGMA,IRANK,WORK,LWORK,IFAIL)
New: CALL F08KAF(M,N,1,A,NRA,B,1,S,RCOND,IRANK,WORK,LWORK,INFO)
c Note workspace requirements are different.
    IF (INFO.NE.0) THEN
C Answer now in B
C Singular values now in S, not WORK.
C The standard error is not computed
    ...
```

### F04JDF

Scheduled for withdrawal at Mark 23 Replaced by F08KAF (DGELSS)

```
Old: CALL F04JDF(M,N,A,NRA,B,TOL,SIGMA,IRANK,WORK,LWORK,IFAIL)
New: CALL F08KAF(M,N,1,A,NRA,B,1,S,RCOND,IRANK,WORK,LWORK,INFO)
c Note workspace requirements are different.
    IF (INFO.NE.0) THEN
C Answer now in B
C Singular values now in S, not WORK.
C The standard error is not computed
    ...
```

### F04JLF

Scheduled for withdrawal at Mark 23 Replaced by F08ZBF (DGGGLM)

```
Old: CALL F04JLF(M,N,P,A,LDA,B,LDB,D,X,Y,WORK,LWORK,IFAIL)
New: CALL F08ZBF(M,N,P,A,LDA,B,LDB,D,X,Y,WORK,LWORK,INFO)
C Slight workspace differences
IF (INFO.NE.0) THEN
...
```

### F04JMF

Scheduled for withdrawal at Mark 23 Replaced by F08ZAF (DGGLSE)

```
Old: CALL F04JMF(M,N,P,A,LDA,B,LDB,C,D,X,WORK,LWORK,IFAIL)
New: CALL F08ZAF(M,N,P,A,LDA,B,LDB,C,D,X,WORK,LWORK,INFO)
C Slight workspace differences
IF (INFO.NE.0) THEN
...
```

### F04KLF

Scheduled for withdrawal at Mark 23 Replaced by F08ZPF (ZGGGLM)

```
Old: CALL F04KLF(M,N,P,A,LDA,B,LDB,D,X,Y,WORK,LWORK,IFAIL)
New: CALL F082PF(M,N,P,A,LDA,B,LDB,D,X,Y,WORK,LWORK,INFO)
IF (INFO.NE.O) THEN
...
```

### F04KMF

Scheduled for withdrawal at Mark 23 Replaced by F08ZNF (ZGGLSE)

```
Old: CALL F04KMF(M,N,P,A,LDA,B,LDB,C,D,X,WORK,LWORK,IFAIL)
New: CALL F08ZNF(M,N,P,A,LDA,B,LDB,C,D,X,WORK,LWORK,INFO)
IF (INFO.NE.0) THEN
...
```

## F04LDF

Withdrawn at Mark 18 Replaced by F07BEF (DGBTRS)

> Old: CALL FO4LDF(N,M1,M2,IR,A,IA,AL,IL,IN,B,IB,IFAIL) New: CALL *sphrs*('No Transpose',N,M1,M2,IR,A,IA,IN,B,IB,IFAIL)

It is assumed that the matrix has been factorized by a call of F07BDF (DGBTRF) rather than F01LBF. The array AL and its associated dimension parameter IL are no longer required.

### F04MAF

Withdrawn at Mark 19 Replaced by F11JCF

Existing programs should be modified to call F11JCF. The interfaces are significantly different and therefore precise details of a replacement call cannot be given. Please consult the appropriate routine document.

### F04MBF

Withdrawn at Mark 19 Replaced by F11GAF, F11GBF and F11GCF (or F11JCF or F11JEF)

If a user-defined preconditioner is required existing programs should be modified to call F11GAF, F11GBF and F11GCF. Otherwise F11JCF or F11JEF may be used. The interfaces for these routines are significantly different from that for F04MBF and therefore precise details of a replacement call cannot be given. Please consult the appropriate routine document.

### F04NAF

```
Withdrawn at Mark 17
Replaced by F06SKF (ZTBSV) and F07BSF (ZGBTRS)
```

```
Old: CALL F04NAF(JOB,N,ML,MU,A,NRA,IN,B,TOL,IFAIL)
New: JOB = ABS(JOB)
IF (JOB.EQ.1) THEN
CALL cgbtrs('No Transpose',N,ML,MU,1,A,NRA,IN,B,N,IFAIL)
ELSE IF (JOB.EQ.2) THEN
CALL cgbtrs('Conjugate Transpose',N,ML,MU,1,A,NRA,IN,B,N,IFAIL)
ELSE IF (JOB.EQ.3) THEN
CALL ctbsv('Upper','No Transpose','Non-unit',N,ML+MU,A,NRA,B,1)
END IF
```

It is assumed that the matrix has been factorized by a call of F07BRF (ZGBTRF) rather than F01NAF. The replacement routines do not have the functionality to perturb diagonal elements of the triangular factor U, as specified by a negative value of JOB in F04NAF. The parameter TOL is therefore no longer useful. If this functionality is genuinely required, please contact NAG.

## **F05** – Orthogonalisation

## F05ABF

Withdrawn at Mark 14 Replaced by F06EJF (DNRM2)

> Old: U = FO5ABF(X,N)New: U = snrm2(N,X,1)

# F06 – Linear Algebra Support Routines

## F06QGF

Withdrawn at Mark 16

```
Replaced by F06RAF, F06RCF and F06RJF
     Old: ANORM = F06QGF(NORM, MATRIX, M, N, A, LDA)
     New: C = MATRIX(1:1)
           IF ( (C.EQ.'G') .OR. (C.EQ.'g') ) THEN
              ANORM = FO6RAF(NORM, M, N, A, LDA, WORK1)
          ELSE IF ( (C.EQ.'H') .OR. (C.EQ.'h') .OR. (C.EQ.'S') .OR.
+ (C.EQ.'s')) THEN
              ANORM = FO6RCF(NORM, 'U', N, A, LDA, WORK2)
          ELSE IF ( (C.EQ.'E') .OR. (C.EQ.'e') .OR. (C.EQ.'Y') .OR.
                        (C.EQ.'y')) THEN
          +
              ANORM = FOGRCF(NORM, 'L', N, N, A, LDA, WORK1)
           ELSE IF ( (C.EQ.'U') .OR. (C.EQ.'u') ) THEN
              ANORM = F06RJF(NORM, 'U', 'N', M, N, A, LDA, WORK1)
           ELSE IF ( (C.EQ.'L') .OR. (C.EQ.'l') ) THEN
              ANORM = F06RJF(NORM, 'L', 'N', M, N, A, LDA, WORK1)
           END IF
```

C must be declared as CHARACTER\*1, WORK1 as a *double precision* array of dimension (1) and WORK2 as a *double precision* array of dimension (N).

## F06VGF

Withdrawn at Mark 16 Replaced by F06UAF, F06UCF and F06UJF

C must be declared as CHARACTER\*1, WORK1 as a *double precision* array of dimension (1) and WORK2 as a *double precision* array of dimension (N).

## F11 – Large Scale Linear Systems

## F11BAF

Withdrawn at Mark 21 Replaced by F11BDF

F11BDF contains two additional parameters as follows:

WORK(LWORK) - *double precision* array.

LWORK - INTEGER.

See the routine document for further information.

### F11BBF

Withdrawn at Mark 21 Replaced by F11BEF

Old: CALL F11BBF(IREVCM,U,V,WORK,LWORK,IFAIL)
New: CALL F11BEF(IREVCM,U,V,WGT,WORK,LWORK,IFAIL)

WGT must be a one-dimensional *double precision* array of length at least n (the order of the matrix) if weights are to be used in the termination criterion, and 1 otherwise. Note that the call to F11BEF requires the weights to be supplied in WGT(1 : n) rather than WORK(1 : n). The minimum value of the parameter LWORK may also need to be changed.

### F11BCF

Withdrawn at Mark 21 Replaced by F11BFF

> Old: CALL F11BCF(ITN, STPLHS, STPRHS, ANORM, SIGMAX, IFAIL) New: CALL F11BFF(ITN, STPLHS, STPRHS, ANORM, SIGMAX, WORK, IFAIL)

F11BFF contains two additional parameters as follows:

WORK(LWORK) – *double precision* array.

LWORK - INTEGER.

See the routine document for further information.

### F11GAF

Scheduled for withdrawal at Mark 22 Replaced by F11GDF

F11GDF contains two additional parameters as follows:

WORK(LWORK) – *double precision* array.

LWORK - INTEGER.

See the routine document for further information.

#### F11GBF

Scheduled for withdrawal at Mark 22 Replaced by F11GEF

Old: CALL F11GBF(IREVCM,U,V,WORK,LWORK,IFAIL)
New: CALL F11GEF(IREVCM,U,V,WGT,WORK,LWORK,IFAIL)

WGT must be a one-dimensional *double precision* array of length at least n (the order of the matrix) if weights are to be used in the termination criterion, and 1 otherwise. Note that the call to F11GEF requires the weights to be supplied in WGT(1 : n) rather than WORK(1 : n). The minimum value of the parameter LWORK may also need to be changed.

### F11GCF

Scheduled for withdrawal at Mark 22 Replaced by F11GFF

F11GFF contains two additional parameters as follows:

WORK(LWORK) – *double precision* array.

LWORK – INTEGER.

See the routine document for further information.

# G01 – Simple Calculations on Statistical Data

### G01ACF

Withdrawn at Mark 9 Replaced by G04BBF

## G01BAF

Withdrawn at Mark 16 Replaced by G01EBF

Old: P = GO1BAF(IDF,T,IFAIL)
New: P = GO1EBF('Lower-tail',T,real(IDF),IFAIL)

#### G01BBF

Withdrawn at Mark 16 Replaced by G01EDF

```
Old: P = G01BBF(I1,I2,A,IFAIL)
New: P = G01EDF('Upper-tail',A,real(I1),real(I2),IFAIL)
```

## G01BCF

Withdrawn at Mark 16 Replaced by G01ECF

Old: P = GO1BCF(X,N,IFAIL)
New: P = GO1ECF('Upper-tail',X,real(N),IFAIL)

### G01BDF

Withdrawn at Mark 16 Replaced by G01EEF

Old: P = G01BDF(X,A,B,IFAIL)
New: CALL G01EEF(X,A,B,TOL,P,Q,PDF,IFAIL)

where TOL is set to the accuracy required by the user and Q and PDF are additional output quantities.

Note: the values of A and B must be  $\leq 106$ .

#### G01CAF

Withdrawn at Mark 16 Replaced by G01FBF

Old: T = GO1CAF(P,N,IFAIL)
New: T = GO1FBF('Lower-tail',P,real(N),IFAIL)

### G01CBF

Withdrawn at Mark 16 Replaced by G01FDF

Old: F = GO1CBF(P,M,N,IFAIL)
New: F = GO1FDF(P,real(M),real(N),IFAIL)

## G01CCF

Withdrawn at Mark 16 Replaced by G01FCF

Old: X = GO1CCF(P,N,IFAIL)
New: X = GO1FCF(P,real(N),IFAIL)

### G01CDF

Withdrawn at Mark 16 Replaced by G01FEF

> Old: X = GO1CDF(P,A,B,IFAIL) New: X = GO1FEF(P,A,B,TOL,IFAIL)

where TOL is set to the accuracy required by the user.

Note: the values of A and B must be  $\leq 106$ .

### G01CEF

Withdrawn at Mark 18 Replaced by G01FAF

```
Old: X = GO1CEF(P,IFAIL)
New: X = GO1FAF('Lower-tail',P,IFAIL)
```

# G02 – Correlation and Regression Analysis

### G02CJF

Withdrawn at Mark 16 Replaced by G02DAF and G02DGF

```
Old:
            CALL G02CJF(X,IX,Y,IY,N,M,IR,THETA,IT,SIGSQ,C,IC,IPIV,
      +
                    WK1,WK2,IFAIL)
New: C
            set the first M elements of ISX to 1
            CALL FO6DBF(M,1,ISX,1)
     С
            THEN
            TOL = XO2AJF()
           CALL G02DAF('Zero', 'Unweighted', N, X, IX, M, ISX, M, Y, WT,
                         RSS, IDF, THETA, SE, COV, RES, H, C, IC, SVD, IRANK,
                         P,TOL,WK,IFAIL)
            SIGSQ(1) = RSS/IDF
            there are two or more dependent variables,
     С
            i.e., IR is greater than or equal to 2 then:
DO 20 I = 2, IR
     С
               CALL G02DGF('Unweighted', N, WT, RSS, IP, IRANK, COV, C, IC, SVD,
              +
                            P,Y(1,I),THETA(1,I),SE,RES,WK,IFAIL)
               SIGSQ(I) = RSS/IDF
        20 CONTINUE
```

For unweighted regression, as is used here, WT may be any *double precision* array and will not be referenced, e.g., SIGSQ could be used.

The array C no longer contains  $(X^{T}X)-1$ ; however,  $(X^{T}X)-1$  scaled by  $\hat{\sigma}^{2}$  is returned in packed form in array COV. The upper triangular part of C will now contain a factorization of  $X^{T}X$ .

The *double precision* arrays SE(M), COV(M × (M + 1)/2), RES(N), H(N), P(M × (M + 2)), the logical variable SVD and the INTEGER variable IRANK are additional outputs. There is also a single *double precision* workspace WK( $5 \times (M - 1) + M \times M$ ).

## **G04** – Analysis of Variance

### G04ADF

Withdrawn at Mark 17 Replaced by G04BCF

```
Old: CALL G04ADF(DATA,VAR,AMR,AMC,AMT,LCODE,IA,N,NN)
New: IFAIL = 0
CALL G04BCF(1,N,N,DATA,N,IT,GMEAN,AMT,TABLE,6,C,NMAX,
+ IREP,RPMEAN,AMR,AMC,R,EF,0.0,0,WK,IFAIL)
```

The arrays AMR, AMC and AMT contain the means of the rows, columns and treatments rather than the totals. The values equivalent to those returned in the array VAR of G04ADF are returned in the second

column of the two-dimensional array TABLE starting at the second row, e.g., VAR(1) = TABLE(2, 2). The two-dimensional integer array LCODE (containing the treatment codes) has been replaced by the onedimensional array IT. These arrays will be the equivalent if IA = N. The following additional declarations are required.

```
double precision GMEAN
INTEGER IFAIL
double precision C(NMAX,NMAX), EF(NMAX), TABLE(6,5), R(NMAX*NMAX),
+ RPMEAN(1), WK(NMAX*NMAX+NMAX)
INTEGER IREP(NMAX), IT(NMAX*NMAX)
```

where NMAX is an integer such that  $NMAX \ge N$ .

### **G04AEF**

Withdrawn at Mark 17 Replaced by G04BBF

```
Old: CALL G04AEF(Y,N,K,NOBS,GBAR,GM,SS,IDF,F,FP,IFAIL)
New: CALL G04BBF(N,Y,O,K,IT,GM,BMEAN,GBAR,TABLE,4,C,KMAX,NOBS,
+ R,EF,0.0D0,0,WK,IFAIL)
```

The values equivalent to those returned by G04AEF in the arrays IDF and SS are returned in the first and second columns of TABLE starting at row 2 and the values equivalent to those returned in the scalars F and FP are returned in TABLE(2,4) and TABLE(2,5) respectively. NOBS is output from G04BBF rather than input. The groups are indicated by the array IT. The following code illustrates how IT can be computed from NOBS.

```
IJ = 0

DO 40 I = 1, K

DO 20 J = 1, NOBS(I)

IJ = IJ + 1

IT(IJ) = I

20 CONTINUE

40 CONTINUE
```

The following additional declarations are required.

```
double precision BMEAN(1),C(KMAX,KMAX),EF(KMAX),R(NMAX),TABLE(4,5),
+ WK(KMAX*KMAX+KMAX)
INTEGER IT(NMAX)
```

NMAX and KMAX are integers such that NMAX  $\geq$  N and KMAX  $\geq$  K.

### **G04AFF**

Withdrawn at Mark 17 Replaced by G04CAF

Y1 is a one-dimensional array containing the observations in the same order as Y, if IY1 = M and IY2 = NR then these are equivalent. LFAC is an integer array such that LFAC(1) = NC and LFAC(2) = NR. The following indicates how the results equivalent to those produced by G04AFF can be extracted from the results produced by G04CAF.

G04AFF G04CAF ROW(i) TMEAN(IMEAN(1)+i), i = 1, 2, ..., NRTMEAN(j), j = 1,2,...,NC TMEAN(IMEAN(2)+(j-1)\*NR+i), i = 1,2,...,NR; j = COL(j) CELL(i,j) 1,2,...,NC GM BMEAN(1) SS(1) TABLE(3,2)SS(2) TABLE(2,2)TABLE(4,2)SS(i) IDF(1) TABLE(3,1) IDF(2) TABLE(2,1)

TABLE(4,1)
TABLE(3,4)
TABLE(2,4)
TABLE(4,4)
TABLE(3,5)
TABLE(2,5)
TABLE(4,5)

Note how rows and columns have swapped.

The following additional declarations are required.

double precision TABLE(6,5), R(NMAX), TMEAN(MAXT), E(MAXT), BMEAN(1),
+ SEMEAN(5)
INTEGER IMEAN(5), IWK(NMAX+6), LFAC(2)

NMAX and MAXT are integers such that NMAX  $\geq$  M  $\times$  NR  $\times$  NC and MAXT  $\geq$  NR + NC + NR  $\times$  NC.

# **G05** – Random Number Generators

# G05AAF

Withdrawn at Mark 7 Replaced by G05CAF

# G05ABF

Withdrawn at Mark 7 Replaced by G05DAF

# G05ACF

Withdrawn at Mark 7 Replaced by G05DBF

# G05ADF

Withdrawn at Mark 7 Replaced by G05DDF

# G05AEF

Withdrawn at Mark 7 Replaced by G05DDF

# G05AFF

Withdrawn at Mark 7 Replaced by G05DEF

## G05AGF

Withdrawn at Mark 7 Replaced by G05DFF

## G05AHF

Withdrawn at Mark 7 Replaced by G05FFF

## G05AJF

Withdrawn at Mark 7 Replaced by G05FFF

## G05AKF

Withdrawn at Mark 7 Replaced by G05FFF **G05ALF** Withdrawn at Mark 7 Replaced by G05FEF

**G05AMF** Withdrawn at Mark 7 Replaced by G05FEF

**G05ANF** Withdrawn at Mark 7 Replaced by G05DHF

**G05APF** Withdrawn at Mark 7 Replaced by G05DJF

**G05AQF** Withdrawn at Mark 7 Replaced by G05DKF

**G05ARF** Withdrawn at Mark 7 Replaced by G05EXF

**G05ASF** Withdrawn at Mark 7 Replaced by G05EDF

**G05ATF** Withdrawn at Mark 7 Replaced by G05EBF

**G05AUF** Withdrawn at Mark 7 Replaced by G05EFF

**G05AVF** Withdrawn at Mark 7 Replaced by G05ECF

**G05AWF** Withdrawn at Mark 7 Replaced by G05EXF

**G05AZF** Withdrawn at Mark 7 Replaced by G05EYF

**G05BAF** Withdrawn at Mark 7 Replaced by G05CBF

**G05BBF** Withdrawn at Mark 7 Replaced by G05CCF

### G05CAF

Scheduled for withdrawal at Mark 22 Replaced by G05KAF

> Old: X = G05CAF(X) New: X = G05KAF(IGEN,ISEED)

The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05CAF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05KAF.

### G05CBF

Scheduled for withdrawal at Mark 22 Replaced by G05KBF

```
Old: CALL G05CBF(I)
New: IGEN = 0
ISEED(1) = I
CALL G05KBF(IGEN,ISEED)
```

The integer parameter IGEN can be set to any number between 0 and 273 inclusive. If IGEN is set to zero then the integer array ISEED, of dimension 4, contains in its first element the integer seed value to initialise the basic generator; otherwise all four elements of ISEED must be set to integers, at least six digits in length.

### G05CCF

Scheduled for withdrawal at Mark 22 Replaced by G05KCF

Old: CALL G05CCF New: CALL G05KCF(IGEN,ISEED)

The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. IGEN can be set to any number between 0 and 273 inclusive.

#### G05CFF

Scheduled for withdrawal at Mark 22 Replaced by F06DFF

```
Old: CALL G05CFF(IA,NI,XA,NX,IFAIL)
New: LGEN = IGEN
CALL F06DFF(4,ISEED,1,LSEED,1)
```

The data defining the generator state for the group of routines G05K-G05Q, can be saved by simply creating local copies of the parameters IGEN and ISEED.

### G05CGF

Scheduled for withdrawal at Mark 22 Replaced by F06DFF

The data defining the generator state for the group of routines G05K-G05Q, can be restored by simply copying back previously saved values contained in the parameters IGEN and ISEED.

### G05DAF

Scheduled for withdrawal at Mark 22 Replaced by G05LGF

Old: DO 10 I = 1, N X(I) = GO5DAF(A,B) 10 CONTINUE

```
New: AA = MIN(A,B)
BB = MAX(A,B)
IFAIL = 0
CALL G05LGF(AA,BB,N,X,IGEN,ISEED,IFAIL)
```

In G05LGF the first parameter must be less than or equal to the second parameter, this does not have to be the case in G05DAF. The *double precision* array X must be at least max(1, N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DAF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LGF.

## G05DBF

Scheduled for withdrawal at Mark 22 Replaced by G05LJF

In G05LJF the first parameter must be non-negative, this does not have to be the case in G05DBF. The *double precision* array X must be at least max(1, N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DBF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LJF.

## G05DCF

Scheduled for withdrawal at Mark 22 Replaced by G05LNF

In G05LNF the second parameter must be positive, this does not have to be the case in G05DCF. The *double precision* array X must be at least max(1,N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DCF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LNF.

### G05DDF

Scheduled for withdrawal at Mark 22 Replaced by G05LAF

In G05LAF the second parameter represents the variance whereas the second parameter in G05DDF represents the standard deviation. The *double precision* array X must be at least max(1, N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DDF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LAF. The algorithm used in G05LAF is different from that used in G05DDF, so the sequence of values produced by G05DDF cannot be reproduced by G05LAF.

### **G05DEF**

Scheduled for withdrawal at Mark 22 Replaced by G05LKF

In G05LKF the the second parameter represents the variance of the corresponding normal distribution whereas the second parameter in G05DEF represents the standard deviation. The *double precision* array X must be at least max(1, N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DEF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LKF. The algorithm used in G05DEF, so the sequence of values produced by G05DEF cannot be reproduced by G05LKF.

### G05DFF

Scheduled for withdrawal at Mark 22 Replaced by G05LLF

In G05LLF the the second parameter must be non-negative, this does not have to be the case in G05DFF. The *double precision* array X must be at least max(1, N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DFF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LLF.

#### G05DGF

Withdrawn at Mark 16 Replaced by G05FFF

Old: X = G05DGF(G,H,IFAIL)
New: CALL G05LFF(A,B,1,X(1),IGEN,ISEED,IFAIL)

where X must now be declared as an array of length at least 1. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DGF could be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LFF.

#### G05DHF

Scheduled for withdrawal at Mark 22 Replaced by G05LCF

The *double precision* array X must be at least max(1,N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DHF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LCF.

## G05DJF

Scheduled for withdrawal at Mark 22 Replaced by G05LBF

The *double precision* array X must be at least max(1,N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DJF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LBF.

## G05DKF

Scheduled for withdrawal at Mark 22 Replaced by G05LDF

The *double precision* array X must be at least max(1,N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DKF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LDF.

### G05DLF

Withdrawn at Mark 16 Replaced by G05FEF

Old: X = G05DLF(G,H,IFAIL)
New: CALL G05LEF(G,H,1,X(1),IGEN,ISEED,IFAIL)

where X must now be declared as an array of length at least 1. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DLF could be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LEF.

## G05DMF

Withdrawn at Mark 16 Replaced by G05FEF

where X must now be declared as an array of length at least 1. If the value of X(1) returned by G05LEF is 1.0, appropriate action should be taken. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DMF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LEF. Alternatively the ratio of gamma variates can be used i.e.,

CALL G05LFF(G,1.0D0,1,X(1),IGEN,ISEED,IFAIL1) CALL G05LFF(H,1.0D0,1,Y(1),IGEN,ISEED,IFAIL2) IF (Y(1).NE.0.0D0) X(1) = X(1)/Y(1)

where Y must be declared as an array of length at least 1.

### **G05DPF**

Scheduled for withdrawal at Mark 22 Replaced by G05LMF

The *double precision* array X must be at least max(1,N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DPF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LMF.

### G05DRF

Scheduled for withdrawal at Mark 22 Replaced by G05MEF

```
Old: DO 10 I = 1, M
IX(I) = G05DRF(ALAMDA(I),IFAIL)
10 CONTINUE
New: CALL G05MEF(M,ALAMDA,IX,IGEN,ISEED,IFAIL)
```

The integer array IX and the *double precision* array ALAMDA must be at least M in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DRF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05MEF.

### G05DYF

Scheduled for withdrawal at Mark 22 Replaced by G05MAF

The integer array IX must be at least max(1,N) in length. In G05MAF the first parameter IA not be greater than the second parameter, this is not the case in G05DYF. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DYF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05MAF.

#### G05DZF

Scheduled for withdrawal at Mark 22 Replaced by G05KEF

```
Old: L = G05DZF(P)
New: PP = MAX(0.0D0,MIN(P,1.0D0))
IFAIL = 0
L = G05KEF(PP,IGEN,ISEED,IFAIL)
```

The *double precision* parameter P in G05KEF must not be less than zero or greater than one. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05DZF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05KEF.

## G05EAF

Scheduled for withdrawal at Mark 22 Replaced by G05LZF

```
Old: CALL G05EAF(A,N,C,IC,EPS,R,NR,IFAIL)
New: MODE = 0
CALL G05LZF(MODE,N,A,C,IC,X,IGEN,ISEED,R,NR,IFAIL)
```

The integer parameter MODE in G05LZF is set to zero to initialise the reference vector only as is done in the call to G05EAF. The *double precision* array X must be at least N in length and will contain a multivariate Normal vector to be generated in a subsequent call to G05LZF with MODE = 1. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EAF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LZF. See also the replacement call for the superseded routine G05EZF.

## G05EBF

The reference vector R and its dimension are not required by G05MAF. The integer array X must be at least N in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EBF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05MAF.

## G05ECF

Scheduled for withdrawal at Mark 22 Replaced by G05MKF

```
Old: CALL G05ECF(T,R,NR,IFAIL)
    DO 10 I = 1, N
        X(I) = G05EYF(R,NR)
    10 CONTINUE
New: CALL G05MKF(0,T,N,X,IGEN,ISEED,R2,NR2,IFAIL)
        CALL G05MKF(1,T,N,X,IGEN,ISEED,R2,NR2,IFAIL)
```

The *double precision* array R2 is the reference vector in G05MKF and this needs two more elements of storage than R, used in G05ECF. Thus for the dimension, NR2, of R2, we have  $NR2 \ge NR + 2$ . The integer vector X must be of length at least N. The first parameter, MODE, in G05MKF can also take the values 2 and 3, see the G05MKF routine document for details. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05ECF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05MKF.

### G05EDF

Scheduled for withdrawal at Mark 22 Replaced by G05MJF

```
Old: CALL G05EDF(M,P,R,NR,IFAIL)
    DO 10 I = 1, N
        X(I) = G05EYF(R,NR)
    10 CONTINUE
New: CALL G05MJF(0,M,P,N,X,IGEN,ISEED,R2,NR2,IFAIL)
        CALL G05MJF(1,M,P,N,X,IGEN,ISEED,R2,NR2,IFAIL)
```

The *double precision* array R2 is the reference vector in G05MJF and this needs two more elements of storage than R, used in G05EDF. Thus for the dimension, NR2, of R2, we have  $NR2 \ge NR + 2$ . The integer vector X must be of length at least N. The first parameter, MODE, in G05MJF can also take the

values 2 and 3, see the G05MJF routine document for details. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EDF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05MJF.

### G05EEF

Scheduled for withdrawal at Mark 22 Replaced by G05MCF

```
Old: CALL G05EEF(M,P,R,NR,IFAIL)
    DO 10 I = 1, N
        X(I) = G05EYF(R,NR)
    10 CONTINUE
New: CALL G05MCF(0,M,P,N,X,IGEN,ISEED,R2,NR2,IFAIL)
        CALL G05MCF(1,M,P,N,X,IGEN,ISEED,R2,NR2,IFAIL)
```

The *double precision* array R2 is the reference vector in G05MCF and this needs two more elements of storage than R, used in G05EEF. Thus for the dimension, NR2, of R2, we have  $NR2 \ge NR + 2$ . The integer vector X must be of length at least N. The first parameter, MODE, in G05MCF can also take the values 2 and 3, see the G05MCF routine document for details. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EEF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05MCF.

### G05EFF

Scheduled for withdrawal at Mark 22 Replaced by G05MLF

```
Old: CALL G05EFF(L,M,NP,NR,IFAIL)
    DO 10 I = 1, N
        X(I) = G05EYF(R,NR)
    10 CONTINUE
New: CALL G05MLF(0,L,M,NP,N,X,IGEN,ISEED,R2,NR2,IFAIL)
        CALL G05MLF(1,L,M,NP,N,X,IGEN,ISEED,R2,NR2,IFAIL)
```

The *double precision* array R2 is the reference vector in G05MLF and this needs two more elements of storage than R, used in G05EFF. Thus for the dimension, NR2, of R2, we have  $NR2 \ge NR + 2$ . The integer vector X must be of length at least N. The first parameter, MODE, in G05MLF can also take the values 2 and 3, see the G05MLF routine document for details. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EFF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05MLF.

#### G05EGF

```
Scheduled for withdrawal at Mark 22
Replaced by G05PAF
Old: CALL G05EGF(E,A,NA,B,NB,R,NR,VAR,IFAIL)
```

```
New: AVAR = B(1)**2
IF (AVAR.GT.O.ODO) THEN
DO 10 I = 1, NB - 1
THETA(I) = -B(I+1)/B(1)
10 CONTINUE
ELSE
DO 20 I = 1, IQ
THETA(I) = 0.0D0
20 CONTINUE
END IF
MODE = 0
CALL G05PAF(MODE,E,NA,A,NB-1,THETA,AVAR,VAR,N,X,IGEN,
+ ISEED,R,NR,IFAIL)
```

The *double precision* vector THETA must be of length at least NB - 1. The integer parameter MODE in G05PAF is set to zero to initialise the reference vector only as is done in the call to G05EGF. The *double precision* array X must be at least N in length where the integer parameter N is the number of terms in the

time series to be generated in a subsequent call to G05PAF with MODE = 1. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EGF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05PAF. See also the replacement call for the superseded routine G05EWF.

## G05EHF

Scheduled for withdrawal at Mark 22 Replaced by G05NAF

Old: CALL G05EHF(INDEX,N,IFAIL)
New: CALL G05NAF(INDEX,N,IGEN,ISEED,IFAIL)

The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EHF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05NAF.

## G05EJF

Scheduled for withdrawal at Mark 22 Replaced by G05NBF

> Old: CALL GO5EJF(IA,N,IZ,M,IFAIL) New: CALL GO5NBF(IA,N,IZ,M,IGEN,ISEED,IFAIL)

The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EJF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05NBF.

### G05EWF

```
Scheduled for withdrawal at Mark 22
Replaced by G05PAF
     Old: CALL G05EGF(E,A,NA,B,NB,R,NR,VAR,IFAIL)
           DO 10 I = 1, N
              X(I) = GO5EWF(R, NR, IFAIL)
        10 CONTINUE
     New: AVAR = B(1) * * 2
           IF (AVAR.GT.0.0D0) THEN
              DO 10 I = 1, NB - 1
                 THETA(I) = -B(I+1)/B(1)
        10
              CONTINUE
           ELSE
              DO 20 I = 1, IQ
                 THETA(I) = 0.0D0
        20
              CONTINUE
           END IF
           MODE = 0
           CALL G05PAF(MODE, E, NA, A, NB-1, THETA, AVAR, VAR, N, X, IGEN,
                        ISEED, R, NR, IFAIL)
          MODE = 1
           CALL G05PAF(MODE, E, NA, A, NB-1, THETA, AVAR, VAR, N, X, IGEN,
                        ISEED,R,NR,IFAIL)
```

The *double precision* vector THETA must be of length at least NB - 1. The integer parameter MODE in G05PAF is set to zero to initialise the reference vector only as is done in the call to G05EGF. The *double precision* array X must be at least N in length where the integer parameter N is the number of terms in the time series to be generated in the subsequent call to G05PAF with MODE = 1. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EWF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05PAF. See also the replacement call for the superseded routine G05EGF.

### G05EXF

Scheduled for withdrawal at Mark 22 Replaced by G05MZF

The *double precision* array R2 is the reference vector in G05MZF and this needs four more elements of storage than R, used in G05EXF. Thus for the dimension, NR2, of R2, we have NR2  $\ge$  NR + 4. The integer vector X must be of length at least N. The first parameter, MODE, in G05MZF can also take the value 2, see the G05MZF routine document for details. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EXF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05MZF.

### G05EYF

Scheduled for withdrawal at Mark 22 Replaced by G05MZF

G05EYF is designed to be used in conjunction with other routines in the G05 chapter that have also been superseded. See the replacement calls for these routines for details.

### G05EZF

Scheduled for withdrawal at Mark 22 Replaced by G05LZF

```
Old: CALL G05EAF(A,N,C,IC,EPS,R,NR,IFAIL)
CALL G05E2F(X,N,R,NR,IFAIL)
New: MODE = 0
CALL G05L2F(MODE,N,A,C,IC,X,IGEN,ISEED,R,NR,IFAIL)
MODE = 1
CALL G05L2F(MODE,N,A,C,IC,X,IGEN,ISEED,R,NR,IFAIL)
```

The integer parameter MODE in G05LZF is set to zero to initialise the reference vector only as is done in the call to G05EAF. The *double precision* array X must be at least N in length and will contain a multivariate Normal vector generated in the subsequent call to G05LZF with MODE = 1. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05EAF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LZF. See also the replacement call for the superseded routine G05EAF.

### G05FAF

Scheduled for withdrawal at Mark 22 Replaced by G05LGF

```
Old: CALL G05FAF(A,B,N,X)
New: AA = MIN(A,B)
BB = MAX(A,B)
IFAIL = 0
CALL G05LGF(AA,BB,N,X,IGEN,ISEED,IFAIL)
```

In G05LGF the first parameter must be less than or equal to the second parameter, this does not have to be the case in G05FAF. The *double precision* array X must be at least max(1, N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05FAF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LGF.

### G05FBF

Scheduled for withdrawal at Mark 22 Replaced by G05LJF

```
Old: CALL G05FBF(A,N,X)
New: AA = ABS(A)
    IFAIL = 0
    CALL G05LJF(AA,N,X,IGEN,ISEED,IFAIL)
```

In G05LJF the first parameter must be non-negative, this does not have to be the case in G05FBF. The *double precision* array X must be at least max(1, N) in length. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05FBF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LJF.

### G05FDF

```
Scheduled for withdrawal at Mark 22
Replaced by G05LAF
```

```
Old: CALL G05FDF(A,B,N,X)
New: BB = B**2
    IFAIL = 0
    CALL G05LAF(A,BB,N,X,IGEN,ISEED,IFAIL)
```

In G05LAF the second parameter represents the variance whereas the second parameter in G05FDF represents the standard deviation. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05FDF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LAF.

### G05FEF

Scheduled for withdrawal at Mark 22 Replaced by G05LEF

> Old: CALL G05FEF(A,B,N,X,IFAIL) New: CALL G05LEF(A,B,N,X,IGEN,ISEED,IFAIL)

The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05FEF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LEF.

#### G05FFF

Scheduled for withdrawal at Mark 22 Replaced by G05LFF Old: CALL G05FFF(A,B,N,X,IFAIL)

New: CALL GO5LFF(A,B,N,X,IGEN,ISEED,IFAIL)

The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05FFF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LFF.

#### G05FSF

Scheduled for withdrawal at Mark 22 Replaced by G05LPF

> Old: CALL G05FSF(A,N,X,IFAIL) New: CALL G05LPF(A,N,X,IGEN,ISEED,IFAIL)

The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05FSF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05LPF.

[NP3657/21]

### G05GAF

Scheduled for withdrawal at Mark 22 Replaced by G05QAF

Old: CALL G05GAF(SIDE,INIT,M,N,A,LDA,WK,IFAIL)
New: CALL G05QAF(SIDE,INIT,M,N,A,LDA,IGEN,ISEED,WK,IFAIL)

The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05GAF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05QAF.

### G05GBF

Scheduled for withdrawal at Mark 22 Replaced by G05QBF

Old: CALL G05GBF(N,D,C,LDC,EPS,WK,IFAIL)
New: CALL G05QBF(N,D,C,LDC,EPS,IGEN,ISEED,WK,IFAIL)

The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05GBF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05QBF.

### G05HDF

Scheduled for withdrawal at Mark 22 Replaced by G05PCF

```
Old: CALL G05HDF(MODE,K,IP,IQ,MEAN,PAR,LPAR,QQ,IK,N,W,REF,LREF,
                 IWORK, LIWORK, IFAIL)
    +
New: IF (MODE.EQ.'S') THEN
        IMODE = 0
     ELSE IF (MODE.EQ.'C') THEN
        IMODE = 1
     ELSE IF (MODE.EQ.'R') THEN
        IMODE = 3
     END IF
     T_{1}T_{1} = 0
     DO 30 L = 1, IP
        DO 20 I = 1, K
           DO 10 J = 1, K
              LL = LL + 1
              PHI(I,J,L) = PAR(LL)
  10
           CONTINUE
  20
        CONTINUE
  30 CONTINUE
     DO 60 L = 1, IQ-1
        DO 50 I = 1, K
           DO 40 J = 1, K
               LL = LL +
                         1
               THETA(I,J,L) = PAR(LL)
  40
           CONTINUE
        CONTINUE
  50
  60 CONTINUE
     IF (MEAN.EQ.'M') THEN
        DO 70 I = 1, K
           LL = LL + 1
           XMEAN(I) = PAR(LL)
  70
        CONTINUE
     ELSE
        DO 80 I = 1, K
           XMEAN(I) = 0.0D0
  80
        CONTINUE
     END IF
     CALL G05PCF(IMODE,K,XMEAN, IP, PHI, IQ, THETA, QQ, IK, N, W, IGEN,
                  ISEED, REF, LREF, IWORK, LIWORK, IFAIL)
    +
```

The integer parameter IMODE should be set to 0, 1 or 3 in place of the parameter MODE having settings of 'S', 'C' or 'R' respectively. The *double precision* array PHI should have length at least max(1, IP × (K × K)); if dimensioned as PHI(K, K, IP) (as in the above example) then PHI(*i*,*j*,*l*) will contain the element PAR((l-1) × k × k + (i-1) × k + j). The *double precision* array THETA should have length at least max(1, IQ × (K × K)); if dimensioned as THETA(K, K, IQ) (as in the above example) then THETA(*i*,*j*,*l*) will contain the element PAR(IP × k × k + (l-1) × k × k + (i-1) × k + j). The *double precision* array XMEAN should have length at least K; if MEAN = 'M' then XMEAN(*i*) will contain the element PAR(IP + IQ × k × k + i), otherwise XMEAN should contain an array of zero values. The integer parameter IGEN contains the generator number to use and the integer array ISEED of dimension 4 contains the current state for that generator. G05HDF can be called without a prior call to one of the initialisation routines G05CBF or G05CCF; in such cases a prior call to G05KBF or G05KCF must precede the first call to G05PCF.

#### G05YAF

Scheduled for withdrawal at Mark 23 Replaced by G05YCF, G05YDF, G05YEF, G05YFF, G05YGF, G05YHF, G05YJF and G05YKF

This routine has been replaced by a suite of smaller routines consisting of initialisation routines and generator routines. So for:

Faure quasi random numbers

Old: CALL G05YAF(.TRUE.,'F',ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YCF(IDIM,IREF,IFAIL)

Old: CALL G05YAF(.FALSE.,'F',ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YDF(N,QUASI,IREF,IFAIL)

### Sobol quasi random numbers

Old: CALL G05YAF(.TRUE.,'S',ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YEF(IDIM,IREF,ISKIP,IFAIL)

Old: CALL G05YAF(.FALSE.,'S',ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YFF(N,QUASI,IREF,IFAIL)

#### Neiderreiter quasi random numbers

Old: CALL G05YAF(.TRUE.,'N',ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YGF(IDIM,IREF,SKIP,IFAIL)

Old: CALL GO5YAF(.FALSE.,'N',ISKIP,IDIM,QUASI,IREF,IFAIL) New: CALL GO5YHF(N,QUASI,IREF,IFAIL)

#### G05YBF

Scheduled for withdrawal at Mark 23

Replaced by G05YCF, G05YDF, G05YEF, G05YFF, G05YGF, G05YHF, G05YJF and G05YKF

This routine has been replaced by a suite of routines consisting of the relevant initialisation routine followed by one of two possible generator routines.

Faure quasi random numbers with Gaussian probability:

Old: CALL G05YBF(.TRUE.,'F',.FALSE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YCF(IDIM,IREF,IFAIL)

Old: CALL G05YBF(.FALSE.,'F',.FALSE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YJF(XMEAN,STD,N,QUASI,IREF,IFAIL)

Sobol quasi random numbers with Gaussian probability:

Old: CALL G05YBF(.TRUE.,'S',.FALSE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YEF(IDIM,IREF,ISKIP,IFAIL)

Old: CALL G05YBF(.FALSE.,'S',.FALSE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL) New: CALL G05YJF(XMEAN,STD,N,QUASI,IREF,IFAIL)

#### Neiderreiter quasi random numbers with Gaussian probability:

Old: CALL G05YBF(.TRUE.,'N',.FALSE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YGF(IDIM,IREF,SKIP,IFAIL)

Old: CALL G05YBF(.FALSE.,'N',.FALSE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YJF(XMEAN,STD,N,QUASI,IREF,IFAIL)

Faure quasi random numbers with log Normal probability:

Old: CALL G05YBF(.TRUE.,'F',.TRUE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YCF(IDIM,IREF,IFAIL)

Old: CALL G05YBF(.FALSE.,'F',.TRUE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YKF(XMEAN,STD,N,QUASI,IREF,IFAIL)

Sobol quasi random numbers with log Normal probability:

Old: CALL G05YBF(.TRUE.,'S',.TRUE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YEF(IDIM,IREF,ISKIP,IFAIL)

Old: CALL G05YBF(.FALSE.,'S',.TRUE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YKF(XMEAN,STD,N,QUASI,IREF,IFAIL)

Neiderreiter quasi random numbers with log Normal probability:

Old: CALL G05YBF(.TRUE.,'N',.TRUE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL) New: CALL G05YGF(IDIM,IREF,SKIP,IFAIL)

```
Old: CALL G05YBF(.FALSE.,'N',.TRUE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YKF(XMEAN,STD,N,QUASI,IREF,IFAIL)
```

#### G05ZAF

Scheduled for withdrawal at Mark 22

## **G08** – Nonparametric Statistics

# G08ABF

```
Withdrawn at Mark 16
Replaced by G08AGF
```

W1 is a *double precision* work array of dimension  $(3 \times N)$ . The *double precision* array W2 is no longer required. WNOR returns the normalized Wilcoxon test statistic. The *double precision* array Z, of dimension (N), contains the difference between the paired sample observations, and by setting the *double precision* variable XME to zero the routine may be used to test whether the medians of the two matched or paired samples are equal.

## G08ADF

Withdrawn at Mark 16 Replaced by G08AHF, G08AJF and G08AKF

The observations from the two independent samples must be stored in two separate *double precision* arrays, of dimensions N1 and N2, where N2 = N - N1, rather than consecutively in one array as in G08ADF.

UNOR returns the normalized Mann–Whitney U statistic. The LOGICAL parameter TIES indicates whether ties were present in the pooled sample or not and RANKS, a *double precision* array of dimension (N1+N2), returns the ranks of the pooled sample.

Both G08ADF and its replacement routine G08AHF return approximate tail probabilities for the test statistic. To compute exact tail probabilities G08AJF may be used if there are no ties in the pooled sample and G08AKF may be used if there are ties in the pooled sample.

### G08CAF

Withdrawn at Mark 16 Replaced by G08CBF

Old: CALL G08CAF(N,X,NULL,NP,P,NEST,NTYPE,D,PROB,S,IND,IFAIL)
New: CALL G08CBF(N,X,DIST,PAR,NEST,NTYPE,D,Z,PROB,S,IFAIL)

The following table indicates how existing choices for the null distribution, indicated through the INTEGER variable NULL in G08CAF, may be made in G08CBF using the character variable DIST.

null distribution	G08CAF – NULL	G08CBF – DIST
uniform	1	'U'
Normal	2	'N'
Poisson	3	'P'
exponential	4	'E'

PAR is a *double precision* array of dimension (1) for both the one and two parameter distributions, but only the first element of PAR is actually referenced (used) if the chosen null distribution has only one parameter. The input parameter NP is no longer required.

On exit S contains the sample observations sorted into ascending order. It no longer contains the sample cumulative distribution function but this may be computed from S.

# G13 – Time Series Analysis

## G13DAF

```
Withdrawn at Mark 17
Replaced by G13DMF
```

Old:		CALL G13DAF(X,NXM,NX,NSM,NS,NL,ICR,CO,C,IFAIL)	
New:	С	First transpose the data matrix X	
	С	note NSM is used as the first dimension of the array W	
		DO 20 I = 1, NS	
		CALL $FO6EFF(NX,X,(1,I),1,W(I,1),NSM)$	
		20 CONTINUE	
	С	then if ICR = 0 in the call to G13DAF	
		CALL G13DMF('V-Covariances',NS,NX,W,NSM,NL,WMEAN,CO,C,IFAIL)	)
	С	else if ICR = 1 in the call to G13DAF	
		CALL G13DMF('R-Correlations',NS,NX,W,NSM,NL,WMEAN,CO,C,IFAIL)	_)

Note that in G13DAF the NS series are stored in the columns of X whereas in G13DMF these series are stored in rows; hence it is necessary to transpose the data array.

The *double precision* array WMEAN must be of length NS, and on output stores the means of each of the NS series.

### **Replacement Calls**

The diagonal elements of C0 store the variances of the series if covariances are requested, but the standard deviations if correlations are requested.

### missing entity H

### H01ABF

Withdrawn at Mark 12 Replaced by E04MFF/E04MFA

### H01ADF

Withdrawn at Mark 12 Replaced by E04MFF/E04MFA

## H01AEF

Withdrawn at Mark 9 Replaced by E04MFF/E04MFA

### H01AFF

Withdrawn at Mark 12 Replaced by E04MFF/E04MFA

## H01BAF

Withdrawn at Mark 12 Replaced by E04MFF/E04MFA

## H02AAF

Withdrawn at Mark 12 Replaced by E04NCF/E04NCA

#### H02BAF

Withdrawn at Mark 15 Replaced by H02BBF

```
Old:
        CALL HO2BAF(A,MM,N1,M,N,200,L,X,NUMIT,OPT,IFAIL)
New: C M, N and MM must be set before these declaration statements
        INTEGER MAXDPT, LIWORK, LRWORK, ITMAX, MSGLVL, MAXNOD, INTFST
        PARAMETER (LIWORK = (25+N+M)*MAXDPT + 5*N + M + 4)
PARAMETER (LRWORK = MAXDPT*(N+2) + 2*N*N + 13*N + 12*M)
        INTEGER
                    INTVAR(N), IWORK(LIWORK)
        double precision BIGBND, TOLFES, TOLIV, ROPT
        double precision RA(MM,N), RX(N), CVEC(N), BL(N+M), BU(N+M),
                     RWORK(LRWORK)
        DO 10 J = 1, N
           INTVAR(J) = 1
           CVEC(J) = A(1,J)
           RX(J) = 1.0D0
           DO 20 I = 1, M
               RA(I,J) = A(I+1,J)
    20
           CONTINUE
       CONTINUE
    10
        BIGBND = 1.0e20
        DO 30 I = 1, N
           BL(I) = 0.0D0
           BU(I) = BIGBND
    30 CONTINUE
        DO 40 I = N+1, N+M
           BU(I) = A(I-N+1,N+1)
           BL(I) = -BIGBND
    40 CONTINUE
        ITMAX = 0
        MSGLVL = 0
        MAXNOD = 0
```

```
INTFST = 0
    TOLIV = 0.0D0
    TOLFES = 0.0D0
    MAXDPT = 3*N/2
    IFAIL = 0
    CALL H02BBF(ITMAX,MSGLVL,N,M,RA,MM,BL,BU,INTVAR,CVEC,MAXNOD,
   +
                INTFST, MAXDPT, TOLIV, TOLFES, BIGBND, RX, ROPT, IWORK,
   +
                LIWORK, RWORK, LRWORK, IFAIL)
   L = 1
    IF (IFAIL.EQ.0) L = 0
    IF (IFAIL.EQ.4) L = 2
    IF (L.EQ.O) THEN
       DO 50 I = 1, N
          X(I) = RX(I)
50
       CONTINUE
       OPT = ROPT
    ENDIF
```

The code indicates the minimum changes necessary, but H02BBF has additional flexibility and users may wish to take advantage of new features. It is strongly recommended that users consult the routine document.

## M01 – Sorting

## M01AAF

Withdrawn at Mark 13 Replaced by M01DAF

> Old: CALL MO1AAF(A,M,N,IP,IST,IFAIL) New: CALL MO1DAF(A(M),1,N-M+1,'A',IP(M),IFAIL)

The array IST is no longer needed.

#### M01ABF

Withdrawn at Mark 13 Replaced by M01DAF

Old: CALL MO1ABF(A,M,N,IP,IST,IFAIL)
New: CALL MO1DAF(A(M),1,N-M+1,'D',IP(M),IFAIL)

The array IST is no longer needed.

### M01ACF

Withdrawn at Mark 13 Replaced by M01DBF

Old: CALL MO1ACF(IA,M,N,IP,IST,IFAIL)
New: CALL MO1DBF(IA(M),1,N-M+1,'A',IP(M),IFAIL)

The array IST is no longer needed.

#### M01ADF

Withdrawn at Mark 13 Replaced by M01DBF

Old: CALL MO1ADF(IA,M,N,IP,IST,IFAIL)
New: CALL MO1DBF(IA(M),1,N-M+1,'D',IP(M),IFAIL)

The array IST is no longer needed.

#### M01AEF

Withdrawn at Mark 13 Replaced by M01DEF and M01EAF

Old: CALL MO1AEF(A,NR,NC,IC,T,TT,IFAIL)
New: CALL MO1DEF(A,NR,1,NR,IC,IC,'A',IRANK,IFAIL)
DO 10 I = 1, NC

CALL MO1EAF(A(1,I),1,NR,IRANK,IFAIL) 10 CONTINUE

The *double precision* arrays T and TT are no longer needed, but a new integer array IRANK of length NR is required.

## M01AFF

Withdrawn at Mark 13 Replaced by M01DEF and M01EAF

```
Old: CALL MO1AFF(A,NR,NC,IC,T,TT,IFAIL)
New: CALL MO1DEF(A,NR,1,NR,IC,IC,'D',IRANK,IFAIL)
DO 10 I = 1, NC
CALL MO1EAF(A(1,I),1,NR,IRANK,IFAIL)
10 CONTINUE
```

The *double precision* arrays T and TT are no longer needed, but a new integer array IRANK of length NR is required.

### M01AGF

Withdrawn at Mark 13 Replaced by M01DFF and M01EBF

```
Old: CALL M01AGF(IA,NR,NC,IC,K,L,IFAIL)
New: CALL M01DFF(IA,NR,1,NR,IC,IC,'A',IRANK,IFAIL)
D0 10 I = 1, NC
CALL M01EBF(IA(1,I),1,NR,IRANK,IFAIL)
10 CONTINUE
```

The integer arrays K and L are no longer needed, but a new integer array IRANK of length NR is required.

#### M01AHF

```
Withdrawn at Mark 13
Replaced by M01DFF and M01EBF
```

```
Old: CALL M01AHF(IA,NR,NC,IC,K,L,IFAIL)
New: CALL M01DFF(IA,NR,1,NR,IC,IC,'D',IRANK,IFAIL)
D0 10 I = 1, NC
CALL M01EBF(IA(1,I),1,NR,IRANK,IFAIL)
10 CONTINUE
```

The integer arrays K and L are no longer needed, but a new integer array IRANK of length NR is required.

#### M01AJF

```
Withdrawn at Mark 16
Replaced by M01CAF, M01DAF and M01ZAF
```

Old: CALL MO1AJF(A,W,IND,INDW,N,NW,IFAIL)
New: CALL MO1DAF(A,1,N,'A',IND,IFAIL)
CALL MO1ZAF(IND,1,N,IFAIL)
CALL MO1CAF(A,1,N,'A',IFAIL)

The arrays W and INDW are no longer needed.

### M01AKF

Withdrawn at Mark 16 Replaced by M01CAF, M01DAF and M01ZAF

Old: CALL MO1AKF(A,W,IND,INDW,N,NW,IFAIL)
New: CALL MO1DAF(A,1,N,'D',IND,IFAIL)
CALL MO1ZAF(IND,1,N,IFAIL)
CALL MO1CAF(A,1,N,'D',IFAIL)

The arrays W and INDW are no longer needed.

**M01ALF** Withdrawn at Mark 13 Replaced by M01CBF, M01DBF and M01ZAF

Old: CALL MO1ALF(IA,IW,IND,INDW,N,NW,IFAIL)
New: CALL MO1DBF(IA,1,N,'A',IND,IFAIL)
CALL MO1ZAF(IND,1,N,IFAIL)
CALL MO1CBF(IA,1,N,'A',IFAIL)

The arrays IW and INDW are no longer needed.

#### M01AMF

Withdrawn at Mark 13 Replaced by M01CBF, M01DBF and M01ZAF

Old: CALL MO1AMF(IA,IW,IND,INDW,N,NW,IFAIL)
New: CALL MO1DBF(IA,1,N,'D',IND,IFAIL)
 CALL MO1ZAF(IND,1,N,IFAIL)
 CALL MO1CBF(IA,1,N,'D',IFAIL)

The arrays IW and INDW are no longer needed.

### M01ANF

Withdrawn at Mark 13 Replaced by M01CAF

> Old: CALL MO1ANF(A,I,J,IFAIL) New: CALL MO1CAF(A,I,J,'A',IFAIL)

#### M01APF

Withdrawn at Mark 16 Replaced by M01CAF

> Old: CALL MO1APF(A,I,J,IFAIL) New: CALL MO1CAF(A,I,J,'D',IFAIL)

### M01AQF

Withdrawn at Mark 13 Replaced by M01CBF

> Old: CALL MO1AQF(IA,I,J,IFAIL) New: CALL MO1CBF(IA,I,J,'A',IFAIL)

### M01ARF

Withdrawn at Mark 13 Replaced by M01CBF

> Old: CALL MO1ARF(IA,I,J,IFAIL) New: CALL MO1CBF(IA,I,J,'D',IFAIL)

The character-sorting routines M01BAF, M01BBF, M01BCF and M01BDF have no exact replacements, because they require the data to be stored in an integer array, whereas the new character-sorting routines require the data to be stored in a character array. The following advice assumes that calling programs are modified so that the data is stored in a character array CH instead of in an integer array IA; *nchar* denotes the machine-dependent number of characters stored in an integer variable. The new routines sort according to the ASCII collating sequence, which may differ from the machine-dependent collating sequence used by the old routines.

#### M01BAF

Withdrawn at Mark 13 Replaced by M01CCF

Old: CALL MO1BAF(IA,I,J,IFAIL)
New: CALL MO1CCF(CH,I,J,1,nchar,'D',IFAIL)

assuming that each element of the character array CH corresponds to one element of the integer array IA.

## M01BBF

Withdrawn at Mark 13 Replaced by M01CCF

Old: CALL MO1BBF(IA,I,J,IFAIL)
New: CALL MO1CCF(CH,I,J,1,nchar,'A',IFAIL)

assuming that each element of the character array CH corresponds to one element of the integer array IA.

## M01BCF

Withdrawn at Mark 13 Replaced by M01CCF

Old: CALL MO1BCF(IA,NR,NC,L1,L2,LC,IUC,IT,ITT,IFAIL)
New: CALL MO1CCF(CH,LC,IUC,(L1-1)\*nchar-1,L2\*nchar,'D',IFAIL)

provided that each element of the character array CH corresponds to a whole column of the integer array IA. The arrays IT and ITT are no longer needed. The call of M01CCF will fail if NR\**nchar* exceeds 255.

## M01BDF

Withdrawn at Mark 13 Replaced by M01CCF

Old: CALL MO1BDF(IA,NR,NC,L1,L2,LC,IUC,IT,ITT,IFAIL)
New: CALL MO1CCF(CH,LC,IUC,(L1-1)\*nchar-1,L2\*nchar,'A',IFAIL)

provided that each element of the character array CH corresponds to a whole column of the integer array IA. The arrays IT and ITT are no longer needed. The call of M01CCF will fail if NR\**nchar* exceeds 255.

# **P01** – Error Trapping

### **P01AAF** Withdrawn at Mark 13 Replaced by P01ABF

Existing programs should be modified to call P01ABF. Please consult the appropriate routine document.

# X02 – Machine Constants

## X02AAF

Withdrawn at Mark 16 Replaced by X02AJF

> Old: X02AAF(X) New: X02AJF()

## X02ABF

Withdrawn at Mark 16 Replaced by X02AKF

> Old: X02ABF(X) New: X02AKF()

## X02ACF

Withdrawn at Mark 16 Replaced by X02ALF

> Old: X02ACF(X) New: X02ALF()

X02ADF

Withdrawn at Mark 14 Replaced by X02AJF and X02AKF

```
Old: X02ADF(X)
New: X02AKF()/X02AJF()
```

### X02AEF

Withdrawn at Mark 14 Replaced by X02AMF

Old: X02AEF(X)
New: LOG(X02AMF())

**Note**: the replacement expressions may not return the same value, but the value will be sufficiently close, and safe, for the purposes for which it is used in the Library.

### X02AFF

```
Withdrawn at Mark 14
Replaced by X02AMF
```

```
Old: X02AFF(X)
New: -LOG(X02AMF())
```

Note: the replacement expressions may not return the same value, but the value will be sufficiently close, and safe, for the purposes for which it is used in the Library.

### X02AGF

Withdrawn at Mark 16 Replaced by X02AMF

```
Old: X02AGF(X)
New: X02AMF()
```

**Note**: the replacement expressions may not return the same value, but the value will be sufficiently close, and safe, for the purposes for which it is used in the Library.

### X02BAF

Withdrawn at Mark 14 Replaced by X02BHF

```
Old: XO2BAF(X)
New: XO2BHF()
```

# X02BCF

Withdrawn at Mark 14 Replaced by X02AMF

Old: X02BCF(X)
New: -LOG(X02AMF())/LOG(2.0)

**Note**: the replacement expressions may not return the same value, but the value will be sufficiently close, and safe, for the purposes for which it is used in the Library.

### X02BDF

Withdrawn at Mark 14 Replaced by X02AMF

```
Old: X02BDF(X)
New: LOG(X02AMF())/LOG(2.0)
```

**Note**: the replacement expressions may not return the same value, but the value will be sufficiently close, and safe, for the purposes for which it is used in the Library.

# X02CAF

Withdrawn at Mark 17 not needed except with F01BTF and F01BXF