

## 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### Advice on Replacement Calls for Withdrawn/Superseded Routines

The following list gives the names of replacement routines for those routines that have been withdrawn or superseded. For routines that have been withdrawn or superseded since Mark 13 replacement calls are also given.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.

#### C02 – Zeros of Polynomials

##### C02ADF

Withdrawn at Mark 15

Replaced by C02AFF

```
Old: CALL C02ADF (AR,AC,N,REZ,IMZ,TOL,IFAIL)
New: CALL C02AFF (A,N-1,SCALE,Z,W,IFAIL)
```

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

##### C02AEF

Withdrawn at Mark 16

Replaced by C02AGF

```
Old: CALL C02AEF (A,N,REZ,IMZ,TOL,IFAIL)
New: CALL C02AGF (A,N-1,SCALE,Z,W,IFAIL)
```

The zeros are returned in the *real* array Z of dimension (2,N) rather than in the arrays REZ and IMZ, and W is a *real* work array of dimension (2 \* (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Withdrawn at Mark 9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Withdrawn at Mark 9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Withdrawn at Mark 9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Withdrawn at Mark 10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Withdrawn at Mark 8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Withdrawn at Mark 9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Withdrawn at Mark 9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Withdrawn at Mark 12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Withdrawn at Mark 12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Withdrawn at Mark 8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Withdrawn at Mark 8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Withdrawn at Mark 9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Withdrawn at Mark 8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Withdrawn at Mark 8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Withdrawn at Mark 8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Withdrawn at Mark 9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Withdrawn at Mark 11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Withdrawn at Mark 8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 D02HAF or D02GAF

**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 or 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: DO 10 L = 1,N
      THRES(L) = TOL
10 CONTINUE
   CALL D02PVF(N,X,Y,XEND,TOL,THRES,2,'usualtask',.FALSE.,
+          0.0e0,W,14*N,IFAIL)
   CALL D02PCF(FCN,XEND,X,Y,YP,YMAX,W,IFAIL)
```

THRES, YP and YMAX are *real* arrays of length N and the length of array W needs extending to length 14\*N.

**D02BBF**

Withdrawn at Mark 18  
Replaced by D02PCF and associated D02P routines

```
Old: CALL D02BBF(X,XEND,N,Y,TOL,IRELAB,FCN,OUTPUT,W,IFAIL)
New: CALL D02PVF(N,X,Y,XEND,TOL,THRES,2,'usualtask',.FALSE.,
+          0.0e0,W,14*N,IFAIL)
      ... set XWANT ...
10 CONTINUE
   CALL D02PCF(FCN,XWANT,X,Y,YP,YMAX,W,IFAIL)
   IF (XWANT.LT.XEND) THEN
      ... reset XWANT ...
      GO TO 10
   ENDIF
```

THRES, YP and YMAX are *real* arrays of length N and the length of array W needs extending to length 14\*N.

**D02BDF**

Withdrawn at Mark 18  
Replaced by D02PCF and associated D02P routines

```
Old: CALL D02BDF(X,XEND,N,Y,TOL,IRELAB,FCN,STIFF,YNORM,W,
+          IW,M,OUTPUT,IFAIL)
New: CALL D02PVF(N,X,Y,XEND,TOL,THRES,2,'usualtask',.TRUE.,
+          0.0e0,W,32*N,IFAIL)
      ... set XWANT ...
10 CONTINUE
   CALL D02PCF(FCN,XWANT,X,Y,YP,YMAX,IFAIL)
   IF (XWANT.LT.XEND) THEN
      ... reset XWANT ...
```

```

      GO TO 10
    ENDIF
    CALL D02PZF(RMSERR,ERRMAX,TERRMX,W,IFAIL)

```

THRES, YP, YMAX and RMSERR are *real* arrays of length N and W is now a *real* one-dimensional array of length 32\*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 *real* 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 *real* 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**

Withdrawn at Mark 18

Replaced by D02CJF

```

Old: CALL D02CGF(X,XEND,N,Y,TOL,HMAX,M,VAL,FCN,W,IFAIL)
New: CALL D02CJF(X,XEND,N,Y,FCN,TOL,'M',D02CJX,G,W,IFAIL)
.
.
.
real FUNCTION G(X,Y)
real X,Y(*)
G = Y(M)-VAL
END

```

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

```

Old: CALL D02EAF(X,XEND,N,Y,TOL,FCN,W,IW,IFAIL)
New: CALL D02EJF(X,XEND,N,Y,FCN,TOL,'M',D02EJX,D02EJW,D02EJY,W,IW,
+           IFAIL)

```

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

**D02EBF**

Withdrawn at Mark 18

Replaced by D02EJF

```
Old: CALL D02EBF(X,XEND,N,Y,TOL,IRELAB,FCN,MPED,PEDERV,OUTPUT,W,IW,
+           IFAIL)
New: CALL D02EJF(X,XEND,N,Y,FCN,PEDERV,TOL,RELABS,OUTPUT,D02EJW,W,IW,
+           IFAIL)
```

D02EJW is a *real* 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

```
Old: CALL D02EGF(X,XEND,N,Y,TOL,HMAX,M,VAL,FCN,W,IW,IFAIL)
New: CALL D02EJF(X,XEND,N,Y,FCN,D02EJY,TOL,'M',D02EJX,G,W,IW,IFAIL)
.
.
.
real FUNCTION G(X,Y)
real X,Y(*)
G = Y(M)-VAL
END
```

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

**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 *real* array of dimension (N1 + 4), MU is a *real* array of dimension (M1 + 4), C is a *real* array of dimension (N1\*M1), WRK is a *real* array of dimension ((N1 + 6) \* (M1 + 6)), A1, B1 and FF are *real* 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 *real* 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

**E04CDF**

Withdrawn at Mark 7

Replaced by E04UCF/E04UCA

**E04CEF**

Withdrawn at Mark 7

Replaced by E04JYF

**E04CFF**

Withdrawn at Mark 8

Replaced by E04UCF/E04UCA

**E04CGF**

Withdrawn at Mark 13

Replaced by E04JYF

```
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**

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(*)
real       XC(N), FC, GC(N), USER(*)
C
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  $(12*N)$  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 E04UCF/E04UCA or E04KDF

**E04DDF**

Withdrawn at Mark 8

Replaced by E04UCF/E04UCA or E04KDF

**E04DEF**

Withdrawn at Mark 13

Replaced by E04KYF

```

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 E04KZF

```

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 E04LYF

```

Old: CALL E04EBF(N,X,F,G,IW,LIW,W,LW,IFAIL)
New: CALL E04LYF(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)
INTEGER      N, IUSER(*)
real       XC(N), FC, GC(N), USER(*)
C
CALL FUNCT2(N,XC,FC,GC)
C
RETURN
END

SUBROUTINE HESS(N,XC,HESLC,LH,HESDC,IUSER,USER)
INTEGER      N, LH, IUSER(*)
real       XC(N), HESLC(LH), HESDC(N), USER(*)
C

```

```

      CALL HESS2(N,XC,HESLC,LH,HESDC)
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.

**E04FAF**

Withdrawn at Mark 8

Replaced by E04FCF or E04FYF

**E04FBF**

Withdrawn at Mark 7

Replaced by E04FCF or E04FYF

**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)

```

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(*)
      real       XC(N), FVECC(M), USER(*)
C
      CALL LSFUN1(M,N,XC,FVECC)
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.

**E04GAF**

Withdrawn at Mark 8

Replaced by E04GBF, E04GYF, E04GDF or E04GZF

**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(*)
      real       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(*)
  real 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(*)
  real XC(N), FVECC(M), FJACC(LJC,N), USER(*)
C
CALL LSFUN2(M,N,XC,FVECC,FJACC,LJC)
C
RETURN
END
C
SUBROUTINE LSHES(M,N,FVECC,XC,B,LB,IUSER,USER)
INTEGER M, N, LB, IUSER(*)
  real FVECC(M), XC(N), B(LB), USER(*)
C
CALL LSHES2(M,N,FVECC,XC,B,LB)
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 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(*)
      real        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**

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 (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(*)
      real        X(N), OBJF, OBJGRD(N), USER(*)
      INTEGER      IFLAG, IW(1)
      real        W(1)
C
      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  $1.0e+6$  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	<b>Minor print level</b>
INTYPE	<b>Cold start/Warm start</b>
MAXCAL	<b>Minor iteration limit</b> (note that this counts iterations rather than function calls)
ETA	<b>Line search tolerance</b>
XTOL	<b>Optimality tolerance</b> (note that this specifies the accuracy in F rather than the accuracy in X)
STEPMX	<b>Step limit</b>
DELTA	<b>Difference interval</b>

**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(*)
      real        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(*)
      real        X(N), OBJF, OBJGRD(N), USER(*)
      INTEGER      IW(1)
      real        W(1)
C
      CALL FUNCT(MODE, N, X, OBJF, OBJGRD, IW, 1, W, 1)
      RETURN
      END
```

**E04KCF**

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(*)
      real        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,BU,X,F,G,IW,LIW,W,LW,IFAIL)
New: CALL E04LYF(N,IBOUND,FUNCT,HESS,BL,BU,X,F,G,IW,LIW,W,LW,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)
      INTEGER      N, IUSER(*)
      real        XC(N), FC, GC(N), USER(*)
C
      CALL FUNCT2(N,XC,FC,GC)
C
      RETURN
      END

      SUBROUTINE HESS(N,XC,HESLC,LH,HESDC,IUSER,USER)
      INTEGER      N, LH, IUSER(*)
      real        XC(N), HESLC(LH), HESDC(N), USER(*)
C
      CALL HESS2(N,XC,HESLC,LH,HESDC)
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.

### E04MBF

Withdrawn at Mark 18

Replaced by E04MFF/E04MFA

```

Old: CALL E04MBF(ITMAX,MSGLVL,N,NCLIN,NCTOTL,NROWA,A,BL,BU,CVEC,
+           LINOBJ,X,ISTATE,OBJLP,CLAMDA,IWORK,LIWORK,WORK,
+           LWORK,IFAIL)
New: CALL E04MFF(N,NCLIN,A,NROWA,BL,BU,CVEC,ISTATE,X,ITER,OBJLP,
+           AX,CLAMDA,IWORK,LIWORK,WORK,LWORK,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(\*) – **real** 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**

Withdrawn at Mark 18

Replaced by E04NFF/E04NFA

```
Old: CALL E04NAF (ITMAX,MSGVLV,N,NCLIN,NCTOTL,NROWA,NROWH,NCOLH,
+             BIGBND,A,BL,BU,CVEC,FEATOL,HESS,QPHESS,COLD,LP,
+             ORTHOG,X,ISTATE,ITER,OBJ,CLAMDA,IWORK,LIWORK,
+             WORK,LWORK,IFAIL)
New: CALL E04NFF (N,NCLIN,A,NROWA,BL,BU,CVEC,HESS,NROWH,QPHESS,
+             ISTATE,X,ITER,OBJ,AX,CLAMDA,IWORK,LIWORK,WORK,
+             LWORK,IFAIL)
```

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
      real         HESS (NROWH,NCOLH), X(N), HX(N)
New: SUBROUTINE QPHESS (N,JTHCOL,HESS,NROWH,X,HX)
      INTEGER      N, JTHCOL, NROWH
      real         HESS (NROWH,*), X(N), HX(N)
```

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

E04NFF/E04NFA contains one additional parameter as follows:

AX(\*) – **real** 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.

**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)
      INTEGER      MODE, N, NSTATE, IUSER(*)
      real         X(N), OBJF, OBJGRD(N), USER(*)
C
      CALL FUNCT1 (MODE,N,X,OBJF)
      RETURN
      END
+     SUBROUTINE CONFUN (MODE,NCNLN,N,NROWJ,NEEDC,X,C,CJAC.NSTATE,
      IUSER,USER)
      INTEGER      MODE, NCNLN, N, NROWJ, NEEDC(*), NSTATE, IUSER(*)
      real         X(X), C(*), CJAC (NROWJ,*), USER(*)
C
      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.

**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 E04USF(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(*)
      real      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(*)
      real      X(N),F(*),FJAC(LDFJ,*),USER(*)
```

See the routine documents for further information.

**E04UPF**

Withdrawn at Mark 19

Replaced by E04USF/E04USA

```
Old: CALL E04UPF(M,N,NCLIN,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 E04USF(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) – *real* array.

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

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(*)
      real      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(*)
      real      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
      real         X(N), OBJF, OBJGRD(N)
New: SUBROUTINE OBJFUN(MODE,N,X,OBJF,OBJGRD,NSTATE,IUSER,USER)
      INTEGER      MODE, N, NSTATE, IUSER(*)
      real         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
      real         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(*)
      real         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.  
 USER(\*) – **real** 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
      real         X(N), OBJF, OBJGRD(N)
New: SUBROUTINE OBJFUN(MODE,N,X,OBJF,OBJGRD,NSTATE,IUSER,USER)
      INTEGER      MODE, N, NSTATE, IUSER(*)
      real         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
      real       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(*)
      real       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(N,N) – real array.
IUSER(*) – INTEGER array of dimension at least 1.
USER(*) – real 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 (SGETRF/DGETRF) and F07AJF (SGETRI/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 (SGETRF/DGETRF) computes the LU factorization of the matrix A, F06QFF copies the factorization from A to X, and F07AJF (SGETRI/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 (SGETRI/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 F01ACF(N,EPS,A,IA,B,IB,Z,L,IFAIL)
New: CALL F01ABF(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 F07FDF (SPOTRF/DPOTRF), F08SEF (SSYGST/DSYGST) and F06EGF (SSWAP/DSWAP)

```
Old: CALL F01AEF(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.0) THEN
          CALL ssygst(1,'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.

**F01AFF**

Withdrawn at Mark 18

Replaced by F06YJF (STRSM/DTRSM) and F06EGF (SSWAP/DSWAP)

```
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+1,1.0e0,B,IB,Z(1,M1),IZ)
      CALL sswap(N,DL,1,B,IB+1)
```

**F01AGF**

Withdrawn at Mark 18

Replaced by F08FEF (SSYTRD/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) = 0.0e0
      DO 10 I = 1, N
          E2(I) = E(I)*E(I)
10    CONTINUE
```

where TAU is a *real* 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 (SSYTRD/DSYTRD) is different from that computed by F01AGF, but it has the same eigenvalues.

**F01AHF**

Withdrawn at Mark 18

Replaced by F08FGF (SORMTR/DORMTR)

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

```
Old: CALL F01AHF(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 *real* array of length at least (M2-M1+1), and LWORK is its actual length.

**F01AJF**

Withdrawn at Mark 18

Replaced by F08FEF (SSYTRD/DSYTRD) and F08FFF (SORGTR/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) = 0.0e0
      CALL F06QFF('L',N,N,A,IA,Z,IZ)
      CALL sorgtr('L',N,Z,IZ,TAU,WORK,LWORK,INFO)

```

where TAU is a *real* 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 (SSYTRD/DSYTRD) and F08FFF (SORGTR/DORGTR) are different from those computed by F01AJF, but they satisfy the same relation  $Q^T A Q = T$ .

**F01AKF**

Withdrawn at Mark 18

Replaced by F08NEF (SGEHRD/DGEHRD)

```

Old: CALL F01AKF(N,K,L,A,IA,INTGER)
New: CALL sgehrd(N,K,L,A,IA,TAU,WORK,LWORK,INFO)

```

where TAU is a *real* 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 (SGEHRD/DGEHRD) is different from that computed by F01AKF, because F08NEF (SGEHRD/DGEHRD) uses orthogonal transformations, whereas F01AKF uses stabilized elementary transformations.

**F01ALF**

Withdrawn at Mark 18

Replaced by F08NGF (SORMHR/DORMHR)

The following replacement is valid only if the previous call to F01AKF has been replaced by a call to F08NEF (SGEHRD/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 *real* array of length at least (IR) and LWORK is its actual length.

**F01AMF**

Withdrawn at Mark 18

Replaced by F08NSF (CGEHRD/ZGEHRD)

```

Old: CALL F01AMF(N,K,L,AR,IAR,AI,IAI,INTGER)
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 cgehrd(N,K,L,A,IA,TAU,WORK,LWORK,INFO)

```

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

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

**F01ANF**

Withdrawn at Mark 18

Replaced by F08NTF (CUNGHR/ZUNGHR)

The following replacement is valid only if the previous call to F01AMF has been replaced by a call to F08NSF (CGEHRD/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)
      DO 20 J = 1, IR
          DO 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** array of dimension (IA,N), TAU is a **complex** array of length at least (N-1), Z is a **complex** array of dimension (IZ,IR), WORK is a **complex** array of length at least (IR) and LWORK is its actual length.

### F01APF

Withdrawn at Mark 18

Replaced by F08NFF (SORGHR/DORGHR) and F06QFF

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

```

Old: CALL F01APF(N,K,L,INTGER,H,IH,V,IV)
New: CALL F06QFF('L',N,N,H,IH,V,IV)
      CALL sorghr(N,K,L,V,IV,TAU,WORK,LWORK,INFO)

```

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

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

### F01ATF

Withdrawn at Mark 18

Replaced by F08NHF (SGEBAL/DGEBAL)

```

Old: CALL F01ATF(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 (SGEBAL/DGEBAL) may be different from that returned by F01ATF.

### F01AUF

Withdrawn at Mark 18

Replaced by F08NJF (SGEBAK/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 (CGEBAL/ZGEBAL)

```

Old: CALL F01AVF(N,IB,AR,IAR,AI,IAI,K,L,D)
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 cgebal('B',N,A,IA,K,L,D,INFO)
      DO 20 J = 1, N
          DO 10 I = 1, N
              AR(I,J) = real(A(I,J))
              AI(I,J) = imag(A(I,J))
          10 CONTINUE
      20 CONTINUE

```

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

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

**F01AWF**

Withdrawn at Mark 18

Replaced by F08NWF (CGEBAK/ZGEBAK)

```

Old: CALL F01AWF(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** array of dimension (IZ,M).

**F01AXF**

Withdrawn at Mark 18

Replaced by F08BEF (SGEQPF/DGEQPF) and F06EFF (SCOPY/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 **real** array of length at least (3\*N).

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

**F01AYF**

Withdrawn at Mark 18

Replaced by F08GEF (SSPTRD/DSPTRD)

```

Old: CALL F01AYF(N,TOL,A,IA,D,E,E2)
New: CALL ssptrd('U',N,A,D,E(2),TAU,INFO)
      E(1) = 0.0e0
      DO 10 I = 1, N
          E2(I) = E(I)*E(I)
10    CONTINUE

```

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

**F01AZF**

Withdrawn at Mark 18

Replaced by F08GGF (SOPMTR/DOPMTR)

The following replacement is valid only if the previous call to F01AYF has been replaced by a call to F08GEF (SSPTRD/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 **real** array of length at least (M2-M1+1).

**F01BCF**

Withdrawn at Mark 18

Replaced by F08FSF (CHETRD/ZHETRD) and F08FTF (CUNGTR/ZUNGTR)

```

Old: CALL F01BCF(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) = 0.0e0

```

```

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

Note that the tridiagonal matrix  $T$  and the unitary matrix  $Q$  computed by F08FSF (CHETRD/ZHETRD) and F08FTF (CUNGTR/ZUNGTR) are different from those computed by F01BCF, but they satisfy the same relation  $Q^H A Q = T$ .

### F01BDF

Withdrawn at Mark 18

Replaced by F07FDF (SPOTRF/DPOTRF), F08SEF (SSYGST/DSYGST) and F06EGF (SSWAP/DSWAP)

```

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.0) 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 (STRMM/DTRMM)

```

Old: CALL F01BEF(N,M1,M2,B,IB,DL,V,IV)
New: CALL sswap(N,DL,1,B,IB+1)
      CALL strmm('L','L','N','N',N,M2-M1+1,1.0e0,B,IB,V(1,M1),IV)
      CALL sswap(N,DL,1,B,IB+1)

```

### F01BFF

Withdrawn at Mark 8

Replaced by F07GDF (SPPTRF/DPPTRF) or F07PDF (SSPTRF/DSPTRF)

### F01BHF

Withdrawn at Mark 9

Replaced by F02WEF

### F01BJF

Withdrawn at Mark 9

Replaced by F08HEF (SSBTRD/DSBTRD)

### F01BKF

Withdrawn at Mark 9

Replaced by F02WDF

### F01BMF

Withdrawn at Mark 9

Replaced by F07BDF (SGBTRF/DGBTRF)

**F01BNF**

Withdrawn at Mark 17

Replaced by F07FRF (CPOTRF/ZPOTRF)

Old: CALL F01BNF(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 *real* 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 (CPOTRF/ZPOTRF) and F07FWF (CPOTRI/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 (SPPTRF/DPPTRF) or F07PDF (SSPTRF/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 (SPPTRF/DPPTRF) and F07PDF (SSPTRF/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 (SSPTRF/DSPTRF), the INTEGER array IPIV of length N must be supplied.

**F01BTF**

Withdrawn at Mark 18

Replaced by F07ADF (SGETRF/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 (SGETRF/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 (SGETRF/DGETRF). If this value is required, it may be calculated after a call of F07ADF (SGETRF/DGETRF) by code similar to the following:



```

DP = 1.0e0
DO 10 I = 1, N
  IF (I.NE.IPIV(I)) DP = -DP
10 CONTINUE

```

**F01BWF**

Withdrawn at Mark 18

Replaced by F08HEF (SSBTRD/DSBTRD)

```

Old: CALL F01BWF(N,M1,A,IA,D,E)
New: CALL sbtrd('N','U',N,M1-1,A,IA,D,E(2),Q,1,WORK,INFO)
     E(1) = 0.0e0

```

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

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

**F01BXF**

Withdrawn at Mark 17

Replaced by F07FDF (SPOTRF/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,0.0e0,0.0e0,A,M)

```

**F01CBF**

Withdrawn at Mark 14

Replaced by F06QHF

```

Old: CALL F01CBF(A,M,N,IFAIL)
New: CALL F06QHF('General',M,N,0.0e0,1.0e0,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,1.0e0,B,M,1.0e0,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,1.0e0,B,M,-1.0e0,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 F01CGF(A,MA,NA,P,Q,B,MB,NB,M1,M2,N1,N2,IFAIL)
New: CALL F01CTF('N','N',M2-M1+1,N2-N1+1,1.0e0,A(P,Q),MA,1.0e0,
+           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+1,1.0e0,A(P,Q),MA,-1.0e0,
+           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 (SGEMM/DGEMM)

```
Old: CALL F01CLF(A,B,C,N,P,M,IFAIL)
New: CALL sgemm('N','T',N,P,M,1.0e0,B,N,C,P,0.0e0,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 (SCOPY/DCOPY)

```
Old: CALL F01CNF(V,M,A,LA,I)
New: CALL scopy(M,V,1,A(I,1),LA)
```

**F01CPF**

Withdrawn at Mark 13

Replaced by F06EFF (SCOPY/DCOPY)

```
Old: CALL F01CPF(A,B,N)
New: CALL scopy(N,A,1,B,1)
```

**F01CQF**

Withdrawn at Mark 13

Replaced by F06FBF

```
Old: CALL F01CQF(A,N)
New: CALL F06FBF(N,0.0e0,A,1)
```

**F01CSF**

Withdrawn at Mark 13

Replaced by F06PEF (SSPMV/DSPMV)

```
Old: CALL F01CSF(A,LA,B,N,C)
New: CALL sspmv('U',N,1.0e0,A,B,1,0.0e0,C,1)
```

**F01DAF**

Withdrawn at Mark 13

Replaced by F06EAF (SDOT/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

Old: D = F01DBF(L,M,C1,IRA,ICB,A,IA,B,IB,N)  
 New: CALL X03AAF(A(IRA,L),(M-L)\*IA+1,B(L,ICB),M-L+1,IA,1,C1,0.0e0,D,  
 + D2,.TRUE.,IFAIL)

(here D2 is a new *real* variable whose value is not used).**F01DCF**

Withdrawn at Mark 13

Replaced by F06GAF (CDOTU/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

Old: CALL F01DDF(L,M,CX,IRA,ICB,A,IA,B,IB,N,CR,CI)  
 New: CALL X03ABF(A(IRA,L),(M-L)\*IA+1,B(L,ICB),M-L+1,IA,1,-CX,DX,  
 + .TRUE.,IFAIL)  
 CR = *-real*(DX)  
 CI = *-imag*(DX)

(here DX is a new *complex* variable).**F01DEF**

Withdrawn at Mark 14

Replaced by F06EAF (SDOT/DDOT)

Old: F01DEF(A,B,N)  
 New: *sdot*(N,A,1,B,1)

**F01LBF**

Withdrawn at Mark 18

Replaced by F07BDF (SGBTRF/DGBTRF)

Old: CALL F01LBF(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 (SGBTRF/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**

Withdrawn at Mark 15

Replaced by F08KEF (SGBTRD/DGBTRD) and F08KFF (SORGBR/DORGBR) or F08KGF (SORMBR/DORMBR)

Old: CALL F01LZF(N,A,NRA,C,NRC,WANTB,B,WANTQ,WANTY,Y,NRY,LY,WANTZ,Z,  
 + NRZ,NCZ,D,E,WORK1,WORK2,IFAIL)  
 New: CALL *sgebrd*(N,N,A,NRA,D,E(2),TAUQ,TAUP,WORK1,LWORK,INFO)

```

IF (WANTB) THEN
  CALL sormbr('Q', 'L', 'T', N, 1, NA, NRA, TAUQ, B, N, WORK1, LWORK, INFO)
ELSE IF (WANTQ) THEN
  CALL sorgbr('Q', N, N, N, A, NRA, TAUQ, WORK, LWORK, INFO)
ELSE IF (WANTY) THEN
  CALL sormbr('Q', 'R', 'N', LY, N, N, A, NRA, TAUQ, Y, NRY, WORK1, LWORK,
+           INFO)
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 (CGBTRF/ZGBTRF)

```

Old: CALL F01NAF(N, ML, MU, A, NRA, TOL, IN, SCALE, IFAIL)
New: CALL cgbrf(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 (CGBTRF/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 (SGEQRF/DGEQRF)

```

Old: CALL F01QAF(M, N, A, NRA, C, NRC, Z, IFAIL)
New: CALL sgqrf(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 (SORGQR/DORGQR) and F08AGF (SORMQR/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 (SGEQRF/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 *real* 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 (SGEQRF/DGEQRF) are not the same as those returned by F01QCF. Subsequent calls to F01QDF or F01QEF must also be replaced by calls to F08AGF (SORMQR/DORMQR) or F08AFF (SORGQR/DORGQR) as shown below.

**F01QDF**

Withdrawn at Mark 18

Replaced by F08AGF (SORMQR/DORMQR)

The following replacement is valid only if the previous call to F01QCF has been replaced by a call to F08AEF (SGEQRF/DGEQRF) as shown above. It also assumes that the second argument of F01QDF (WHERE) 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 (SORGQR/DORGQR)

The following replacement is valid only if the previous call to F01QCF has been replaced by a call to F08AEF (SGEQRF/DGEQRF) as shown above. It also assumes that the first argument of F01QEF (WHERE) 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 (SGEQPF/DGEQPF)

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

```
Old: CALL F01QFF('C',M,N,A,LDA,ZETA,PERM,WORK,IFAIL)
New: DO 10 I = 1, N
      PERM(I) = 0
10 CONTINUE
      CALL sgeqpf(M,N,A,LDA,PERM,ZETA,WORK,INFO)
```

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

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

**F01RCF**

Withdrawn at Mark 18

Replaced by F08ASF (CGEQRF/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* 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 (CGEQRF/ZGEQRF) are not the same as those returned by F01RCF. Subsequent calls to F01RDF or F01REF must also be replaced by calls to F08AUF (CUNMQR/ZUNMQR) or F08ATF (CUNGQR/ZUNGQR) as shown below.

**F01RDF**

Withdrawn at Mark 18

Replaced by F08AUF (CUNMQR/ZUNMQR)

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

```
Old: CALL F01RDF(TRANS,'S',M,N,A,LDA,THETA,NCOLB,B,LDB,WORK,IFAIL)
New: CALL cunmqr('L',TRANS,M,NCOLB,N,A,LDA,THETA,B,LDB,WORK,LWORK,
+ INFO)
```

where LWORK is the actual length of WORK.

**F01REF**

Withdrawn at Mark 18

Replaced by F08ATF (CUNGQR/ZUNGQR)

The following replacement is valid only if the previous call to F01RCF has been replaced by a call to F08ASF (CGEQRF/ZGEQRF) as shown above. It also assumes that the first argument of F01REF (WHERE) 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 (CGEQPF/ZGEQPF)

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

```
Old: CALL F01RFF('C',M,N,A,LDA,THETA,PERM,WORK,IFAIL)
New: DO 10 I = 1, N
      PERM(I) = 0
10 CONTINUE
   CALL cgeqpf(M,N,A,LDA,PERM,THETA,CWORK,WORK,INFO)
```

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

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

## F02 – Eigenvalues and Eigenvectors

### Notes:

1. Replacement routines require complex matrices to be stored in *complex* arrays, whereas most of the corresponding old routines require the real and imaginary parts to be stored separately in two *real* arrays.
2. Replacement routines for computing eigenvectors may scale the eigenvectors in a different manner from the old routines, and hence at first glance the eigenvectors may appear to disagree completely; they may indeed be different, but they are equally acceptable as eigenvectors; some replacement routines may also return the eigenvalues (and the corresponding eigenvectors) in a different order.
3. Replacement routines in Chapter F07 and F08 have a parameter INFO, which has a different specification to the usual NAG error-handling parameter IFAIL. See the F07 or F08 Chapter Introduction for details.

### 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 *real* array of length at least (3\*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 *real* array of length at least (3\*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 *real* array of length at least (3\*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

```
Old: CALL F02AEF(A,IA,B,IB,N,R,V,IV,DL,E,IFAIL)
New: CALL F06QFF('U',N,N,A,IA,V,IV)
      CALL F02FDF(1,'V','U',N,V,IV,B,IB,R,WORK,LWORK,IFAIL)
```

where WORK is a *real* array of length at least (3\*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 *real* array of length at least (4\*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 *real* array of length at least (4\*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: 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('N', N, A, IA, R, V, 1, RWORK, WORK, LWORK, IFAIL)
      DO 30 I = 1, N
          RR(I) = real(R(I))
          RI(I) = imag(R(I))
30     CONTINUE
```

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



**F02ALF**

Withdrawn at Mark 8  
Replaced by F02GCF

**F02AMF**

Withdrawn at Mark 18  
Replaced by F08JEF (SSTEQR/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 *real* array of length at least  $(2*(N-1))$ .

**F02ANF**

Withdrawn at Mark 18  
Replaced by F08PSF (CHSEQR/ZHSEQR)

```
Old: CALL F02ANF(N,EPS,HR,IHR,HI,IHI,RR,RI,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('E','N',N,1,N,H,IH,R,Z,1,WORK,1,INFO)
      DO 30 I = 1, N
          RR(I) = real(R(I))
          RI(I) = imag(R(I))
30    CONTINUE
```

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

**F02APF**

Withdrawn at Mark 18  
Replaced by F08PEF (SHSEQR/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 *real* array of length (1) (not used in this call), and WORK is a *real* array of length at least  $(3 * N)$ ; the iteration counts (returned by F02APF in the array ICNT) are not available from F08PEF (SHSEQR/DHSEQR).

**F02AQF**

Withdrawn at Mark 18  
Replaced by F08PEF (SHSEQR/DHSEQR) and F08QKF (STREVC/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 *real* array of length at least  $(3*N)$ ; the iteration counts (returned by F02AQF in the array INTGER) are not available from F08PEF (SHSEQR/DHSEQR); M is an integer which is set to N by F08QKF (STREVC/DTREVC).

**F02ARF**

Withdrawn at Mark 18  
Replaced by F08PSF (CHSEQR/ZHSEQR) and F08QXF (CTREVC/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** array of dimension (IH,N), R is a **complex** array of length (N), V is a **complex** array of dimension (IV,N), WORK is a **complex** array of length at least (2\*N) and RWORK is a **real** array of length at least (N); M is an integer which is set to N by F08QXF (CTREVC/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 (CGEHRD/ZGEHRD) and F08NTF (CUNGHR/ZUNGHR).

**F02ATF**

Withdrawn at Mark 8

Replaced by F08PKF (SHSEIN/DHSEIN)

**F02AUF**

Withdrawn at Mark 8

Replaced by F08PXF (CHSEIN/ZHSEIN)

**F02AVF**

Withdrawn at Mark 18

Replaced by F08JFF (SSTERF/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

```

Old: CALL F02AWF(AR,IAR,AI,IAI,N,R,WK1,WK2,WK3,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 F02HAF('N','L',N,A,IA,R,RWORK,WORK,LWORK,IFAIL)

```

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

**F02AXF**

Withdrawn at Mark 18

Replaced by F02HAF

```

Old: CALL F02AXF(AR,IAR,AI,IAI,N,R,VR,IVR,VI,IVI,WK1,WK2,WK3,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 F06TFF('L',N,N,A,IA,V,IV)
    CALL F02HAF('V','L',N,V,IV,R,RWORK,WORK,LWORK,IFAIL)
DO 40 J = 1, N
  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** array of dimension (IA,N), V is a **complex** array of dimension (IV,N), RWORK is a **real** array of length at least (3\*N), WORK is a **complex** array of length at least (2\*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 (CSTEQR/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) = real(V(I,J))
          VI(I,J) = imag(V(I,J))
        30 CONTINUE
      40 CONTINUE
```

where V is a **complex** 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

```
Old: CALL F02BBF(A,IA,N,ALB,UB,M,MM,R,V,IV,D,E,E2,X,G,C,
+           ICOUNT,IFAIL)
New: CALL F02FCF('Vectors','Value','Lower',N,A,IA,ALB,UB,0,0,
+           M,MM,R,V,IV,WORK,LWORK,IWORK,IFAIL)
```

where R must have dimension (N), WORK is a **real** array of length at least (8\*N), LWORK is its actual length, and IWORK is an integer array of length at least (5\*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** array of dimension (IA,N), R is a **complex** array of dimension (N), V is a **complex** array of dimension (IV,M), WORK is a **complex** array of length at least (N\*(N+2)), LWORK is its actual length, and RWORK is a **real** array of length at least (2\*N).

**F02BEF**

Withdrawn at Mark 18

Replaced by F08JJF (SSTEBZ/DSTEBZ) and F08JKF (SSTEIN/DSTEIN)

```

Old: CALL F02BEF(N,D,ALB,UB,EPS,EPS1,E,E2,M,MM,R,V,IV,ICOUNT,X,C,
+          IFAIL)
New: CALL sstebz('V','B',N,ALB,UB,0,0,EPS1,D,E(2),MM,NSPLIT,R,IBLOCK,
+          ISPLIT,X,IWORK,INFO)
      CALL sstein(N,D,E(2),MM,R,IBLOCK,ISPLIT,V,IV,X,IWORK,IFAILV,INFO)

```

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\*N).

**F02BFF**

Withdrawn at Mark 18

Replaced by F08JJF (SSTEBZ/DSTEBZ)

```

Old: CALL F02BFF(D,E,E2,N,M1,M2,MM12,EPS1,EPS,EPS2,IZ,R,WU)
New: CALL sstebz('I','E',N,0.0e0,0.0e0,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 *real* array of length at least (4\*N), and IWORK is an integer array of length at least (3\*N).

**F02BKF**

Withdrawn at Mark 18

Replaced by F08PKF (SHSEIN/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 (SHSEIN/DHSEIN) if there are complex conjugate pairs of eigenvalues.

**F02BLF**

Withdrawn at Mark 18

Replaced by F08PXF (CHSEIN/ZHSEIN)

```

Old: CALL F02BLF(N,M,HR,IHR,HI,IHI,RI,C,RR,VR,IVR,VI,I,VI,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))
10    CONTINUE
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* array of dimension (IH,N), R is a *complex* array of length (N), V is a *complex* array of dimension (IV,M), M2 is an integer variable, WORK is a *complex* array of length at least (N\*N), RWORK is a *real* array of length at least (N), and IFAILR is an integer array of length at least (N).

**F02BMF**

Withdrawn at Mark 9

Replaced by F08HEF (SSBTRD/DSBTRD) and F08JJF (SSTEBZ/DSTEBZ)

**F02SWF**

Withdrawn at Mark 18

Replaced by F08KEF (SGEBRD/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: DO 20 J = 1, N
      DO 10 I = J+1, N
          A(I,J) = 0.0e0
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,
+                WORK,LWORK,INFO)
      END IF

```

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

**F02SXF**

Withdrawn at Mark 18

Replaced by F08KFF (SORGBR/DORGBR) or F08KGF (SORMBR/DORMBR)

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

```

Old: CALL F02SXF(N,A,LDA,NCOLY,Y,LDY,WORK,IFAIL)
New: IF (NCOLY.EQ.0) THEN
      CALL sorgbr('P',N,N,N,A,LDA,TAUP,WORK,LWORK,INFO)
    ELSE
      CALL sormbr('P','L','T',N,NCOLY,N,A,LDA,TAUP,Y,LDY,WORK,
+                LWORK,INFO)
    END IF

```

**F02SYF**

Withdrawn at Mark 18

Replaced by F08MEF (SBDSQR/DBDSQR)

```

Old: CALL F02SYF(N,D,E,NCOLB,B,LDB,NROWY,Y,LDY,NCOLZ,Z,LDZ,WORK,
+                IFAIL)
New: CALL sbdqr('U',N,NCOLZ,NROWY,NCOLB,D,E,Z,LDZ,Y,LDY,B,LDB,WORK,
+                INFO)

```

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

**F02SZF**

Withdrawn at Mark 15

Replaced by F08MEF (SBDSQR/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
    END IF

```

```

ELSE
  NCVT = 0
END IF
CALL sbsqr('U',N,NCVT,NRU,NCC,D,E(2),Z,NRZ,Y,NRY,B,N,WORK,INFO)

```

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

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

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

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

### F02UWF

Withdrawn at Mark 18

Replaced by F08KSF (CGEBRD/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,WANTQ,Q,LDQ,WORK,IFAIL)
New: DO 20 J = 1, N
      DO 10 I = J+1, N
        A(I,J) = 0.0e0
10    CONTINUE
20    CONTINUE
      CALL cgebrd(N,N,A,LDA,D,E,TAUQ,TAUP,WORK,LWORK,INFO)
      IF (WANTQ) THEN
        CALL F06TFF('L',N,N,A,LDA,Q,LDQ)
        CALL cungbr('Q',N,N,N,Q,LDQ,TAUQ,WORK,LWORK,INFO)
      END IF
      IF (NCOLY.GT.0) 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* arrays of length at least (N), and LWORK is the actual length of WORK.

### F02UXF

Withdrawn at Mark 18

Replaced by F08KTF (CUNGBR/ZUNGBR) or F08KUF (CUNMBR/ZUNMBR)

The following replacement is valid only if the previous call to F02UWF has been replaced by a call to F08KSF (CGEBRD/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 (CBDSQR/ZBDSQR)

```

Old: CALL F02UYF(N,D,E,NCOLB,B,LDB,NROWY,Y,LDY,NCOLZ,Z,LDZ,WORK,
+          IFAIL)
New: CALL cbdsqr('U',N,NCOLZ,NROWY,NCOLB,D,E,Z,LDZ,Y,LDY,B,LDB,WORK,
+          INFO)

```

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

**F02WAF**

Withdrawn at Mark 16

Replaced by F02WEF

```

Old: CALL F02WAF(M,N,A,NRA,WANTB,B,SV,WORK,LWORK,IFAIL)
New: IF (WANTB) THEN
      NCOLB = 1
    ELSE
      NCOLB = 0
    END IF
    CALL F02WEF(M,N,A,NRA,NCOLB,B,M,.FALSE.,WORK,1,SV,.TRUE.,
+           WORK,1,RWORK,IFAIL)

```

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

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

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

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

**F02WBF**

Withdrawn at Mark 14

Replaced by F02WEF

```

Old: CALL F02WBF(M,N,A,NRA,WANTB,B,SV,WORK,LWORK,IFAIL)
New: IF (WANTB) THEN
      NCOLB = 1
    ELSE
      NCOLB = 0
    END IF
    CALL F02WEF(M,N,A,NRA,NCOLB,B,M,.FALSE.,WORK,1,SV,.TRUE.,
+           WORK,1,RWORK,IFAIL)

```

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

$$lwork = \max(3 \times (M - 1), 1) \text{ when } M = N \text{ and WANTB is false;}$$

$$lwork = \max(5 \times (M - 1), 1) \text{ when } M = N \text{ and WANTB is true;}$$

$$lwork = M^2 + 3 \times (M - 1) \text{ when } M < N \text{ and WANTB is false;}$$

$$lwork = M^2 + 5 \times (M - 1) \text{ when } M < N \text{ and WANTB is true.}$$

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**

Withdrawn at Mark 14

Replaced by F02WEF

```

Old: CALL F02WCF(M,N,MINMN,A,NRA,Q,NRQ,SV,PT,NRPT,WORK,LWORK,
+           IFAIL)
New: IF (M.GE.N) THEN
      CALL F06QFF('General',M,N,A,NRA,Q,NRQ)
      CALL F02WEF(M,N,Q,NRQ,0,WORK,1,.TRUE.,WORK,1,SV,.TRUE.,
+           PT,NRPT,RWORK,IFAIL)
    ELSE
      CALL F06QFF('General',M,N,A,NRA,PT,NRPT)
      CALL F02WEF(M,N,PT,NRPT,0,WORK,1,.TRUE.,Q,NRQ,SV,.TRUE.,
+           WORK,1,RWORK,IFAIL)
    END IF

```

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

$$lwork = N^2 + 5 \times (N - 1) \text{ when } M \geq N;$$

$$lwork = M^2 + 5 \times (M - 1) \text{ when } M < N.$$

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

## F03 – Determinants

### F03AGF

Withdrawn at Mark 17

Replaced by F07HDF (SPBTRF/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 (SPBTRF/DPBTRF), the array A holds the matrix packed using a different scheme to that used by F03AGF; see the routine document for details. F07HDF (SPBTRF/DPBTRF) overwrites A with the Cholesky factor  $L$  (without reciprocating diagonal elements) rather than returning  $L$  in the array RL. F07HDF (SPBTRF/DPBTRF) does not compute the determinant of the input matrix, returned as  $D1 \times 2.0^{ID}$  by F03AGF. If this is required, it may be calculated after the call of F07HDF (SPBTRF/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 = 1.0e0
ID = 0
DO 30 I = 1, N
  D1 = D1*A(1,I)**2
10  IF (D1.GE.1.0e0) THEN
    D1 = D1*0.0625e0
    ID = ID + 4
    GO TO 10
  END IF
20  IF (D1.LT.0.0625e0) THEN
    D1 = D1*16.0e0
    ID = ID - 4
    GO TO 20
  END IF
30 CONTINUE
```

### F03AHF

Withdrawn at Mark 17

Replaced by F07ARF (CGETRF/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 (CGETRF/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 (CGETRF/ZGETRF) does not compute the determinant of the input matrix, returned as **cmplx**(DETR, DETI) $\times 2.0^{ID}$  by F03AHF. If this is required, it may be calculated after a call of F07ARF (CGETRF/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(1.0e0,0.0e0)
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.1.0e0) 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*16.0e0
```



```

        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 (SGBTRF/DGBTRF)

**F03AMF**

Withdrawn at Mark 17

Replaced by none; see Chapter F03

```

Old: CALL F01BNF(N,A,IA,P,IFAIL)
     CALL F03AMF(N,TEN,P,D1,D2)
New: CALL cpotrf('Upper',N,A,IA,IFAIL)
     D1 = 1.0e0
     D2 = 0.0e0
     DO 30 I = 1, N
         D1 = D1*real(A(I,I))**2
10     IF (D1.GE.1.0e0) THEN
         D1 = D1*0.0625e0
         D2 = D2 + 4
         GO TO 10
     END IF
20     IF (D1.LT.0.0625e0) THEN
         D1 = D1*16.0e0
         D2 = D2 - 4
         GO TO 20
     END IF
30 CONTINUE
     IF (TEN) THEN
         I = D2
         D2 = D2*LOG10(2.0e0)
         D1 = D1*2.0e0**(I-D2/LOG10(2.0e0))
     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 (CPOTRF/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 (CPOTRF/ZPOTRF), array A contains the upper triangle of the matrix rather than the lower triangle.

**F04 – Simultaneous Linear Equations****F04AKF**

Withdrawn at Mark 17

Replaced by F07ASF (CGETRS/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 (CGETRF/ZGETRF) rather than F03AHF; see the F03 Chapter Introduction for details. IPIV is an INTEGER array of length N, as returned by F07ARF (CGETRF/ZGETRF), and the array P is no longer required. INFO is an INTEGER diagnostic parameter; see the F07ASF (CGETRS/ZGETRS) routine document for details.

**F04ALF**

Withdrawn at Mark 17

Replaced by F07HEF (SPBTRS/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 spbtrs('Lower',N,M,IR,A,IA,X,IX,INFO)
```

It is assumed that the matrix has been factorized by a call of F07HDF (SPBTRF/DPBTRF) rather than F03AGF; see the F03 Chapter Introduction for details. A is the factorized matrix as returned by F07HDF (SPBTRF/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 (SPBTRS/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 (SPBTRS/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 F08AGF (SORMQR/DORMQR), F06PJF (STRSV/DTRSV) and F06EFF (SCOPY/DCOPY)

```
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)
      DO 10 I = 1, N
          X(IPIV(I)) = B(I)
      10 CONTINUE
```

where Y must be the same *real* 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 (SGEQPF/DGEQPF) as shown above.

**F04APF**

Withdrawn at Mark 8

Replaced by F04AXF

**F04AQF**

Withdrawn at Mark 16

Replaced by F07GEF (SPPTRS/DPPTRS) or F07PEF (SSPTRS/DSPTRS)

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

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

```
Old: CALL F04AQF(N,M,RL,D,B,X)
New: CALL scopy(N,B,1,X,1)
      CALL spbtrs('Lower',N,1,RL,X,N,INFO)
```

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

```
Old: CALL F04AQF(N,M,RL,D,B,X)
New: CALL scopy(N,B,1,X,1)
      CALL spbtrs('Lower',N,1,RL,IPIV,X,N,INFO)
```

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 (SSPTRF/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 (SCOPY/DCOPY), which simply copies array B to X, is not necessary. References to X in the calls of F07GEF (SPPTRS/DPPTRS) and F07PEF (SSPTRS/DSPTRS) may then be replaced by references to B, in which case B will be overwritten by the solution vector.

**F04AUF**

Withdrawn at Mark 9  
Replaced by F04JGF

**F04AVF**

Withdrawn at Mark 9  
Replaced by F07BEF (SGBTRS/DGBTRS)

**F04AWF**

Withdrawn at Mark 17  
Replaced by F07FSF (CPOTRS/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 (CPOTRF/ZPOTRF) rather than F01BNF; see the the F01 Chapter Introduction for details. A is the factorized matrix as returned by F07FRF (CPOTRF/ZPOTRF). The array P is no longer required. INFO is an INTEGER diagnostic parameter; see the F07FSF (CPOTRS/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 (CPOTRS/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 (SGETRS/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 (SGETRF/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 (SPOTRS/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 (SPOTRF/DPOTRF) rather than F01BXF. The array P is no longer required.

**F04LDF**

Withdrawn at Mark 18  
Replaced by F07BEF (SGBTRS/DGBTRS)

Old: CALL F04LDF(N,M1,M2,IR,A,IA,AL,IL,IN,B,IB,IFAIL)  
New: CALL *sgbtrs*('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 (SGBTRF/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 F11GDF, F11GEF and F11GFF (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 F07BSF (CGBTRS/ZGBTRS) and F06SKF (CTBSV/ZTBSV)

```
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 (CGBTRF/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 (SNRM2/DNRM2)

```
Old: U = F05ABF(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 = F06RAF(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 = F06RCF(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 = F06RCF(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 *real* array of dimension (1) and WORK2 as a *real* array of dimension (N).

**F06VGF**

Withdrawn at Mark 16

Replaced by F06UAF, F06UCF and F06UJF

```
Old: ANORM = F06VGF(NORM, MATRIX, M, N, A, LDA)
New: C = MATRIX(1:1)
     IF ( (C.EQ.'G') .OR. (C.EQ.'g') ) THEN
       ANORM = F06UAF(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 = F06UCF(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 = F06UCF(NORM, 'L', N, A, LDA, WORK1)
     ELSE IF ( (C.EQ.'U') .OR. (C.EQ.'u') ) THEN
       ANORM = F06UJF(NORM, 'U', 'N', M, N, A, LDA, WORK1)
     ELSE IF ( (C.EQ.'L') .OR. (C.EQ.'l') ) THEN
       ANORM = F06UJF(NORM, 'L', 'N', M, N, A, LDA, WORK1)
     END IF
```

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

**F11 – Sparse Linear Algebra****F11BAF**

Scheduled for withdrawal at Mark 21

Replaced by F11BDF

```
Old: CALL F11BAF(METHOD, PRECON, NORM, WEIGHT, ITERM, N, M, TOL, MAXITN,
+              ANORM, SIGMAX, MONIT, LWREQ, IFAIL)
New: CALL F11BDF(METHOD, PRECON, NORM, WEIGHT, ITERM, N, M, TOL, MAXITN,
+              ANORM, SIGMAX, MONIT, WORK, LWORK, LWREQ, IFAIL)
```

F11BDF contains two additional parameters as follows:

WORK(LWORK) – *real* array.

LWORK – INTEGER. See the routine document for further information.

**F11BBF**

Scheduled for withdrawal 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 *real* 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**

Scheduled for withdrawal at Mark 21

Replaced by F11BFF

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

F11BFF contains two additional parameters as follows:

WORK(LWORK) – *real* array.

LWORK – INTEGER. See the routine document for further information.

**F11GAF**

Scheduled for withdrawal at Mark 22

Replaced by F11GDF

```

Old: CALL F11GAF(METHOD,PRECON,SIGCMP,NORM,WEIGHT,ITERM,N,TOL,MAXITN,
+              ANORM,SIGMAX,SIGTOL,MAXITS,MONIT,LWREQ,IFAIL)
New: CALL F11GDF(METHOD,PRECON,SIGCMP,NORM,WEIGHT,ITERM,N,TOL,MAXITN,
+              ANORM,SIGMAX,MAXITS,MONIT,MONIT,LWREQ,WORK,LWORK,IFAIL)

```

F11GDF contains two additional parameters as follows:

WORK(LWORK) – *real* 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 *real* 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

```

Old: CALL F11GCF(ITN,STPLHS,STPRHS,ANORM,SIGMAX,ITS,SIGERR,IFAIL)
New: CALL F11GFF(ITN,STPLHS,STPRHS,ANORM,SIGMAX,ITS,SIGERR,
+              WORK,LWORK,IFAIL)

```

F11GFF contains two additional parameters as follows:

WORK(LWORK) – *real* 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 = G01BAF(IDF,T,IFAIL)
New: P = G01EBF('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 = G01BCF(X,N,IFAIL)
New: P = G01ECF('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  $\leq 10^6$ .

**G01CAF**

Withdrawn at Mark 16

Replaced by G01FBF

```
Old: T = G01CAF(P,N,IFAIL)
New: T = G01FBF('Lower-tail',P,real(N),IFAIL)
```

**G01CBF**

Withdrawn at Mark 16

Replaced by G01FDF

```
Old: F = G01CBF(P,M,N,IFAIL)
New: F = G01FDF(P,real(M),real(N),IFAIL)
```

**G01CCF**

Withdrawn at Mark 16

Replaced by G01FCF

```
Old: X = G01CCF(P,N,IFAIL)
New: X = G01FCF(P,real(N),IFAIL)
```

**G01CDF**

Withdrawn at Mark 16

Replaced by G01FEF

```
Old: X = G01CDF(P,A,B,IFAIL)
New: X = G01FEF(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  $\leq 10^6$ .

**G01CEF**

Withdrawn at Mark 18

Replaced by G01FAF

```
Old: X = G01CEF(P,IFAIL)
New: X = G01FAF('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 F06DBF(M,1,ISX,1)
        C  THEN
        TOL = X02AJF()
        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
        C  there are two or more dependent variables,
        C  i.e., IR is greater than or equal to 2 then:
```

```

DO 20 I = 2, IR
  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 *real* 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 *real* 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 *real* workspace WK(5 \* (M - 1) + M \* 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 one-dimensional array IT. These arrays will be the equivalent if IA = N. The following additional declarations are required.

```

real      GMEAN
INTEGER    IFAIL
real      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  $NMAX \geq N$ .

### 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,0.0e0,0,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.

```

real      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

```
Old: CALL G04AFF (Y, IY1, IY2, M, NR, NC, ROW, COL, CELL, ICELL, GM, SS, IDF, F, FP,
+             IFAIL)
New: CALL G04CAF (M*NR*NC, Y1, 2, LFAC, 1, 2, 0, 6, TABLE, ITOTAL, TMEAN, MAXT, E,
+             IMEAN, SEMEAN, BMEAN, R, IWK, IFAIL)
```

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, ..., NR
COL(j)	TMEAN(j), j = 1, 2, ..., NC
CELL(i, j)	TMEAN(IMEAN(2)+(j-1)*NR+i), i = 1, 2, ..., NR; j = 1, 2, ..., NC
GM	BMEAN(1)
SS(1)	TABLE(3, 2)
SS(2)	TABLE(2, 2)
SS(i)	TABLE(4, 2)
IDF(1)	TABLE(3, 1)
IDF(2)	TABLE(2, 1)
IDF(i)	TABLE(4, 1)
F(1)	TABLE(3, 4)
F(2)	TABLE(2, 4)
F(3)	TABLE(4, 4)
FP(1)	TABLE(3, 5)
FP(2)	TABLE(2, 5)
FP(3)	TABLE(4, 5)

Note how rows and columns have swapped.

The following additional declarations are required.

```
real      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 G05KAF

**G05ABF**

Withdrawn at Mark 7

Replaced by G05LGF

**G05ACF**

Withdrawn at Mark 7

Replaced by G05LJF

**G05ADF**

Withdrawn at Mark 7

Replaced by G05LAF

**G05AEF**

Withdrawn at Mark 7  
Replaced by G05LAF

**G05AFF**

Withdrawn at Mark 7  
Replaced by G05LKF

**G05AGF**

Withdrawn at Mark 7  
Replaced by G05LLF

**G05AHF**

Withdrawn at Mark 7  
Replaced by G05LFF

**G05AJF**

Withdrawn at Mark 7  
Replaced by G05LFF

**G05AKF**

Withdrawn at Mark 7  
Replaced by G05LFF

**G05ALF**

Withdrawn at Mark 7  
Replaced by G05LEF

**G05AMF**

Withdrawn at Mark 7  
Replaced by G05LEF

**G05ANF**

Withdrawn at Mark 7  
Replaced by G05LCF

**G05APF**

Withdrawn at Mark 7  
Replaced by G05LBF

**G05AQF**

Withdrawn at Mark 7  
Replaced by G05LDF

**G05ARF**

Withdrawn at Mark 7  
Replaced by G05MZF

**G05ASF**

Withdrawn at Mark 7  
Replaced by G05MJF

**G05ATF**

Withdrawn at Mark 7  
Replaced by G05MAF

**G05AUF**

Withdrawn at Mark 7  
Replaced by G05MLF

**G05AVF**

Withdrawn at Mark 7  
Replaced by G05MKF

**G05AWF**

Withdrawn at Mark 7  
Replaced by G05MZF

**G05AZF**

Withdrawn at Mark 7  
Replaced by G05MZF

**G05BAF**

Withdrawn at Mark 7  
Replaced by G05KBF

**G05BBF**

Withdrawn at Mark 7  
Replaced by G05KCF

**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

```
Old: CALL G05CGF(IA,NI,XA,NX,IFAIL)
New: IGEN = LGEN
      CALL F06DFF(4,LSEED,1,ISEED,1)
```

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) = G05DAF(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 *real* 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

```
Old: DO 10 I = 1, N
      X(I) = G05DBF(A)
10 CONTINUE
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 G05DBF. The *real* 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

```
Old: DO 10 I = 1, N
      X(I) = G05DCF(A,B)
10 CONTINUE
New: BB = ABS(B)
      IFAIL = 0
      CALL G05LNF(A,BB,N,X,IGEN,ISEED,IFAIL)
```

In G05LNF the second parameter must be positive, this does not have to be the case in G05DCF. The *real* 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

```

Old: DO 10 I = 1, N
      X(I) = G05DDF(A,B)
10 CONTINUE
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 G05DDF represents the standard deviation. The *real* 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

```

Old: DO 10 I = 1, N
      X(I) = G05DEF(A,B)
10 CONTINUE
New: BB = B**2
      IFAIL = 0
      CALL G05LKF(A, BB, N, X, IGEN, ISEED, IFAIL)

```

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 *real* 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 G05LKF is different from that 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

```

Old: DO 10 I = 1, N
      X(I) = G05DFF(A,B)
10 CONTINUE
New: BB = ABS(B)
      IFAIL = 0
      CALL G05LLF(A, BB, N, X, IGEN, ISEED, IFAIL)

```

In G05LLF the the second parameter must be non-negative, this does not have to be the case in G05DFF. The *real* 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 G05LFF

```

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

```
Old: DO 10 I = 1, N
      X(I) = G05DHF(DF,IFAIL)
      10 CONTINUE
New: CALL G05LCF(DF,N,X,IGEN,ISEED,IFAIL)
```

The *real* 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

```
Old: DO 10 I = 1, N
      X(I) = G05DJF(DF,IFAIL)
      10 CONTINUE
New: CALL G05LBF(DF,N,X,IGEN,ISEED,IFAIL)
```

The *real* 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

```
Old: DO 10 I = 1, N
      X(I) = G05DKF(DF1,DF2,IFAIL)
      10 CONTINUE
New: CALL G05LDF(DF1,DF2,N,X,IGEN,ISEED,IFAIL)
```

The *real* 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 G05LEF

```
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 G05LEF

```
Old: X = G05DMF(G,H,IFAIL)
New: CALL G05LEF(G,H,1,X(1),IGEN,ISEED,IFAIL)
      IF (X(1).LT.1.0e0) X(1) = X(1)/(1.0e0-X(1))
```

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,1.0e0,1,X(1),IGEN,ISEED,IFAIL1)
CALL G05LFF(H,1.0e0,1,Y(1),IGEN,ISEED,IFAIL2)
IF (Y(1).NE.0.0e0) 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

```
Old: DO 10 I = 1, N
      X(I) = G05DPF(A,B,IFAIL)
10 CONTINUE
New: CALL G05LMF(A,B,N,X,IGEN,ISEED,IFAIL)
```

The *real* 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 *real* 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

```
Old: DO 10 I = 1, M
      IX(I) = G05DYF(IA,IB)
10 CONTINUE
New: IFAIL = 0
      CALL G05MAF(IA,IB,N,IX,IGEN,ISEED,IFAIL)
```

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(0.0e0,MIN(P,1.0e0))
      IFAIL = 0
      L = G05KEF(PP,IGEN,ISEED,IFAIL)
```

The *real* 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 *real* 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**

Scheduled for withdrawal at Mark 22

Replaced by G05MAF

```
Old: CALL G05EBF(IA,IB,R,NR,IFAIL)
      DO 10 I = 1, N
          X(I) = G05EYF(R,NR)
      10 CONTINUE
New: CALL G05MAF(IA,IB,N,X,IGEN,ISEED,IFAIL)
```

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 *real* 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  $NR2 \geq NR + 2$ . 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 *real* 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  $NR2 \geq NR + 2$ . 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 *real* 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  $NR2 \geq NR + 2$ . 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 *real* 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  $NR2 \geq NR + 2$ . 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.0.0e0) THEN
          DO 10 I = 1, NB - 1
              THETA(I) = -B(I+1)/B(1)
      10 CONTINUE
      ELSE
          DO 20 I = 1, IQ
              THETA(I) = 0.0e0
      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 *real* 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 *real* 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 G05EJF(IA,N,IZ,M,IFAIL)
New: CALL G05NBF(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) = G05EWF(R,NR,IFAIL)
      10 CONTINUE
New: AVAR = B(1)**2
      IF (AVAR.GT.0.0e0) THEN
          DO 10 I = 1, NB - 1
              THETA(I) = -B(I+1)/B(1)
          10 CONTINUE
      ELSE
          DO 20 I = 1, IQ
              THETA(I) = 0.0e0
          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 *real* 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 *real* 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

```

Old: CALL G05EXF(P,NP,IP,LP,R,NR,IFAIL)
      DO 10 I = 1, N
          X(I) = G05EYF(R,NR)
      10 CONTINUE
New: CALL G05MZF(0,P,NP,IP,LP,N,X,IGEN,ISEED,R2,NR2,IFAIL)
      CALL G05MZF(1,P,NP,IP,LP,N,X,IGEN,ISEED,R2,NR2,IFAIL)

```

The *real* 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  $NR2 \geq NR + 4$ . 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 G05EZF(X,N,R,NR,IFAIL)
New: MODE = 0
      CALL G05LZF(MODE,N,A,C,IC,X,IGEN,ISEED,R,NR,IFAIL)
      MODE = 1
      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 *real* 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 *real* 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 *real* 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 G05LFF(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.

**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
    LL = 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
50  CONTINUE
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) = 0.0e0
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 *real* array PHI should have length at least  $\max(1, IP \times (K \times K))$ ; if

dimensioned as PHI(K,K,IP) (as in the above example) then  $\text{PHI}(i,j,l)$  will contain the element  $\text{PAR}((l-1) \times k \times k + (i-1) \times k + j)$ . The *real* array THETA should have length at least  $\max(1, \text{IQ} \times (K \times K))$ ; if dimensioned as THETA(K,K,IQ) (as in the above example) then  $\text{THETA}(i,j,l)$  will contain the element  $\text{PAR}(\text{IP} \times k \times k + (l-1) \times k \times k + (i-1) \times k + j)$ . The *real* array XMEAN should have length at least K; if MEAN='M' then  $\text{XMEAN}(i)$  will contain the element  $\text{PAR}(\text{IP} + \text{IQ} \times k \times k + i)$ , 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.

## G08 – Nonparametric Statistics

### G08ABF

Withdrawn at Mark 16

Replaced by G08AGF

```
Old: CALL G08ABF(X,Y,N,W1,W2,W,N1,P,IFAIL)
New: DO 20 I = 1, N
      Z(I) = X(I) - Y(I)
20 CONTINUE
XME = 0.0e0
CALL G08AGF(N,Z,XME,'Lower-tail','No-zeros',W,WNOR,P,
+          N1,W1,IFAIL)
```

W1 is a *real* work array of dimension (3\*N). The *real* array W2 is no longer required. WNOR returns the normalized Wilcoxon test statistic. The *real* array Z, of dimension (N), contains the difference between the paired sample observations, and by setting the *real* 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

```
Old: CALL G08ADF(X,N,N1,W,U,P,IFAIL)
New: N2 = N - N1
CALL G08AHF(N1,X,N2,X(N1+1),'Lower-tail',U,UNOR,P,
+          TIES,RANKS,W,IFAIL)
```

The observations from the two independent samples must be stored in two separate *real* 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 *real* 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 *real* 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: C    First transpose the data matrix X
      C    note NSM is used as the first dimension of the array W
      DO 20 I = 1, NS
          CALL F06EFF(NX,X,(1,I),1,W(I,1),NSM)
      20 CONTINUE
      C    then if ICR = 0 in the call to G13DAF
          CALL G13DMF('V-Covariances',NS,NX,W,NSM,NL,WMEAN,CO,C,IFAIL)
      C    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 *real* array WMEAN must be of length NS, and on output stores the means of each of the NS series.

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

## H – Operations Research

### 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 H02BAF(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, MSGGLVL, 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)
      real        BIGBND, TOLFES, TOLIV, ROPT
      real        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) = 1.0e0
         DO 20 I = 1, M
            RA(I,J) = A(I+1,J)
20      CONTINUE
10     CONTINUE
      BIGBND = 1.0e20
      DO 30 I = 1, N
         BL(I) = 0.0e0
         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
      MSGGLVL = 0
      MAXNOD = 0
      INTFST = 0
      TOLIV = 0.0e0
      TOLFES = 0.0e0
      MAXDPT = 3*N/2
      IFAIL = 0
      CALL H02BBF(ITMAX,MSGGLVL,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.0) 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 M01AAF(A,M,N,IP,IST,IFAIL)
New: CALL M01DAF(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 M01ABF(A,M,N,IP,IST,IFAIL)
New: CALL M01DAF(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 M01ACF(IA,M,N,IP,IST,IFAIL)
New: CALL M01DBF(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 M01ADF(IA,M,N,IP,IST,IFAIL)
New: CALL M01DBF(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 M01AEF(A,NR,NC,IC,T,TT,IFAIL)
New: CALL M01DEF(A,NR,1,NR,IC,IC,'A',IRANK,IFAIL)
      DO 10 I = 1, NC
          CALL M01EAF(A(1,I),1,NR,IRANK,IFAIL)
      10 CONTINUE
```

The *real* 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 M01AFF(A,NR,NC,IC,T,TT,IFAIL)
New: CALL M01DEF(A,NR,1,NR,IC,IC,'D',IRANK,IFAIL)
      DO 10 I = 1, NC
          CALL M01EAF(A(1,I),1,NR,IRANK,IFAIL)
      10 CONTINUE
```

The *real* 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)
      DO 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)
      DO 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 M01DAF, M01ZAF and M01CAF

```

Old: CALL M01AJF(A,W,IND,INDW,N,NW,IFAIL)
New: CALL M01DAF(A,1,N,'A',IND,IFAIL)
      CALL M01ZAF(IND,1,N,IFAIL)
      CALL M01CAF(A,1,N,'A',IFAIL)

```

The arrays W and INDW are no longer needed.

**M01AKF**

Withdrawn at Mark 16

Replaced by M01DAF, M01ZAF and M01CAF

```

Old: CALL M01AKF(A,W,IND,INDW,N,NW,IFAIL)
New: CALL M01DAF(A,1,N,'D',IND,IFAIL)
      CALL M01ZAF(IND,1,N,IFAIL)
      CALL M01CAF(A,1,N,'D',IFAIL)

```

The arrays W and INDW are no longer needed.

**M01ALF**

Withdrawn at Mark 13

Replaced by M01DBF, M01ZAF and M01CBF

```

Old: CALL M01ALF(IA,IW,IND,INDW,N,NW,IFAIL)
New: CALL M01DBF(IA,1,N,'A',IND,IFAIL)
      CALL M01ZAF(IND,1,N,IFAIL)
      CALL M01CBF(IA,1,N,'A',IFAIL)

```

The arrays IW and INDW are no longer needed.

**M01AMF**

Withdrawn at Mark 13

Replaced by M01DBF, M01ZAF and M01CBF

```

Old: CALL M01AMF(IA,IW,IND,INDW,N,NW,IFAIL)
New: CALL M01DBF(IA,1,N,'D',IND,IFAIL)
      CALL M01ZAF(IND,1,N,IFAIL)
      CALL M01CBF(IA,1,N,'D',IFAIL)

```

The arrays IW and INDW are no longer needed.

**M01ANF**

Withdrawn at Mark 13

Replaced by M01CAF

```

Old: CALL M01ANF(A,I,J,IFAIL)
New: CALL M01CAF(A,I,J,'A',IFAIL)

```

**M01APF**

Withdrawn at Mark 16

Replaced by M01CAF

```

Old: CALL M01APF(A,I,J,IFAIL)
New: CALL M01CAF(A,I,J,'D',IFAIL)

```

**M01AQF**

Withdrawn at Mark 13

Replaced by M01CBF

Old: CALL M01AQF(IA,I,J,IFAIL)  
 New: CALL M01CBF(IA,I,J,'A',IFAIL)

**M01ARF**

Withdrawn at Mark 13

Replaced by M01CBF

Old: CALL M01ARF(IA,I,J,IFAIL)  
 New: CALL M01CBF(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 M01BAF(IA,I,J,IFAIL)  
 New: CALL M01CCF(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 M01BBF(IA,I,J,IFAIL)  
 New: CALL M01CCF(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 M01BCF(IA,NR,NC,L1,L2,LC,IUC,IT,ITT,IFAIL)  
 New: CALL M01CCF(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 M01BDF(IA,NR,NC,L1,L2,LC,IUC,IT,ITT,IFAIL)  
 New: CALL M01CCF(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: X02BAF(X)

New: X02BHF()

**X02BCF**

Withdrawn at Mark 14

Replaced by X02AMF

Old: X02BCF(X)

New:  $-\text{LOG}(\text{X02AMF}()) / \text{LOG}(2.0)$

**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:  $\text{LOG}(\text{X02AMF}()) / \text{LOG}(2.0)$

**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

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