# **NAG Library**

# Advice on Replacement Calls for Withdrawn/Superseded Routines

The following list gives the names of routines that are suitable replacments for routines that have either been withdrawn or superseded since Mark 17.

The list indicates the minimum change necessary, but many of the replacement routines have additional flexibility and you may wish to take advantage of new features. It is strongly recommended that you consult the routine documents.

# C05 - Roots of One or More Transcendental Equations

### C05ADF

```
Scheduled for withdrawal at Mark 25. Replaced by C05AYF.
```

# C05AGF

Scheduled for withdrawal at Mark 25. Replaced by C05AUF.

```
Old: FUNCTION F(XX)
...
END FUNCTION F
...
CALL C05AGF(X,H,EPS,ETA,F,A,B,IFAIL)
New: FUNCTION F(XX,IUSER,RUSER)
...
INTEGER, INTENT(INOUT) :: IUSER(*)
REAL (KIND=nag_wp), INTENT(INOUT) :: RUSER(*)
...
END FUNCTION F
...
INTEGER :: IUSER(1)
REAL (KIND=nag_wp) :: RUSER(1)
...
CALL C05AUF(X,H,EPS,ETA,F,A,B,IUSER,RUSER,IFAIL)
```

### C05AJF

Scheduled for withdrawal at Mark 25. Replaced by C05AWF.

```
Old: FUNCTION F(XX)
...
END FUNCTION F
```

```
CALL CO5AJF(X, EPS, ETA, F, NFMAX, IFAIL)
New: FUNCTION F(XX, IUSER, RUSER)
        INTEGER,
                             INTENT(INOUT) :: IUSER(*)
        REAL (KIND=nag_wp), INTENT(INOUT) :: RUSER(*)
     END FUNCTION F
     . . .
     INTEGER
                         :: IUSER(1)
     REAL (KIND=nag_wp) :: RUSER(1)
     CALL CO5AWF(X, EPS, ETA, F, NFMAX, IUSER, RUSER, IFAIL)
C05NBF
Scheduled for withdrawal at Mark 25.
Replaced by C05OBF.
Old: SUBROUTINE FCN(N,X,FVEC,IFLAG)
     END SUBROUTINE FCN
     CALL CO5NBF(FCN,N,X,FVEC,XTOL,WA,LWA,IFAIL)
New: SUBROUTINE FCN(N,X,FVEC,IUSER,RUSER,IFLAG)
        INTEGER,
                             INTENT(INOUT) :: IUSER(*)
        REAL (KIND=nag_wp), INTENT(INOUT) :: RUSER(*)
     END FUNCTION FCN
     INTEGER
                        :: IUSER(1)
     REAL (KIND=nag_wp) :: RUSER(1)
     CALL CO5QBF(FCN,N,X,FVEC,XTOL,IUSER,RUSER,IFAIL)
C05NCF
Scheduled for withdrawal at Mark 25.
Replaced by C05QCF.
Old: SUBROUTINE FCN(N,X,FVEC,IFLAG)
     END SUBROUTINE FCN
     REAL (KIND=nag_wp) :: FJAC(LDFJAC,N)
     CALL CO5NCF(FCN,N,X,FVEC,XTOL,MAXFEV,ML,MU,EPSFCN,DIAG,MODE,FACTOR, &
                  NPRINT, NFEV, FJAC, LDFJAC, R, LR, QTF, W, IFAIL)
New: SUBROUTINE FCN(N,X,FVEC,IUSER,RUSER,IFLAG)
        INTEGER,
                             INTENT(INOUT) :: IUSER(*)
        REAL (KIND=nag_wp), INTENT(INOUT) :: RUSER(*)
     END FUNCTION FCN
                         :: IUSER(1)
     INTEGER
     REAL (KIND=nag_wp) :: FJAC(N,N), RUSER(1)
     CALL CO5QCF(FCN,N,X,FVEC,XTOL,MAXFEV,ML,MU,EPSFCN,MODE,DIAG,FACTOR, &
                  NPRINT, NFEV, FJAC, R, QTF, IUSER, RUSER, IFAIL)
C05NDF
Scheduled for withdrawal at Mark 25.
Replaced by C05QDF.
Old: REAL (KIND=nag_wp) :: FJAC(LDFJAC,N)
     CALL CO5NDF(IREVCM,N,X,FVEC,XTOL,ML,MU,EPSFCN,DIAG,MODE,FACTOR, &
                  FJAC,LDFJAC,R,LR,QTF,W,IFAIL)
```

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```
New: REAL (KIND=nag_wp) :: FJAC(N,N), RWSAV(4*N+20)
     INTEGER
                        :: IWSAV(17)
     CALL CO5QDF(IREVCM,N,X,FVEC,XTOL,ML,MU,EPSFCN,MODE,DIAG,FACTOR, &
                 FJAC,R,QTF,IWSAV,RWSAV,IFAIL)
C05PBF/C05PBA
Scheduled for withdrawal at Mark 25.
Replaced by C05RBF.
Old: SUBROUTINE FCN_CO5PBF(N,X,FVEC,FJAC,LDFJAC,IFLAG)
     END SUBROUTINE FCN_C05PBF
     REAL (KIND=nag_wp) :: FJAC(LDFJAC,N)
     CALL CO5PBF(FCN_CO5PBF,N,X,FVEC,FJAC,LDFJAC,XTOL,WA,LWA,IFAIL)
        or
     SUBROUTINE FCN_CO5PBA(N,X,FVEC,FJAC,LDFJAC,IFLAG,IUSER,RUSER)
     END SUBROUTINE FCN_CO5PBA
     REAL (KIND=nag_wp) :: FJAC(LDFJAC,N)
     CALL CO5PBA(FCN_CO5PBA,N,X,FVEC,FJAC,LDFJAC,XTOL,WA,LWA,IUSER,RUSER,IFAIL)
New: SUBROUTINE FCN(N,X,FVEC,FJAC,IUSER,RUSER,IFLAG)
     END SUBROUTINE FCN
     REAL (KIND=nag_wp) :: FJAC(N,N)
     CALL CO5RBF(FCN,N,X,FVEC,FJAC,XTOL,IUSER,RUSER,IFAIL)
C05PCF/C05PCA
Scheduled for withdrawal at Mark 25.
Replaced by C05RCF.
Old: SUBROUTINE FCN_CO5PCF(N,X,FVEC,FJAC,LDFJAC,IFLAG)
     END SUBROUTINE FCN_CO5PCF
     REAL (KIND=nag_wp) :: FJAC(LDFJAC,N)
     CALL CO5PCF(FCN_CO5PCF,N,X,FVEC,FJAC,LDFJAC,XTOL,MAXFEV,DIAG,MODE,FACTOR, &
                 NPRINT, NFEV, NJEV, R, LR, QTF, W, IFAIL)
        OΥ
     SUBROUTINE FCN_CO5PCA(N,X,FVEC,FJAC,LDFJAC,IFLAG,IUSER,RUSER)
     END SUBROUTINE FCN_CO5PCA
     REAL (KIND=nag_wp) :: FJAC(LDFJAC,N)
     CALL CO5PCA(FCN_CO5PCA,N,X,FVEC,FJAC,LDFJAC,XTOL,MAXFEV,DIAG,MODE,FACTOR, &
                 NPRINT, NFEV, NJEV, R, LR, QTF, W, IUSER, RUSER, IFAIL)
New: SUBROUTINE FCN(N,X,FVEC,FJAC,IUSER,RUSER,IFLAG)
        INTEGER.
                             INTENT(INOUT) :: IUSER(*)
        REAL (KIND=nag_wp), INTENT(INOUT) :: RUSER(*)
     END FUNCTION FCN
     REAL (KIND=nag_wp) :: FJAC(N,N)
```

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CALL CO5RCF(FCN,N,X,FVEC,FJAC,XTOL,MAXFEV,MODE,DIAG,FACTOR, & NPRINT,NFEV,NJEV,R,QTF,IUSER,RUSER,IFAIL)

# C05PDF/C05PDA

Scheduled for withdrawal at Mark 25. Replaced by C05RDF.

### C05ZAF

Scheduled for withdrawal at Mark 25. Replaced by C05ZDF.

The array XP must now have dimension N regardless of the value of MODE, and likewise ERR must now have dimension M regardless. The parameter IFAIL is the standard NAG parameter for error trapping. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction for details.

# C06 – Summation of Series

# C06DBF

Scheduled for withdrawal at Mark 25. Replaced by C06DCF.

```
Old: DO I = 1, LX
    RES(I) = CO6DBF(X(I),C,N,S)
    END DO

New: XMIN = -1.0D0
    XMAX = 1.0D0

SELECT CASE (S)
    CASE (1,2,3)
        S_USE = S
    CASE DEFAULT
        S_USE = 2
    END SELECT

IFAIL = 0
    CALL CO6DCF(X,LX,XMIN,XMAX,C,N,S_USE,RES,IFAIL)
```

The old routine C06DBF returns a single sum at a time, whereas the new routine C06DCF returns a vector of LX values at once. The parameter IFAIL is the standard NAG parameter for error trapping. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction for details.

### C06EAF

Scheduled for withdrawal at Mark 26. Replaced by C06PAF.

```
Old: CALL CO6EAF(X,N,IFAIL)
New: CALL CO6PAF('F',X,N,WORK,IFAIL)
```

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where WORK is a real array of length  $3 \times N + 100$  and X(0: N+1) has been extended by 2 elements from the original X(0: N-1). The output values X are stored in a different order with real and imaginary parts stored contiguously. The mapping of output elements is as follows:

```
X(2 \times i) \leftarrow X(i), for i = 0, 1, ..., N/2 and X(2 + i + 1) \leftarrow X(N - i), for i = 1, 2, ..., (N + 1)/2.
```

### C06EBF

Scheduled for withdrawal at Mark 26.

```
Replaced by C06PAF.
```

```
Old: CALL CO6EBF(X,N,IFAIL)
New: CALL CO6PAF('B',X,N,WORK,IFAIL)
```

where WORK is a real array of length  $3 \times N + 100$  and X(0: N+1) has been extended by 2 elements from the original X(0: N-1). The input values of X are stored in a different order with real and imaginary parts stored contiguously. Also C06PAF performs the inverse transform without the need to first conjugate. If prior conjugation of original array X is assumed then the mapping of input elements is:

```
X(2 \times i) \leftarrow X(i), for i = 0, 1, ..., N/2 and X(2 \times i + 1) \leftarrow X(N - i), for i = 1, 2, ..., (N - 1)/2.
```

# C06ECF

Scheduled for withdrawal at Mark 26.

Replaced by C06PCF.

```
Old: CALL CO6ECF(X,Y,N,IFAIL)
New: CALL CO6PCF('F',Z,N,WORK,IFAIL)
```

where WORK is a complex array of length  $2 \times N + 15$  and Z is a complex array of length N such that Z(i) = CMPLX(X(i), Y(i)), for i = 0, 1, ..., N - 1 on input and output.

# C06EKF

Scheduled for withdrawal at Mark 26. Replaced by C06FKF.

```
replaced by Coolini.
```

```
Old: CALL CO6EKF(IJOB,X,Y,N,IFAIL)
New: CALL CO6FKF(IJOB,X,Y,N,WORK,IFAIL)
```

where WORK is a real array of length N.

# C06FRF

Scheduled for withdrawal at Mark 26.

Replaced by C06PSF.

where cx and cwork are complex arrays of lengths  $m \times n$  and  $n \times m + 2 \times n + 15$  respectively.

# C06FUF

Scheduled for withdrawal at Mark 26.

Replaced by C06PUF.

```
Call CO6PUF('F',m,n,cx,cwork,ifail)
x(1:m*n) = real(cx(1:m*n))
y(1:m*n) = aimag(cx(1:m*n))
```

where cx and cwork are complex arrays of lengths  $m \times n$  and  $n \times m + 2 \times n + 2 \times m + 30$  respectively.

### C06GBF

Scheduled for withdrawal at Mark 26. There is no replacement for this routine.

## C06GCF

Scheduled for withdrawal at Mark 26. There is no replacement for this routine.

# C06GOF

Scheduled for withdrawal at Mark 26. There is no replacement for this routine.

### C06GSF

Scheduled for withdrawal at Mark 26. There is no replacement for this routine.

### C06HAF

Scheduled for withdrawal at Mark 26. Replaced by C06RAF.

where y and rwork are real arrays of lengths  $m \times (n+2)$  and  $m \times n + 2 \times n + 15$  respectively.

# C06HBF

Scheduled for withdrawal at Mark 26.

Replaced by C06RAF.

where y and rwork are real arrays of lengths  $m \times (n+3)$  and  $m \times n + 2 \times n + 15$  respectively.

### C06HCF

Scheduled for withdrawal at Mark 26. Replaced by C06RCF.

```
Old: Call c06hcf(direct,m,n,x,init,trig,work,ifail)
New: y(1:m*n) = x(1:m*n)
        Call c06raf(direct,m,n,y,rwork,ifail)
        x(1:m*n) = y(1:m*n)
```

where y and rwork are real arrays of lengths  $m \times (n+2)$  and  $m \times n + 2 \times n + 15$  respectively.

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# C06HDF

Scheduled for withdrawal at Mark 26. Replaced by C06RDF.

```
Old: Call c06hdf(direct,m,n,x,init,trig,work,ifail)
New: y(1:m*n) = x(1:m*n)
        Call c06raf(direct,m,n,y,rwork,ifail)
        x(1:m*n) = y(1:m*n)
```

where y and rwork are real arrays of lengths  $m \times (n+2)$  and  $m \times n + 2 \times n + 15$  respectively.

# **D01 – Quadrature**

### D01BAF

Scheduled for withdrawal at Mark 26. Replaced by D01UAF.

```
Old: FUNCTION FUN(x)
       real(kind=nag_wp) :: FUN
       real(kind=nag_wp), intent(in) :: X
       FUN = ...
       END FUNCTION
       DINEST = D01BAF(D01XXX,A,B,N,FUN,IFAIL)
New : SUBROUTINE F(X,NX,FV,IFLAG,IUSER,RUSER)
      ! see example below
       END SUBROUTINE F
        integer :: key
        integer, allocatable :: iuser(:)
        real(kind=nag_wp), allocatable :: ruser(:)
       ! set KEY according to quadrature formula
       ! KEY = 0 : (D01XXX = D01BAZ)
       ! KEY = -3 : (D01XXX=D01BAY)
       ! KEY = -4 : (D01XXX=D01BAW)
       ! KEY = -5 : (D01XXX=D01BAX)
       ! KEY = ABS(KEY) for normal weights
       KEY = 0
       allocate(iuser(liuser), ruser(lruser))
       CALL DO1UAF(KEY, A, B, N, F, DINEST, IUSER, RUSER, IFAIL)
```

IUSER and RUSER are arrays available to allow you to pass information to the user-supplied subroutine F.

IFLAG is an integer which you may use to force an immediate exit from D01UAF in case of an error in the user-supplied subroutine F.

F may be used to call the original FUN as follows, although it may be more efficient to recode the integrand.

```
SUBROUTINE F(X,NX,FV,IFLAG,IUSER,RUSER)
...
integer, intent(in) :: NX
integer, intent(inout) :: iflag
real(kind=nag_wp), intent(in) :: X(NX)
real(kind=nag_wp), intent(out) :: fv(nx)
real(kind=wp) , intent(inout) :: ruser(*)
integer, intent(inout) :: iuser(*)
integer :: j
external FUN
```

```
do j=1,nx
  FV(j) = FUN(x(j))
enddo

END SUBROUTINE F
```

### D01BBF

Scheduled for withdrawal at Mark 26. Replaced by D01TBF.

The supplied subroutines D01XXX and the parameter ITYPE have been combined into a single parameter KEY. KEY < 0 is equivalent to ITYPE = 1 (adjusted weights). KEY > 0 is equivalent to ITYPE = 0 (normal weights). |KEY| indicates the quadrature rule.

```
|KEY| = 0: Gauss-Legendre (D01XXX = D01BAZ)

|KEY| = 3: Gauss-Laguerre (D01XXX = D01BAX)

|KEY| = 4: Gauss-Hermite (D01XXX = D01BAW)

|KEY| = 5: Rational Gauss (D01XXX = D01BAY)
```

# **D02 – Ordinary Differential Equations**

## D02BAF

Withdrawn at Mark 18.

Replaced by D02PEF and associated D02P routines.

IWSAV is an integer array of length 130 and RWSAV is a real array of length  $350 + 32 \times N$ .

IUSER and RUSER are arrays available to allow you to pass information to the user defined routine F2.

The definition of F2 can use the original routine FCN as follows:

```
SUBROUTINE F2(T,N,Y,YP,IUSER,RUSER)
       .. Scalar Arguments ..
!
      Real (Kind=wp), Intent (In)
                                               :: t
      Integer, Intent (In)
!
       .. Array Arguments ..
      Real (Kind=wp), Intent (Inout) :: ruser(1)
      Real (Kind=wp), Intent (In)
Real (Kind=wp), Intent (Out)
Integer, Intent (Inout)
                                           :: y(n)
                                              :: yp(n)
:: iuser(1)
       .. Procedure Arguments ..
      External
                                              :: fcn
       .. Executable Statements ..
       Continue
      Call fcn(t,y,yp)
    End Subroutine F2
```

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### D02BBF

Withdrawn at Mark 18.

Replaced by D02PEF and associated D02P routines.

IWSAV is an integer array of length 130 and RWSAV is a real array of length  $350 + 32 \times N$ .

IUSER and RUSER are arrays available to allow you to pass information to the user defined routine F2.

The definition of F2 can use the original routine FCN as follows:

```
SUBROUTINE F2(T,N,Y,YP,IUSER,RUSER)
!
      .. Scalar Arguments ..
     Real (Kind=wp), Intent (In)
                                       :: t
     Integer, Intent (In)
      .. Array Arguments ..
!
     Real (Kind=wp), Intent (Inout) :: ruser(1)
                                    :: y(n)
     Real (Kind=wp), Intent (In)
     Real (Kind=wp), Intent (Out)
                                      :: yp(n)
     Integer, Intent (Inout)
                                       :: iuser(1)
      .. Procedure Arguments ..
     External
                                       :: fcn
      .. Executable Statements ..
      Continue
     Call fcn(t,y,yp)
   End Subroutine F2
```

# D02BDF

Withdrawn at Mark 18.

Replaced by D02PEF and associated D02P routines.

IWSAV is an integer array of length 130 and RWSAV is a real array of length  $350 + 32 \times N$ .

IUSER and RUSER are arrays available to allow you to pass information to the user defined function F2.

The definition of F2 can use the original function FCN as follows:

```
SUBROUTINE F2(T,N,Y,YP,IUSER,RUSER)

! .. Scalar Arguments ..
Real (Kind=wp), Intent (In) :: t
Integer, Intent (In) :: n

! .. Array Arguments ..
Real (Kind=wp), Intent (Inout) :: ruser(1)
Real (Kind=wp), Intent (In) :: y(n)
Real (Kind=wp), Intent (Out) :: yp(n)
Integer, Intent (Inout) :: iuser(1)
```

## D02CAF

Withdrawn at Mark 18. Replaced by D02CJF.

```
Old: CALL DO2CAF(X,XEND,N,Y,TOL,FCN,W,IFAIL)
New: CALL DO2CJF(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 or USEd from the nag\_library MODULE. The array W needs to be 5 elements greater in length.

### D02CBF

Withdrawn at Mark 18. Replaced by D02CJF.

```
Old: CALL DO2CBF(X,XEND,N,Y,TOL,IRELAB,FCN,OUTPUT,W,IFAIL)
New: CALL DO2CJF(X,XEND,N,Y,FCN,TOL,RELABS,OUTPUT,DO2CJW,W,IFAIL)
```

D02CJW is a real function provided in the NAG Fortran Library and must be declared as EXTERNAL or USEd from the nag\_library MODULE. 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 (KIND=nag_wp) FUNCTION G(X,Y)
REAL (KIND=nag_wp) X,Y(*)
G = Y(M)-VAL
END
```

D02CJX is a subroutine provided in the NAG Fortran Library and must be declared as EXTERNAL or USEd from the nag\_library MODULE. 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 DO2CHF(X,XEND,N,Y,TOL,IRELAB,HMAX,FCN,G,W,IFAIL)
New: CALL DO2CJF(X,XEND,N,Y,FCN,TOL,RELABS,DO2CJX,G,W,IFAIL)
```

D02CJX is a subroutine provided by the NAG Fortran Library and must be declared as EXTERNAL or USEd from the nag\_library MODULE. The functionality of HMAX can be provided as described

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under the replacement call for D02CGF. 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,D02EJY,TOL,'M',D02EJX,D02EJW,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 or USEd from the nag\_library MODULE.

#### D02EBF

Withdrawn at Mark 18. Replaced by D02EJF.

```
Old: CALL DO2EBF(X,XEND,N,Y,TOL,IRELAB,FCN,MPED,PEDERV,OUTPUT,W,IW, & IFAIL)

New: CALL DO2EJF(X,XEND,N,Y,FCN,PEDERV,TOL,RELABS,OUTPUT,DO2EJW,W,IW, & IFAIL)
```

D02EJW is a real function provided in the NAG Fortran Library and must be declared as EXTERNAL or USEd from the nag\_library MODULE. 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 must be declared as EXTERNAL or USEd from the nag\_library MODULE.

#### D02EGF

Withdrawn at Mark 18. Replaced by D02EJF.

D02EJY and D02EJX are subroutines provided in the NAG Fortran Library and must be declared as EXTERNAL or USEd from the nag\_library MODULE. 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 DO2EHF(X,XEND,N,Y,TOL,IRELAB,HMAX,MPED,PEDERV,FCN,G,W,IFAIL)
New: CALL DO2EJF(X,XEND,N,Y,FCN,PEDERV,TOL,RELABS,DO2EJX,G,W,IW,IFAIL)
```

D02EJX is a subroutine provided by the NAG Fortran Library and must be declared as EXTERNAL or USEd from the nag\_library MODULE. The functionality of HMAX can be provided as described under the replacement call for D02EGF. 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 must be declared as EXTERNAL or USEd from the nag\_library MODULE.

### D02PAF

Withdrawn at Mark 18.

Replaced by D02PEF and associated D02P routines.

Existing programs should be modified to call D02PQF and D02PEF. The interfaces are significantly different and therefore precise details of a replacement call cannot be given. Please consult the appropriate routine documents.

### D02PCF

Scheduled for withdrawal at Mark 26.

Replaced by D02PEF and associated D02P routines.

IWSAV is an integer array of length 130 and RWSAV is a real array of length  $350 + 32 \times N$ .

IUSER and RUSER are arrays available to allow you to pass information to the user defined routine F2.

The definition of F2 can use the original routine F as follows:

```
SUBROUTINE F2(T,N,Y,YP,IUSER,RUSER)
!
      .. Scalar Arguments ..
     Real (Kind=wp), Intent (In)
                                       :: t
     Integer, Intent (In)
                                       :: n
!
     .. Array Arguments ..
     Real (Kind=wp), Intent (Inout)
                                       :: ruser(1)
     Real (Kind=wp), Intent (In)
                                       :: y(n)
     Real (Kind=wp), Intent (Out)
                                      :: yp(n)
     Integer, Intent (Inout)
                                      :: iuser(1)
     .. Procedure Arguments ..
     External
                                       :: f
     .. Executable Statements ..
     Continue
     Call f(t,y,yp)
     Return
   End Subroutine F2
```

### D02PDF

Scheduled for withdrawal at Mark 26.

Replaced by D02PFF and associated D02P routines.

IWSAV is an integer array of length 130 and RWSAV is a real array of length  $350 + 32 \times N$ .

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IUSER and RUSER are arrays available to allow you to pass information to the user defined routine F2. The definition of F2 can use the original routine F as follows:

```
SUBROUTINE F2(T,N,Y,YP,IUSER,RUSER)
!
      .. Scalar Arguments ..
      Real (Kind=wp), Intent (In)
                                          :: t
      Integer, Intent (In)
                                          :: n
!
      .. Array Arguments ..
      Real (Kind=wp), Intent (Inout) :: ruser(1)
      Real (Kind=wp), Intent (In)
Real (Kind=wp), Intent (Out)
                                          :: y(n)
                                          :: yp(n)
      Integer, Intent (Inout)
                                          :: iuser(1)
      .. Procedure Arguments ..
      External
                                          :: f
1
      .. Executable Statements ..
      Continue
      Call f(t,y,yp)
      Return
   End Subroutine F2
```

### D02PVF

Scheduled for withdrawal at Mark 26. Replaced by D02PQF.

See D02PCF and D02PDF for further information.

## D02PWF

Scheduled for withdrawal at Mark 26.
Replaced by D02PRF.

```
Old: CALL DO2PWF(TENDNU,IFAIL)
New: CALL DO2PRF(TENDNU,IWSAV,RWSAV,IFAIL)
```

IWSAV is an integer array of length 130 and RWSAV is a real array of length 350.

## D02PXF

Scheduled for withdrawal at Mark 26. Replaced by D02PSF.

IWSAV is an integer array of length 130 and RWSAV is a real array of length  $350 + 32 \times N$ .

IUSER and RUSER are arrays available to allow you to pass information to the user defined routine F2.

The definition of F2 can use the original routine F as follows:

```
SUBROUTINE F2(T,N,Y,YP,IUSER,RUSER)
! .. Scalar Arguments ..
Real (Kind=wp), Intent (In) :: t
Integer, Intent (In) :: n
```

```
! .. Array Arguments ..
Real (Kind=wp), Intent (Inout) :: ruser(1)
Real (Kind=wp), Intent (In) :: y(n)
Real (Kind=wp), Intent (Out) :: yp(n)
Integer, Intent (Inout) :: iuser(1)
! .. Procedure Arguments ..
External :: f
! .. Executable Statements ..
Continue

Call f(t,y,yp)

Return
End Subroutine F2
```

## D02PYF

Scheduled for withdrawal at Mark 26. Replaced by D02PTF.

```
Old: Call DO2PYF(TOTFCN,STPCST,WASTE,STPSOK,HNEXT,IFAIL)
New: Call DO2PTF(TOTFCN,STPCST,WASTE,STPSOK,HNEXT,IWSAV, & RWSAV,IFAIL)
```

IWSAV is an integer array of length 130 and RWSAV is a real array of length 350.

## D02PZF

Scheduled for withdrawal at Mark 26. Replaced by D02PUF.

```
Old: Call DO2PZF(RMSERR, ERRMAX, TERRMX, WORK, IFAIL)
New: Call DO2PUF(N, RMSERR, ERRMAX, TERRMX, IWSAV, RWSAV, IFAIL)
```

N must be unchanged from that passed to D02PQF.

IWSAV is an integer array of length 130 and RWSAV is a real array of length  $350 + 32 \times N$ .

# D02QDF

Withdrawn at Mark 17. Replaced by D02NBF or D02NCF.

Existing programs should be modified to call D02NSF, D02NVF and D02NBF, or D02NVF, 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. Replaced by D02NBF or D02NCF.

# D02XAF

Withdrawn at Mark 18.

Replaced by D02PSF and associated D02P routines.

Not needed except with D02PAF.

# D02XBF

Withdrawn at Mark 18.

Replaced by D02PSF and associated D02P routines.

Not needed except with D02PAF.

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# D02YAF

Withdrawn at Mark 18.

Replaced by D02PFF and associated D02P routines.

There is no precise equivalent to this routine.

# **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

### 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.

# E04 - Minimizing or Maximizing a Function

### E04CCF/E04CCA

```
Withdrawn at Mark 24. Replaced by E04CBF.
```

```
Old: CALL E04CCF(N,X,F,TOL,IW,W1,W2,W3,W4,W5,W6,FUNCT,MONIT,MAXCAL, & IFAIL)

Or

CALL E04CCA(N,X,F,TOL,IW,W1,W2,W3,W4,W5,W6,FUNCT2,MONIT2,MAXCAL, & IUSER,RUSER,IFAIL)

New: CALL E04CBF(N,X,F,TOLF,TOLX,FUNCT2,MONIT3,MAXCAL,IUSER,RUSER, & IFAIL)
```

The new routine can be derived from the old as follows:

```
SUBROUTINE MONIT3(FMIN,FMAX,SIM,N,NCALL,SERROR,VRATIO,IUSER,
RUSER)

INTEGER N, NCALL, IUSER(*)
REAL (KIND=nag_wp) FMIN, FMAX, SIM(N+1,N), SERROR, VRATIO, RUSER(*)

CALL MONIT2(FMIN,FMAX,SIM,N,N+1,NCALL,IUSER,RUSER)

! Add code here to monitor the values of SERROR and VRATIO, if necessary
RETURN
END
```

### 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 or be a module subprogram USEd 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 (KIND=nag_wp) XC(N), FVECC(M), USER(*)

CALL LSFUN1(M,N,XC,FVECC)

RETURN
END
```

In general the extra parameters, IUSER and USER, should be declared in the calling program as IUSER(1) and USER(1), but will not need initializing. If however, a COMMON block was used to pass information into LSFUN1, or get information from LSFUN1, then the arrays IUSER and USER should be declared appropriately and used for this purpose.

# 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 or be a module subprogram USEd in the calling (sub)program. In

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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 (KIND=nag_wp) XC(N), FVECC(M), FJACC(LJC,N), USER(*)

CALL LSFUN2(M,N,XC,FVECC,FJACC,LJC)

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 initializing. If however, a COMMON block was used to pass information through E04GCF into LSFUN2, or get information from LSFUN2, then the arrays IUSER and USER 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 or be a module subprogram USEd 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 (KIND=nag_wp) XC(N), FVECC(M), FJACC(LJC,N), USER(*)
CALL LSFUN2(M,N,XC,FVECC,FJACC,LJC)
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 initializing. If however, a COMMON block was used to pass information through E04GEF into LSFUN2, or get information from LSFUN2, then the arrays IUSER and USER should be declared appropriately and used for this purpose.

# E04HFF

Withdrawn at Mark 19. Replaced by E04HYF.

```
Old: CALL EO4HFF(M,N,X,FSUMSQ,IW,LIW,W,LW,IFAIL)
New: CALL EO4HYF(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 be declared as EXTERNAL or be a module subprogram USEd 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 (KIND=nag_wp) XC(N), FVECC(M), FJACC(LJC,N), USER(*)

CALL LSFUN2(M,N,XC,FVECC,FJACC,LJC)

RETURN
END

SUBROUTINE LSHES(M,N,FVECC,XC,B,LB,IUSER,USER)
INTEGER M, N, LB, IUSER(*)
REAL (KIND=nag_wp) FVECC(M), XC(N), B(LB), USER(*)
```

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```
CALL LSHES2(M,N,FVECC,XC,B,LB)
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 initializing. If, however, a COMMON block was used to pass information through E04HFF into LSFUN2 or LSHES2, or to get information from LSFUN2 or LSHES2, then the arrays IUSER and RUSER 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 or be a module subprogram USEd 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 (KIND=nag_wp) XC(N), FC, USER(*)

CALL FUNCT1(N,XC,FC)

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 initializing.

# E04KAF

Withdrawn at Mark 19. Replaced by E04KYF.

```
Old: CALL EO4KAF(N, IBOUND, BL, BU, X, F, G, IW, LIW, W, LW, IFAIL)
New: CALL EO4KYF(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 or be a module subprogram USEd 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 (KIND=nag_wp) XC(N), FC, GC(N), USER(*)

CALL FUNCT2(N,XC,FC,GC)

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 initializing.

# E04KCF

Withdrawn at Mark 19. Replaced by E04KZF.

```
Old: CALL EO4KCF(N, IBOUND, BL, BU, X, F, G, IW, LIW, W, LW, IFAIL)
New: CALL EO4KZF(N, IBOUND, FUNCT, BL, BU, X, F, G, IW, LIW, W, LW, IUSER, USER, IFAIL)
```

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FUNCT appears in the parameter list instead of the fixed-name subroutine FUNCT2 of E04KCF. FUNCT must be declared as EXTERNAL or be a module subprogram USEd 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 (KIND=nag_wp) XC(N), FC, GC(N), USER(*)

CALL FUNCT2(N,XC,FC,GC)

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 initializing.

#### E04LAF

Withdrawn at Mark 19. Replaced by E04LYF.

```
Old: CALL EO4LAF(N, IBOUND, BL, BU, X, F, G, IW, LIW, W, LW, IFAIL)

New: CALL EO4LYF(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 be declared as EXTERNAL or be a module subprogram USEd in the calling (sub)program. In addition they have an extra two parameters, IUSER and USER, over and above those of FUNCT2 and HESS2. They may be derived from FUNCT2 and HESS2 as follows:

```
FUNCT(N, XC, FC, GC, IUSER, USER)
SUBROUTINE
INTEGER
                    N, IUSER(*)
REAL (KIND=nag_wp) XC(N), FC, GC(N), USER(*)
CALL FUNCT2(N,XC,FC,GC)
RETURN
END
                    HESS(N, XC, HESLC, LH, HESDC, IUSER, USER)
SUBROUTINE
                    N, LH, IUSER(*)
TNTEGER
REAL (KIND=nag_wp) XC(N), HESLC(LH), HESDC(N), USER(*)
CALL HESS2(N,XC,HESLC,LH,HESDC)
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 initializing.

# E04MBF

Withdrawn at Mark 18. Replaced by E04MFF/E04MFA.

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

New: CALL EO4MFF(N,NCLIN,A,NROWA,BL,BU,CVEC,ISTATE,X,ITER,OBJLP, & AX,CLAMDA,IWORK,LIWORK,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.

## E04MZF

Scheduled for withdrawal at Mark 26. Replaced by E04MXF.

```
014.
mpslst = .false.
                     ! or = .true.
Call E04MZF(infile,maxn,maxm,maxnnz,xbldef,xbudef,mpslst,n,m,nnz,iobj, &
         ncolh,a,irowa,iccola,bl,bu,start,pnames,nname,crname,xs,istate,ifail)
 if (ifail==1 .or. ifail==2 .or. ifail==3) then
  ! not enough memory, allocate bigger arrays as given in M, N, NNZ
   ! and call EO4MZF again
 else if (ifail>=4 .and. ifail<=16) then
   ! MPS input file formating error
   ! stop
 else if (ifail==17) then
   ! wrong arguments to EO4MZF
   ! stop
 else if (ifail==0) then
  ! data successfully read, call solver
 end if
New:
mpslst = 0
                 ! or = 1
 Call E04MXF(infile, maxn, maxm, maxnnz, maxncolh, maxnnzh, maxlintvar, &
       mpslst,n,m,nnz,ncolh,nnzh,lintvar,iobj,a,irowa,iccola,bl,bu,pnames, &
       nname,crname,h,irowh,iccolh,minmax,intvar,ifail)
 if (ifail==2) then
   ! not enough memory, allocate bigger arrays as given in M, N, NNZ, NCOLH,
   ! NNZH, LINTVAR and call EO4MXF again
 else if (ifail>=3 .and. ifail<=35) then
   ! MPS input file formatting error
 else if (ifail==36) then
   ! wrong input argument
   ! stop
 else if (ifail=-999) then
   ! internal memory allocation error
 else if (ifail==0 .or. ifail==1) then
   ! data successfully read (with possible warning)
   start = 'C'
   do j=1,n
    xs(j) = min(max(0.0_nag_wp,bl(j)),bu(j))
     istate(j) = 0.0_nag_wp
   end do
   ! call solver
end if
```

E04MXF has extended the functionality of E04MZF and the interface has changed substantially. If there are integer variables, a quadratic part of the objective function or OBJSENSE section, E04MXF will read them and return them in the new parameters (LINTVAR, INTVAR, NCOLH, NNZH, H, IROWH, ICCOLH and MINMAX), with E04MZF these caused a file formatting error. The new routine E04MXF might also accept a slightly misformatted input files and return a warning IFAIL = 1.

The type of parameter MPSLST has changed from logical to integer.

Parameters XBLDEF, XBUDEF from E04MZF were removed and fixed in E04MXF to their default values 0 and  $10^{20}$ , respectively. Note that value  $10^{20}$  within bounds is interpreted in our solvers as  $+\infty$  (unconstrained).

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Parameters START, XS, ISTATE were present in E04MZF only for the convenience of calling the solver routine E04NKF/E04NKA and have been removed from E04MXF.

Should you need any assistance, please do not hesitate to contact NAG.

#### **E04NAF**

Withdrawn at Mark 18. Replaced by E04NFF/E04NFA.

```
Old: CALL EO4NAF(ITMAX,MSGLVL,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 EO4NFF(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 (KIND=nag_wp) HESS(NROWH,NCOLH), X(N), HX(N)

New: SUBROUTINE QPHESS(N,JTHCOL,HESS,NROWH,X,HX)

INTEGER N, JTHCOL, NROWH

REAL (KIND=nag_wp) HESS(NROWH,*), X(N), HX(N)
```

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

E04NFF/E04NFA contains one additional parameter as follows:

```
AX(*) – 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.

# E04UNF

Withdrawn at Mark 22. Replaced by E04USF/E04USA.

```
Old: CALL EO4UNF(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, & RUSER,IFAIL)

New: CALL EO4USF(M,N,NCLIN,NCNLN,LDA,LDCJ,LDFJ, & LDR,A,BL,BU,Y,CONFUN,OBJFUN,ITER, & ISTATE,C,CJAC,F,FJAC,CLAMDA,OBJF, & R,X,IWORK,LIWORK,WORK,LWORK,IUSER, & RUSER,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,RUSER)
INTEGER MODE,M,N,LDFJ,NSTATE,IUSER(*)
REAL (KIND=nag_wp) X(N),F(*),FJAC(LDFJ,*),RUSER(*)

New: SUBROUTINE OBJFUN(MODE,M,N,LDFJ,NEEDFI,X,F,FJAC,NSTATE, & IUSER,RUSER)
INTEGER MODE,M,N,LDFJ,NEEDFI,NSTATE,IUSER(*)
REAL (KIND=nag_wp) X(N),F(*),FJAC(LDFJ,*),RUSER(*)
```

See the routine documents for further information.

## E04UPF

Withdrawn at Mark 19. Replaced by E04USF/E04USA.

```
Old: CALL EO4UPF(M,N,NCLIN,NCNLN,LDA,LDCJ,LDFJ,LDR,A,BL,BU, & CONFUN,OBJFUN,ITER,ISTATE,C,CJAC,F,FJAC, & CLAMDA,OBJF,R,X,IWORK,LIWORK,WORK,LWORK, & IUSER,USER,IFAIL)

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

E04USF/E04USA contains one additional parameter as follows:

```
Y(M) – 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, ..., 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 (KIND=nag_wp) 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 (KIND=nag_wp) X(N),F(*),FJAC(LDFJ,*),USER(*)
```

See the routine documents for further information.

### E04VCF

Withdrawn at Mark 17. Replaced by E04UCF/E04UCA.

```
Old: CALL EO4VCF(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 EO4UCF(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 (KIND=nag_wp) X(N), OBJF, OBJGRD(N)

New: SUBROUTINE OBJFUN(MODE,N,X,OBJF,OBJGRD,NSTATE,IUSER,USER)
INTEGER Mode, N, NSTATE, IUSER(*)
REAL (KIND=nag_wp) 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 (KIND=nag_wp) 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 (KIND=nag_wp) X(N), C(NCNLN), CJAC(NROWJ,N), USER(*)
```

If NCNLN = 0, then the name of the dummy routine E04VDM/E54VDM may need to be changed to E04UDM 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:

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```
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.

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 (KIND=nag_wp) X(N), OBJF, OBJGRD(N)

New: SUBROUTINE OBJFUN(MODE,N,X,OBJF,OBJGRD,NSTATE,IUSER,USER)
INTEGER MODE, N, NSTATE, IUSER(*)
REAL (KIND=nag_wp) 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 (KIND=nag_wp) 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 (KIND=nag_wp) X(N), C(NCNLN), CJAC(NROWJ,N), USER(*)
```

If NCNLN = 0, then the name of the dummy routine E04VDM/E54VDM may need to be changed to E04UDM 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(LDR,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.

# E04ZCF/E04ZCA

Withdrawn at Mark 24.

There is no replacement for this routine.

# F01 - Matrix Operations, Including Inversion

## F01AAF

Withdrawn at Mark 17.

Replaced by F07ADF (DGETRF) and F07AJF (DGETRI).

```
Old: CALL F01AAF(A,IA,N,X,IX,WKSPCE,IFAIL)

New: CALL DGETRF(N,N,A,IA,IPIV,INFO)

CALL F06QFF('General',N,N,A,IA,X,IX)

CALL DGETRI(N,X,IX,IPIV,WKSPCE,LWORK,INFO)
```

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

### F01AEF

Withdrawn at Mark 18.

Replaced by F07FDF (DPOTRF), F08SEF (DSYGST) and F06EGF (DSWAP).

INFO is set to a positive value if the matrix B is not positive definite. It is essential to test IFAIL.

# F01AFF

Withdrawn at Mark 18.

Replaced by F06EGF (DSWAP) and F06YJF (DTRSM).

## F01AGF

Withdrawn at Mark 18.

Replaced by F08FEF (DSYTRD).

```
Old: CALL F01AGF(N,TOL,A,IA,D,E,E2)
New: CALL DSYTRD('L',N,A,IA,D,E(2),TAU,WORK,LWORK,INFO)
        E(1) = 0.0D0
        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 (DSYTRD) is different from that computed by F01AGF, but it has the same eigenvalues.

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# F01AHF

Withdrawn at Mark 18.

Replaced by F08FGF (DORMTR).

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

```
Old: CALL FO1AHF(N,M1,M2,A,IA,E,Z,IZ)
New: CALL DORMTR('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 (DSYTRD) and F08FFF (DORGTR).

```
Old: CALL F01AJF(N,TOL,A,IA,D,E,Z,IZ)
New: CALL DSYTRD('L',N,A,IA,D,E(2),TAU,WORK,LWORK,INFO)
    E(1) = 0.0D0
    CALL F06QFF('L',N,N,A,IA,Z,IZ)
    CALL DORGTR('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 (DSYTRD) and F08FFF (DORGTR) are different from those computed by F01AJF, but they satisfy the same relation  $Q^{T}AQ = T$ .

## F01AKF

Withdrawn at Mark 18.

Replaced by F08NEF (DGEHRD).

```
Old: CALL FO1AKF(N,K,L,A,IA,INTGER)
New: CALL DGEHRD(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 (DGEHRD) is different from that computed by F01AKF, because F08NEF (DGEHRD) uses orthogonal transformations, whereas F01AKF uses stabilized elementary transformations.

## F01ALF

Withdrawn at Mark 18.

Replaced by F08NGF (DORMHR).

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

```
Old: CALL F01ALF(K,L,IR,A,IA,INTGER,Z,IZ,N)
New: CALL DORMHR('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 (ZGEHRD).

```
10 CONTINUE
20 CONTINUE
CALL ZGEHRD(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 (ZGEHRD) is different from that computed by F01AMF, because F08NSF (ZGEHRD) uses orthogonal transformations, whereas F01AMF uses stabilized elementary transformations.

### F01ANF

Withdrawn at Mark 18. Replaced by F08NUF (ZUNMHR).

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

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 F06QFF and F08NFF (DORGHR).

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

```
Old: CALL FO1APF(N,K,L,INTGER,H,IH,V,IV)

New: CALL FO6QFF('L',N,N,H,IH,V,IV)

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

### F01ATF

Withdrawn at Mark 18.

Replaced by F08NHF (DGEBAL).

```
Old: CALL FO1ATF(N,IB,A,IA,K,L,D)
New: CALL DGEBAL('B',N,A,IA,K,L,D,INFO)
```

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

### F01AUF

```
Withdrawn at Mark 18.
```

Replaced by F08NJF (DGEBAK).

```
Old: CALL FO1AUF(N,K,L,M,D,Z,IZ)
New: CALL DGEBAK('B','R',N,K,L,D,M,Z,IZ,INFO)
```

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# F01AVF

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

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

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

### F01AWF

Withdrawn at Mark 18.

Replaced by F08NWF (ZGEBAK).

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

# F01AXF

Withdrawn at Mark 18.

Replaced by F06EFF (DCOPY) and F08BEF (DGEQPF).

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

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

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

# F01AYF

Withdrawn at Mark 18.

Replaced by F08GEF (DSPTRD).

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

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

### F01AZF

Withdrawn at Mark 18. Replaced by F08GGF (DOPMTR).

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

```
Old: CALL FO1AZF(N,M1,M2,A,IA,Z,IZ) New: CALL DOPMTR('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 (ZHETRD) and F08FTF (ZUNGTR).

```
Old: CALL FO1BCF(N, TOL, AR, IAR, AI, IAI, D, E, WK1, WK2)
New: DO 20 J = 1, N
        DO 10 I = 1, N
           A(I,J) = CMPLX(AR(I,J),AI(I,J),KIND=nag\_wp)
  10
        CONTINUE
  20 CONTINUE
     CALL ZHETRD('L',N,A,IA,D,E(2),TAU,WORK,LWORK,INFO)
     E(1) = 0.0D0
     CALL ZUNGTR('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) = AIMAG(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 (ZHETRD) and F08FTF (ZUNGTR) are different from those computed by F01BCF, but they satisfy the same relation  $Q^{H}AQ = T$ .

# F01BDF

Withdrawn at Mark 18.

Replaced by F07FDF (DPOTRF), F08SEF (DSYGST) and F06EGF (DSWAP).

```
Old: CALL FO1BDF(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 DPOTRF('L',N,B,IB,INFO)
     IF (INFO.EQ.O) THEN
        CALL DSYGST(2,'L',N,A,IA,B,IB,INFO)
     ELSE
        IFAIL = 1
     END IF
     CALL DSWAP(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.

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## F01BEF

Withdrawn at Mark 18.

Replaced by F06YFF (DTRMM) and F06EGF (DSWAP).

#### F01BNF

Withdrawn at Mark 17. Replaced by F07FRF (ZPOTRF).

```
Old: CALL FO1BNF(N,A,IA,P,IFAIL)
New: CALL ZPOTRF('Upper',N,A,IA,INFO)
```

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 (ZPOTRF) and F07FWF (ZPOTRI).

```
Old: CALL FO1BPF(N,A,IA,V,IFAIL)

New: CALL ZPOTRF('Upper',N,A,IA,INFO)

CALL ZPOTRI('Upper',N,A,IA,INFO)
```

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.

### F01BTF

Withdrawn at Mark 18. Replaced by F07ADF (DGETRF).

```
Old: CALL FO1BTF(N,A,IA,P,DP,IFAIL)
New: CALL DGETRF(N,N,A,IA,IPIV,INFO)
```

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

# F01BWF

Withdrawn at Mark 18.

Replaced by F08HEF (DSBTRD).

```
Old: CALL F01BWF(N,M1,A,IA,D,E)

New: CALL DSBTRD('N','U',N,M1-1,A,IA,D,E(2),Q,1,WORK,INFO)

E(1) = 0.0D0
```

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

### F01BXF

Withdrawn at Mark 17. Replaced by F07FDF (DPOTRF).

```
Old: CALL FO1BXF(N,A,IA,P,IFAIL)
New: CALL DPOTRF('Upper',N,A,IA,INFO)
```

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).

# F01LBF

Withdrawn at Mark 18. Replaced by F07BDF (DGBTRF).

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

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

#### F01MAF

Withdrawn at Mark 19. Replaced by F11JAF.

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

# F01NAF

Withdrawn at Mark 17. Replaced by F07BRF (ZGBTRF).

```
Old: CALL FO1NAF(N,ML,MU,A,NRA,TOL,IN,SCALE,IFAIL)
New: CALL ZGBTRF(N,N,ML,MU,A,NRA,IN,INFO)
```

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

# F01QCF

Withdrawn at Mark 18. Replaced by F08AEF (DGEQRF).

```
Old: CALL FO1QCF(M,N,A,LDA,ZETA,IFAIL)
New: CALL DGEQRF(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 (DGEQRF) are not the same as those returned by F01QCF. Subsequent calls to F01QDF or F01QEF must also be replaced by calls to F08AFF (DORGQR) or F08AGF (DORMQR) as shown below.

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# F01QDF

Withdrawn at Mark 18. Replaced by F08AGF (DORMQR).

The following replacement is valid only if the previous call to F01QCF has been replaced by a call to F08AEF (DGEQRF) as shown below or if the previous call to F01QFF has been replaced by a call to F08BEF (DGEQPF) as shown below. It also assumes that the second argument of F01QDF is set to WHERET = '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 DORMQR('L',TRANS,M,NCOLB,N,A,LDA,ZETA,B,LDB,WORK,LWORK,INFO)
```

where LWORK is the actual length of WORK.

# F01QEF

Withdrawn at Mark 18. Replaced by F08AFF (DORGQR).

The following replacement is valid only if the previous call to F01QCF has been replaced by a call to F08AEF (DGEQRF) as shown above or if the previous call to F01QFF has been replaced by a call to F08BEF (DGEQPF) as shown below. It also assumes that the first argument of F01QEF is set to WHERET = 'S', which is appropriate if the contents of A and ZETA have not been changed after the call of F01QCF.

```
Old: CALL FO1QEF('S',M,N,NCOLQ,A,LDA,ZETA,WORK,IFAIL)
New: CALL DORGQR(M,NCOLQ,N,A,LDA,ZETA,WORK,LWORK,INFO)
```

where LWORK is the actual length of WORK.

## F01QFF

Withdrawn at Mark 18. Replaced by F08BEF (DGEQPF).

The following replacement assumes that the first argument of F01QFF (PIVOT) is  $^{\prime}$ C'. There is no direct replacement if PIVOT =  $^{\prime}$ 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 DGEQPF(M,N,A,LDA,PERM,ZETA,WORK,INFO)
```

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

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

### F01RCF

Withdrawn at Mark 18. Replaced by F08ASF (ZGEQRF).

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

```
Old: CALL FO1RCF(M,N,A,LDA,THETA,IFAIL)
New: CALL ZGEQRF(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.

## F01RDF

Withdrawn at Mark 18. Replaced by F08AUF (ZUNMQR).

The following replacement is valid only if the previous call to F01RCF has been replaced by a call to F08ASF (ZGEQRF) as shown below or if the previous call to F01RFF has been replaced by a call to F08BSF (ZGEQPF) as shown below. It also assumes that the second argument of F01RDF is set to WHERET = 'S', which is appropriate if the contents of A and THETA have not been changed after the call of F01RCF.

```
Old: CALL FO1RDF(TRANS,'S',M,N,A,LDA,THETA,NCOLB,B,LDB,WORK,IFAIL)
New: CALL ZUNMQR('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 (ZUNGQR).

The following replacement is valid only if the previous call to F01RCF has been replaced by a call to F08ASF (ZGEQRF) as shown below or if the previous call to F01RFF has been replaced by a call to F08BSF (ZGEQPF) as shown below. It also assumes that the first argument of F01REF is set to WHERET = 'S', which is appropriate if the contents of A and THETA have not been changed after the call of F01RCF.

```
Old: CALL FO1REF('S',M,N,NCOLQ,A,LDA,THETA,WORK,IFAIL)
New: CALL ZUNGQR(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 (ZGEOPF).

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

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

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

# F02 – Eigenvalues and Eigenvectors

# F02AAF

```
Withdrawn at Mark 18.
Replaced by F08FAF (DSYEV).
```

```
Old: CALL F02AAF(A,IA,N,R,E,IFAIL)
New: CALL DSYEV('N','L',N,A,IA,R,WORK,LWORK,INFO)
IF (INFO.NE.O) THEN ...
```

where WORK is a real array of length at least  $(3 \times N)$  and LWORK is its actual length. Larger values of LWORK, up to some optimal value, may improve performance.

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## F02ABF

```
Withdrawn at Mark 18.

Replaced by F08FAF (DSYEV).

Old: CALL F02ABF(A,IA,N,R,V,IV,E,IFAIL)

New: CALL F06QFF('L',N,N,A,IA,V,IV)

CALL DSYEV('V','L',N,V,IV,R,WORK,LWORK,INFO)

IF (INFO.NE.O) THEN ...
```

where WORK is a real array of length at least  $(3 \times N)$  and LWORK is its actual length. Larger values of LWORK, up to some optimal value, may improve performance. 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 F08SAF (DSYGV).

Old: CALL F02ADF(A,IA,B,IB,N,R,DE,IFAIL)

New: CALL DSYGV(1,'N','U',N,A,IA,B,IB,R,WORK,LWORK,INFO)

IF (INFO.NE.O) THEN ...
```

where WORK is a real array of length at least  $(3 \times N)$  and LWORK is its actual length. Larger values of LWORK, up to some optimal value, may improve performance.

Note that the call to F08SAF (DSYGV) 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 F08SAF (DSYGV).

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 DSYGV(1,'V','U',N,V,IV,B,IB,R,WORK,LWORK,INFO)

IF (INFO.NE.O) THEN
```

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

Note that the call to F08SAF (DSYGV) will overwrite the upper triangle of the array B and leave the subdiagonal elements unchanged, whereas the call to F02AEF 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 F08NAF (DGEEV).

Old: CALL F02AFF(A,IA,N,RR,RI,INTGER,IFAIL)
New: CALL DGEEV('N','N',N,A,IA,RR,RI,VR,1,VI,1, & WORK,LWORK,INFO)
IF (INFO.EQ.O) THEN
```

where VR and VI are real arrays of length (1) (not used in this call), WORK is a real array of length at least  $(4 \times N)$  and LWORK is its actual length; the iteration counts (returned by F02AFF in the array INTGER) are not available from F08NAF (DGEEV). Larger values of LWORK, up to some optimal value, may improve performance.

### F02AGF

Withdrawn at Mark 18. Replaced by F08NAF (DGEEV).

where WORK is a real array of length at least  $(4 \times N)$  and LWORK is its actual length; the iteration counts (returned by F02AGF in the array INTGER) are not available from F08NAF (DGEEV). Larger values of LWORK, up to some optimal value, may improve performance.

### F02AJF

Withdrawn at Mark 18. Replaced by F08NNF (ZGEEV).

where A is a complex array of dimension (LDA, N), LDA must be at least max(1,N), R is a complex array of dimension (N), VR and VL are dummy complex array of length (1) (not used in this call), RWORK is a real array of length at least  $(2 \times N)$ , WORK is a complex array of length at least  $(2 \times N)$  and LWORK is its actual length. Larger values of LWORK, up to some optimal value, may improve performance. The iteration counts (returned by F02AJF in the array INTGER) are not available from F08NNF (ZGEEV).

### F02AKF

Withdrawn at Mark 18. Replaced by F08NNF (ZGEEV).

```
Old: CALL FO2AKF(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),KIND=nag_wp)
  10
        CONTINUE
  20 CONTINUE
     CALL ZGEEV('N','V',N,A,LDA,R,VL,LDVL,VR1,LDVR,
                  WORK, LWORK, RWORK, INFO)
     IF (INFO.EQ.O) THEN
        DO 40 J = 1, N
           RR(J) = REAL(R(J))
           RI(J) = AIMAG(R(J))
           DO 30 I = 1, N
               VR(I,J) = REAL(VR1(I,J))
               VI(I,J) = AIMAG(VR1(I,J))
  30
           CONTINUE
```

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```
40 CONTINUE
```

where A is a complex array of dimension (LDA, N), LDA is at least max(1, N), R is a complex array of length (N), VL is a complex array of dimension (1,1), LDVL is 1, VR1 is a complex array of dimension (LDVR, N), LDVR is at least max(1, N), RWORK is a real array of length at least  $(2 \times N)$ , WORK is a complex array of length at least  $(2 \times N)$  and LWORK is its actual length. Larger values of LWORK, up to some optimal value, may improve performance. The iteration counts (returned by F02AKF in the array INTGER) are not available from F08NNF (ZGEEV).

## F02AMF

```
Withdrawn at Mark 18. Replaced by F08JEF (DSTEQR). Old: CALL F02AMF(N,EPS,D,E,V,IV,IFAIL) New: CALL DSTEQR('V',N,D,E(2),V,IV,WORK,INFO) where WORK is a real array of length at least (2 \times (N-1)).
```

### F02ANF

Withdrawn at Mark 18. Replaced by F08PSF (ZHSEQR).

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 (DHSEQR).

Old: CALL F02APF(N,EPS,H,IH,RR,RI,ICNT,IFAIL)

New: CALL DHSEQR('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  $(3 \times N)$ ; the iteration counts (returned by F02APF in the array ICNT) are not available from F08PEF (DHSEQR).

### F02AQF

Withdrawn at Mark 18.

Replaced by F08PEF (DHSEOR) and F08OKF (DTREVC).

```
Old: CALL FO2AQF(N,K,L,EPS,H,IH,V,IV,RR,RI,INTGER,IFAIL)

New: CALL DHSEQR('S','V',N,K,L,H,IH,RR,RI,V,IV,WORK,1,INFO)

CALL DTREVC('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  $(3 \times N)$ ; the iteration counts (returned by F02AQF in the array INTGER) are not available from F08PEF (DHSEQR); M is an integer which is set to N by F08QKF (DTREVC).

## F02ARF

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

```
Old: CALL FO2ARF(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),KIND=nag_wp)
  10
        CONTINUE
  20 CONTINUE
     CALL ZHSEQR('S','V',N,K,L,H,IH,R,V,IV,WORK,1,INFO)
     CALL ZTREVC('R','O',SELECT,N,H,IH,V,IV,V,IV,N,M,WORK,RWORK,INFO)
     DO 40 J = 1, N
        RR(J) = REAL(R(J))
        RI(J) = AIMAG(R(J))
        DO 30 I = 1, N
           VR(I,J) = REAL(V(I,J))
           VI(I,J) = AIMAG(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  $(2 \times N)$  and RWORK is a real array of length at least (N); M is an integer which is set to N by F08QXF (ZTREVC).

If F02ARF was preceded by a call to F01AMF to reduce a full complex matrix to Hessenberg form, then the call to F01AMF must also be replaced by calls to F08NSF (ZGEHRD) and F08NTF (ZUNGHR). IH must be  $\geq \max(1, N)$  and IV must be  $\geq \max(1, N)$ .

## F02AVF

```
Withdrawn at Mark 18.
Replaced by F08JFF (DSTERF).

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

### F02AWF

Withdrawn at Mark 18. Replaced by F08FNF (ZHEEV).

where A is a complex array of dimension (LDA, N), LDA is at least max(1, N) RWORK is a real array of length at least  $max(1, 3 \times N - 2)$ , WORK is a complex array of length at least  $(2 \times N)$  and LWORK is its actual length. Larger values of LWORK, up to some optimal value, may improve performance.

### F02AXF

```
Withdrawn at Mark 18.
Replaced by F08FNF (ZHEEV).
```

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```
CALL F06TFF('L',N,N,A,LDA,V,LDV)

CALL ZHEEV('V','L',N,V,LDV,R,WORK,LWORK,RWORK,INFO)

IF (INFO.EQ.0) THEN

DO 40 J = 1, N

DO 30 I = 1, N

VR(I,J) = REAL(V(I,J))

VI(I,J) = AIMAG(V(I,J))

CONTINUE

40 CONTINUE
```

where A is a complex array of dimension (LDA, N), LDA is at least max(1,N), V is a complex array of dimension (LDV, N), LDV is at least max(1,N), RWORK is a real array of length at least  $max(1,3\times N-2)$ , WORK is a complex array of length at least  $(2\times N)$  and LWORK is its actual length. If F02AXF was called with the same arrays supplied for VR and AR and for VI and AI, then the call to F06TFF may be omitted.

#### F02AYF

Withdrawn at Mark 18. Replaced by F08JSF (ZSTEQR).

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

# F02BBF

Withdrawn at Mark 19. Replaced by F08FBF (DSYEVX).

```
Old: CALL FO2BBF(A,LDA,N,RLB,RUB,M,MM,R,V,LDV,D,E,E2,X,G,C, & ICOUNT,IFAIL)

New: CALL DSYEVX('V','V','L',N,A,LDA,RLB,RUB, & 0,0,2*XO2AMF(),MM,R,V,LDV,WORK,LWORK,IWORK, & JFAIL,INFO)
```

where R must have dimension at least max(1,N), WORK is a real array of length at least  $(4 \times N)$ , LWORK is its actual length, JFAIL is an integer array of length at least max(1,N), and IWORK is an integer array of length at least  $(5 \times N)$ . Note that in the call to F02BBF R needs only to be of dimension (M). Larger values of LWORK, up to some optimal value, may improve performance. Arguments C, ICOUNT, X, G, E2, E and D are not used.

#### F02BCF

Withdrawn at Mark 19. Replaced by F02ECF.

```
Old: CALL FO2BCF(A,IA,N,ALB,UB,M,MM,RR,RI,VR,IVR,VI,IVI, & INTGER,ICNT,C,B,IB,U,V,IFAIL)

New: CALL FO2ECF('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  $(N \times (N+4))$  and LWORK is its actual length.

### F02BDF

Withdrawn at Mark 19. Replaced by F02GCF.

```
Old: CALL FO2BDF(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),KIND=nag_wp)
        CONTINUE
  10
  20 CONTINUE
     CALL FO2GCF('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) = AIMAG(R(I))
  30 CONTINUE
     DO 50 J = 1, MM
        DO 40 I = 1, N
           VR(I,J) = REAL(V(I,J))
           VI(I,J) = AIMAG(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  $(N \times (N+2))$ , LWORK is its actual length, and RWORK is a real array of length at least  $(2 \times N)$ .

# F02BEF

Withdrawn at Mark 18.

Replaced by F08JJF (DSTEBZ) and F08JKF (DSTEIN).

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

## F02BFF

Withdrawn at Mark 18.

Replaced by F08JJF (DSTEBZ).

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  $(4 \times N)$ , and IWORK is an integer array of length at least  $(3 \times N)$ .

# F02BJF

```
Withdrawn at Mark 23.
```

Replaced by F08WAF (DGGEV).

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### F02BKF

```
Withdrawn at Mark 18.
Replaced by F08PKF (DHSEIN).
```

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

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

### F02BLF

Withdrawn at Mark 18. Replaced by F08PXF (ZHSEIN).

```
Old: CALL FO2BLF(N,M,HR,IHR,HI,IHI,RI,C,RR,VR,IVR,VI,IVI,BR,IBR,BI, &
                 IBI,U,W,IFAIL)
New: DO 20 J = 1, N
        R(J) = CMPLX(RR(J),RI(J),KIND=nag_wp)
        DO 10 I = 1, N
           H(I,J) = CMPLX(HR(I,J),HI(I,J),KIND=nag\_wp)
  10
        CONTINUE
  20 CONTINUE
     CALL ZHSEIN('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) = AIMAG(V(I,J))
        CONTINUE
  40
  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  $\times$  N), RWORK is a real array of length at least (N), and IFAILR is an integer array of length at least (N).

# F02EAF

Withdrawn at Mark 23. Replaced by F08PAF (DGEES).

```
Old: CALL FO2EAF(JOB,N,A,LDA,WR,WI,Z,LDZ,WORK,LWORK,IFAIL)
New: LOGICAL SELECT
     EXTERNAL SELECT
     IF (JOB.EQ.'N') THEN
       JOBVS = 'N'
     ELSE
       JOBVS = 'V'
     END IF
     CALL DGEES (JOBVS, 'N', SELECT, N, A, LDA, O, WR, WI, Z, LDZ, WORK, &
                  LWORK, BWORK, INFO)
     IF (INFO.EQ.O) THEN
     LOGICAL FUNCTION SELECT (AR, AI)
     REAL (KIND=nag_wp) :: AR, AI
     SELECT = .TRUE.
     RETURN
     ENDK
```

Withdrawn at Mark 23.

#### F02EBF

```
Replaced by F08NAF (DGEEV).
Old: CALL FO2EBF(JOB, N, A, LDA, WR, WI, VR, LDVR, VI, LDVI, WORK, LWORK, &
                  IFAIL)
New: IF (JOB.EQ.'N') THEN
        JOBVR = 'N'
     ELSE
        JOBVR = 'V'
     END IF
     CALL DGEEV('N', JOBVR, N, A, LDA, WR, WI, VL, LDVL, VR1, LDVR1,
                 WORK, LWORK, INFO)
     IF (INFO.EQ.O) THEN
!
        Eigenvector information is stored differently.
1
        For complex conjugate pairs (that is, corresponding
!
        to the j-th eigenvector such that WI(j) is nonzero,
!
        and WI(j) = -WI(j+1), the real and imaginary parts
        of the first of the pair of eigenvectors are stored
!
        as consecutive columns of VR1: VR1(:,j), VR1(:,j+1).
        The second in the pair is just the conjugate of the
!
        first, so can be constructed by negating the
!
        elements in VR1(:,j+1).
        If the j-th eigenvector is real (WI(j)=0), the
1
        corresponding real eigenvector is stored in the
        j-th column of VR1, VR1(1:N,j).
```

#### F02FAF

```
Withdrawn at Mark 23.
Replaced by F08FAF (DSYEV).

Old: CALL F02FAF(JOB, UPLO, N, A, LDA, W, WORK, LWORK, IFAIL)

New: CALL DSYEV(JOB, UPLO, N, A, LDA, W, WORK, LWORK, INFO)

IF (INFO.EQ.O) THEN
```

The minimum workspace requirement has not increased but the requirement for optimal performance might be different. The workspace query mechanism (LWORK = -1) should be used to determine the requirement for optimal performance.

## F02FCF

```
Withdrawn at Mark 23.
Replaced by F08FBF (DSYEVX).

Old: CALL F02FCF(JOB,RANGE,UPLO,N,A,LDA,WL,WU,IL,IU,MEST,M, & W,Z,LDZ,WORK,LWORK,IWORK,IFAIL)

New: CALL DSYEVX(JOB,RANGE,UPLO,N,A,LDA,WL,WU,IL,IU,ABSTOL,M, & W,Z,LDZ,WORK,LWORK,IWORK,JFAIL,INFO)

IF (INFO.EQ.0) THEN
```

The minimum workspace requirement has not increased but the requirement for optimal performance might be different. The workspace query mechanism (LWORK = -1) should be used to determine the requirement for optimal performance.

# F02FDF

```
Withdrawn at Mark 23.
Replaced by F08SAF (DSYGV).

Old: CALL F02FDF(ITYPE, JOB, UPLO, N, A, LDA, B, LDB, W, WORK, LWORK, IFAIL)

New: CALL DSYGV(ITYPE, JOB, UPLO, N, A, LDA, B, LDB, W, WORK, LWORK, INFO)

IF (INFO.EQ.0) THEN
```

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The minimum workspace requirement has not increased but the requirement for optimal performance might be different. The workspace query mechanism (LWORK = -1) should be used to determine the requirement for optimal performance.

#### F02FHF

```
Withdrawn at Mark 23.
Replaced by F08UAF (DSBGV).

Old: CALL F02FHF(N,MA,A,LDA,MB,B,LDB,D,WORK,LWORK,IFAIL)

New: CALL DSBGV('N','U',N,MA,MB,A,LDA,B,LDB,D,Z,LDZ,WORK,INFO)

IF (INFO.EQ.O) THEN

...
```

The order of eigenvalues in D changes from descending to ascending.

The minimum workspace requirement has changed to become LWORK =  $3 \times N$ 

### F02GAF

```
Withdrawn at Mark 23.
Replaced by F08PNF (ZGEES).
Old: CALL FO2GAF(JOB,N,A,LDA,W,Z,LDZ,RWORK,WORK,LWORK,IFAIL)
New: LOGICAL BWORK(1)
     LOGICAL SELECT
     EXTERNAL SELECT
     IF (JOB.EQ.'N') THEN
        JOBVS = 'N'
     ELSE
        JOBVS = 'V'
     END IF
     CALL ZGEES(JOBVS,'N', SELECT, N, A, LDA, O, W, Z, LDZ,
                  WORK, LWORK, RWORK, BWORK, INFO)
     IF (INFO.NE.O) THEN
     LOGICAL FUNCTION SELECT(C)
     COMPLEX*16 C
     SELECT = .TRUE.
     RETURN
```

The minimum workspace requirement has not increased but the requirement for optimal performance might be different. The workspace query mechanism (LWORK = -1) should be used to determine the requirement for optimal performance.

```
Withdrawn at Mark 23.
Replaced by F08NNF (ZGEEV).

Old: CALL F02GBF(JOB,N,A,LDA,W,V,LDV,RWORK,WORK,LWORK,IFAIL)
New: CALL ZGEEV('N',JOB,N,A,LDA,W,VL,LDVL,V,LDV,
WORK,LWORK,RWORK,INFO)
IF (INFO.EQ.O) THEN
...

F02GJF

Withdrawn at Mark 23.
Replaced by F08WNF (ZGGEV).

Old: CALL F02GJF(N,AR,LDAR,AI,LDAI,BR,LDBR,BI,LDBI,EPS1,ALFR,
ALFI,BETA,MATV,VR,LDVR,VI,LDVI,ITER,IFAIL)

New: IF (MATV) THEN
JOBVR = 'V'
```

JOBVR = 'N'

Note that the separated real and imaginary parts of input and output data in F02GJF has been replaced by combined complex types in F08WNF (ZGGEV).

#### F02HAF

```
Withdrawn at Mark 23.
Replaced by F08FNF (ZHEEV).

Old: CALL F02HAF(JOB,UPLO,N,A,LDA,W,RWORK,WORK,LWORK,IFAIL)
New: CALL ZHEEV(JOB,UPLO,N,A,LDA,W,WORK,LWORK,RWORK,INFO)
IF (INFO.EQ.O) THEN
```

The minimum workspace requirement has not increased but the requirement for optimal performance might be different. The workspace query mechanism (LWORK = -1) should be used to determine the requirement for optimal performance.

#### F02HCF

```
Withdrawn at Mark 23.
Replaced by F08FPF (ZHEEVX).

Old: CALL F02HCF(JOB,RANGE,UPLO,N,A,LDA,WL,WU,IL,IU,MEST,M,W,Z,LDZ,WORK,LWORK,RWORK,IWORK,IFAIL)
```

```
Old: CALL FO2HCF(JOB,RANGE,UPLO,N,A,LDA,WL,WU,IL,IU,MEST,M, & W,Z,LDZ,WORK,LWORK,RWORK,IWORK,IFAIL)

New: CALL ZHEEVX(JOB,RANGE,UPLO,N,A,LDA,WL,WU,IL,IU,ABSTOL,M, & W,Z,LDZ,WORK,LWORK,RWORK,IWORK,JFAIL,INFO)

IF (INFO.EQ.O) THEN

...
```

The minimum workspace requirement has not increased but the requirement for optimal performance might be different. The workspace query mechanism (LWORK = -1) should be used to determine the requirement for optimal performance.

# F02HDF

Withdrawn at Mark 23. Replaced by F08SNF (ZHEGV).

```
Old: CALL F02HDF(ITYPE, JOB, UPLO, N, A, LDA, B, LDB, W, RWORK, WORK, & LWORK, IFAIL)

New: CALL ZHEGV(ITYPE, JOB, UPLO, N, A, LDA, B, LDB, W, WORK, LWORK, & RWORK, INFO)

IF (INFO.EQ.0) THEN

...
```

The minimum workspace requirement has not increased but the requirement for optimal performance might be different. The workspace query mechanism (LWORK = -1) should be used to determine the requirement for optimal performance.

### F02SWF

```
Withdrawn at Mark 18.
Replaced by F08KEF (DGEBRD).
```

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

```
Old: CALL F02SWF(N,A,LDA,D,E,NCOLY,Y,LDY,WANTQ,Q,LDQ,IFAIL) 
 New: DO 20 J = 1, N DO 10 I = J+1, N
```

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```
A(I,J) = 0.0D0

10 CONTINUE

20 CONTINUE

CALL DGEBRD(N,N,A,LDA,D,E,TAUQ,TAUP,WORK,LWORK,INFO)

IF (WANTQ) THEN

CALL F06QFF('L',N,N,A,LDA,Q,LDQ)

CALL DORGBR('Q',N,N,N,Q,LDQ,TAUQ,WORK,LWORK,INFO)

END IF

IF (NCOLY.GT.O) THEN

CALL DORMBR('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 (DORGBR) and F08KGF (DORMBR).

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

```
Old: CALL F02SXF(N,A,LDA,NCOLY,Y,LDY,WORK,IFAIL)

New: IF (NCOLY.EQ.O) THEN

CALL DORGBR('P',N,N,N,A,LDA,TAUP,WORK,LWORK,INFO)

ELSE

CALL DORMBR('P','L','T',N,NCOLY,N,A,LDA,TAUP,Y,LDY,WORK, & LWORK,INFO)

END IF
```

#### F02SYF

Withdrawn at Mark 18.

Replaced by F08MEF (DBDSQR).

```
Old: CALL FO2SYF(N,D,E,NCOLB,B,LDB,NROWY,Y,LDY,NCOLZ,Z,LDZ,WORK, & IFAIL)

New: CALL DBDSQR('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  $(4 \times (N-1))$  unless NCOLB = NROWY = NCOLZ = 0.

# F02UWF

Withdrawn at Mark 18.

Replaced by F08KSF (ZGEBRD), F06TFF, F08KTF (ZUNGBR) and F08KUF (ZUNMBR).

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.

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 (ZUNGBR) or F08KUF (ZUNMBR).

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

where LWORK is the actual length of CWORK.

#### F02UYF

Withdrawn at Mark 18.

Replaced by F08MSF (ZBDSQR).

```
Old: CALL F02UYF(N,D,E,NCOLB,B,LDB,NROWY,Y,LDY,NCOLZ,Z,LDZ,WORK, IFAIL) &
New: CALL ZBDSQR('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  $(4 \times (N-1))$  unless NCOLB = NROWY = NCOLZ = 0.

#### F02WEF

Withdrawn at Mark 23.

Replaced by F08KBF (DGESVD).

```
CALL FO2WEF(M,N,A,LDA,NCOLB,B,LDB,WANTQ,Q,LDQ,SV,WANTP,
                   PT,LDPT,WORK,IFAIL)
New:
      IF (WANTQ) THEN
         JOBU = 'A'
      ELSE
         JOBU = 'N'
      END IF
      IF (WANTP) THEN
          JOBVT = 'A'
      ELSE
         JOBVT = 'N'
      END IF
      LWORK = -1
      CALL DGESVD(JOBU, JOBVT, M, N, A, LDA, SV, Q, LDQ, PT, LDPT, WORK, LWORK, INFO)
      LWORK = ANINT(WORK(1))
      ALLOCATE (W(LWORK))
      CALL DGESVD(JOBU, JOBVT, M, N, A, LDA, SV, Q, LDQ, PT, LDPT, W, LWORK, INFO)
      DEALLOCATE (W)
```

WORK must be a one-dimensional real array of length at least *lwork* given by  $\max(1, 3 \times \min(M, N) + \max(M, N), 5 \times \min(M, N))$ 

Larger values of LWORK, up to some optimal value, may improve performance.

Please note that the facility to return  $Q^TB$  is not provided so arguments WANTB and B are not required. Instead, F08KBF (DGESVD) has an option to return the entire M \* M orthogonal matrix Q, referred to as U in its documentation, through its 8th argument.

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# F02XEF

```
Withdrawn at Mark 23.
Replaced by F08KPF (ZGESVD).
```

```
Old: CALL FO2XEF(M,N,A,LDA,NCOLB,B,LDB,WANTQ,Q,LDQ,SV,WANTP,
                   PH, LDPH, RWORK, CWORK, IFAIL)
New: IF (WANTQ) THEN
         JOBU = 'A'
      ELSE
         JOBU = 'N'
      END IF
      IF (WANTP) THEN
          JOBVT = 'A'
      ELSE
         JOBVT = 'N'
      END IF
      LWORK = -1
      CALL ZGESVD(JOBU, JOBVT, M, N, A, LDA, SV, Q, LDQ, PT, LDPT, WORK,
                   LWORK, RWORK, INFO)
      LWORK = ANINT(WORK(1))
      ALLOCATE (W(LWORK))
      CALL ZGESVD(JOBU, JOBVT, M, N, A, LDA, SV, Q, LDQ, PT, LDPT, W,
                                                                            æ
                   LWORK, RWORK, INFO)
      DEALLOCATE (W)
```

WORK must be a one-dimensional complex array of length at least *lwork* given by  $\max(1, 2 \times \min(M, N) + \max(M, N))$ 

RWORK must be a one-dimensional real array of length  $max(1, 5 \times min(M, N))$ 

Larger values of LWORK, up to some optimal value, may improve performance.

Please note that the facility to return  $Q^HB$  is not provided so arguments WANTB and B are not required. Instead, F08KPF (ZGESVD) has an option to return the entire M \* M unitary matrix Q, referred to as U in its documentation, through its 8th argument.

# F03 – Determinants

## F03AAF

Scheduled for withdrawal at Mark 25. Replaced by F07ADF (DGETRF) and F03BAF.

**Note:** the real array WKSPCE has been replaced by the integer array IPIV for holding the pivots of the factorization.

# F03ABF

Scheduled for withdrawal at Mark 25. Replaced by F07FDF (DPOTRF) and F03BFF.

```
CALL F03BFF(N,A,LDA,D,ID,IFAIL)
DET = D*2**ID
```

**Note:** the real array WKSPCE is no longer required. Also the upper triangular part of A, stored in A, has been replaced here by its Cholesky factorization; the lower triangular part of A can be used and overwritten by replacing 'U' by 'L' in the call to DPOTRF above.

### F03ACF

Scheduled for withdrawal at Mark 25. Replaced by F07HDF (DPBTRF) and F03BHF.

**Note:** the storage of A in arrays A and AB is different. In fact AB(i,j) = A(j,i), for i = 1, 2, ..., m and  $j = \max(1, i - m), ..., i$  which conforms to the LAPACK banded storage scheme. The factorization is returned in AB rather than in a separate array (RL). The upper part of matrix A can also be stored in AB on input to DPBTRF.

#### F03ADF

Scheduled for withdrawal at Mark 25. Replaced by F07ARF (ZGETRF) and F03BNF.

**Note:** the real array WKSPCE has been replaced by the integer array IPIV for holding the pivots of the factorization. The real and imaginary parts of the determinant are independently scaled.

### F03AEF

Scheduled for withdrawal at Mark 25. Replaced by F07FDF (DPOTRF) and F03BFF.

**Note:** the upper triangular part of A, stored in A, has been replaced here by its Cholesky factorization; the lower triangular part of A can be used and overwritten by replacing UPLO = 'U' by UPLO = 'L' in the call to F07FDF (DPOTRF) above.

# F03AFF

Scheduled for withdrawal at Mark 25. Replaced by F07ADF (DGETRF) and F03BAF.

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Note: real array P has been replaced by the integer array IPIV for holding the pivots of the factorization.

#### F03AGF

Withdrawn at Mark 17.
Replaced by F07HDF (DPBTRF).

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

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

```
D1 = 1.0_nag_wp
   ID = 0
   DO 30 I = 1, N
      D1 = D1*A(1,I)**2
10
      IF (D1.GE.1.0_nag_wp) THEN
         D1 = D1*0.0625_nag_wp
         ID = ID + 4.0
         GO TO 10
      END IF
20
      IF (D1.LT.0.0625_nag_wp) THEN
         D1 = D1*16.0_nag_wp
         ID = ID - 4.0
         GO TO 20
      END IF
30 CONTINUE
```

### F03AHF

Withdrawn at Mark 17. Replaced by F07ARF (ZGETRF).

```
Old: CALL FO3AHF(N,A,IA,DETR,DETI,ID,RINT,IFAIL)
New: CALL ZGETRF(N,N,A,IA,IPIV,INFO)
```

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

```
DET = CMPLX(1.0_nag_wp,KIND=nag_wp)
   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(AIMAG(DET))).GE.1.0_nag_wp) THEN
         DET = DET*0.062_nag_wp
         ID = ID + 4
         GO TO 10
      END IF
      IF (MAX(ABS(REAL(DET)), ABS(AIMAG(DET))).LT.0.0625_nag_wp) THEN
20
         DET = DET*16.0_nag_wp
         ID = ID - 4
         GO TO 20
```

```
END IF
30 CONTINUE
DETR = REAL(DET)
DETI = AIMAG(DET)
```

#### F03AMF

Withdrawn at Mark 17.

There is no replacement for this routine.

```
Old: CALL FO1BNF(N,A,IA,P,IFAIL)
     CALL FO3AMF(N,TEN,P,D1,D2)
New: CALL ZPOTRF('Upper', N, A, IA, INFO)
     D1 = 1.0_nag_wp
     D2 = 0.0_nag_wp
     DO 30 I = 1, N
        D1 = D1*REAL(A(I,I))**2
  10
        IF (D1.GE.1.0_nag_wp) THEN
           D1 = D1*0.0625_nag_wp
           D2 = D2 + 4.0 \underline{\text{nag\_wp}}
           GO TO 10
        END IF
  20
        IF (D1.LT.0.0625_nag_wp) THEN
           D1 = D1*16.0  nag wp
           D2 = D2 - 4.0_nag_wp
           GO TO 20
        END IF
  30 CONTINUE
     IF (TEN) THEN
        I = D2
        D2 = D2*LOG10(2.0_nag_wp)
        D1 = D1*2.0_nag_wp**(I-D2/LOG10(2.0_nag_wp))
```

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

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

# F04 – Simultaneous Linear Equations

### F04AAF

# F04ACF

```
Withdrawn at Mark 23. Replaced by F07HAF (DPBSV).
```

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### F04ADF

Withdrawn at Mark 23. Replaced by F07ANF (ZGESV).

```
Old: CALL FO4ADF(A,LDA,B,LDB,N,M,C,LDC,WKSPCE,IFAIL)

New: CALL ZGESV(N,M,A,LDA,IPIV,B,LDB,INFO)

IF (INFO.EQ.O) THEN

! Answer now in B
```

#### F04AFF

Scheduled for withdrawal at Mark 25.

There is no replacement for this routine.

The factorization and solution of a positive definite linear system can be handled by calls to routines from Chapter F07, e.g., F07FBF (DPOSVX).

For example:

#### F04AGF

Scheduled for withdrawal at Mark 25.

There is no replacement for this routine.

The factorization and solution of a positive definite linear system can be handled by calls to routines from Chapter F07, e.g., F07FAF (DPOSV).

For example:

# F04AHF

Scheduled for withdrawal at Mark 25.

There is no replacement for this routine.

The factorization and solution of a real general linear system can be handled by calls to routines from the Chapter F07, e.g., F07ABF (DGESVX).

For example:

# F04AJF

Scheduled for withdrawal at Mark 25.

There is no replacement for this routine.

The factorization and solution of a real general linear system can be handled by calls to routines from Chapter F07, e.g., F07AAF (DGESV).

For example:

#### F04AKF

Withdrawn at Mark 17. Replaced by F07ASF (ZGETRS).

```
Old: CALL FO4AKF(N,IR,A,IA,P,B,IB)
New: CALL ZGETRS('No Transpose',N,IR,A,IA,IPIV,B,IB,INFO)
```

#### F04ALF

Withdrawn at Mark 17. Replaced by F07HEF (DPBTRS).

```
Old: CALL F04ALF(N,M,IR,RL,IRL,M1,B,IB,X,IX)

New: CALL F06QFF('General',N,IR,B,IB,X,IX)

CALL DPBTRS('Lower',N,M,IR,A,IA,X,IX,INFO)
```

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

# F04ANF

Withdrawn at Mark 18.

Replaced by F06EFF (DCOPY), F06PJF (DTRSV) and F08AGF (DORMQR).

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 (DGEQPF) as shown above.

# F04ARF

```
Withdrawn at Mark 23.
Replaced by F07AAF (DGESV).

Old: CALL F04ARF(A,LDA,B,N,C,WKSPCE,IFAIL)
New: CALL DGESV(N,1,A,LDA,IPIV,B,N,INFO)
IF (INFO.EQ.O) THEN
! Answer now in B
```

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# F04AWF

Withdrawn at Mark 17.
Replaced by F07FSF (ZPOTRS).
Old: CALL F04AWF(N,IR,A,IA,P,B,IB,X,IX)

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

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

# F04AYF

Withdrawn at Mark 18. Replaced by F07AEF (DGETRS).

```
Old: CALL FO4AYF(N,IR,A,IA,P,B,IB,IFAIL)
New: CALL DGETRS('No Transpose',N,IR,A,IA,IPIV,B,IB,INFO)
```

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

### F04AZF

Withdrawn at Mark 17. Replaced by F07FEF (DPOTRS).

```
Old: CALL FO4AZF(N,IR,A,IA,P,B,IB,IFAIL)
New: CALL DPOTRS('Upper',N,IR,A,IA,B,IB,INFO)
```

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

#### F04EAF

```
Withdrawn at Mark 23. Replaced by F07CAF (DGTSV).
```

```
Old: CALL F04EAF(N,D,DU,DL,B,IFAIL)

New: CALL DGTSV(N,1,DL(2),D,DU(2),B,N,INFO)

IF (INFO.EQ.0) THEN

! Answer now in B
```

### F04FAF

Withdrawn at Mark 23.

Replaced by F07JAF (DPTSV), or F07JDF (DPTTRF) and F07JEF (DPTTRS).

```
Old: CALL FO4FAF(JOB,N,D,E,B,IFAIL)
New: CALL DPTSV(N,1,D,E(2),B,1,INFO)
```

# F04JAF

Withdrawn at Mark 23.

Replaced by F08KAF (DGELSS).

```
Old: CALL F04JAF(M,N,A,LDA,B,TOL,SIGMA,IRANK,WORK,LWORK,IFAIL)

New: CALL DGELSS(M,N,1,A,LDA,B,1,S,RCOND,IRANK,WORK,LWORK,INFO)

IF (INFO.EQ.O) THEN

! Answer now in B
! Singular values now in S, not WORK.
```

```
! The standard error is not computed
```

The minimum workspace requirement has changed from  $4 \times N$  to  $3 \times \min(N, M) + \max(2 \times \min(N, M), \max(M, N), 1)$ .

### F04JDF

Withdrawn at Mark 23.

Replaced by F08KAF (DGELSS).

```
Old: CALL F04JDF(M,N,A,LDA,B,TOL,SIGMA,IRANK,WORK,LWORK,IFAIL)

New: CALL DGELSS(M,N,1,A,LDA,B,1,S,RCOND,IRANK,WORK,LWORK,INFO)

! Note workspace requirements are different.

IF (INFO.EQ.0) THEN

! Answer now in B

! Singular values now in S, not WORK.

! The standard error is not computed
```

The minimum workspace requirement has changed from  $N \times (M+4)$  to  $3 \times \min(N, M) + \max(2 \times \min(N, M), \max(M, N), 1)$ .

#### F04JLF

Withdrawn at Mark 23.

Replaced by F08ZBF (DGGGLM).

```
Old: CALL F04JLF(M,N,P,A,LDA,B,LDB,D,X,Y,WORK,LWORK,IFAIL)
New: CALL DGGGLM(M,N,P,A,LDA,B,LDB,D,X,Y,WORK,LWORK,INFO)
IF (INFO.EQ.O) THEN
...
```

The minimum workspace requirement has not increased but the requirement for optimal performance might be different. The workspace query mechanism (LWORK = -1) should be used to determine the requirement for optimal performance.

# F04JMF

```
Withdrawn at Mark 23.
Replaced by F08ZAF (DGGLSE).
```

```
Old: CALL F04JMF(M,N,P,A,LDA,B,LDB,C,D,X,WORK,LWORK,IFAIL)
New: CALL DGGLSE(M,N,P,A,LDA,B,LDB,C,D,X,WORK,LWORK,INFO)
IF (INFO.EQ.0) THEN
```

The minimum workspace requirement has not increased but the requirement for optimal performance might be different. The workspace query mechanism (LWORK = -1) should be used to determine the requirement for optimal performance.

# F04KLF

```
Withdrawn at Mark 23.
Replaced by F08ZPF (ZGGGLM).
```

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

## F04KMF

Withdrawn at Mark 23. Replaced by F08ZNF (ZGGLSE).

```
Old: CALL FO4KMF(M,N,P,A,LDA,B,LDB,C,D,X,WORK,LWORK,IFAIL)
New: CALL ZGGLSE(M,N,P,A,LDA,B,LDB,C,D,X,WORK,LWORK,INFO)
```

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```
IF (INFO.EQ.O) THEN
```

#### F04LDF

Withdrawn at Mark 18. Replaced by F07BEF (DGBTRS).

```
Old: CALL FO4LDF(N,M1,M2,IR,A,IA,AL,IL,IN,B,IB,IFAIL)
New: CALL DGBTRS('No Transpose',N,M1,M2,IR,A,IA,IN,B,IB,INFO)
```

It is assumed that the matrix has been factorized by a call of F07BDF (DGBTRF). 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 F11GDF, F11GEF and F11GFF. Otherwise F11JCF or F11JEF may be used. The interfaces for these routines are significantly different from that for F04MBF and therefore precise details of a replacement call cannot be given. Please consult the appropriate routine document.

#### F04NAF

Withdrawn at Mark 17.

Replaced by F06SKF (ZTBSV) and F07BSF (ZGBTRS).

It is assumed that the matrix has been factorized by a call of F07BRF (ZGBTRF). 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.

# F04YCF

Scheduled for withdrawal at Mark 26. Replaced by F04YDF.

```
Old: CALL F04YCF(ICASE,N,X,ESTNRM,WORK,IWORK,IFAIL)
New: CALL F04YDF(IREVCM,M,N,X,LDX,Y,LDY,ESTNRM,T,SEED,WORK,IWORK,IFAIL)
```

F04YDF returns an estimate of the 1-norm of a rectangular  $M \times N$  matrix, whereas F04YCF only works with square matrices. The real array X, which was previously used to return matrix-vector products to F04YCF, has been replaced with two real arrays X(LDX,\*) and Y(LDY,\*) which are used to return matrix-matrix products to F04YDF. Here,  $LDX \ge N$ ,  $LDY \ge M$  and the second dimensions of X and Y are at least of size T, where you can choose parameter T. The sizes of the workspace arrays WORK and

IWORK have been increased to  $M \times T$  and  $2 \times N + 5 \times T + 20$  respectively. The integer SEED provides a seed for the random number generator used by F04YDF. The integer ICASE has been replaced by IREVCM, which can take the values 0, 1 or 2. See the routine documentation for F04YDF further details about the reverse communication interface.

#### F04ZCF

Scheduled for withdrawal at Mark 26. Replaced by F04ZDF.

```
Old: CALL FO4ZCF(ICASE,N,X,ESTNRM,WORK,IWORK,IFAIL)
New: CALL FO4ZDF(IREVCM,M,N,X,LDX,Y,LDY,ESTNRM,T,SEED,WORK,RWORK,IWORK,IFAIL)
```

F04ZDF returns an estimate of the 1norm of a rectangular  $M \times N$  matrix, whereas F04ZCF only works with square matrices. The complex array X, which was previously used to return matrix–vector products to F04ZCF, has been replaced with two complex arrays X(LDX,\*) and Y(LDY,\*) which are used to return matrix-matrix products to F04ZDF. Here,  $LDX \ge N$ ,  $LDY \ge M$  and the second dimensions of X and Y are at least of size T, where you can choose the parameter T. The sizes of the workspace arrays WORK and IWORK have been increased to  $M \times T$  and  $2 \times N + 5 \times T + 20$  respectively and there is an additional real workspace array RWORK of size  $2 \times N$ . The integer SEED provides a seed for the random number generator used by F04ZDF. The integer ICASE has been replaced by IREVCM, which can take the values 0, 1 or 2. See the routine documentation for F04ZDF for further details about the reverse communication interface.

# F11 – Large Scale Linear Systems

## F11BAF

Withdrawn 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

Withdrawn at Mark 21. Replaced by F11BEF.

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

WGT must be a one-dimensional 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

Withdrawn at Mark 21. Replaced by F11BFF.

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

F11BFF contains two additional parameters as follows:

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```
WORK(LWORK) – real array. 
 LWORK – integer.
```

See the routine document for further information.

#### F11GAF

Withdrawn 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, SIGTOL, MAXITS, 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

Withdrawn 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

Withdrawn 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**

# **G01AAF**

Scheduled for withdrawal at Mark 26. Replaced by G01ATF.

#### G01CEF

```
Withdrawn at Mark 18.

Replaced by G01FAF.

Old: X = G01CEF(P,IFAIL)

New: X = G01FAF('Lower-tail',P,IFAIL)
```

```
G04 – Analysis of Variance
```

# **G04ADF**

Withdrawn at Mark 17. Replaced by G04BCF.

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 TABL starting at the second row, e.g., VAR(1) = TABL(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.

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

# **G04AEF**

Withdrawn at Mark 17. Replaced by G04BBF.

```
Old: CALL GO4AEF(Y,N,K,NOBS,GBAR,GM,SS,IDF,F,FP,IFAIL)

New: CALL GO4BBF(N,Y,O,K,IT,GM,BMEAN,GBAR,TABL,4,C,KMAX,NOBS, & R,EF,O.ODO,O,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 TABL starting at row 2 and the values equivalent to those returned in the scalars F and FP are returned in TABL(2,4) and TABL(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

CONTINUE
40 CONTINUE
```

The following additional declarations are required.

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

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### **G04AFF**

Withdrawn at Mark 17. Replaced by G04CAF.

```
Old: CALL GO4AFF(Y,IY1,IY2,M,NR,NC,ROW,COL,CELL,ICELL,GM,SS,IDF,F,FP, & IFAIL)

New: CALL GO4CAF(M*NR*NC,Y1,2,LFAC,1,2,0,6,TABL,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
              BMEAN(1)
GM
SS(1)
              TABL(3,2)
              TABL(2,2)
SS(2)
              TABL(4,2)
SS(i)
              TABL(3,1)
IDF(1)
IDF(2)
              TABL(2,1)
IDF(i)
              TABL(4,1)
F(1)
              TABL(3,4)
F(2)
              TABL(2,4)
              TABL(4,4)
F(3)
FP(1)
              TABL(3,5)
              TABL(2,5)
FP(2)
              TABL(4,5)
FP(3)
```

Note how rows and columns have swapped.

The following additional declarations are required.

```
REAL (KIND=nag_wp) TABL(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

### **G05CAF**

Withdrawn at Mark 22. Replaced by G05SAF.

```
Old: DO 20 I = 1, N
            X(I) = G05CAF(X(I))
20 CONTINUE
New: CALL G05SAF(N,STATE,X,IFAIL)
```

The integer array STATE in the call to G05SAF contains information on the base generator being used. This array must have been initialized prior to calling G05SAF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SAF is likely to be different from those produced by G05CAF.

# G05CBF

Withdrawn at Mark 22. Replaced by G05KFF.

```
Old: CALL G05CBF(I)
New: LSEED = 1
```

```
SEED(1) = I
GENID = 1
SUBID = 1
CALL G05KFF(GENID, SUBID, SEED, LSEED, STATE, LSTATE, IFAIL)
```

The integer array STATE in the call to G05KFF contains information on the base generator being used. The base generator is chosen via the integer parameters GENID and SUBID. The required length of the array STATE depends on the base generator chosen. Due to changes in the underlying code a sequence of values produced by using a random number generator initialized via a call to G05KFF is likely to be different from a sequence produced by a generator initialized by G05CBF, even if the same value for I is used.

#### G05CCF

Withdrawn at Mark 22. Replaced by G05KGF.

```
Old: CALL G05CCF
New: GENID = 1
    SUBID = 1
    CALL G05KGF(GENID, SUBID, STATE, LSTATE, IFAIL)
```

The integer array STATE in the call to G05KGF contains information on the base generator being used. The base generator is chosen via the integer parameters GENID and SUBID. The required length of the array STATE depends on the base generator chosen.

### **G05CFF**

Withdrawn at Mark 22. Replaced by F06DFF.

The state of the base generator for the group of routines G05KFF, G05KGF, G05KHF, G05KJF, G05NCF, G05NDF, G05PDF–G05PZF, G05RCF–G05RZF, G05S and G05T can be saved by simply creating a local copy of the array STATE. The first element of the STATE array contains the number of elements that are used by the random number generating routines, therefore either this number of elements can be copied, or the whole array (as defined in the calling program).

### **G05CGF**

Withdrawn at Mark 22. Replaced by F06DFF.

The state of the base generator for the group of routines G05KFF, G05KGF, G05KHF, G05KJF, G05NCF, G05NDF, G05PDF–G05PZF, G05RCF–G05RZF, G05S and G05T can be restored by simply copying back the previously saved copy of the STATE array. The first element of the STATE array contains the number of elements that are used by the random number generating routines, therefore either this number of elements can be copied, or the whole array (as defined in the calling program).

#### G05DAF

Withdrawn at Mark 22. Replaced by G05SQF.

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```
IFAIL = 0
CALL G05SQF(N,A,B,STATE,X,IFAIL)
```

The old routine G05DAF returns a single variate at a time, whereas the new routine G05SQF returns a vector of N values in one go. In G05SQF the minimum value must be held in the parameter A and the maximum in parameter B, therefore A < B. This was not the case for the equivalent parameters in G05DAF.

The integer array STATE in the call to G05SQF contains information on the base generator being used. This array must have been initialized prior to calling G05SQF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SQF is likely to be different from those produced by G05DAF.

### G05DBF

Withdrawn at Mark 22. Replaced by G05SFF.

The old routine G05DBF returns a single variate at a time, whereas the new routine G05SFF returns a vector of N values in one go. In G05SFF parameter A must be non-negative, this was not the case for the equivalent parameter in G05DBF.

The integer array STATE in the call to G05SFF contains information on the base generator being used. This array must have been initialized prior to calling G05SFF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SFF is likely to be different from those produced by G05DBF.

# G05DCF

Withdrawn at Mark 22. Replaced by G05SLF.

The old routine G05DCF returns a single variate at a time, whereas the new routine G05SLF returns a vector of N values in one go. In G05SLF the spread (parameter A) must be positive, this was not the case for the equivalent parameters in G05DCF.

The integer array STATE in the call to G05SLF contains information on the base generator being used. This array must have been initialized prior to calling G05SLF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SLF is likely to be different from those produced by G05DCF.

### G05DDF

Withdrawn at Mark 22. Replaced by G05SKF.

```
IFAIL = 0
CALL G05SKF(N,XMU,VAR,STATE,X,IFAIL)
```

The old routine G05DDF returns a single variate at a time, whereas the new routine G05SKF returns a vector of N values in one go. G05SKF expects the variance of the Normal distribution (parameter VAR), compared to G05DDF which expected the standard deviation.

The integer array STATE in the call to G05SKF contains information on the base generator being used. This array must have been initialized prior to calling G05SKF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SKF is likely to be different from those produced by G05DDF.

### **G05DEF**

Withdrawn at Mark 22. Replaced by G05SMF.

The old routine G05DEF returns a single variate at a time, whereas the new routine G05SMF returns a vector of N values in one go. G05SMF expects the variance of the corresponding Normal distribution (parameter VAR), compared to G05DEF which expected the standard deviation.

The integer array STATE in the call to G05SMF contains information on the base generator being used. This array must have been initialized prior to calling G05SMF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SMF is likely to be different from those produced by G05DEF.

### **G05DFF**

Withdrawn at Mark 22. Replaced by G05SCF.

The old routine G05DFF returns a single variate at a time, whereas the new routine G05SCF returns a vector of N values in one go. G05SCF expects the semi-interquartile range (parameter SEMIQR) to be non-negative, this was not the case for the equivalent parameter in G05DFF.

The integer array STATE in the call to G05SCF contains information on the base generator being used. This array must have been initialized prior to calling G05SCF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SCF is likely to be different from those produced by G05DFF.

### **G05DHF**

Withdrawn at Mark 22. Replaced by G05SDF.

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The old routine G05DHF returns a single variate at a time, whereas the new routine G05SDF returns a vector of N values in one go.

The integer array STATE in the call to G05SDF contains information on the base generator being used. This array must have been initialized prior to calling G05SDF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SDF is likely to be different from those produced by G05DHF.

#### G05DJF

Withdrawn at Mark 22. Replaced by G05SNF.

The old routine G05DJF returns a single variate at a time, whereas the new routine G05SNF returns a vector of N values in one go.

The integer array STATE in the call to G05SNF contains information on the base generator being used. This array must have been initialized prior to calling G05SNF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SNF is likely to be different from those produced by G05DJF.

#### G05DKF

Withdrawn at Mark 22. Replaced by G05SHF.

The old routine G05DKF returns a single variate at a time, whereas the new routine G05SHF returns a vector of N values in one go.

The integer array STATE in the call to G05SHF contains information on the base generator being used. This array must have been initialized prior to calling G05SHF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SHF is likely to be different from those produced by G05DKF.

#### G05DPF

Withdrawn at Mark 22. Replaced by G05SSF.

The old routine G05DPF returns a single variate at a time, whereas the new routine G05SSF returns a vector of N values in one go.

The integer array STATE in the call to G05SSF contains information on the base generator being used. This array must have been initialized prior to calling G05SSF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SSF is likely to be different from those produced by G05DPF.

#### **G05DRF**

Withdrawn at Mark 22. Replaced by G05TKF.

The old routine G05DRF returns a single variate at a time, whereas the new routine G05TJF returns a vector of N values in one go. For efficiency, the new routine can make use of a reference vector, R. If, as in this case, the integer parameter MODE is set to 3, the real reference vector R is not referenced, and its length, LR, need only be at least one.

The integer array STATE in the call to G05TJF contains information on the base generator being used. This array must have been initialized prior to calling G05TJF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05TJF is likely to be different from those produced by G05DRF.

#### G05DYF

Withdrawn at Mark 22. Replaced by G05TLF.

The old routine G05DYF returns a single variate at a time, whereas the new routine G05TLF returns a vector of N values in one go. In G05TLF the minimum value must be held in the parameter A and the maximum in parameter B, therefore  $A \leq B$ . This was not the case for the equivalent parameters in G05DYF.

The integer array STATE in the call to G05TLF contains information on the base generator being used. This array must have been initialized prior to calling G05TLF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05TLF is likely to be different from those produced by G05DYF.

### **G05DZF**

Withdrawn at Mark 22. Replaced by G05TBF.

The old routine G05DZF returns a single variate at a time, whereas the new routine G05TBF returns a vector of N values in one go. The real parameter P in G05TBF must not be less than zero or greater than one, this was not the case for the equivalent parameter in G05DZF.

The integer array STATE in the call to G05TBF contains information on the base generator being used. This array must have been initialized prior to calling G05TBF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05TBF is likely to be different from those produced by G05DZF.

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### **G05EAF**

Withdrawn at Mark 22. Replaced by G05RZF.

The old routine G05EAF sets up a reference vector for use by G05EZF. The functionality of both these routines has been combined into the single new routine G05RZF. Setting MODE = 0 in the call to G05RZF only sets up the real reference vector R and hence mimics the functionality of G05EAF.

The length of the real reference vector, R, in G05RZF must be at least  $M \times (M+1) + 1$ . In contrast to the equivalent parameter in G05EAF, this array must be allocated in the calling program.

# G05EBF

Withdrawn at Mark 22. Replaced by G05TLF.

There is no direct replacement for routine G05EBF. G05EBF sets up a reference vector for use by G05EYF, this reference vector is no longer required. The replacement routine for G05EYF is G05TLF.

### G05ECF

Withdrawn at Mark 22. Replaced by G05TJF.

```
Old: CALL GO5ECF(LAMBDA,R1,LR1,IFAIL)
    DO 10 I = 1, N
        X(I) = GO5EYF(R1,LR1)
10 CONTINUE
New: MODE = 2
    CALL GO5TJF(MODE,N,LAMBDA,R,LR,STATE,X,IFAIL)
```

The old routine G05ECF sets up a reference vector for use by G05EYF. The replacement routine G05TJF is now used to both set up a reference vector and generate the required variates. Setting MODE = 0 in the call to G05TJF sets up the real reference vector R and hence mimics the functionality of G05ECF. Setting MODE = 1 generates a series of variates from a reference vector mimicking the functionality of G05EYF for this particular distribution. Setting MODE = 2 initializes the reference vector and generates the variates in one go.

The routine G05EYF returns a single variate at a time, whereas the new routine G05TJF returns a vector of N values in one go.

The length of the real reference vector, R, in G05TJF, must be allocated in the calling program in contrast to the equivalent parameter in G05ECF, see the documentation for more details.

The integer array STATE in the call to G05TJF contains information on the base generator being used. This array must have been initialized prior to calling G05TJF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05TJF is likely to be different from those produced by a combination of G05ECF and G05EYF.

#### G05EDF

Withdrawn at Mark 22. Replaced by G05TAF.

```
Old: CALL G05EDF(M,P,R1,LR1,IFAIL)
        DO 10 I = 1, N
            X(I) = G05EYF(R1,LR1)
        10 CONTINUE
New: MODE = 2
      CALL G05TAF(MODE,N,M,P,R,LR,STATE,X,IFAIL)
```

The old routine G05EDF sets up a reference vector for use by G05EYF. The replacement routine G05TAF is now used to both set up a reference vector and generate the required variates. Setting MODE = 0 in the call to G05TAF sets up the real reference vector R and hence mimics the functionality of G05EDF. Setting MODE = 1 generates a series of variates from a reference vector mimicking the functionality of G05EYF for this particular distribution. Setting MODE = 2 initializes the reference vector and generates the variates in one go.

The routine G05EYF returns a single variate at a time, whereas the new routine G05TAF returns a vector of N values in one go.

The length of the real reference vector, R, in G05TAF, needs to be a different length from the equivalent parameter in G05EDF, see the documentation for more details.

The integer array STATE in the call to G05TAF contains information on the base generator being used. This array must have been initialized prior to calling G05TAF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05TAF is likely to be different from those produced by a combination of G05EDF and G05EYF.

#### G05EEF

Withdrawn at Mark 22. Replaced by G05THF.

```
Old: CALL G05EEF(M,P,R1,LR1,IFAIL)
   DO 10 I = 1, N
       X(I) = G05EYF(R1,LR1)
   10 CONTINUE
New: MODE = 2
   CALL G05THF(MODE,N,M,P,R,LR,STATE,X,IFAIL)
```

The old routine G05EEF sets up a reference vector for use by G05EYF. The replacement routine G05THF is now used to both set up a reference vector and generate the required variates. Setting MODE = 0 in the call to G05THF sets up the real reference vector R and hence mimics the functionality of G05EEF. Setting MODE = 1 generates a series of variates from a reference vector mimicking the functionality of G05EYF for this particular distribution. Setting MODE = 2 initializes the reference vector and generates the variates in one go.

The routine G05EYF returns a single variate at a time, whereas the new routine G05THF returns a vector of N values in one go.

The length of the real reference vector, R, in G05THF, needs to be a different length from the equivalent parameter in G05EEF, see the documentation for G05THF for more details.

The integer array STATE in the call to G05THF contains information on the base generator being used. This array must have been initialized prior to calling G05THF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05THF is likely to be different from those produced by a combination of G05EEF and G05EYF.

## G05EFF

Withdrawn at Mark 22. Replaced by G05TEF.

```
Old: CALL G05EFF(NS,M,NP,R1,LR1,IFAIL)
        DO 10 I = 1, N
            X(I) = G05EYF(R1,LR1)
        10 CONTINUE
New: MODE = 2
        CALL G05TEF(MODE,N,NS,NP,M,R,LR,STATE,X,IFAIL)
```

The old routine G05EFF sets up a reference vector for use by G05EYF. The replacement routine G05TEF is now used to both set up a reference vector and generate the required variates. Setting MODE = 0 in the call to G05TEF sets up the real reference vector R and hence mimics the functionality of G05EFF. Setting MODE = 1 generates a series of variates from a reference vector mimicking the functionality of G05EYF

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for this particular distribution. Setting MODE = 2 initializes the reference vector and generates the variates in one go.

The routine G05EYF returns a single variate at a time, whereas the new routine G05TEF returns a vector of N values in one go.

The length of the real reference vector, R, in G05TEF, needs to be a different length from the equivalent parameter in G05EFF, see the documentation for more details.

The integer array STATE in the call to G05TEF contains information on the base generator being used. This array must have been initialized prior to calling G05TEF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05TEF is likely to be different from those produced by a combination of G05EFF and G05EYF.

#### G05EGF

Withdrawn at Mark 22. Replaced by G05PHF.

```
Old: CALL GO5EGF(E,A,NA,B,NB,R,NR,VAR,IFAIL)
New: AVAR = B(1)**2
     IQ = NB - 1
     IF (AVAR.GT.0.0D0) THEN
        DO 10 I = 1, IQ
           THETA(I) = -B(I+1)/B(1)
  10
        CONTINUE
     ELSE
        DO 20 I = 1, IQ
           THETA(I) = 0.0D0
  2.0
        CONTINUE
     END IF
     MODE = 0
     CALL GO5PHF (MODE, N, E, NA, A, IQ, THETA, AVAR, R, LR, STATE, VAR, X, IFAIL)
```

The real vector THETA must be of length at least IQ = NB - 1.

The old routine G05EGF sets up a reference vector for use by G05EWF. The replacement routine G05PHF is now used to both set up a reference vector and generate the required variates. Setting MODE=0 in the call to G05PHF sets up the real reference vector R and hence mimics the functionality of G05EGF. When MODE=0, the integer array STATE in the call to G05PHF need not be set.

#### **G05EHF**

Withdrawn at Mark 22. Replaced by G05NCF.

```
Old: CALL GO5EHF(INDEX,N,IFAIL)
New: CALL GO5NCF(INDEX,N,STATE,IFAIL)
```

The integer array STATE in the call to G05NCF contains information on the base generator being used. This array must have been initialized prior to calling G05NCF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05NCF is likely to be different from those produced by G05EHF.

### G05EJF

Withdrawn at Mark 22. Replaced by G05NDF.

```
Old: CALL GO5EJF(IA,N,IZ,M,IFAIL)
New: CALL GO5NDF(IA,N,IZ,M,STATE,IFAIL)
```

The integer array STATE in the call to G05NDF contains information on the base generator being used. This array must have been initialized prior to calling G05NDF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization.

Due to changes in the underlying code the sequence of values produced by G05NDF is likely to be different from those produced by G05EJF.

#### **G05EWF**

Withdrawn at Mark 22. Replaced by G05PHF.

```
Old: CALL GO5EGF(E,A,NA,B,NB,R,NR,VAR,IFAIL)
     DO 10 I = 1, N
        X(I) = GO5EWF(R,NR,IFAIL)
  10 CONTINUE
New: AVAR = B(1)**2
     IQ = NB - 1
     IF (AVAR.GT.O.ODO) THEN
        DO 10 I = 1, IQ
           THETA(I) = -B(I+1)/B(1)
  10
        CONTINUE
     ELSE
        DO 20 I = 1, IQ
           THETA(I) = 0.0D0
  20
        CONTINUE
     END IF
     MODE = 2
     CALL GO5PHF(MODE, N, E, NA, A, NB-1, THETA, AVAR, VAR, R, LR, STATE, X, IFAIL)
```

The real vector THETA must be of length at least IQ = NB - 1.

The old routine G05EGF sets up a reference vector for use by G05EWF. The replacement routine G05PHF is now used to both set up a reference vector and generate the required variates. Setting the integer parameter MODE to 0 in the call to G05PHF sets up the real reference vector R and hence mimics the functionality of G05EGF. Setting MODE to 1 generates a series of variates from a reference vector mimicking the functionality of G05EWF. Setting MODE to 2 initializes the reference vector and generates the variates in one go.

The integer array STATE in the call to G05PHF contains information on the base generator being used. This array must have been initialized prior to calling G05PHF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05PHF is likely to be different from those produced by G05EGF.

### **G05EXF**

Withdrawn at Mark 22. Replaced by G05TDF.

```
Old: CALL G05EXF(P,NP,IP1,ITYPE,R1,LR1,IFAIL)
    DO 10 I = 1, N
        X(I) = G05EYF(R1,LR1)
10 CONTINUE
New: MODE = 2
    CALL G05TDF(MODE,N,P,NP,IP1,ITYPE,R,LR,STATE,X,IFAIL)
```

The old routine G05EXF sets up a reference vector for use by G05EYF. The replacement routine G05TDF is now used to both set up a reference vector and generate the required variates. Setting MODE = 0 in the call to G05TDF sets up the real reference vector R and hence mimics the functionality of G05EXF. Setting MODE = 1 generates a series of variates from a reference vector mimicking the functionality of G05EYF for this particular distribution. Setting MODE = 2 initializes the reference vector and generates the variates in one go.

The routine G05EYF returns a single variate at a time, whereas the new routine G05TDF returns a vector of N values in one go.

The length of the real reference vector, R, in G05TDF must be allocated in the calling program in contrast to the equivalent parameter in G05EXF, see the documentation for more details.

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The integer array STATE in the call to G05TDF contains information on the base generator being used. This array must have been initialized prior to calling G05TDF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05TDF is likely to be different from those produced by a combination of G05EXF and G05EYF.

#### G05EYF

Withdrawn at Mark 22. Replaced by G05TDF.

There is no direct replacement routine for G05EYF.

G05EYF is designed to generate random draws from a distribution defined by a reference vector. These reference vectors are created by other routines in Chapter G05, for example G05EBF, which have themselves been superseded. In order to replace a call to G05EYF you must identify which NAG routine generated the reference vector being used and look up its replacement. For example, to replace a call to G05EYF preceded by a call to G05EBF, as in:

```
CALL G05EBF(M, IB, R, NR, IFAIL)
X = G05EYF(R, NR)
```

you would need to look at the replacement routine for G05EBF.

#### G05EZF

Withdrawn at Mark 22. Replaced by G05RZF.

The old routine G05EAF sets up a reference vector for use by G05EZF. The functionality of both these routines has been combined into the single new routine G05RZF. Setting MODE = 2 in the call to G05RZF sets up the real reference vector R and generates the draws from the multivariate Normal distribution in one go.

The old routine G05EZF returns a single (M-dimensional vector) draw from the multivariate Normal distribution at a time, whereas the new routine G05RZF returns an N by M matrix of N draws in one go.

The integer array STATE in the call to G05RZF contains information on the base generator being used. This array must have been initialized prior to calling G05RZF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05RZF is likely to be different from those produced by G05EZF.

# G05FAF

Withdrawn at Mark 22. Replaced by G05SQF.

```
Old: CALL GO5FAF(AA,BB,N,X)
New: A = MIN(AA,BB)
B = MAX(AA,BB)
IFAIL = 0
CALL GO5SQF(N,A,B,STATE,X,IFAIL)
```

In G05SQF the minimum value must be held in the parameter A and the maximum in parameter B, therefore  $A \le B$ . This was not the case for the equivalent parameters in G05FAF.

The integer array STATE in the call to G05SQF contains information on the base generator being used. This array must have been initialized prior to calling G05SQF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SQF is likely to be different from those produced by G05FAF.

### G05FBF

Withdrawn at Mark 22. Replaced by G05SFF.

In G05SFF parameter A must be non-negative, this was not the case for the equivalent parameter in G05FBF.

The integer array STATE in the call to G05SFF contains information on the base generator being used. This array must have been initialized prior to calling G05SFF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SFF is likely to be different from those produced by G05FBF.

### **G05FDF**

Withdrawn at Mark 22. Replaced by G05SKF.

G05SKF expects the variance of the Normal distribution (parameter VAR), compared to G05FDF which expected the standard deviation.

The integer array STATE in the call to G05SKF contains information on the base generator being used. This array must have been initialized prior to calling G05SKF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SKF is likely to be different from those produced by G05FDF.

#### **G05FEF**

Withdrawn at Mark 22. Replaced by G05SBF.

```
Old: CALL GO5FEF(A,B,N,X,IFAIL)
New: CALL GO5SBF(N,A,B,STATE,X,IFAIL)
```

The integer array STATE in the call to G05SBF contains information on the base generator being used. This array must have been initialized prior to calling G05SBF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SBF is likely to be different from those produced by G05FEF.

### **G05FFF**

Withdrawn at Mark 22. Replaced by G05SJF.

```
Old: CALL GO5FFF(A,B,N,X,IFAIL)
New: CALL GO5SJF(N,A,B,STATE,X,IFAIL)
```

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The integer array STATE in the call to G05SJF contains information on the base generator being used. This array must have been initialized prior to calling G05SJF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SJF is likely to be different from those produced by G05FFF.

#### G05FSF

Withdrawn at Mark 22.
Replaced by G05SRF.

Old: CALL G05FSF(VK,N,X,IFAIL)
New: CALL G05SRF(N,VK,STATE,X,IFAIL)

The integer array STATE in the call to G05SRF contains information on the base generator being used. This array must have been initialized prior to calling G05SRF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05SRF is likely to be different from those produced by G05FSF.

### **G05GAF**

Withdrawn at Mark 22. Replaced by G05PXF.

```
Old: CALL G05GAF(SIDE, INIT, M, N, A, LDA, WK, IFAIL)
New: CALL G05PXF(SIDE, INIT, M, N, STATE, A, LDA, IFAIL)
```

The integer array STATE in the call to G05PXF contains information on the base generator being used. This array must have been initialized prior to calling G05PXF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05PXF is likely to be different from those produced by G05GAF.

### **G05GBF**

Withdrawn at Mark 22. Replaced by G05PYF.

```
Old: CALL G05GBF(N,D,C,LDC,EPS,WK,IFAIL)
New: CALL G05PYF(N,D,EPS,STATE,C,LDC,IFAIL)
```

The integer array STATE in the call to G05PYF contains information on the base generator being used. This array must have been initialized prior to calling G05PYF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05PYF is likely to be different from those produced by G05GBF.

### G05HDF

Withdrawn at Mark 22. Replaced by G05PJF.

```
LL = LL + 1
             PHI(I,J,L) = PAR(LL)
10
         CONTINUE
20
      CONTINUE
30 CONTINUE
   DO 60 L = 1, IQ-1
      DO 50 I = 1, K
         DO 40 J = 1, K
             LL = LL + 1
             THETA(I,J,L) = PAR(LL)
40
          CONTINUE
      CONTINUE
50
60 CONTINUE
   IF (MEAN.EQ.'M') THEN
      DO 70 I = 1, K
         LL = LL + 1
         XMEAN(I) = PAR(LL)
70
      CONTINUE
   ELSE
      DO 80 I = 1, K
         XMEAN(I) = 0.0D0
80
      CONTINUE
   END IF
   LDW = N
   CALL GO5PJF(IMODE, N, K, XMEAN, IP, PHI, IQ, THETA, QQ, LDQQ, REF, LREF, &
                STATE, W, LDW, 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  $\max(1, \operatorname{IP} \times (K \times K))$ ; if dimensioned as  $\operatorname{PHI}(K, K, \operatorname{IP})$  (as in the above example) then  $\operatorname{PHI}(i, j, l)$  will contain the element  $\operatorname{PAR}((l-1) \times k \times k + (i-1) \times k + j)$ . The real array THETA should have length at least  $\max(1, \operatorname{IQ} \times (K \times K))$ ; if dimensioned as  $\operatorname{THETA}(K, K, \operatorname{IQ})$  (as in the above example) then  $\operatorname{THETA}(i, j, l)$  will contain the element  $\operatorname{PAR}(\operatorname{IP} \times k \times k + (l-1) \times k \times k + (i-1) \times k + j)$ . The real array XMEAN should have length at least K; if  $\operatorname{MEAN} = \operatorname{'M'}$  then  $\operatorname{XMEAN}(i)$  will contain the element  $\operatorname{PAR}(\operatorname{IP} + \operatorname{IQ} \times k \times k + i)$ , otherwise XMEAN should contain an array of zero values.

The integer array STATE in the call to G05PJF contains information on the base generator being used. This array must have been initialized prior to calling G05PJF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05PJF is likely to be different from those produced by G05HDF.

## **G05HKF**

Withdrawn at Mark 24. Replaced by G05PDF.

```
Old: CALL GO5HKF(DIST,NUM,IP,IQ,THETA,GAMMA,DF,HT,ET,FCALL,RVEC,IGEN, & ISEED,RWSAV,IFAIL)

New: CALL GO5PDF(DIST,NUM,IP,IQ,THETA,GAMMA,DF,HT,ET,FCALL,R,LR,STATE, & IFAIL)
```

The integer array STATE in the call to G05PDF contains information on the base generator being used. This array must have been initialized prior to calling G05PDF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05PDF is likely to be different from those produced by G05HKF.

#### **G05HLF**

Withdrawn at Mark 24. Replaced by G05PEF.

```
Old: CALL GO5HLF(DIST,NUM,IP,IQ,THETA,GAMMA,DF,HT,ET,FCALL,RVEC,IGEN, & ISEED,RWSAV,IFAIL)

New: CALL GO5PEF(DIST,NUM,IP,IQ,THETA,GAMMA,DF,HT,ET,FCALL,R,LR,STATE, & IFAIL)
```

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The integer array STATE in the call to G05PEF contains information on the base generator being used. This array must have been initialized prior to calling G05PEF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05PEF is likely to be different from those produced by G05HLF.

#### G05HMF

Withdrawn at Mark 24. Replaced by G05PFF.

```
Old: CALL GO5HMF(DIST,NUM,IP,IQ,THETA,GAMMA,DF,HT,ET,FCALL,RVEC,IGEN, & ISEED,RWSAV,IFAIL)

New: CALL GO5PFF(DIST,NUM,IP,IQ,THETA,GAMMA,DF,HT,ET,FCALL,R,LR,STATE, & IFAIL)
```

The integer array STATE in the call to G05PFF contains information on the base generator being used. This array must have been initialized prior to calling G05PFF with a call to either G05KFF or G05KGF. The required length of the array STATE will depend on the base generator chosen during initialization. Due to changes in the underlying code the sequence of values produced by G05PFF is likely to be different from those produced by G05HMF.

#### **G05HNF**

Withdrawn at Mark 24. Replaced by G05PGF.

```
Old: CALL GO5HNF(DIST,NUM,IP,IQ,THETA,DF,HT,ET,FCALL,RVEC,IGEN,ISEED, & RWSAV,IFAIL)

New: CALL GO5PGF(DIST,NUM,IP,IQ,THETA,DF,HT,ET,FCALL,RVEC,STATE, IFAIL)
```

#### **G05KAF**

Withdrawn at Mark 24. Replaced by G05SAF.

```
Old: DO 20 I = 1, N
            X(I) = G05KAF(IGEN,ISEED)
20 CONTINUE
New: CALL G05SAF(N,STATE,X,IFAIL)
```

The old routine G05KAF returns a single variate at a time, whereas the new routine G05SAF returns a vector of N values in one go.

### G05KBF

Withdrawn at Mark 24. Replaced by G05KFF.

# G05KCF

Withdrawn at Mark 24. Replaced by G05KGF.

```
CALL GO5KGF(2,IGEN,STATE,LSTATE,IFAIL) END IF
```

### G05KEF

Withdrawn at Mark 24. Replaced by G05TBF.

The old routine G05KEF returns a single variate at a time, whereas the new routine G05TBF returns a vector of N values in one go.

#### G05LAF

Withdrawn at Mark 24. Replaced by G05SKF.

```
Old: CALL GO5LAF(XMU, VAR, N, X, IGEN, ISEED, IFAIL)
New: CALL GO5SKF(N, XMU, VAR, STATE, X, IFAIL)
```

# G05LBF

Withdrawn at Mark 24. Replaced by G05SNF.

```
Old: CALL GO5LBF(DF,N,X,IGEN,ISEED,IFAIL)
New: CALL GO5SNF(N,DF,STATE,X,IFAIL)
```

#### **G05LCF**

Withdrawn at Mark 24. Replaced by G05SDF.

```
Old: CALL GO5LCF(DF,N,X,IGEN,ISEED,IFAIL)
New: CALL GO5SDF(N,DF,STATE,X,IFAIL)
```

### **G05LDF**

Withdrawn at Mark 24. Replaced by G05SHF.

```
Old: CALL GO5LDF(DF1,DF2,N,X,IGEN,ISEED,IFAIL)
New: CALL GO5SHF(N,DF1,DF2,STATE,X,IFAIL)
```

### **G05LEF**

Withdrawn at Mark 24. Replaced by G05SBF.

```
Old: CALL GO5LEF(A,B,N,X,IGEN,ISEED,IFAIL)
New: CALL GO5SBF(N,A,B,STATE,X,IFAIL)
```

### **G05LFF**

Withdrawn at Mark 24. Replaced by G05SJF.

```
Old: CALL G05LFF(A,B,N,X,IGEN,ISEED,IFAIL)
New: CALL G05SJF(N,A,B,STATE,X,IFAIL)
```

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# **G05LGF**

Withdrawn at Mark 24. Replaced by G05SQF.

Old: CALL GO5LGF(A,B,N,X,IGEN,ISEED,IFAIL)
New: CALL GO5SQF(N,A,B,STATE,X,IFAIL)

#### G05LHF

Withdrawn at Mark 24. Replaced by G05SPF.

Old: CALL GO5LHF(XMIN,XMAX,XMED,N,X,IGEN,ISEED,IFAIL)
New: CALL GO5SPF(N,XMIN,XMED,XMAX,STATE,X,IFAIL)

### G05LJF

Withdrawn at Mark 24. Replaced by G05SFF.

Old: CALL G05LJF(A,N,X,IGEN,ISEED,IFAIL)
New: CALL G05SFF(N,A,STATE,X,IFAIL)

#### **G05LKF**

Withdrawn at Mark 24. Replaced by G05SMF.

Old: CALL GO5LKF(XMU, VAR, N, X, IGEN, ISEED, IFAIL)
New: CALL GO5SMF(N, XMU, VAR, STATE, X, IFAIL)

### G05LLF

Withdrawn at Mark 24. Replaced by G05SJF.

Old: CALL GO5LLF(XMED, SEMIQR, N, X, IGEN, ISEED, IFAIL)
New: CALL GO5SCF(N, XMED, SEMIQR, STATE, X, IFAIL)

# **G05LMF**

Withdrawn at Mark 24. Replaced by G05SSF.

Old: CALL G05LMF(A,B,N,X,IGEN,ISEED,IFAIL)
New: CALL G05SSF(N,A,B,STATE,X,IFAIL)

# G05LNF

Withdrawn at Mark 24. Replaced by G05SLF.

Old: CALL GO5LNF(A,B,N,X,IGEN,ISEED,IFAIL)
New: CALL GO5SLF(N,A,B,STATE,X,IFAIL)

## **G05LPF**

Withdrawn at Mark 24. Replaced by G05SRF.

Old: CALL GO5LPF(VK,N,X,IGEN,ISEED,IFAIL)
New: CALL GO5SRF(N,VK,STATE,X,IFAIL)

### **G05LQF**

```
Withdrawn at Mark 24.
Replaced by G05SGF.
```

```
Old: CALL G05LQF(NMIX,A,WGT,N,X,IGEN,ISEED,IFAIL)
New: CALL G05SGF(N,NMIX,A,WGT,STATE,X,IFAIL)
```

#### G05LXF

Withdrawn at Mark 24. Replaced by G05RYF.

```
Old: CALL GO5LXF(MODE,DF,M,XMU,C,LDC,N,X,LDX,IGEN,ISEED,R,LR,IFAIL)
New: CALL GO5RYF(MODE,N,DF,M,XMU,C,LDC,R,LR,STATE,X,LDX,IFAIL)
```

### **G05LYF**

Withdrawn at Mark 24. Replaced by G05RZF.

```
Old: GO5LYF(MODE,M,XMU,C,LDC,N,X,LDX,IGEN,ISEED,R,LR,IFAIL)
New: GO5RZF(MODE,N,M,XMU,C,LDC,R,LR,STATE,X,LDX,IFAIL)
```

#### G05LZF

Withdrawn at Mark 24. Replaced by G05RZF.

```
Old: CALL GO5LZF(MODE,M,XMU,C,LDC,X,IGEN,ISEED,R,LR,IFAIL)
New: N = 1
    LDX = 1
    CALL GO5RZF(MODE,N,M,XMU,C,LDC,R,LR,STATE,X,LDX,IFAIL)
```

# G05MAF

Withdrawn at Mark 24. Replaced by G05TLF.

```
Old: CALL GO5MAF(A,B,N,X,IGEN,ISEED,IFAIL)
New: CALL GO5TLF(N,A,B,STATE,X,IFAIL)
```

# G05MBF

Withdrawn at Mark 24.

Replaced by G05TCF.

```
Old: CALL G05MBF(MODE,P,N,X,IGEN,ISEED,R,NR,IFAIL)
New: CALL G05TCF(MODE,N,P,R,LR,STATE,X,IFAIL)
        DO 20 I = 1, N
        X(I) = X(I) + 1
20 CONTINUE
```

G05MBF returned the number of trials required to get the first success, whereas G05TCF returns the number of failures before the first success, therefore the value returned by G05TCF is one less than the equivalent value returned from G05MBF.

# G05MCF

Withdrawn at Mark 24. Replaced by G05THF.

```
Old: CALL GO5MCF(MODE,M,P,N,X,IGEN,ISEED,R,NR,IFAIL)
New: CALL GO5THF(MODE,N,M,P,R,LR,STATE,X,IFAIL)
```

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# **G05MDF**

Withdrawn at Mark 24. Replaced by G05TFF.

Old: CALL GO5MDF(MODE,A,N,X,IGEN,ISEED,R,NR,IFAIL)
New: CALL GO5TFF(MODE,N,A,R,LR,STATE,X,IFAIL)

#### G05MEF

Withdrawn at Mark 24. Replaced by G05TKF.

Old: CALL GO5MEF(M, VLAMDA, X, IGEN, ISEED, IFAIL)
New: CALL GO5TKF(M, VLAMDA, STATE, X, IFAIL)

### G05MJF

Withdrawn at Mark 24. Replaced by G05TAF.

Old: CALL GO5MJF(MODE,M,P,N,X,IGEN,ISEED,R,NR,IFAIL)
New: CALL GO5TAF(MODE,N,M,P,R,LR,STATE,X,IFAIL)

#### G05MKF

Withdrawn at Mark 24. Replaced by G05TJF.

Old: CALL GO5MKF(MODE,LAMBDA,N,X,IGEN,ISEED,R,NR,IFAIL)
New: CALL GO5TJF(MODE,N,LAMBDA,R,LR,STATE,X,IFAIL)

#### G05MLF

Withdrawn at Mark 24. Replaced by G05TEF.

Old: CALL GO5MLF(MODE,NS,NP,M,N,X,IGEN,ISEED,R,NR,IFAIL)
New: CALL GO5TEF(MODE,N,NS,NP,M,R,LR,STATE,X,IFAIL)

# **G05MRF**

Withdrawn at Mark 24. Replaced by G05TGF.

Old: CALL G05MRF(MODE,M,K,P,N,X,LDX,IGEN,ISEED,R,NR,IFAIL)
New: CALL G05TGF(MODE,N,M,K,P,R,LR,STATE,X,LDX,IFAIL)

# G05MZF

Withdrawn at Mark 24. Replaced by G05TDF.

Old: CALL GO5MZF(MODE,P,NP,IP1,ITYPE,N,X,IGEN,ISEED,R,NR,IFAIL)
New: CALL GO5TDF(MODE,N,P,NP,IP1,ITYPE,R,LR,STATE,X,IFAIL)

## **G05NAF**

Withdrawn at Mark 24. Replaced by G05NCF.

Old: CALL GO5NAF(INDEX,N,IGEN,ISEED,IFAIL)
New: CALL GO5NCF(INDEX,N,STATE,IFAIL)

### **G05NBF**

```
Withdrawn at Mark 24. Replaced by G05NDF.
```

```
Old: CALL GO5NBF(IPOP,N,ISAMPL,M,IGEN,ISEED,IFAIL)
New: CALL GO5NDF(IPOP,N,ISAMPL,M,STATE,IFAIL)
```

#### G05PAF

Withdrawn at Mark 24. Replaced by G05PHF.

```
Old: CALL GO5PAF(MODE,XMEAN,IP,PHI,IQ,THETA,AVAR,VAR,N,X,IGEN,ISEED,R, & NR,IFAIL)

New: CALL GO5PHF(MODE,N,XMEAN,IP,PHI,IQ,THETA,AVAR,R,LR,STATE,VAR,X, & IFAIL)
```

### **G05PCF**

Withdrawn at Mark 24. Replaced by G05PJF.

```
Old: CALL GO5PCF(MODE,K,XMEAN,IP,PHI,IQ,THETA,VAR,LDV,N,X,IGEN,ISEED,R, & NR,IWORK,LIWORK,IFAIL)

New: CALL GO5PJF(MODE,N,K,XMEAN,IP,PHI,IQ,THETA,VAR,LDV,R,LR,STATE,X,LDX, & IFAIL)
```

# **G05QAF**

Withdrawn at Mark 24. Replaced by G05PXF.

```
Old: CALL G05QAF(SIDE, INIT, M, N, A, LDA, IGEN, ISEED, WK, IFAIL)
New: CALL G05PXF(SIDE, INIT, M, N, STATE, A, LDA, IFAIL)
```

# G05QBF

Withdrawn at Mark 24. Replaced by G05PYF.

```
Old: CALL G05QBF(N,D,C,LDC,EPS,IGEN,ISEED,WK,IFAIL)
New: CALL G05PYF(N,D,EPS,STATE,C,LDC,IFAIL)
```

# **G05QDF**

Withdrawn at Mark 24. Replaced by G05PZF.

```
Old: CALL G05QDF(MODE,NROW,NCOL,TOTR,TOTC,X,LDX,IGEN,ISEED,R,NR,IW,LIW, & IFAIL)

New: CALL G05PZF(MODE,NROW,NCOL,TOTR,TOTC,R,LR,STATE,X,LDX,IFAIL)
```

# **G05RAF**

Withdrawn at Mark 24. Replaced by G05RDF.

```
Old: CALL GO5RAF(MODE,M,C,LDC,N,X,LDX,IGEN,ISEED,R,LR,IFAIL)
New: CALL GO5RDF(MODE,N,M,C,LDC,R,LR,STATE,X,LDX,IFAIL)
```

### **G05RBF**

Withdrawn at Mark 24. Replaced by G05RCF.

```
Old: CALL GO5RBF(MODE,DF,M,C,LDC,N,X,LDX,IGEN,ISEED,R,LR,IFAIL)
New: CALL GO5RCF(MODE,N,DF,M,C,LDC,R,LR,STATE,X,LDX,IFAIL)
```

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#### **G05YAF**

```
Withdrawn at Mark 23.
Replaced by G05YLF and G05YMF.
Faure quasi-random numbers
Old: CALL GO5YAF(.TRUE., 'F', ISKIP, IDIM, QUAS, IREF, IFAIL)
New: CALL G05YLF(4, IDIM, IREF, LIREF, ISKIP, IFAIL)
Old: CALL GO5YAF(.FALSE., 'F', ISKIP, IDIM, QUAS, IREF, IFAIL)
New: CALL GO5YMF(1,2,QUAS,LDQUAS,IREF,IFAIL)
Sobol quasi-random numbers
Old: CALL GO5YAF(.TRUE.,'S', ISKIP, IDIM, QUAS, IREF, IFAIL)
New: CALL GO5YLF(2,IDIM,IREF,LIREF,ISKIP,IFAIL)
Old: CALL GO5YAF(.FALSE.,'S', ISKIP, IDIM, QUAS, IREF, IFAIL)
New: CALL G05YMF(1,2,QUAS,LDQUAS,IREF,IFAIL)
Neiderreiter quasi-random numbers
Old: CALL GO5YAF(.TRUE.,'N', ISKIP, IDIM, QUAS, IREF, IFAIL)
New: CALL GO5YLF(3, IDIM, IREF, LIREF, ISKIP, IFAIL)
Old: CALL GO5YAF(.FALSE.,'N',ISKIP,IDIM,QUAS,IREF,IFAIL)
New: CALL G05YMF(1,2,QUAS,LDQUAS,IREF,IFAIL)
G05YBF
Withdrawn at Mark 23.
Replaced by G05YLF and either G05YJF or G05YKF.
This routine has been replaced by a suite of routines consisting of the relevant initialization routine
followed by one of two possible generator routines.
Faure quasi-random numbers with Gaussian probability:
Old: CALL GO5YBF(.TRUE.,'F',.FALSE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL GO5YLF(4,IDIM,IREF,LIREF,ISKIP,IFAIL)
Old: CALL GO5YBF(.FALSE., 'F', .FALSE., MEAN, STD, ISKIP, IDIM, QUASI, IREF, IFAIL)
New: CALL G05YJF(MEAN,STD,N,QUASI,IREF,IFAIL)
Sobol quasi-random numbers with Gaussian probability:
Old: CALL GO5YBF(.TRUE.,'S',.FALSE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL GO5YLF(2, IDIM, IREF, LIREF, ISKIP, IFAIL)
Old: CALL GO5YBF(.FALSE.,'S',.FALSE., MEAN, STD, ISKIP, IDIM, QUASI, IREF, IFAIL)
New: CALL G05YJF(MEAN, STD, N, QUASI, IREF, IFAIL)
Neiderreiter quasi-random numbers with Gaussian probability:
Old: CALL GO5YBF(.TRUE.,'N',.FALSE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YLF(3, IDIM, IREF, LIREF, ISKIP, IFAIL)
Old: CALL GO5YBF(.FALSE.,'N',.FALSE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YJF(MEAN, STD, N, QUASI, IREF, IFAIL)
Faure quasi-random numbers with log Normal probability:
Old: CALL GO5YBF(.TRUE., 'F', .TRUE., MEAN, STD, ISKIP, IDIM, QUASI, IREF, IFAIL)
New: CALL GO5YLF(4,IDIM,IREF,LIREF,ISKIP,IFAIL)
```

```
Old: CALL GO5YBF(.FALSE., 'F', .TRUE., MEAN, STD, ISKIP, IDIM, QUASI, IREF, IFAIL)
New: CALL G05YKF(MEAN,STD,N,QUASI,IREF,IFAIL)
Sobol quasi-random numbers with log Normal probability:
Old: CALL GO5YBF(.TRUE.,'S',.TRUE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL GO5YLF(2,IDIM,IREF,LIREF,ISKIP,IFAIL)
Old: CALL G05YBF(.FALSE.,'S',.TRUE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL GO5YKF(MEAN,STD,N,QUASI,IREF,IFAIL)
Neiderreiter quasi-random numbers with log Normal probability:
Old: CALL GO5YBF(.TRUE.,'N',.TRUE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL G05YLF(3,IDIM,IREF,LIREF,ISKIP,IFAIL)
Old: CALL GO5YBF(.FALSE.,'N',.TRUE.,MEAN,STD,ISKIP,IDIM,QUASI,IREF,IFAIL)
New: CALL GO5YKF (MEAN, STD, N, QUASI, IREF, IFAIL)
G05YCF
Withdrawn at Mark 24.
Replaced by G05YLF.
Old: CALL GO5YCF(IDIM, IREF, IFAIL)
New: GENID = 4
     CALL GO5YLF(GENID, IDIM, IREF, LIREF, ISKIP, IFAIL)
G05YDF
Withdrawn at Mark 24.
Replaced by G05YMF.
Old: CALL GO5YDF(N,QUASI,IREF,IFAIL)
New: CALL GO5YMF(N,QUAS,LDQUAS,IREF,IFAIL)
G05YEF
Withdrawn at Mark 24.
Replaced by G05YLF.
Old: CALL GO5YEF(IDIM, IREF, ISKIP, IFAIL)
New: GENID = 2
     CALL GO5YLF(GENID, IDIM, IREF, LIREF, ISKIP, IFAIL)
G05YFF
Withdrawn at Mark 24.
Replaced by G05YMF.
Old: CALL GO5YFF(N,QUASI,IREF,IFAIL)
New: CALL G05YMF(N,QUAS,LDQUAS,IREF,IFAIL)
G05YGF
Withdrawn at Mark 24.
Replaced by G05YLF.
Old: CALL GO5YGF(IDIM, IREF, ISKIP, IFAIL)
New: GENID = 3
     CALL GO5YLF(GENID, IDIM, IREF, LIREF, ISKIP, IFAIL)
```

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### **G05YHF**

```
Withdrawn at Mark 24. Replaced by G05YMF.
```

```
Old: CALL GO5YHF(N,QUASI,IREF,IFAIL)
New: CALL GO5YMF(N,RCORD,QUAS,LDQUAS,IREF,IFAIL)
```

#### G05ZAF

Withdrawn at Mark 22.

There is no replacement for this routine.

# **G13** – Time Series Analysis

### G13DAF

Withdrawn at Mark 17. Replaced by G13DMF.

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

# G13DCF

Withdrawn at Mark 24. Replaced by G13DDF.

```
Old: CALL G13DCF(K,N,IP,IQ,MEAN,PAR,NPAR,QQ,KMAX,W,PARHLD,EXACT,IPRINT, & CGETOL,MAXCAL,ISHOW,NITER,RLOGL,V,G,CM,LDCM,WORK,LWORK, & IW,LIW,IFAIL)

New: CALL G13DDF(K,N,IP,IQ,MEAN,PAR,NPAR,QQ,KMAX,W,PARHLD,EXACT,IPRINT, & CGETOL,MAXCAL,ISHOW,NITER,RLOGL,V,G,CM,LDCM,IFAIL)
```

The workspace arguments WORK, LWORK, IW and LIW are no longer required in the call to G13DDF.

# P01 – Error Trapping

### P01ABF

Withdrawn at Mark 24.

There is no replacement for this routine.

# **X02** – Machine Constants

## X02DAF

Withdrawn at Mark 24.

There is no replacement for this routine.

Replacement Calls NAG Library Manual

# X02DJF

Withdrawn at Mark 24. There is no replacement for this routine.

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Mark 24