NAG Fortran Library Routine Document

F12FGF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details.

1 Purpose

F12FGF is the main solver routine in a suite of routines consisting of F12FGF, F12FDF and F12FFF, that must be called following an initial call to F12FFF and following any calls to F12FDF.

F12FGF returns approximations to selected eigenvalues, and (optionally) the corresponding eigenvectors, of a standard or generalized eigenvalue problem defined by real banded symmetric matrices. The banded matrix must be stored using the LAPACK storage format for real banded **non**symmetric matrices.

2 Specification

```
 SUBROUTINE F12FGF (KL, KU, AB, LDAB, MB, LDMB, SIGMA, NCONV, D, Z, LDZ,
1                   RESID, V, LDV, COMM, ICOMM, IFAIL)
 INTEGER            KL, KU, LDAB, LDMB, NCONV, LDZ, LDV, ICOMM(*), IFAIL
 double precision   AB(LDAB,*), MB(LDMB,*), SIGMA, D(*), Z(LDZ,*),
1                   RESID(*), V(LDV,*), COMM(*)
```

3 Description

The suite of routines is designed to calculate some of the eigenvalues, λ, (and optionally the corresponding eigenvectors, x) of a standard eigenvalue problem $Ax = \lambda x$, or of a generalized eigenvalue problem $Ax = \lambda Bx$ of order n, where n is large and the coefficient matrices A and B are banded, real and symmetric.

Following a call to the initialization routine F12FFF, F12FGF returns the converged approximations to eigenvalues and (optionally) the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace. The eigenvalues (and eigenvectors) are selected from those of a standard or generalized eigenvalue problem defined by real banded symmetric matrices. There is negligible additional computational cost to obtain eigenvectors; an orthonormal basis is always computed, but there is an additional storage cost if both are requested.

The banded matrices A and B must be stored using the LAPACK storage format for banded **non**symmetric matrices; please refer to the f07 Chapter Introduction for details on this storage format.

F12FGF is based on the banded driver routines **dsbdr1** to **dsbdr6** from the ARPACK package, which uses the Implicitly Restarted Lanczos iteration method. The method is described in Lehoucq and Sorensen (1996) and Lehoucq (2001) while its use within the ARPACK software is described in great detail in Lehoucq *et al.* (1998). This suite of routines offers the same functionality as the ARPACK banded driver software for real symmetric problems, but the interface design is quite different in order to make the option setting clearer to the user and to combine the different drivers into a general purpose routine.

F12FGF, is a general purpose forward communication routine that must be called following initialization by F12FFF. F12FGF uses options, set either by default or explicitly by calling F12FDF, to return the converged approximations to selected eigenvalues and (optionally):

the corresponding approximate eigenvectors;

an orthonormal basis for the associated approximate invariant subspace;

both.

4 References

Lehoucq R B (2001) Implicitly Restarted Arnoldi Methods and Subspace Iteration *SIAM Journal on Matrix Analysis and Applications* **23** 551–562

Lehoucq R B and Scott J A (1996) An evaluation of software for computing eigenvalues of sparse nonsymmetric matrices *Preprint MCS-P547-1195* Argonne National Laboratory

Lehoucq R B and Sorensen D C (1996) Deflation Techniques for an Implicitly Restarted Arnoldi Iteration *SIAM Journal on Matrix Analysis and Applications* **17** 789–821

Lehoucq R B, Sorensen D C and Yang C (1998) *ARPACK Users' Guide: Solution of Large-Scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods* SIAM, Philidelphia

5 Parameters

1: KL – INTEGER *Input*

On entry: the number of subdiagonals of the matrices A and B.

Constraint: $\mathrm{KL} \geq 0$.

2: KU – INTEGER *Input*

On entry: the number of superdiagonals of the matrices A and B. Since A and B are symmetric, the normal case is $\mathrm{KU} = \mathrm{KL}$.

Constraint: $\mathrm{KU} \geq 0$.

3: AB(LDAB,$*$) – ***double precision*** array *Input*

Note: the second dimension of the array AB must be at least $\max(1, \mathrm{N})$.

On entry: AB must contain the matrix A in LAPACK banded storage format for nonsymmetric matrices.

4: LDAB – INTEGER *Input*

On entry: the first dimension of the array LDAB as declared in the (sub)program from which F12FGF is called.

Constraint: $\mathrm{LDAB} \geq 2 \times \mathrm{KL} + \mathrm{KU} + 1$.

5: MB(LDMB,$*$) – ***double precision*** array *Input*

Note: the second dimension of the array MB must be at least $\max(1, \mathrm{N})$.

On entry: MB must contain the matrix B in LAPACK banded storage format for nonsymmetric matrices.

6: LDMB – INTEGER *Input*

On entry: the first dimension of the array LDMB as declared in the (sub)program from which F12FGF is called.

7: SIGMA – ***double precision*** *Input*

On entry: if one of the **Shifted** modes has been selected then SIGMA contains the real shift used; otherwise SIGMA is not referenced.

8: NCONV – INTEGER *Output*

On exit: the number of converged eigenvalues.

9: D(∗) – ***double precision*** array *Output*

Note: the dimension of the array D must be at least NEV.

On exit: the first NCONV locations of the array D contain the the converged approximate eigenvalues.

10: Z(LDZ,∗) – ***double precision*** array *Output*

Note: the second dimension of the array Z must be at least NEV + 1 if the default option **Vectors** = Ritz has been selected and at least 1 if the option **Vectors** = None or Schur has been selected.

On exit: if the default option **Vectors** = Ritz has been selected then Z contains the final set of eigenvectors corresponding to the eigenvalues held in D. The real eigenvector associated with an eigenvalue is stored in the corresponding column of Z.

11: LDZ – INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F12FGF is called.

Constraints:

if the default option **Vectors** = Ritz has been selected, LDZ ≥ N;
if the option **Vectors** = None or Schur has been selected, LDZ ≥ 1.

12: RESID(∗) – ***double precision*** array *Input/Output*

Note: the dimension of the array RESID must be at least N.

On entry: RESID need not be set unless the option **Initial Residual** has been set in a prior call to F12FDF in which case RESID should contain an initial residual vector.

On exit: RESID contains the final residual vector.

13: V(LDV,∗) – ***double precision*** array *Output*

Note: the second dimension of the array V must be at least max(1, NCV).

On exit: if the option **Vectors** = Schur has been set or the option **Vectors** = Ritz has been set and a separate array Z has been passed then the first NCONV columns of V will contain approximate Schur vectors that span the desired invariant subspace.

14: LDV – INTEGER *Input*

On entry: the first dimension of the array V as declared in the (sub)program from which F12FGF is called.

Constraint: LDV ≥ n.

15: COMM(∗) – ***double precision*** array *Communication Array*

COMM, on initial entry, must remain unchanged from a prior call to F12FFF or F12FDF.

16: ICOMM(∗) – INTEGER array *Communication Array*

ICOMM, on initial entry, must remain unchanged from the prior call to F12FBF or F12FDF.

17: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

For environments where it might be inappropriate to halt program execution when an error is detected, the value −1 or 1 is recommended. If the output of error messages is undesirable, then

the value 1 is recommended. Otherwise, for users not familiar with this parameter the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

6 Error Indicators and Warnings

If on entry IFAIL $= 0$ or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL $= 1$

On entry, KL < 0.

IFAIL $= 2$

On entry, KU < 0.

IFAIL $= 3$

On entry, LDAB $< 2 \times$ KL $+$ KU $+ 1$.

IFAIL $= 4$

iteration limit < 0.

IFAIL $= 5$

The options **Generalized** and **Regular** are incompatible.

IFAIL $= 6$

Eigenvalues from **both ends** of the spectrum were requested, but only one eigenvalue (NEV) is requested.

IFAIL $= 7$

The option **Initial Residual** was selected but the starting vector held in RESID is zero.

IFAIL $= 8$

On entry, LDZ $< \max(1, \mathrm{N})$ or LDZ < 1 when no vectors are required.

IFAIL $= 9$

On entry, the option **Vectors** $=$ Select was selected, but this is not yet implemented.

IFAIL $= 10$

The number of eigenvalues found to sufficient accuracy is zero.

IFAIL $= 11$

Could not build an Lanczos factorization. Consider changing NCV or NEV in the initialization routine (see Section 5 of the document for F12FAF for details of these parameters).

IFAIL $= 12$

Unexpected error in internal call to compute eigenvalues and corresponding error bounds of the current symmetric tridiagonal matrix. Please contact NAG.

IFAIL = 13

Unexpected error during calculation of a real Schur form: there was a failure to compute all the converged eigenvalues. Please contact NAG.

IFAIL = 14

Failure during internal factorization of real banded matrix. Please contact NAG.

IFAIL = 15

Failure during internal solution of real banded system. Please contact NAG.

IFAIL = 16

The maximum number of iterations has been reached. Some Ritz values may have converged; NCONV returns the number of converged values.

IFAIL = 17

No shifts could be applied during a cycle of the implicitly restarted Lanczos iteration. One possibility is to increase the size of NCV relative to NEV (see Section 5 of the document for F12FFF for details of these parameters).

IFAIL = 18

An unexpected error has occurred. Please contact NAG.

IFAIL = 19

The routine was unable to dynamically allocate sufficient internal workspace. Please contact NAG.

7 Accuracy

The relative accuracy of a Ritz value, λ, is considered acceptable if its Ritz estimate $\leq$ **Tolerance** $\times |\lambda|$. The default **Tolerance** used is the ***machine precision*** given by X02AJF.

8 Further Comments

None.

9 Example

The example solves $Ax = \lambda x$ in regular mode, where A is obtained from the standard central difference discretization of the two-dimensional convection-diffusion operator $\frac{d^2u}{dx^2} + \frac{d^2u}{dy^2} = \rho\frac{du}{dx}$ on the unit square with zero Dirichlet boundary conditions. A is stored in LAPACK banded storage format.

9.1 Program Text

```
*     F12FGF Example Program Text
*     Mark 21 Release. NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          LICOMM, NIN, NOUT
      PARAMETER        (LICOMM=134,NIN=5,NOUT=6)
      INTEGER          MAXBDW, MAXN, MAXNCV, LDAB, LDV
      PARAMETER        (MAXBDW=50,MAXN=1000,MAXNCV=50,LDAB=MAXBDW,
     +                 LDV=MAXN)
      INTEGER          LCOMM
      PARAMETER        (LCOMM=60)
      DOUBLE PRECISION ONE, ZERO
      PARAMETER        (ONE=1.0D+0,ZERO=0.0D+0)
*     .. Local Scalars ..
      DOUBLE PRECISION H2, SIGMA
      INTEGER          I, IDIAG, IFAIL, IFAIL1, ISUB, ISUP, J, KL, KU,
```

```
     +                 LO, N, NCONV, NCV, NEV, NX
*     .. Local Arrays ..
      DOUBLE PRECISION AB(LDAB,MAXN), AX(MAXN), COMM(LCOMM),
     +                 D(MAXNCV,2), MB(1), RESID(MAXN), V(LDV,MAXNCV)
      INTEGER          ICOMM(LICOMM)
*     .. External Functions ..
      DOUBLE PRECISION DNRM2
      EXTERNAL         DNRM2
*     .. External Subroutines ..
      EXTERNAL         DAXPY, DGBMV, F06QHF, F12FFF, F12FGF, X04ABF,
     +                 X04CAF
*     .. Intrinsic Functions ..
*
      INTRINSIC        DABS
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F12FGF Example Program Results'
      WRITE (NOUT,*)
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) NX, NEV, NCV
      N = NX*NX
      IF (N.LT.1 .OR. N.GT.MAXN) THEN
         WRITE (NOUT,99999) 'N is out of range: N = ', N
      ELSE IF (NCV.GT.MAXNCV) THEN
         WRITE (NOUT,99999) 'NCV is out of range: NCV = ', NCV
      ELSE
         IFAIL = 0
*     Initialize communication arrays.
         CALL F12FFF(N,NEV,NCV,ICOMM,LICOMM,COMM,LCOMM,IFAIL)
*
*     Construct the matrix A in banded form and store in AB.
*     Zero out AB.
         CALL F06QHF('G',LDAB,N,ZERO,ZERO,AB,LDAB)
*     KU, KL are number of superdiagonals and subdiagonals within the
*     band of matrices A and M.
         KL = NX
         KU = NX
*     Main diagonal of A.
         H2 = ONE/((NX+1)*(NX+1))
         IDIAG = KL + KU + 1
         DO 20 J = 1, N
            AB(IDIAG,J) = 4.0D+0/H2
   20    CONTINUE
*     First subdiagonal and superdiagonal of A.
         ISUP = KL + KU
         ISUB = KL + KU + 2
         DO 60 I = 1, NX
            LO = (I-1)*NX
            DO 40 J = LO + 1, LO + NX - 1
               AB(ISUP,J+1) = -ONE/H2
               AB(ISUB,J) = -ONE/H2
   40       CONTINUE
   60    CONTINUE
*     KL-th subdiagonal and KU-th super-diagonal.
         ISUP = KL + 1
         ISUB = 2*KL + KU + 1
         DO 100 I = 1, NX - 1
            LO = (I-1)*NX
            DO 80 J = LO + 1, LO + NX
               AB(ISUP,NX+J) = -ONE/H2
               AB(ISUB,J) = -ONE/H2
   80       CONTINUE
  100    CONTINUE
*
*     Find eigenvalues of largest magnitude and the corresponding
*     eigenvectors.
         IFAIL = 1
         CALL F12FGF(KL,KU,AB,LDAB,MB,1,SIGMA,NCONV,D,V,LDV,RESID,V,LDV,
     +               COMM,ICOMM,IFAIL)
         IF (IFAIL.EQ.0) THEN
*        Compute the residual norm  ||A*x - lambda*x||.
```

```
            DO 120 J = 1, NCONV
               CALL DGBMV('NoTranspose',N,N,KL,KU,ONE,AB(KL+1,1),LDAB,
     +                    V(1,J),1,ZERO,AX,1)
               CALL DAXPY(N,-D(J,1),V(1,J),1,AX,1)
               D(J,2) = DNRM2(N,AX,1)
               D(J,2) = D(J,2)/DABS(D(J,1))
  120       CONTINUE
            WRITE (NOUT,*)
            CALL X04ABF(1,NOUT)
            CALL X04CAF('G','N',NCONV,2,D,MAXNCV,
     +                  ' Ritz values and residuals',IFAIL1)
         ELSE
            WRITE (NOUT,99998) IFAIL
         END IF
      END IF
*
99999 FORMAT (1X,A,I5)
99998 FORMAT (1X,' NAG Routine F12FGF Returned with IFAIL = ',I6)
      END
```

9.2 Program Data

```
F12FGF Example Program Data
 10 4 10 : Values for NX NEV and NCV
```

9.3 Program Results

```
 F12FGF Example Program Results

  Ritz values and residuals
                1           2
 1    8.9117E+02   1.0059E-15
 2    9.1978E+02   1.3507E-15
 3    9.1978E+02   1.2715E-15
 4    9.4839E+02   1.3676E-15
```