

NAG Library Routine Document

F04CGF

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

F04CGF computes the solution to a complex system of linear equations $AX = B$, where A is an n by n Hermitian positive-definite tridiagonal matrix and X and B are n by r matrices. An estimate of the condition number of A and an error bound for the computed solution are also returned.

2 Specification

```
SUBROUTINE F04CGF(N, NRHS, D, E, B, LDB, RCOND, ERBND, IFAIL)
INTEGER          N, NRHS, LDB, IFAIL
double precision D(*), RCOND, ERBND
complex*16      E(*), B(LDB,*)
```

3 Description

A is factorized as $A = LDL^H$, where L is a unit lower bidiagonal matrix and D is a real diagonal matrix, and the factored form of A is then used to solve the system of equations.

4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia <http://www.netlib.org/lapack/lug>

Higham N J (2002) *Accuracy and Stability of Numerical Algorithms* (2nd Edition) SIAM, Philadelphia

5 Parameters

- 1: N – INTEGER *Input*
On entry: the number of linear equations n , i.e., the order of the matrix A .
Constraint: $N \geq 0$.
- 2: NRHS – INTEGER *Input*
On entry: the number of right-hand sides r , i.e., the number of columns of the matrix B .
Constraint: $NRHS \geq 0$.
- 3: D(*) – **double precision** array *Input/Output*
Note: the dimension of the array D must be at least $\max(1, N)$.
On entry: must contain the n diagonal elements of the tridiagonal matrix A .
On exit: if $IFAIL = 0$ or $N + 1$, D is overwritten by the n diagonal elements of the diagonal matrix D from the LDL^H factorization of A .

- 4: $E(*)$ – **complex*16** array *Input/Output*
Note: the dimension of the array E must be at least $\max(1, N - 1)$.
On entry: must contain the $(n - 1)$ subdiagonal elements of the tridiagonal matrix A .
On exit: if $IFAIL = 0$ or $N + 1$, E is overwritten by the $(n - 1)$ subdiagonal elements of the unit lower bidiagonal matrix L from the LDL^H factorization of A . (E can also be regarded as the conjugate of the superdiagonal of the unit upper bidiagonal factor U from the $U^H DU$ factorization of A .)
- 5: $B(LDB,*)$ – **complex*16** array *Input/Output*
Note: the second dimension of the array B must be at least $\max(1, NRHS)$. To solve the equations $Ax = b$, where b is a single right-hand side, B may be supplied as a one-dimensional array with length $LDB = \max(1, N)$.
On entry: the n by r matrix of right-hand sides B .
On exit: if $IFAIL = 0$ or $N + 1$, the n by r solution matrix X .
- 6: LDB – **INTEGER** *Input*
On entry: the first dimension of the array B as declared in the (sub)program from which F04CGF is called.
Constraint: $LDB \geq \max(1, N)$.
- 7: $RCOND$ – **double precision** *Output*
On exit: if $IFAIL = 0$ or $N + 1$, an estimate of the reciprocal of the condition number of the matrix A , computed as $RCOND = 1 / (\|A\|_1, \|A^{-1}\|_1)$.
- 8: $ERRBND$ – **double precision** *Output*
On exit: if $IFAIL = 0$ or $N + 1$, an estimate of the forward error bound for a computed solution $\hat{x}$, such that $\|\hat{x} - x\|_1 / \|x\|_1 \leq ERRBND$, where $\hat{x}$ is a column of the computed solution returned in the array B and x is the corresponding column of the exact solution X . If $RCOND$ is less than **machine precision**, then $ERRBND$ is returned as unity.
- 9: $IFAIL$ – **INTEGER** *Input/Output*
On entry: $IFAIL$ must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction 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, if you are 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:

$IFAIL < 0$ and $IFAIL \neq -999$

If $IFAIL = -i$, the i th argument had an illegal value.

IFAIL = -999

Allocation of memory failed. The **double precision** allocatable memory required is N. In this case the factorization and the solution X have been computed, but RCOND and ERRBND have not been computed.

IFAIL > 0 and IFAIL ≤ N

If IFAIL = i , the leading minor of order i of A is not positive-definite. The factorization could not be completed, and the solution has not been computed.

IFAIL = N + 1

RCOND is less than **machine precision**, so that the matrix A is numerically singular. A solution to the equations $AX = B$ has nevertheless been computed.

7 Accuracy

The computed solution for a single right-hand side, $\hat{x}$, satisfies an equation of the form

$$(A + E)\hat{x} = b,$$

where

$$\|E\|_1 = O(\epsilon)\|A\|_1$$

and ϵ is the **machine precision**. An approximate error bound for the computed solution is given by

$$\frac{\|\hat{x} - x\|_1}{\|x\|_1} \leq \kappa(A) \frac{\|E\|_1}{\|A\|_1},$$

where $\kappa(A) = \|A^{-1}\|_1 \|A\|_1$, the condition number of A with respect to the solution of the linear equations. F04CGF uses the approximation $\|E\|_1 = \epsilon \|A\|_1$ to estimate ERRBND. See Section 4.4 of Anderson *et al.* (1999) for further details.

8 Further Comments

The total number of floating-point operations required to solve the equations $AX = B$ is proportional to nr . The condition number estimation requires $O(n)$ floating-point operations.

See Section 15.3 of Higham (2002) for further details on computing the condition number of tridiagonal matrices.

The real analogue of F04CGF is F04BGF.

9 Example

This example solves the equations

$$AX = B,$$

where A is the Hermitian positive-definite tridiagonal matrix

$$A = \begin{pmatrix} 16.0 & 16.0 + 16.0i & 0 & 0 \\ 16.0 - 16.0i & 41.0 & 18.0 - 9.0i & 0 \\ 0 & 18.0 + 9.0i & 46.0 & 1.0 - 4.0i \\ 0 & 0 & 1.0 + 4.0i & 21.0 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 64.0 + 16.0i & -16.0 - 32.0i \\ 93.0 + 62.0i & 61.0 - 66.0i \\ 78.0 - 80.0i & 71.0 - 74.0i \\ 14.0 - 27.0i & 35.0 + 15.0i \end{pmatrix}.$$

An estimate of the condition number of A and an approximate error bound for the computed solutions are also printed.

9.1 Program Text

```
*      F04CGF Example Program Text
*      Mark 21 Release. NAG Copyright 2004.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, NRHSMX
      PARAMETER        (NMAX=8,NRHSMX=2)
      INTEGER          LDB
      PARAMETER        (LDB=NMAX)
*      .. Local Scalars ..
      DOUBLE PRECISION ERRBND, RCOND
      INTEGER          I, IERR, IFAIL, J, N, NRHS
*      .. Local Arrays ..
      COMPLEX *16      B(LDB,NRHSMX), E(NMAX-1)
      DOUBLE PRECISION D(NMAX)
      CHARACTER        CLABS(1), RLABS(1)
*      .. External Subroutines ..
      EXTERNAL          F04CGF, X04DBF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F04CGF Example Program Results'
      WRITE (NOUT,*)
*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, NRHS
      IF (N.LE.NMAX .AND. NRHS.LE.NRHSMX) THEN
*
*          Read A from data file
*
*          READ (NIN,*) (D(I),I=1,N)
*          READ (NIN,*) (E(I),I=1,N-1)
*
*          Read B from data file
*
*          READ (NIN,*) ((B(I,J),J=1,NRHS),I=1,N)
*
*          Solve the equations AX = B for X
*
*          IFAIL = 1
*          CALL F04CGF(N,NRHS,D,E,B,LDB,RCOND,ERRBND,IFAIL)
*
*          IF (IFAIL.EQ.0) THEN
*
*              Print solution, estimate of condition number and approximate
*              error bound
*
*              IERR = 0
*              CALL X04DBF('General',' ',N,NRHS,B,LDB,'Bracketed',' ',
+                'Solution','Integer',RLABS,'Integer',CLABS,80,0,
+                IERR)
*
*              WRITE (NOUT,*)
*              WRITE (NOUT,*) 'Estimate of condition number'
*              WRITE (NOUT,99999) 1.0D0/RCOND
*              WRITE (NOUT,*)
*              WRITE (NOUT,*)
+              'Estimate of error bound for computed solutions'
*              WRITE (NOUT,99999) ERRBND
*              ELSE IF (IFAIL.EQ.N+1) THEN
*
*                  Matrix A is numerically singular. Print estimate of
*                  reciprocal of condition number and solution
*
*                  WRITE (NOUT,*)
*                  WRITE (NOUT,*) 'Estimate of reciprocal of condition number'
*                  WRITE (NOUT,99999) RCOND
```

```

*
      WRITE (NOUT,*)
      IERR = 0
      CALL X04DBF('General',' ',N,NRHS,B,LDB,'Bracketed',' ',
+               'Solution','Integer',RLABS,'Integer',CLABS,80,0,
+               IERR)
*
      ELSE IF (IFAIL.GT.0 .AND. IFAIL.LE.N) THEN
        WRITE (NOUT,99998) 'The leading minor of order ', IFAIL,
+        ' is not positive definite'
      ELSE
        WRITE (NOUT,99997) IFAIL
      END IF
    ELSE
      WRITE (NOUT,*) 'NMAX and/or NRHSMX too small'
    END IF
*
99999 FORMAT (8X,1P,E9.1)
99998 FORMAT (1X,A,I3,A)
99997 FORMAT (1X,' ** F04CGF returned with IFAIL = ',I5)
      END

```

9.2 Program Data

F04CGF Example Program Data

```

      4              2                               :Values of N and NRHS

      16.0          41.0          46.0          21.0 :End of diagonal D
( 16.0, 16.0) ( 18.0, -9.0) ( 1.0, -4.0)           :End of sub-diagonal E

( 64.0, 16.0) (-16.0,-32.0)
( 93.0, 62.0) ( 61.0,-66.0)
( 78.0,-80.0) ( 71.0,-74.0)
( 14.0,-27.0) ( 35.0, 15.0)                       :End of matrix B

```

9.3 Program Results

F04CGF Example Program Results

Solution

```

                                1              2
1 ( 2.0000, 1.0000) ( -3.0000, -2.0000)
2 ( 1.0000, 1.0000) ( 1.0000, 1.0000)
3 ( 1.0000, -2.0000) ( 1.0000, -2.0000)
4 ( 1.0000, -1.0000) ( 2.0000, 1.0000)

```

Estimate of condition number
9.2E+03

Estimate of error bound for computed solutions
1.0E-12
