

NAG Fortran Library Routine Document

F04CFF

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

F04CFF computes the solution to a complex system of linear equations $AX = B$, where A is an n by n Hermitian positive-definite band matrix of band width $2k + 1$, 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 F04CFF (UPLO, N, KD, NRHS, AB, LDAB, B, LDB, RCOND, ERBND,
1                IFAIL)
    INTEGER          N, KD, NRHS, LDAB, LDB, IFAIL
    double precision RCOND, ERBND
    complex*16      AB(LDAB,*), B(LDB,*)
    CHARACTER*1     UPLO
  
```

3 Description

The Cholesky factorization is used to factor A as $A = U^H U$, if $UPLO = 'U'$, or $A = LL^H$, if $UPLO = 'L'$, where U is an upper triangular band matrix with k super-diagonals, and L is a lower triangular band matrix with k sub-diagonals. The factored form of A is then used to solve the system of equations $AX = B$.

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 URL: <http://www.netlib.org/lapack/lug>

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

5 Parameters

- 1: UPLO – CHARACTER*1 *Input*
On entry: if UPLO = 'U', the upper triangle of the matrix A is stored, if UPLO = 'L', the lower triangle of the matrix A is stored.
Constraint: UPLO = 'U' or 'L'.
- 2: N – INTEGER *Input*
On entry: the number of linear equations n , i.e., the order of the matrix A .
Constraint: $N \geq 0$.
- 3: KD – INTEGER *Input*
On entry: the number of super-diagonals k (and the number of sub-diagonals) of the band matrix A .
Constraint: $KD \geq 0$.

- 4: NRHS – INTEGER *Input*
On entry: the number of right-hand sides r , i.e., the number of columns of the matrix B .
Constraint: NRHS ≥ 0 .
- 5: AB(LDAB,*) – **complex*16** array *Input/Output*
Note: the second dimension of the array AB must be at least $\max(1, N)$.
On entry: the n by n symmetric band matrix A . The upper or lower triangular part of the Hermitian matrix is stored in the first $KD + 1$ rows of the array. The j th column of A is stored in the j th column of the array AB as follows:
 if UPLO = 'U', $AB(k + 1 + i - jj) = a_{ij}$ for $\max(1, j - k) \leq i \leq j$;
 if UPLO = 'L', $AB(1 + i - jj) = a_{ij}$ for $j \leq i \leq \min(n, j + k)$.
 See Section 8 below for further details.
On exit: if IFAIL = 0 or $N + 1$, the factor U or L from the Cholesky factorization $A = U^H U$ or $A = LL^H$, in the same storage format as A .
- 6: LDAB – INTEGER *Input*
On entry: the first dimension of the array AB as declared in the (sub)program from which F04CFF is called.
Constraint: LDAB $\geq KD + 1$.
- 7: 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 .
- 8: LDB – INTEGER *Input*
On entry: the first dimension of the array B as declared in the (sub)program from which F04CFF is called.
Constraint: LDB $\geq \max(1, N)$.
- 9: 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 $RCOND = 1 / (\|A\|_1 \|A^{-1}\|_1)$.
- 10: 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.
- 11: 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 < 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 , and the *complex*16* allocatable memory required is $2 \times N$. Allocation failed before the solution could be computed.

IFAIL > 0 and IFAIL \leq 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. F04CFF 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 band storage scheme for the array AB is illustrated by the following example, when $n = 6$, $k = 2$, and UPLO = 'U':

On entry:

$$\begin{array}{cccccc} * & * & a_{13} & a_{24} & a_{35} & a_{46} \\ * & a_{12} & a_{23} & a_{34} & a_{45} & a_{56} \\ a_{11} & a_{22} & a_{33} & a_{44} & a_{55} & a_{66} \end{array}$$

On exit:

$$\begin{array}{cccccc} * & * & u_{13} & u_{24} & u_{35} & u_{46} \\ * & u_{12} & u_{23} & u_{34} & u_{45} & u_{56} \\ u_{11} & u_{22} & u_{33} & u_{44} & u_{55} & u_{66} \end{array}$$

Similarly, if UPLO = 'L' the format of AB is as follows:

On entry:

$$\begin{array}{cccccc} a_{11} & a_{22} & a_{33} & a_{44} & a_{55} & a_{66} \\ a_{21} & a_{32} & a_{43} & a_{54} & a_{65} & * \\ a_{31} & a_{42} & a_{53} & a_{64} & * & * \end{array}$$

On exit:

$$\begin{array}{cccccc} l_{11} & l_{22} & l_{33} & l_{44} & l_{55} & l_{66} \\ l_{21} & l_{32} & l_{43} & l_{54} & l_{65} & * \\ l_{31} & l_{42} & l_{53} & l_{64} & * & * \end{array}$$

Array elements marked * need not be set and are not referenced by the routine.

Assuming that $n \gg k$, the total number of floating-point operations required to solve the equations $AX = B$ is approximately $n(k+1)^2$ for the factorization and $4nkr$ for the solution following the factorization. The condition number estimation typically requires between four and five solves and never more than eleven solves, following the factorization.

In practice the condition number estimator is very reliable, but it can underestimate the true condition number; see Section 15.3 of Higham (2002) for further details.

The real analogue of F04CFF is F04BFF.

9 Example

To solve the equations

$$AX = B,$$

where A is the Hermitian positive-definite band matrix

$$A = \begin{pmatrix} 9.39 & 1.08 - 1.73i & 0 & 0 \\ 1.08 + 1.73i & 1.69 & -0.04 + 0.29i & 0 \\ 0 & -0.04 - 0.29i & 2.65 & -0.33 + 2.24i \\ 0 & 0 & -0.33 - 2.24i & 2.17 \end{pmatrix}$$

and

$$B = \begin{pmatrix} -12.42 + 68.42i & 54.30 - 56.56i \\ -9.93 + 0.88i & 18.32 + 4.76i \\ -27.30 - 0.01i & -4.40 + 9.97i \\ 5.31 + 23.63i & 9.43 + 1.41i \end{pmatrix}.$$

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

9.1 Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*      F04CFF Example Program Text
*      Mark 21 Release. NAG Copyright 2004.
*      .. Parameters ..
INTEGER          NIN, NOUT
PARAMETER       (NIN=5,NOUT=6)
INTEGER          KDMAX, NMAX, NRHSMX
PARAMETER       (KDMAX=4,NMAX=8,NRHSMX=2)
```

```

INTEGER          LDAB, LDB
PARAMETER        (LDAB=KDMAX+1,LDB=NMAX)
CHARACTER        UPLO
PARAMETER        (UPLO='U')
*
.. Local Scalars ..
DOUBLE PRECISION ERRBND, RCOND
INTEGER          I, IERR, IFAIL, J, KD, N, NRHS
*
.. Local Arrays ..
COMPLEX *16      AB(LDAB,NMAX), B(LDB,NRHSMX)
CHARACTER        CLABS(1), RLABS(1)
*
.. External Subroutines ..
EXTERNAL         F04CFF, X04DBF
*
.. Intrinsic Functions ..
INTRINSIC        MAX, MIN
*
.. Executable Statements ..
WRITE (NOUT,*) 'F04CFF Example Program Results'
WRITE (NOUT,*)
*
Skip heading in data file
READ (NIN,*)
READ (NIN,*) N, KD, NRHS
IF (N.LE.NMAX .AND. KD.LE.KDMAX .AND. NRHS.LE.NRHSMX) THEN
*
*   Read the upper or lower triangular part of the band matrix A
*   from data file
*
      IF (UPLO.EQ.'U') THEN
        DO 20 I = 1, N
          READ (NIN,*) (AB(KD+1+I-J,J),J=I,MIN(N,I+KD))
20      CONTINUE
      ELSE IF (UPLO.EQ.'L') THEN
        DO 40 I = 1, N
          READ (NIN,*) (AB(1+I-J,J),J=MAX(1,I-KD),I)
40      CONTINUE
      END IF
*
*   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 F04CFF(UPLO,N,KD,NRHS,AB,LDAB,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','F7.4',
+                   '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','F7.4',
+              'Solution','Integer',RLABS,'Integer',CLABS,80,0,
+              IERR)
*
      ELSE IF (IFAIL.GT.0 .AND. IFAIL.LE.N) THEN
*
      The matrix A is not positive definite to working precision
*
      WRITE (NOUT,99998) 'The leading minor of order ', IFAIL,
+      ' is not positive definite'
      END IF
      ELSE
      WRITE (NOUT,*)
+      'One or more of NMAX, KDMAX and NRHSMX is too small'
      END IF
      STOP
*
99999 FORMAT (4X,1P,E9.1)
99998 FORMAT (1X,A,I3,A)
      END

```

9.2 Program Data

F04CFF Example Program Data

```

      4          1          2          :Values of N, KD and NRHS
(  9.39,  0.00) (  1.08, -1.73)
              (  1.69,  0.00) ( -0.04,  0.29)
                              (  2.65,  0.00) ( -0.33,  2.24)
                                          (  2.17,  0.00) :End of A

(-12.42, 68.42) ( 54.30,-56.56)
(- 9.93,  0.88) ( 18.32,  4.76)
(-27.30, -0.01) ( -4.40,  9.97)
(  5.31, 23.63) (  9.43,  1.41)                               :End of B

```

9.3 Program Results

F04CFF Example Program Results

Solution

```

      1          2
1 (-1.0000, 8.0000) ( 5.0000,-6.0000)
2 (  2.0000,-3.0000) (  2.0000,  3.0000)
3 (-4.0000,-5.0000) (-8.0000,  4.0000)
4 (  7.0000,  6.0000) (-1.0000,-7.0000)

```

Estimate of condition number

1.3E+02

Estimate of error bound for computed solutions

1.5E-14