

NAG Library Routine Document

F04CEF

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

F04CEF computes the solution to a complex system of linear equations $AX = B$, where A is an n by n Hermitian positive-definite matrix, stored in packed format, 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 F04CEF(UPLO, N, NRHS, AP, B, LDB, RCOND, ERBND, IFAIL)
```

```
INTEGER N, NRHS, LDB, IFAIL
```

```
double precision RCOND, ERBND
```

```
complex*16 AP(*), 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 matrix and L is a lower triangular matrix. 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 <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: NRHS – INTEGER *Input*
On entry: the number of right-hand sides r , i.e., the number of columns of the matrix B .
Constraint: $NRHS \geq 0$.

- 4: AP(*) – **complex*16** array Input/Output

Note: the dimension of the array AP must be at least $\max(1, N \times (N + 1)/2)$.

On entry: the n by n Hermitian matrix A . The upper or lower triangular part of the Hermitian matrix is packed column-wise in a linear array. The j th column of A is stored in the array AP as follows:

if UPLO = 'U', $AP(i + (j - 1)j/2) = a_{ij}$ for $1 \leq i \leq j$;

if UPLO = 'L', $AP(i + (j - 1)(2n - j)/2) = a_{ij}$ for $j \leq i \leq n$.

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 .

- 5: B(LDB,*) – **complex*16** array Input/Output

Note: the second dimension of the array B must be at least $\max(1, \text{NRHS})$. 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 $\text{LDB} = \max(1, N)$.

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 F04CEF is called.

Constraint: $\text{LDB} \geq \max(1, N)$.

- 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 $\text{RCOND} = 1 / (\|A\|_1 \|A^{-1}\|_1)$.

- 8: ERBND – **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 $\|\hat{x} - x\|_1 / \|x\|_1 \leq \text{ERBND}$, 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 ERBND 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, 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

COND 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. F04CEF 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 packed storage scheme is illustrated by the following example when $n = 4$ and UPLO = 'U'. Two-dimensional storage of the Hermitian matrix A :

$$\begin{array}{cccc} a_{11} & a_{12} & a_{13} & a_{14} \\ & a_{22} & a_{23} & a_{24} \\ & & a_{33} & a_{34} \\ & & & a_{44} \end{array} \quad (a_{ij} = \bar{a}_{ji})$$

Packed storage of the upper triangle of A :

$$AP = [a_{11}, a_{12}, a_{22}, a_{13}, a_{23}, a_{33}, a_{14}, a_{24}, a_{34}, a_{44}]$$

The total number of floating-point operations required to solve the equations $AX = B$ is proportional to $(\frac{1}{3}n^3 + n^2r)$. 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 F04CEF is F04BEF.

9 Example

This example solves the equations

$$AX = B,$$

where A is the Hermitian positive-definite matrix

$$A = \begin{pmatrix} 3.23 & 1.51 - 1.92i & 1.90 + 0.84i & 0.42 + 2.50i \\ 1.51 + 1.92i & 3.58 & -0.23 + 1.11i & -1.18 + 1.37i \\ 1.90 - 0.84i & -0.23 - 1.11i & 4.09 & 2.33 - 0.14i \\ 0.42 - 2.50i & -1.18 - 1.37i & 2.33 + 0.14i & 4.29 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 3.93 - 6.14i & 1.48 + 6.58i \\ 6.17 + 9.42i & 4.65 - 4.75i \\ -7.17 - 21.83i & -4.91 + 2.29i \\ 1.99 - 14.38i & 7.64 - 10.79i \end{pmatrix}.$$

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

9.1 Program Text

```
*      F04CEF 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)
      CHARACTER        UPLO
      PARAMETER        (UPLO='U')
*      .. Local Scalars ..
      DOUBLE PRECISION ERRBND, RCOND
      INTEGER          I, IERR, IFAIL, J, N, NRHS
*      .. Local Arrays ..
      COMPLEX *16      AP((NMAX*(NMAX+1))/2), B(LDB,NRHSMX)
      CHARACTER        CLABS(1), RLABS(1)
*      .. External Subroutines ..
      EXTERNAL         F04CEF, X04DBF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F04CEF 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 the upper or lower triangular part of the matrix A from
*          data file
*
          IF (UPLO.EQ.'U') THEN
              READ (NIN,*) ((AP(I+(J*(J-1))/2),J=I,N),I=1,N)
          ELSE IF (UPLO.EQ.'L') THEN
              READ (NIN,*) ((AP(I+((2*N-J)*(J-1))/2),J=1,I),I=1,N)
          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 F04CEF(UPLO,N,NRHS,AP,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) ERBND
      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'
      ELSE
          WRITE (NOUT,99997) IFAIL
      END IF
      ELSE
          WRITE (NOUT,*) 'NMAX and/or NRHSMX too small'
      END IF
*
99999 FORMAT (4X,1P,E9.1)
99998 FORMAT (1X,A,I3,A)
99997 FORMAT (1X,' ** F04CEF returned with IFAIL = ',I5)
      END

```

9.2 Program Data

F04CEF Example Program Data

```

      4              2                               :Values of N and NRHS
( 3.23,  0.00) ( 1.51, -1.92) ( 1.90,  0.84) ( 0.42,  2.50)
              ( 3.58,  0.00) (-0.23,  1.11) (-1.18,  1.37)
                      ( 4.09,  0.00) ( 2.33, -0.14)
                                ( 4.29,  0.00) :End of matrix A

```

```
( 3.93, -6.14) ( 1.48,  6.58)
( 6.17,  9.42) ( 4.65, -4.75)
(-7.17,-21.83) (-4.91,  2.29)
( 1.99,-14.38) ( 7.64,-10.79)
```

```
:End of matrix B
```

9.3 Program Results

F04CEF Example Program Results

Solution

```
1      1      2
1 ( 1.0000,-1.0000) (-1.0000, 2.0000)
2 ( 0.0000, 3.0000) ( 3.0000,-4.0000)
3 (-4.0000,-5.0000) (-2.0000, 3.0000)
4 ( 2.0000, 1.0000) ( 4.0000,-5.0000)
```

Estimate of condition number

1.5E+02

Estimate of error bound for computed solutions

1.7E-14
