NAG Fortran Library Routine Document F07FVF (CPORFS/ZPORFS)

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

F07FVF (CPORFS/ZPORFS) returns error bounds for the solution of a complex Hermitian positive-definite system of linear equations with multiple right-hand sides, AX = B. It improves the solution by iterative refinement, in order to reduce the backward error as much as possible.

2 Specification

```
SUBROUTINE FO7FVF(UPLO, N, NRHS, A, LDA, AF, LDAF, B, LDB, X, LDX, FERR, BERR, WORK, RWORK, INFO)

ENTRY cporfs (UPLO, N, NRHS, A, LDA, AF, LDAF, B, LDB, X, LDX, FERR, BERR, WORK, RWORK, INFO)

INTEGER N, NRHS, LDA, LDAF, LDB, LDX, INFO

real FERR(*), BERR(*), RWORK(*)

complex A(LDA,*), AF(LDAF,*), B(LDB,*), X(LDX,*), WORK(*)

CHARACTER*1 UPLO
```

The ENTRY statement enables the routine to be called by its LAPACK name.

3 Description

This routine returns the backward errors and estimated bounds on the forward errors for the solution of a complex Hermitian positive-definite system of linear equations with multiple right-hand sides AX = B. The routine handles each right-hand side vector (stored as a column of the matrix B) independently, so we describe the function of the routine in terms of a single right-hand side b and solution x.

Given a computed solution x, the routine computes the *component-wise backward error* β . This is the size of the smallest relative perturbation in each element of A and b such that x is the exact solution of a perturbed system

$$(A + \delta A)x = b + \delta b$$

$$|\delta a_{ij}| \le \beta |a_{ij}| \quad \text{and} \quad |\delta b_i| \le \beta |b_i|.$$

Then the routine estimates a bound for the *component-wise forward error* in the computed solution, defined by:

$$\max_i |x_i - \hat{x}_i| / \max_i |x_i|$$

where \hat{x} is the true solution.

For details of the method, see the F07 Chapter Introduction.

4 References

Golub G H and van Loan C F (1996) Matrix Computations (3rd Edition) Johns Hopkins University Press, Baltimore

5 Parameters

1: UPLO - CHARACTER*1

Input

On entry: indicates whether the upper or lower triangular part of A is stored and how A has been factorized, as follows:

if UPLO = 'U', the upper triangular part of A is stored and A is factorized as U^HU , where U is upper triangular;

if UPLO = 'L', the lower triangular part of A is stored and A is factorized as LL^H , where L is lower triangular.

Constraint: UPLO = 'U' or 'L'.

2: N – INTEGER

Input

On entry: n, the order of the matrix A.

Constraint: $N \geq 0$.

3: NRHS – INTEGER

Input

On entry: r, the number of right-hand sides.

Constraint: NRHS ≥ 0 .

4: A(LDA,*) - complex array

Input

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

On entry: the n by n original Hermitian positive-definite matrix A as supplied to F07FRF (CPOTRF/ZPOTRF).

5: LDA – INTEGER

Input

On entry: the first dimension of the array A as declared in the (sub)program from which F07FVF (CPORFS/ZPORFS) is called.

Constraint: LDA $\geq \max(1, N)$.

6: AF(LDAF,*) - complex array

Input

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

On entry: the Cholesky factor of A, as returned by F07FRF (CPOTRF/ZPOTRF).

7: LDAF – INTEGER

Input

On entry: the first dimension of the array AF as declared in the (sub)program from which F07FVF (CPORFS/ZPORFS) is called.

Constraint: LDAF $\geq \max(1, N)$.

8: B(LDB,*) - complex array

Input

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

On entry: the n by r right-hand side matrix B.

9: LDB – INTEGER

Input

On entry: the first dimension of the array B as declared in the (sub)program from which F07FVF (CPORFS/ZPORFS) is called.

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

10: X(LDX,*) - complex array

Input/Output

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

On entry: the n by r solution matrix X, as returned by F07FSF (CPOTRS/ZPOTRS).

On exit: the improved solution matrix X.

11: LDX – INTEGER

On entry: the first dimension of the array X as declared in the (sub)program from which F07FVF (CPORFS/ZPORFS) is called.

Constraint: LDX $\geq \max(1, N)$.

12: FERR(*) - real array

Output

Input

Note: the dimension of the array FERR must be at least max(1, NRHS).

On exit: FERR(j) contains an estimated error bound for the jth solution vector, that is, the jth column of X, for j = 1, 2, ..., r.

13: BERR(*) - real array

Output

Note: the dimension of the array BERR must be at least max(1, NRHS).

On exit: BERR(j) contains the component-wise backward error bound β for the jth solution vector, that is, the jth column of X, for j = 1, 2, ..., r.

14: WORK(*) - complex array

Workspace

Note: the dimension of the array WORK must be at least max(1, 2 * N).

15: RWORK(*) - real array

Workspace

Note: the dimension of the array RWORK must be at least max(1, N).

16: INFO – INTEGER

Output

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

6 Error Indicators and Warnings

Errors or warnings detected by the routine:

INFO < 0

If INFO = -i, the *i*th parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

7 Accuracy

The bounds returned in FERR are not rigorous, because they are estimated, not computed exactly; but in practice they almost always overestimate the actual error.

8 Further Comments

For each right-hand side, computation of the backward error involves a minimum of $16n^2$ real floating-point operations. Each step of iterative refinement involves an additional $24n^2$ real operations. At most 5 steps of iterative refinement are performed, but usually only 1 or 2 steps are required.

Estimating the forward error involves solving a number of systems of linear equations of the form Ax = b; the number is usually 5 and never more than 11. Each solution involves approximately $8n^2$ real operations.

The real analogue of this routine is F07FHF (SPORFS/DPORFS).

9 Example

To solve the system of equations AX = B using iterative refinement and to compute the forward and backward error bounds, where

$$A = \begin{pmatrix} 3.23 + 0.00i & 1.51 - 1.92i & 1.90 + 0.84i & 0.42 + 2.50i \\ 1.51 + 1.92i & 3.58 + 0.00i & -0.23 + 1.11i & -1.18 + 1.37i \\ 1.90 - 0.84i & -0.23 - 1.11i & 4.09 + 0.00i & 2.33 - 0.14i \\ 0.42 - 2.50i & -1.18 - 1.37i & 2.33 + 0.14i & 4.29 + 0.00i \end{pmatrix}$$

and}

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

Here A is Hermitian positive-definite and must first be factorized by F07FRF (CPOTRF/ZPOTRF).

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.

```
FO7FVF Example Program Text
Mark 16 Release. NAG Copyright 1993.
.. Parameters ..
INTEGER
                  NIN, NOUT
                (NIN=5,NOUT=6)
NMAX, NRHMAX, LDA, LDAF, LDB, LDX
PARAMETER
INTEGER
PARAMETER
+
                 (NMAX=8,NRHMAX=NMAX,LDA=NMAX,LDAF=NMAX,LDB=NMAX,
                  LDX=NMAX)
.. Local Scalars ..
          I, IFAIL, INFO, J, N, NRHS
UPLO
INTEGER
CHARACTER
.. Local Arrays ..
complex A(LDA,NMAX), AF(LDAF,NMAX), B(LDB,NRHMAX),
                 WORK(2*NMAX), X(LDX,NMAX)
BERR(NRHMAX), FERR(NRHMAX), RWORK(NMAX)
real BERR(NRHMAX), FERR
CHARACTER CLABS(1), RLABS(1)
.. External Subroutines ..
EXTERNAL FO6TFF, XO4DBF, cporfs, cpotrf, cpotrs
.. Executable Statements ..
WRITE (NOUT, *) 'F07FVF Example Program Results'
Skip heading in data file
READ (NIN, *)
READ (NIN, *) N, NRHS
IF (N.LE.NMAX .AND. NRHS.LE.NRHMAX) THEN
   Read A and B from data file, and copy A to AF and B to X
   READ (NIN, *) UPLO
   IF (UPLO.EQ.'U') THEN
      READ (NIN,*) ((A(I,J),J=I,N),I=1,N)
   ELSE IF (UPLO.EQ.'L') THEN
      READ (NIN, *) ((A(I,J), J=1,I), I=1,N)
   END IF
   READ (NIN,*) ((B(I,J),J=1,NRHS),I=1,N)
   CALL F06TFF(UPLO,N,N,A,LDA,AF,LDAF)
   CALL F06TFF('General', N, NRHS, B, LDB, X, LDX)
   Factorize A in the array AF
   CALL cpotrf(UPLO,N,AF,LDAF,INFO)
   WRITE (NOUT, *)
   IF (INFO.EQ.O) THEN
```

```
Compute solution in the array X
            CALL cpotrs (UPLO, N, NRHS, AF, LDAF, X, LDX, INFO)
            Improve solution, and compute backward errors and
            estimated bounds on the forward errors
            CALL cporfs (UPLO, N, NRHS, A, LDA, AF, LDAF, B, LDB, X, LDX, FERR, BERR,
                         WORK, RWORK, INFO)
            Print solution
            IFAIL = 0
            CALL XO4DBF('General',' ',N,NRHS,X,LDX,'Bracketed','F7.4',
                         'Solution(s)','Integer', RLABS,'Integer', CLABS,
                         80,0,IFAIL)
            WRITE (NOUT, *)
            WRITE (NOUT,*) 'Backward errors (machine-dependent)'
            WRITE (NOUT, 99999) (BERR(J), J=1, NRHS)
            WRITE (NOUT, *)
              'Estimated forward error bounds (machine-dependent)'
            WRITE (NOUT, 99999) (FERR(J), J=1, NRHS)
            WRITE (NOUT,*) 'A is not positive-definite'
         END IF
      END IF
      STOP
99999 FORMAT ((5x,1p,4(e11.1,7x)))
      END
```

9.2 Program Data

9.3 Program Results

```
F07FVF Example Program Results

Solution(s)

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)

Backward errors (machine-dependent)
4.3E-17 4.3E-17

Estimated forward error bounds (machine-dependent)
5.9E-14 7.2E-14
```