NAG Fortran Library Routine Document

F07HHF (SPBRFS/DPBRFS)

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

F07HHF (SPBRFS/DPBRFS) returns error bounds for the solution of a real symmetric positive-definite band 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 F07HHF(UPLO, N, KD, NRHS, AB, LDAB, AFB, LDAFB, B, LDB, X,
1                  LDX, FERR, BERR, WORK, IWORK, INFO)
 ENTRY      spbrfs (UPLO, N, KD, NRHS, AB, LDAB, AFB, LDAFB, B, LDB, X,
1                  LDX, FERR, BERR, WORK, IWORK, INFO)
 INTEGER           N, KD, NRHS, LDAB, LDAFB, LDB, LDX, IWORK(*), INFO
 real              AB(LDAB,*), AFB(LDAFB,*), B(LDB,*), X(LDX,*), FERR(*),
1                  BERR(*), 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 real symmetric positive-definite band 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

$$(A + \delta A)x = b + \delta b$$
$$|\delta a_{ij}| \leq \beta |a_{ij}| \quad \text{and} \quad |\delta b_i| \leq \beta |b_i|.$$

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, 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^TU, where U is upper triangular;

if UPLO = 'L', the lower triangular part of A is stored and A is factorized as LL^T, 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 ≥ 0.

3: KD – INTEGER *Input*

On entry: k, the number of super-diagonals or sub-diagonals of the matrix A.

Constraint: KD ≥ 0.

4: NRHS – INTEGER *Input*

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

Constraint: NRHS ≥ 0.

5: AB(LDAB,*) – ***real*** array *Input*

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

On entry: the n by n original symmetric band matrix A as supplied to F07HDF (SPBTRF/DPBTRF).

6: LDAB – INTEGER *Input*

On entry: the first dimension of the array AB as declared in the (sub)program from which F07HHF (SPBRFS/DPBRFS) is called.

Constraint: LDAB $\geq$ KD + 1.

7: AFB(LDAFB,*) – ***real*** array *Input*

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

On entry: the Cholesky factor of A, as returned by F07HDF (SPBTRF/DPBTRF).

8: LDAFB – INTEGER *Input*

On entry: the first dimension of the array AFB as declared in the (sub)program from which F07HHF (SPBRFS/DPBRFS) is called.

Constraint: LDAFB $\geq$ KD + 1.

9: B(LDB,*) – ***real*** 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.

10: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F07HHF (SPBRFS/DPBRFS) is called.

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

11: X(LDX,*) – ***real*** array *Input/Output*

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

On entry: the n by r solution matrix X, as returned by F07HEF (SPBTRS/DPBTRS).

On exit: the improved solution matrix X.

12: LDX – INTEGER *Input*

On entry: the first dimension of the array X as declared in the (sub)program from which F07HHF (SPBRFS/DPBRFS) is called.

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

13: FERR($*$) – ***real*** array *Output*

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

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

14: BERR($*$) – ***real*** array *Output*

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

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 $j = 1, 2, \ldots, r$.

15: WORK($*$) – ***real*** array *Workspace*

Note: the dimension of the array WORK must be at least $\max(1, 3 * \mathrm{N})$.

16: IWORK($*$) – INTEGER array *Workspace*

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

17: 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 ith 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 $8nk$ floating-point operations. Each step of iterative refinement involves an additional $12nk$ operations. This assumes $n \gg k$. 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 4 or 5 and never more than 11. Each solution involves approximately $4nk$ operations.

The complex analogue of this routine is F07HVF (CPBRFS/ZPBRFS).

9 Example

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

$$A = \begin{pmatrix} 5.49 & 2.68 & 0.00 & 0.00 \\ 2.68 & 5.63 & -2.39 & 0.00 \\ 0.00 & -2.39 & 2.60 & -2.22 \\ 0.00 & 0.00 & -2.22 & 5.17 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 22.09 & 5.10 \\ 9.31 & 30.81 \\ -5.24 & -25.82 \\ 11.83 & 22.90 \end{pmatrix}.$$

Here A is symmetric and positive-definite, and is treated as a band matrix, which must first be factorized by F07HDF (SPBTRF/DPBTRF).

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.

```
*     F07HHF Example Program Text
*     Mark 15 Release. NAG Copyright 1991.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      real             ZERO
      PARAMETER        (ZERO=0.0e0)
      INTEGER          NMAX, NRHMAX, KDMAX, LDAB, LDAFB, LDB, LDX
      PARAMETER        (NMAX=8,NRHMAX=NMAX,KDMAX=8,LDAB=KDMAX+1,
     +                 LDAFB=KDMAX+1,LDB=NMAX,LDX=NMAX)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INFO, J, KD, N, NRHS
      CHARACTER        UPLO
*     .. Local Arrays ..
      real             AB(LDAB,NMAX), AFB(LDAFB,NMAX), B(LDB,NRHMAX),
     +                 BERR(NRHMAX), FERR(NRHMAX), WORK(3*NMAX),
     +                 X(LDX,NMAX)
      INTEGER          IWORK(NMAX)
*     .. External Subroutines ..
      EXTERNAL         F06QFF, F06QHF, spbrfs, spbtrf, spbtrs, X04CAF
*     .. Intrinsic Functions ..
      INTRINSIC        MAX, MIN
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F07HHF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, KD, NRHS
      IF (N.LE.NMAX .AND. KD.LE.KDMAX .AND. NRHS.LE.NRHMAX) THEN
*
*        Set A to zero to avoid referencing uninitialized elements
*
         CALL F06QHF('General',KD+1,N,ZERO,ZERO,AB,LDAB)
*
*        Read A and B from data file, and copy A to AFB and B to X
*
         READ (NIN,*) UPLO
         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 (NIN,*) ((B(I,J),J=1,NRHS),I=1,N)
*
         CALL F06QFF('General',KD+1,N,AB,LDAB,AFB,LDAFB)
*
         CALL F06QFF('General',N,NRHS,B,LDB,X,LDX)
*
*        Factorize A in the array AFB
*
         CALL spbtrf(UPLO,N,KD,AFB,LDAFB,INFO)
*
         WRITE (NOUT,*)
         IF (INFO.EQ.0) THEN
*
*           Compute solution in the array X
*
            CALL spbtrs(UPLO,N,KD,NRHS,AFB,LDAFB,X,LDX,INFO)
*
*           Improve solution, and compute backward errors and
*           estimated bounds on the forward errors
*
            CALL spbrfs(UPLO,N,KD,NRHS,AB,LDAB,AFB,LDAFB,B,LDB,X,LDX,
     +                  FERR,BERR,WORK,IWORK,INFO)
*
*           Print solution
*
            IFAIL = 0
*
            CALL X04CAF('General',' ',N,NRHS,X,LDX,'Solution(s)',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)
         ELSE
            WRITE (NOUT,*) 'A is not positive-definite'
         END IF
      END IF
      STOP
*
99999 FORMAT ((3X,1P,7e11.1))
      END
```

9.2 Program Data

```
F07HHF Example Program Data
  4  1  2                       :Values of N, KD and NRHS
  'L'                           :Value of UPLO
  5.49
  2.68   5.63
        -2.39   2.60
               -2.22   5.17     :End of matrix A
 22.09   5.10
  9.31  30.81
 -5.24 -25.82
 11.83  22.90                   :End of matrix B
```

9.3 Program Results

```
F07HHF Example Program Results

Solution(s)
            1          2
1      5.0000    -2.0000
2     -2.0000     6.0000
3     -3.0000    -1.0000
4      1.0000     4.0000

Backward errors (machine-dependent)
      4.9E-17    6.1E-17
Estimated forward error bounds (machine-dependent)
      2.0E-14    3.0E-14
```