

NAG Library Routine Document

F07HNF (ZPBSV)

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

F07HNF (ZPBSV) 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 bandwidth $(2k_d + 1)$ and X and B are n by r matrices.

2 Specification

```
SUBROUTINE F07HNF(UPLO, N, KD, NRHS, AB, LDAB, B, LDB, INFO)
INTEGER          N, KD, NRHS, LDAB, LDB, INFO
complex*16      AB(LDAB,*), B(LDB,*)
CHARACTER*1      UPLO
```

The routine may be called by its LAPACK name ***zpbsv***.

3 Description

F07HNF (ZPBSV) uses the Cholesky decomposition 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, and L is a lower triangular band matrix, with the same number of superdiagonals or subdiagonals as A . 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>

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: if $UPLO = 'U'$, the upper triangle of A is stored.
 If $UPLO = 'L'$, the lower triangle of A is stored.
Constraint: $UPLO = 'U'$ or $'L'$.
- 2: N – INTEGER *Input*
On entry: n , the number of linear equations, i.e., the order of the matrix A .
Constraint: $N \geq 0$.

- 3: KD – INTEGER *Input*
On entry: k_d , the number of superdiagonals of the matrix A if UPLO = 'U', or the number of subdiagonals if UPLO = 'L'.
Constraint: $KD \geq 0$.
- 4: NRHS – INTEGER *Input*
On entry: r , the number of right-hand sides, i.e., the number of columns of the matrix B .
Constraint: $NRHS \geq 0$.
- 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 upper or lower triangle of the Hermitian band matrix A .
The matrix is stored in rows 1 to $k_d + 1$, more precisely,
if UPLO = 'U', the elements of the upper triangle of A within the band must be stored with element A_{ij} in $AB(k_d + 1 + i - j, j)$ for $\max(1, j - k_d) \leq i \leq j$;
if UPLO = 'L', the elements of the lower triangle of A within the band must be stored with element A_{ij} in $AB(1 + i - j, j)$ for $j \leq i \leq \min(n, j + k_d)$.
On exit: if INFO = 0, the triangular factor U or L from the Cholesky factorization $A = U^H U$ or $A = L L^H$ of the band matrix A , 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 F07HNF (ZPBSV) 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 $\max(1, NRHS)$.
On entry: the n by r right-hand side matrix B .
On exit: if INFO = 0, 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 F07HNF (ZPBSV) is called.
Constraint: $LDB \geq \max(1, N)$.
- 9: 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 argument had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO = i , the leading minor of order i of A is not positive-definite, so the factorization could not be completed, and the solution has not 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. See Section 4.4 of Anderson *et al.* (1999) for further details.

F07HPF (ZPBSVX) is a comprehensive LAPACK driver that returns forward and backward error bounds and an estimate of the condition number. Alternatively, F04CFF solves $Ax = b$ and returns a forward error bound and condition estimate. F04CFF calls F07HNF (ZPBSV) to solve the equations.

8 Further Comments

When $n \gg k$, the total number of floating-point operations is approximately $4n(k+1)^2 + 16nkr$, where k is the number of superdiagonals and r is the number of right-hand sides.

The real analogue of this routine is F07HAF (DPBSV).

9 Example

This example solves 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

$$b = \begin{pmatrix} -12.42 + 68.42i \\ -9.93 + 0.88i \\ -27.30 - 0.01i \\ 5.31 + 23.63i \end{pmatrix}.$$

Details of the Cholesky factorization of A are also output.

9.1 Program Text

```
*      F07HNF Example Program Text
*      Mark 21 Release. NAG Copyright 2004.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5, NOUT=6)
      INTEGER          NMAX, KDMAX
      PARAMETER        (NMAX=8, KDMAX=4)
      INTEGER          LDAB
```

```

      PARAMETER      (LDAB=KDMAX+1)
      CHARACTER      UPLO
      PARAMETER      (UPLO='U')
*   .. Local Scalars ..
      INTEGER        I, IFAIL, INFO, J, KD, N
*   .. Local Arrays ..
      COMPLEX *16    AB(LDAB,NMAX), B(NMAX)
      CHARACTER      CLABS(1), RLABS(1)
*   .. External Subroutines ..
      EXTERNAL       X04DFF, ZPBSV
*   .. Intrinsic Functions ..
      INTRINSIC      MAX, MIN
*   .. Executable Statements ..
      WRITE (NOUT,*) 'F07HNF Example Program Results'
      WRITE (NOUT,*)
*   Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, KD
      IF (N.LE.NMAX .AND. KD.LE.KDMAX) THEN
*
*       Read the upper or lower triangular part of the band matrix A
*       from data file
*
*       IF (UPLO.EQ.'U') THEN
*         READ (NIN,*) ((AB(KD+1+I-J,J),J=I,MIN(N,I+KD)),I=1,N)
*       ELSE IF (UPLO.EQ.'L') THEN
*         READ (NIN,*) ((AB(1+I-J,J),J=MAX(1,I-KD),I),I=1,N)
*       END IF
*
*       Read b from data file
*
*       READ (NIN,*) (B(I),I=1,N)
*
*       Solve the equations Ax = b for x
*
*       CALL ZPBSV(UPLO,N,KD,1,AB,LDAB,B,N,INFO)
*
*       IF (INFO.EQ.0) THEN
*
*         Print solution
*
*         WRITE (NOUT,*) 'Solution'
*         WRITE (NOUT,99999) (B(I),I=1,N)
*
*         Print details of factorization
*
*         WRITE (NOUT,*)
*         IFAIL = 0
*         IF (UPLO.EQ.'U') THEN
*           CALL X04DFF(N,N,0,KD,AB,LDAB,'Bracketed','F7.4',
+             'Cholesky factor U','Integer',RLABS,
+             'Integer',CLABS,80,0,IFAIL)
*         ELSE IF (UPLO.EQ.'L') THEN
*           CALL X04DFF(N,N,KD,0,AB,LDAB,'Bracketed','F7.4',
+             'Cholesky factor L','Integer',RLABS,
+             'Integer',CLABS,80,0,IFAIL)
*         END IF
*
*       ELSE
*         WRITE (NOUT,99998) 'The leading minor of order ', INFO,
+           ' is not positive definite'
*       END IF
*     ELSE
*       WRITE (NOUT,*) 'NMAX and/or KDMAX too small'
*     END IF
*
99999 FORMAT ((3X,4(' (',F7.4,',',F7.4,')',:)))
99998 FORMAT (1X,A,I3,A)
      END

```

9.2 Program Data

F07HNF Example Program Data

```

      4              1                                :Values of N and KD
(  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 matrix A

(-12.42,68.42) ( -9.93, 0.88) (-27.30,-0.01) (  5.31,23.63) :End of vector b

```

9.3 Program Results

F07HNF Example Program Results

```

Solution
(-1.0000, 8.0000) ( 2.0000,-3.0000) (-4.0000,-5.0000) ( 7.0000, 6.0000)

Cholesky factor U
      1              2              3              4
1  ( 3.0643, 0.0000) ( 0.3524,-0.5646)
2              ( 1.1167, 0.0000) (-0.0358, 0.2597)
3              ( 1.6066, 0.0000) (-0.2054, 1.3942)
4              ( 0.4289, 0.0000)

```
