

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 (KIND=nag_wp) 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 $A = L L^H$ 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 (KIND=nag_wp) 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 $A = LL^H$ 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 (KIND=nag_wp) 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

INFO < 0

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

INFO > 0

The leading minor of order $\langle value \rangle$ 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, F04CFE solves $Ax = b$ and returns a forward error bound and condition estimate. F04CFE calls F07HNF (ZPBSV) to solve the equations.

8 Parallelism and Performance

F07HNF (ZPBSV) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

F07HNF (ZPBSV) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 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).

10 Example

This example solves the equations

$$Ax = b,$$

where A is the Hermitian positive definite band matrix

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

and

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

Details of the Cholesky factorization of A are also output.

10.1 Program Text

```

Program f07hnfe

!      F07HNF Example Program Text

!      Mark 25 Release. NAG Copyright 2014.

!      .. Use Statements ..
Use nag_library, Only: nag_wp, x04dff, zpbsv
!      .. Implicit None Statement ..
Implicit None
!      .. Parameters ..
Integer, Parameter          :: nin = 5, nout = 6
Character (1), Parameter   :: uplo = 'U'
!      .. Local Scalars ..
Integer                    :: i, ifail, info, j, kd, ldab, n
!      .. Local Arrays ..
Complex (Kind=nag_wp), Allocatable :: ab(:,,:), b(:)
Character (1)              :: clabs(1), rlabs(1)
!      .. Intrinsic Procedures ..
Intrinsic                  :: max, min
!      .. Executable Statements ..
Write (nout,*) 'F07HNF Example Program Results'
Write (nout,*)
!      Skip heading in data file
Read (nin,*)
Read (nin,*) n, kd
ldab = kd + 1
Allocate (ab(ldab,n),b(n))

!      Read the upper or lower triangular part of the band matrix A
!      from data file

      If (uplo=='U') Then
         Read (nin,*)((ab(kd+1+i-j,j),j=i,min(n,i+kd)),i=1,n)
      Else If (uplo=='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(1:n)

!      Solve the equations Ax = b for x
!      The NAG name equivalent of zpbsv is f07hnf
Call zpbsv(uplo,n,kd,1,ab,ldab,b,n,info)

      If (info==0) Then

!         Print solution

         Write (nout,*) 'Solution'
         Write (nout,99999) b(1:n)

!         Print details of factorization

         Write (nout,*)
         Flush (nout)

!         ifail: behaviour on error exit
!         =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
         ifail = 0
         If (uplo=='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=='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

99999 Format ((3X,4(' (',F7.4,',',F7.4,')':)))
99998 Format (1X,A,I3,A)
      End Program f07hnfe

```

10.2 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

```

10.3 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)

```
