NAG Library Routine Document

F07PNF (ZHPSV)

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

F07PNF (ZHPSV) computes the solution to a complex system of linear equations

$$AX = B,$$

where A is an n by n Hermitian matrix stored in packed format and X and B are n by r matrices.

2 Specification

```
SUBROUTINE F07PNF (UPLO, N, NRHS, AP, IPIV, B, LDB, INFO)

INTEGER                 N, NRHS, IPIV(N), LDB, INFO
COMPLEX (KIND=nag_wp) AP(*), B(LDB,*)
CHARACTER(1)            UPLO
```

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

3 Description

F07PNF (ZHPSV) uses the diagonal pivoting method to factor A as $A = UDU^{\mathrm{H}}$ if UPLO = 'U' or $A = LDL^{\mathrm{H}}$ if UPLO = 'L', where U (or L) is a product of permutation and unit upper (lower) triangular matrices, D is Hermitian and block diagonal with 1 by 1 and 2 by 2 diagonal blocks. 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

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 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: NRHS – INTEGER *Input*

On entry: r, the number of right-hand sides, i.e., the number of columns of the matrix B.

Constraint: NRHS ≥ 0.

4: AP$(*)$ – COMPLEX (KIND=nag_wp) array *Input/Output*

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

On entry: the n by n Hermitian matrix A, packed by columns.

More precisely,

if UPLO = 'U', the upper triangle of A must be stored with element A_{ij} in AP$(i + j(j-1)/2)$ for $i \leq j$;

if UPLO = 'L', the lower triangle of A must be stored with element A_{ij} in AP$(i + (2n-j)(j-1)/2)$ for $i \geq j$.

On exit: the block diagonal matrix D and the multipliers used to obtain the factor U or L from the factorization $A = UDU^{\mathrm{H}}$ or $A = LDL^{\mathrm{H}}$ as computed by F07PRF (ZHPTRF), stored as a packed triangular matrix in the same storage format as A.

5: IPIV(N) – INTEGER array *Output*

On exit: details of the interchanges and the block structure of D. More precisely,

if IPIV$(i) = k > 0$, d_{ii} is a 1 by 1 pivot block and the ith row and column of A were interchanged with the kth row and column;

if UPLO = 'U' and IPIV$(i-1) =$ IPIV$(i) = -l < 0$, $\begin{pmatrix} d_{i-1,i-1} & \bar{d}_{i,i-1} \\ \bar{d}_{i,i-1} & d_{ii} \end{pmatrix}$ is a 2 by 2 pivot block and the $(i-1)$th row and column of A were interchanged with the lth row and column;

if UPLO = 'L' and IPIV$(i) =$ IPIV$(i+1) = -m < 0$, $\begin{pmatrix} d_{ii} & d_{i+1,i} \\ d_{i+1,i} & d_{i+1,i+1} \end{pmatrix}$ is a 2 by 2 pivot block and the $(i+1)$th row and column of A were interchanged with the mth row and column.

6: B(LDB,$*$) – COMPLEX (KIND=nag_wp) array *Input/Output*

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

Note: 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 LDB $= \max(1, \mathrm{N})$.

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

On exit: if INFO $= 0$, the n by r solution matrix X.

7: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F07PNF (ZHPSV) is called.

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

8: 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 argument had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO $= i$, d_{ii} is exactly zero. The factorization has been completed, but the block diagonal matrix D is exactly singular, so the solution could not be 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 $\kappa(A) = \left\|A^{-1}\right\|_1\|A\|_1$, the condition number of A with respect to the solution of the linear equations. See Section 4.4 of Anderson *et al.* (1999) and Chapter 11 of Higham (2002) for further details.

F07PPF (ZHPSVX) is a comprehensive LAPACK driver that returns forward and backward error bounds and an estimate of the condition number. Alternatively, F04CJF solves $AX = B$ and returns a forward error bound and condition estimate. F04CJF calls F07PNF (ZHPSV) to solve the equations.

8 Further Comments

The total number of floating point operations is approximately $\frac{4}{3}n^3 + 8n^2r$, where r is the number of right-hand sides.

The real analogue of this routine is F07PAF (DSPSV). The complex symmetric analogue of this routine is F07QNF (ZSPSV).

9 Example

This example solves the equations

$$Ax = b,$$

where A is the Hermitian matrix

$$A = \begin{pmatrix} -1.84 & 0.11 - 0.11i & -1.78 - 1.18i & 3.91 - 1.50i \\ 0.11 + 0.11i & -4.63 & -1.84 + 0.03i & 2.21 + 0.21i \\ -1.78 + 1.18i & -1.84 - 0.03i & -8.87 & 1.58 - 0.90i \\ 3.91 + 1.50i & 2.21 - 0.21i & 1.58 + 0.90i & -1.36 \end{pmatrix}$$

and

$$b = \begin{pmatrix} 2.98 - 10.18i \\ -9.58 + 3.88i \\ -0.77 - 16.05i \\ 7.79 + 5.48i \end{pmatrix}.$$

Details of the factorization of A are also output.

9.1 Program Text

```
    Program f07pnfe

!     F07PNF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: nag_wp, x04ddf, zhpsv
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
      Character (1), Parameter         :: uplo = 'U'
!     .. Local Scalars ..
      Integer                          :: i, ifail, info, j, n
!     .. Local Arrays ..
      Complex (Kind=nag_wp), Allocatable :: ap(:), b(:)
      Integer, Allocatable             :: ipiv(:)
      Character (1)                    :: clabs(1), rlabs(1)
!     .. Executable Statements ..
      Write (nout,*) 'F07PNF Example Program Results'
      Write (nout,*)
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) n

      Allocate (ap((n*(n+1))/2),b(n),ipiv(n))

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

      If (uplo=='U') Then
        Read (nin,*)((ap(i+(j*(j-1))/2),j=i,n),i=1,n)
      Else If (uplo=='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(1:n)

!     Solve the equations Ax = b for x
!     The NAG name equivalent of zhpsv is f07pnf
      Call zhpsv(uplo,n,1,ap,ipiv,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
        Call x04ddf(uplo,'Non-unit diagonal',n,ap,'Bracketed','F7.4', &
          'Details of factorization','Integer',rlabs,'Integer',clabs,80,0, &
          ifail)

!       Print pivot indices
```

```
        Write (nout,*)
        Write (nout,*) 'Pivot indices'
        Write (nout,99998) ipiv(1:n)

      Else
        Write (nout,99997) 'The diagonal block ', info, ' of D is zero'
      End If

99999 Format ((3X,4(' (',F7.4,',',F7.4,')':)))
99998 Format (1X,7I11)
99997 Format (1X,A,I3,A)
    End Program f07pnfe
```

9.2 Program Data

```
F07PNF Example Program Data
    4                                                          :Value of N
 ( -1.84,  0.00) (  0.11, -0.11) ( -1.78, -1.18) (  3.91, -1.50)
                 ( -4.63 , 0.00) ( -1.84,  0.03) (  2.21,  0.21)
                                 ( -8.87,  0.00) (  1.58, -0.90)
                                                 ( -1.36 , 0.00) :End matrix A
 (  2.98,-10.18) ( -9.58,  3.88) ( -0.77,-16.05) (  7.79,  5.48) :End vector b
```

9.3 Program Results

```
 F07PNF Example Program Results

 Solution
    ( 2.0000, 1.0000) ( 3.0000,-2.0000) (-1.0000, 2.0000) ( 1.0000,-1.0000)

 Details of factorization
                    1                   2                   3                   4
 1  (-7.1028, 0.0000) ( 0.2997, 0.1578) ( 0.3397, 0.0303) (-0.1518, 0.3743)
 2                    (-5.4176, 0.0000) ( 0.5637, 0.2850) ( 0.3100, 0.0433)
 3                                      (-1.8400, 0.0000) ( 3.9100,-1.5000)
 4                                                        (-1.3600, 0.0000)

 Pivot indices
           1          2         -1         -1
```