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 ≥ 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: $\text{NRHS} \geq 0$.

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

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

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 $A = UDU^{\text{H}}$ or $A = LDL^{\text{H}}$ 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 $\text{IPIV}(i) = k > 0$, 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 $\text{IPIV}(i-1) = \text{IPIV}(i) = -l < 0$, $\begin{pmatrix} d_{i-1,i-1} & \bar{d}_{i,i-1} \\ \bar{d}_{i,i-1} & d_{ii} \end{pmatrix}$ 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 $\text{IPIV}(i) = \text{IPIV}(i+1) = -m < 0$, $\begin{pmatrix} d_{ii} & d_{i+1,i} \\ d_{i+1,i} & d_{i+1,i+1} \end{pmatrix}$ 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$(\text{LDB}, *)$ – COMPLEX (KIND=nag_wp) array *Input/Output*

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

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 $\text{LDB} = \max(1, \text{N})$.

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

On exit: if $\text{INFO} = 0$, 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: $\text{LDB} \geq \max(1, \text{N})$.

8: INFO – INTEGER *Output*

On exit: $\text{INFO} = 0$ 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

Element $\langle value \rangle$ of the diagonal 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 Parallelism and Performance

F07PNF (ZHPSV) is not threaded by NAG in any implementation.

F07PNF (ZHPSV) 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

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).

10 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.

10.1 Program Text

```
    Program f07pnfe

!     F07PNF Example Program Text

!     Mark 25 Release. NAG Copyright 2014.

!     .. 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
```

10.2 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
```

10.3 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
```