NAG Library Routine Document

F07GNF (ZPPSV)

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

F07GNF (ZPPSV) computes the solution to a complex system of linear equations

$$AX = B,$$

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

2 Specification

```
SUBROUTINE F07GNF(UPLO, N, NRHS, AP, B, LDB, INFO)
INTEGER            N, NRHS, LDB, INFO
complex*16         AP(*), B(LDB,*)
CHARACTER*1        UPLO
```

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

3 Description

F07GNF (ZPPSV) uses the Cholesky decomposition to factor A as $A = U^{\mathrm{H}}U$ if UPLO = 'U' or $A = LL^{\mathrm{H}}$ if UPLO = 'L', where U is an upper triangular matrix and L is a lower triangular matrix. 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, Philadelphiahttp://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: 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.

4: AP($*$) – ***complex*16*** 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: if INFO $= 0$, the factor U or L from the Cholesky factorization $A = U^{\mathrm{H}}U$ or $A = LL^{\mathrm{T}}$, in the same storage format as A.

5: B(LDB,$*$) – ***complex*16*** array *Input/Output*

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

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.

6: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F07GNF (ZPPSV) is called.

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

7: 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 $= i$, 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.

F07GPF (ZPPSVX) is a comprehensive LAPACK driver that returns forward and backward error bounds and an estimate of the condition number. Alternatively, F04CEF solves $Ax = b$ and returns a forward error bound and condition estimate. F04CEF calls F07GNF (ZPPSV) 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 F07GAF (DPPSV).

9 Example

This example solves the equations

$$Ax = b,$$

where A is the symmetric positive-definite matrix

$$A = \begin{pmatrix} 3.23 & 1.51 - 1.92i & 1.90 + 0.84i & 0.42 + 2.50i \\ 1.51 + 1.92i & 3.58 & -0.23 + 1.11i & -1.18 + 1.37i \\ 1.90 - 0.84i & -0.23 - 1.11i & 4.09 & 2.33 - 0.14i \\ 0.42 - 2.50i & -1.18 - 1.37i & 2.33 + 0.14i & 4.29 \end{pmatrix}$$

and

$$b = \begin{pmatrix} 3.93 - 6.14i \\ 6.17 + 9.42i \\ -7.17 - 21.83i \\ 1.99 - 14.38i \end{pmatrix}.$$

Details of the Cholesky factorization of A are also output.

9.1 Program Text

```
*     F07GNF Example Program Text
*     Mark 21 Release. NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX
      PARAMETER        (NMAX=8)
      CHARACTER        UPLO
      PARAMETER        (UPLO='U')
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INFO, J, N
*     .. Local Arrays ..
      COMPLEX *16      AP((NMAX*(NMAX+1))/2), B(NMAX)
      CHARACTER        CLABS(1), RLABS(1)
*     .. External Subroutines ..
      EXTERNAL         X04DDF, ZPPSV
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F07GNF Example Program Results'
      WRITE (NOUT,*)
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*        Read the upper or lower triangular part of the matrix A from
*        data file
*
         IF (UPLO.EQ.'U') THEN
```

```
            READ (NIN,*) ((AP(I+(J*(J-1))/2),J=I,N),I=1,N)
         ELSE IF (UPLO.EQ.'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(I),I=1,N)
*
*        Solve the equations Ax = b for x
*
         CALL ZPPSV(UPLO,N,1,AP,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
            CALL X04DDF(UPLO,'Non-unit diagonal',N,AP,'Bracketed',
     +                  'F7.4','Cholesky factor','Integer',RLABS,
     +                  'Integer',CLABS,80,0,IFAIL)
*
         ELSE
            WRITE (NOUT,99998) 'The leading minor of order ', INFO,
     +        ' is not positive definite'
         END IF
      ELSE
         WRITE (NOUT,*) 'NMAX too small'
      END IF
*
99999 FORMAT ((3X,4(' (',F7.4,',',F7.4,')',:)))
99998 FORMAT (1X,A,I3,A)
      END
```

9.2 Program Data

```
F07GNF Example Program Data
   4                                                          :Value of N
 ( 3.23,  0.00) ( 1.51, -1.92) ( 1.90,  0.84) ( 0.42,  2.50)
                ( 3.58,  0.00) (-0.23,  1.11) (-1.18,  1.37)
                               ( 4.09,  0.00) ( 2.33, -0.14)
                                              ( 4.29,  0.00) :End of matrix A
 ( 3.93, -6.14) ( 6.17,  9.42) (-7.17,-21.83) ( 1.99,-14.38) :End of vector b
```

9.3 Program Results

```
 F07GNF Example Program Results

 Solution
    ( 1.0000,-1.0000) ( 0.0000, 3.0000) (-4.0000,-5.0000) ( 2.0000, 1.0000)

 Cholesky factor
                    1                  2                  3                  4
 1  ( 1.7972, 0.0000) ( 0.8402,-1.0683) ( 1.0572, 0.4674) ( 0.2337, 1.3910)
 2                    ( 1.3164, 0.0000) (-0.4702,-0.3131) ( 0.0834,-0.0368)
 3                                      ( 1.5604, 0.0000) ( 0.9360,-0.9900)
 4                                                        ( 0.6603, 0.0000)
```