

# F07FSFP (PZPOTRS)

## NAG Parallel Library Routine Document

**Note:** before using this routine, please read the Users' Note for your implementation to check for implementation-dependent details. You are advised to enclose any calls to NAG Parallel Library routines between calls to Z01AAFP and Z01ABFP.

### 1 Description

F07FSFP (PZPOTRS) solves an  $n$  by  $n$  complex Hermitian positive-definite system of linear equations with multiple right-hand sides, i.e.,  $A_s X = B_s$ , where  $A_s$  is a submatrix of a larger  $m_A$  by  $n_A$  matrix  $A$ , i.e.,

$$A_s(1:n, 1:n) \equiv A(i_A : i_A + n - 1, j_A : j_A + n - 1),$$

and  $B_s$  is a ( $r$  right-hand sides) submatrix of a larger  $m_B$  by  $n_B$  matrix  $B$ , i.e.,

$$B_s(1:n, 1:r) \equiv B(i_B : i_B + n - 1, j_B : j_B + r - 1).$$

The matrix  $A_s$  must have been previously factorized by a call to F07FRFP (PZPOTRF). F07FRFP (PZPOTRF) performs a Cholesky factorization and F07FSFP (PZPOTRS) solves the system of equations by forward and backward substitution.

### 2 Specification

```

SUBROUTINE F07FSFP(UPLO, N, NRHS, A, IA, JA, IDESCA, B, IB, JB,
1             IDESCB, INFO)
ENTRY       PZPOTRS(UPLO, N, NRHS, A, IA, JA, IDESCA, B, IB, JB,
1             IDESCB, INFO)
COMPLEX*16  A(*), B(*)
INTEGER     N, NRHS, IA, JA, IDESCA(*), IB, JB, IDESCB(*),
1          INFO
CHARACTER*1 UPLO

```

The ENTRY statement enables the routine to be called by its ScaLAPACK name.

### 3 Usage

#### 3.1 Definitions

The following definitions are used in describing the data distribution within this document:

- $m_p$  – the number of rows in the Library Grid.
- $n_p$  – the number of columns in the Library Grid.
- $p_r$  – the row grid coordinate of the calling processor.
- $p_c$  – the column grid coordinate of the calling processor.
- $M_b^X$  – the blocking factor for the distribution of the rows of a matrix  $X$ .
- $N_b^X$  – the blocking factor for the distribution of the columns of a matrix  $X$ .
- $\text{numroc}(\alpha, b_\ell, q, s, k)$  – a function which gives the **number of rows or columns** of a distributed matrix owned by the processor with the row or column coordinate  $q$  ( $p_r$  or  $p_c$ ), where  $\alpha$  is the total number of rows or columns of the matrix,  $b_\ell$  is the blocking factor used ( $M_b^X$  or  $N_b^X$ ),  $s$  is the row or column coordinate of the processor that possesses the first row or column of the distributed matrix and  $k$  is either  $m_p$  or  $n_p$ . The Library provides the function Z01CAFP (NUMROC) for the evaluation of this function.

#### 3.2 Global and Local Arguments

The following global **input** arguments must have the same value on entry to the routine on each processor and the global **output** arguments will have the same value on exit from the routine on each processor:

Global input arguments: UPLO, N, NRHS, IA, JA, IB, JB, IDESCA(1), IDESCA(3:8), IDESCB(1), IDESCB(3:8)

Global output arguments: INFO

The remaining arguments are local.

### 3.3 Distribution Strategy

The array  $A$  must contain the Cholesky factorization of the matrix  $A_s$ , previously factorized by F07FRFP (PZPOTRF). The Cholesky factors must be stored in a cyclic two-dimensional block distribution (described in the F07 Chapter Introduction), as returned by F07FRFP (PZPOTRF). The right-hand sides of the equation,  $B_s$  are stored in the array  $B$ , in a cyclic two-dimensional block distribution.

### 3.4 Related Routines

The Library provides many support routines for the generation, scattering/gathering and input/output of matrices/vectors in cyclic two-dimensional block form. The following routines may be used in conjunction with F07FSFP (PZPOTRS):

Complex matrix generation: F01ZVFP  
 Complex matrix input: X04BRFP  
 Complex matrix output: X04BSFP  
 Complex matrix gather: F01WGFP  
 Complex matrix scatter: F01WUFP

## 4 Arguments

- 1: UPLO — CHARACTER\*1 *Global Input*  
*On entry:* indicates whether  $A_s$  has been factorized as  $U^H U$  or  $LL^H$  as follows:
  - if UPLO = 'U', then  $A_s = U^H U$ , where  $U$  is upper triangular;
  - if UPLO = 'L', then  $A_s = LL^H$ , where  $L$  is lower triangular.*Constraint:* UPLO = 'U' or 'L'.
- 2: N — INTEGER *Global Input*  
*On entry:*  $n$ , the order of the matrix  $A_s$ .  
*Constraint:*  $0 \leq N \leq \min(\text{IDESCA}(3), \text{IDESCA}(4), \text{IDESCB}(3))$ .
- 3: NRHS — INTEGER *Global Input*  
*On entry:*  $r$ , the number of right-hand sides.  
*Constraint:*  $0 \leq \text{NRHS} \leq \text{IDESCB}(4)$ .
- 4: A(\*) — COMPLEX\*16 array *Local Input*  
**Note:** the array  $A$  is formally defined as a vector. However, you may find it more convenient to consider  $A$  as a two-dimensional array of dimension  $(\text{IDESCA}(9), \gamma)$ , where  $\gamma \geq \text{numroc}(\text{JA} + \text{N} - 1, \text{IDESCA}(6), p_c, \text{IDESCA}(8), n_p)$ .  
*On entry:* the local part of the Cholesky factorization of the matrix  $A_s$  as returned by F07FRFP (PZPOTRF).
- 5: IA — INTEGER *Global Input*  
*On entry:*  $i_A$ , the row index of matrix  $A$  that identifies the first row of the Cholesky factorization of  $A_s$ .  
*Constraints:*  $1 \leq \text{IA} \leq \text{IDESCA}(3) - \text{N} + 1$  and  $\text{mod}(\text{IA} - 1, \text{IDESCA}(5)) = 0$ .

- 6:** JA — INTEGER *Global Input*  
*On entry:*  $j_A$ , the column index of matrix  $A$  that identifies the first column of the Cholesky factorization of  $A_s$ .  
*Constraints:*  $1 \leq JA \leq \text{IDESCA}(4) - N + 1$  and  $\text{mod}(JA-1, \text{IDESCA}(6)) = 0$ .
- 7:** IDESCA(\*) — INTEGER array *Local Input*  
**Note:** the dimension of the array IDESCA must be at least 9.  
*Distribution:* the array elements IDESCA(1) and IDESCA(3),...,IDESCA(8) must be global to the processor grid and the array elements IDESCA(2) and IDESCA(9) are local to each processor.  
*On entry:* the description array for the matrix  $A$ . This array must contain details of the distribution of the matrix  $A$  and the logical processor grid.  
 IDESCA(1), the descriptor type. For this routine, which uses a cyclic two-dimensional block distribution, IDESCA(1) = 1;  
 IDESCA(2), the Library context, usually returned by a call to the Library Grid initialisation routine Z01AAFP;  
 IDESCA(3), the number of rows,  $m_A$ , of the matrix  $A$ ;  
 IDESCA(4), the number of columns,  $n_A$ , of the matrix  $A$ ;  
 IDESCA(5), the blocking factor,  $M_b^A$ , used to distribute the rows of the matrix  $A$ ;  
 IDESCA(6), the blocking factor,  $N_b^A$ , used to distribute the columns of the matrix  $A$ ;  
 IDESCA(7), the processor row index over which the first row of the matrix  $A$  is distributed;  
 IDESCA(8), the processor column index over which the first column of the matrix  $A$  is distributed;  
 IDESCA(9), the leading dimension of the conceptual two-dimensional array  $A$ .  
*Constraints:*  
 IDESCA(1) = 1;  
 IDESCA(3)  $\geq$  0; IDESCA(4)  $\geq$  0;  
 IDESCA(5) = IDESCA(6); IDESCA(5)  $\geq$  1; IDESCA(6)  $\geq$  1;  
 $0 \leq \text{IDESCA}(7) \leq m_p - 1$ ;  $0 \leq \text{IDESCA}(8) \leq n_p - 1$ ;  
 IDESCA(9)  $\geq \max(1, \text{numroc}(\text{IDESCA}(3), \text{IDESCA}(5), p_r, \text{IDESCA}(7), m_p))$ .
- 8:** B(\*) — COMPLEX\*16 array *Local Input/Local Output*  
**Note:** array B is formally defined as a vector. However, you may find it more convenient to consider B as a two-dimensional array of dimension (IDESCB(9), $\gamma$ ), where  $\gamma \geq \text{numroc}(\text{JB} + \text{NRHS} - 1, \text{IDESCB}(6), p_c, \text{IDESCB}(8), n_p)$ .  
*On entry:* the local part of the right-hand side matrix  $B$  which may contain parts of the  $n$  by  $r$  submatrix  $B_s$ .  
*On exit:* the  $n$  by  $r$  solution matrix  $X$  distributed in the same cyclic two-dimensional block distribution.
- 9:** IB — INTEGER *Global Input*  
*On entry:*  $i_B$ , the row index of matrix  $B$  that identifies the first row of the submatrix  $B_s$ .  
*Constraints:*  $1 \leq IB \leq \text{IDESCB}(3) - N + 1$  and  $\text{mod}(IB-1, \text{IDESCB}(5)) = 0$ .  
 The I $A$ th row of the array A and the IBth row of the array B must be located on the same row of the processor grid, i.e.,  

$$\text{mod}(\text{IDESCA}(7) + (\text{IA} - 1)/\text{IDESCA}(5), n_p) = \text{mod}(\text{IDESCB}(7) + (\text{IB} - 1)/\text{IDESCB}(5), n_p)$$
.
- 10:** JB — INTEGER *Global Input*  
*On entry:*  $j_B$ , the column index of matrix  $B$  that identifies the first column of the submatrix  $B_s$ .  
*Constraint:*  $1 \leq JB \leq \text{IDESCB}(4) - \text{NRHS} + 1$ .

**11: IDESCB(\*)** — INTEGER array*Local Input***Note:** the dimension of the array IDESCB must be at least 9.*Distribution:* the array elements IDESCB(1) and IDESCB(3),...,IDESCB(8) must be global to the processor grid and the array elements IDESCB(2) and IDESCB(9) are local to each processor.*On entry:* the description array for the matrix  $B$ . This array must contain details of the distribution of the matrix  $B$  and the logical processor grid.

IDESCB(1), the descriptor type. For this routine, which uses a cyclic two-dimensional block distribution, IDESCB(1) = 1;

IDESCB(2), the Library context, usually returned by a call to the Library Grid initialisation routine Z01AAFP;

IDESCB(3), the number of rows,  $m_B$ , of the matrix  $B$ ;IDESCB(4), the number of columns,  $n_B$ , of the matrix  $B$ ;IDESCB(5), the blocking factor,  $M_b^B$ , used to distribute the rows of the matrix  $B$ ;IDESCB(6), the blocking factor,  $N_b^B$ , used to distribute the columns of the matrix  $B$ ;IDESCB(7), the processor row index over which the first row of the matrix  $B$  is distributed;IDESCB(8), the processor column index over which the first column of the matrix  $B$  is distributed;IDESCB(9), the leading dimension of the conceptual two-dimensional array  $B$ .*Constraints:*

IDESCB(1) = 1;

IDESCB(3)  $\geq$  0; IDESCB(4)  $\geq$  0;

IDESCB(2) = IDESCA(2);

IDESCB(5) = IDESCB(6); IDESCB(5)  $\geq$  1; IDESCB(6)  $\geq$  1;0  $\leq$  IDESCB(7)  $\leq$   $m_p - 1$ ; 0  $\leq$  IDESCB(8)  $\leq$   $n_p - 1$ ;IDESCB(9)  $\geq$  max(1,numroc(IDESCB(3),IDESCB(5), $p_r$ ,IDESCB(7), $m_p$ )).**12: INFO** — INTEGER*Global Output*

The NAG Parallel Library provides a mechanism, via the routine Z02EAFP, to reduce the amount of parameter validation performed by this routine. For a full description refer to the Z02 Chapter Introduction.

*On exit:* INFO = 0 (or -9999 if reduced error checking is enabled) unless the routine detects an error (see Section 5).

## 5 Errors and Warnings

If INFO  $\neq$  0 explanatory error messages are output from the root processor (or processor {0,0} when the root processor is not available) on the current error message unit (as defined by X04AAF).

INFO &lt; 0

On entry, one of the arguments was invalid:

if the  $k$ th argument is a scalar INFO =  $-k$ ;if the  $k$ th argument is an array and its  $j$ th element is invalid, INFO =  $-(100 \times k + j)$ .

This error occurred either because a global argument did not have the same value on all logical processors, or because its value on one or more processors was incorrect.

## 6 Further Comments

The total number of floating-point operations is approximately  $8n^2r$ .

## 6.1 Algorithmic Detail

Forward and backward substitution is used.

If UPLO = 'U',  $A = U^H U$ , where  $U$  is upper triangular; the solution  $X$  is computed by solving  $U^H Y = B$  and then  $UX = Y$ .

If UPLO = 'L',  $A = LL^H$ , where  $L$  is lower triangular; the solution  $X$  is computed by solving  $LY = B$  and then  $L^H X = Y$ .

## 6.2 Parallelism Detail

The Level-3 BLAS operations are carried out in parallel.

## 6.3 Accuracy

For each right-hand side vector  $b$ , the computed solution  $x$  is the exact solution of a perturbed system of equations  $(A + E)x = b$ , where

$$|E| \leq c(n)\epsilon|U^H| \cdot |U| \quad \text{if UPLO = 'U'},$$

$$|E| \leq c(n)\epsilon|L| \cdot |L^H| \quad \text{if UPLO = 'L'},$$

$c(n)$  is a modest linear function of  $n$  and  $\epsilon$  is the *machine precision*. If  $x$  is the true solution, then the computed solution  $\hat{x}$  satisfies a forward error bound of the form

$$\frac{\|x - \hat{x}\|_\infty}{\|x\|_\infty} \leq \epsilon c(n) \kappa(A),$$

where  $\kappa(A)$  is the condition number of  $A$ . See the F07 Chapter Introduction.

## 7 References

- [1] Golub G H and van Loan C F (1996) *Matrix Computations* Johns Hopkins University Press (3rd Edition), Baltimore

## 8 Example

To solve the system of equations  $AX = B$ , where

$$A = \begin{pmatrix} 3.23 + 0.00i & 1.51 - 1.92i & 1.90 + 0.84i & 0.42 + 2.50i \\ 1.51 + 1.92i & 3.58 + 0.00i & -0.23 + 1.11i & -1.18 + 1.37i \\ 1.90 - 0.84i & -0.23 - 1.11i & 4.09 + 0.00i & 2.33 - 0.14i \\ 0.42 - 2.50i & -1.18 - 1.37i & 2.33 + 0.14i & 4.29 + 0.00i \end{pmatrix} \quad \text{and}$$

$$B = \begin{pmatrix} 3.93 - 6.14i & 1.48 + 6.58i \\ 6.17 + 9.42i & 4.65 - 4.75i \\ -7.17 - 21.83i & -4.91 + 2.29i \\ 1.99 - 14.38i & 7.64 - 10.79i \end{pmatrix}.$$

Here  $A$  is Hermitian positive-definite and must first be factorized by F07FRFP (PZPOTRF). The example uses a 2 by 2 logical processor grid and a block size of 2.

**Note:** the listing of the Example Program presented below does not give a full pathname for the data file being opened, but in general the user must give the full pathname in this and any other OPEN statement.

## 8.1 Example Text

```

*   F07FSFP Example Program Text
*   NAG Parallel Library Release 2. NAG Copyright 1996.
*   .. Parameters ..
INTEGER          NIN, NOUT
PARAMETER        (NIN=5,NOUT=6)
INTEGER          DT
PARAMETER        (DT=1)
INTEGER          MB, NB
PARAMETER        (MB=2,NB=MB)
INTEGER          NMAX, IAROW, IACOL, LDA, LDB, NRHMAX, LW
PARAMETER        (NMAX=8,IAROW=0,IACOL=0,LDA=NMAX,LDB=NMAX,
+               NRHMAX=2,LW=NMAX)
*   .. Local Scalars ..
INTEGER          IA, IB, ICNTXT, IFAIL, INFO, JA, JB, MP, N, NP,
+               NRHS
LOGICAL          ROOT
CHARACTER        UPLO
CHARACTER*80     FORMAT
*   .. Local Arrays ..
COMPLEX*16       A(LDA,NMAX), B(LDB,NRHMAX), WORK(LW)
INTEGER          IDESCA(9), IDESCB(9)
*   .. External Functions ..
LOGICAL          Z01ACFP
EXTERNAL         Z01ACFP
*   .. External Subroutines ..
EXTERNAL         F07FRFP, F07FSFP, X04BRFP, X04BSFP, Z01AAFP,
+               Z01ABFP
*   .. Executable Statements ..
ROOT = Z01ACFP()
IF (ROOT) THEN
    WRITE (NOUT,*) 'F07FSFP Example Program Results'
    WRITE (NOUT,*)
END IF

*
MP = 2
NP = 2
IFAIL = 0

*
CALL Z01AAFP(ICNTXT,MP,NP,IFAIL)

*
OPEN (NIN,FILE='f07fsfpe.d')
*   Skip heading in data file
READ (NIN,*)
READ (NIN,*) N, NRHS, UPLO, FORMAT

*
IF (N.LE.NMAX .AND. NRHS.LE.NRHMAX) THEN
*
*   Set the array descriptor of A
*
    IDESCA(1) = DT
    IDESCA(2) = ICNTXT
    IDESCA(3) = N
    IDESCA(4) = N
    IDESCA(5) = MB
    IDESCA(6) = NB
    IDESCA(7) = IAROW

```

```

      IDESCA(8) = IACOL
      IDESCA(9) = LDA
      IA = 1
      JA = 1
*
*      Read A from the data file
*
      IFAIL = 0
      CALL X04BRFP(NIN,N,N,A,1,1,IDESCA,IFAIL)
*
*      Factorize the matrix
*
      CALL F07FRFP(UPLO,N,A,IA,JA,IDESCA,INFO)
*
      IF (INFO.EQ.0) THEN
*
*          Set the array descriptor of B
*
          IDESCB(1) = DT
          IDESCB(2) = IDESCA(2)
          IDESCB(3) = N
          IDESCB(4) = NRHS
          IDESCB(5) = MB
          IDESCB(6) = NB
          IDESCB(7) = IAROW
          IDESCB(8) = IACOL
          IDESCB(9) = LDB
          IB = 1
          JB = 1
*
*          Read B from data file
*
          IFAIL = 0
          CALL X04BRFP(NIN,N,NRHS,B,1,1,IDESCB,IFAIL)
*
          CALL F07FSFP(UPLO,N,NRHS,A,IA,JA,IDESCA,B,IB,JB,IDESCB,INFO)
          IF (INFO.EQ.0) THEN
*
*              Print solution(s)
*
              IF (ROOT) THEN
                  WRITE (NOUT,*) 'Solution(s)'
                  WRITE (NOUT,*)
              END IF
              IFAIL = 0
*
              CALL X04BSFP(NOUT,N,NRHS,B,IB,JB,IDESCB,FORMAT,WORK,
+                  IFAIL)
*
              ELSE
                  IF (ROOT) WRITE (NOUT,*)
+                  'Unable to solve triangular system'
              END IF
          ELSE
              IF (ROOT) WRITE (NOUT,*)
+              'Matrix is not positive-definite'
          END IF
*

```

```

      END IF
*
      CLOSE (NIN)
*
      IFAIL = 0
      CALL Z01ABFP(ICNTXT,'N',IFAIL)
*
      STOP
      END

```

## 8.2 Example Data

F07FSFP Example Program Data

```

4 2 'L' '(2(:,' (','F7.4,'','F7.4,'')))' :Value of N, NRHS, UPLO and FORMAT
(3.23, 0.00) ( 0.0 , 0.0 ) ( 0.0 , 0.0 ) ( 0.0 , 0.0 )
(1.51, 1.92) ( 3.58, 0.00) ( 0.0 , 0.0 ) ( 0.0 , 0.0 )
(1.90,-0.84) (-0.23,-1.11) ( 4.09, 0.00) ( 0.0 , 0.0 )
(0.42,-2.50) (-1.18,-1.37) ( 2.33, 0.14) ( 4.29, 0.00) :End of matrix A
( 3.93, -6.14) ( 1.48, 6.58)
( 6.17, 9.42) ( 4.65, -4.75)
(-7.17,-21.83) (-4.91, 2.29)
( 1.99,-14.38) ( 7.64,-10.79) :End of matrix B

```

## 8.3 Example Results

F07FSFP Example Program Results

Solution(s)

```

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

```