

# NAG Library Routine Document

## F01EPF

**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

F01EPF computes the principal matrix square root,  $A^{1/2}$ , of a real upper quasi-triangular  $n$  by  $n$  matrix  $A$ .

### 2 Specification

```
SUBROUTINE F01EPF (N, A, LDA, IFAIL)
  INTEGER          N, LDA, IFAIL
  REAL (KIND=nag_wp) A(LDA,*)
```

### 3 Description

A square root of a matrix  $A$  is a solution  $X$  to the equation  $X^2 = A$ . A nonsingular matrix has multiple square roots. For a matrix with no eigenvalues on the closed negative real line, the principal square root, denoted by  $A^{1/2}$ , is the unique square root whose eigenvalues lie in the open right half-plane.

F01EPF computes  $A^{1/2}$ , where  $A$  is an upper quasi-triangular matrix, with  $1 \times 1$  and  $2 \times 2$  blocks on the diagonal. Such matrices arise from the Schur factorization of a real general matrix, as computed by F08PEF (DHSEQR), for example. F01EPF does not require  $A$  to be in the canonical Schur form described in F08PEF (DHSEQR), it merely requires  $A$  to be upper quasi-triangular.  $A^{1/2}$  then has the same block triangular structure as  $A$ .

The algorithm used by F01EPF is described in Higham (1987). In addition a blocking scheme described in Deadman *et al.* (2013) is used.

### 4 References

Björck D and Hammarling S (1983) A Schur method for the square root of a matrix *Linear Algebra Appl.* **52/53** 127–140

Deadman E, Higham N J and Ralha R (2013) Blocked Schur Algorithms for Computing the Matrix Square Root *Applied Parallel and Scientific Computing: 11th International Conference, (PARA 2012, Helsinki, Finland)* P. Manninen and P. Uster, Eds *Lecture Notes in Computer Science* **7782** 171–181 Springer–Verlag

Higham N J (1987) Computing real square roots of a real matrix *Linear Algebra Appl.* **88/89** 405–430

Higham N J (2008) *Functions of Matrices: Theory and Computation* SIAM, Philadelphia, PA, USA

### 5 Arguments

- 1: N – INTEGER *Input*  
*On entry:*  $n$ , the order of the matrix  $A$ .  
*Constraint:*  $N \geq 0$ .
- 2: A(LDA,\*) – REAL (KIND=nag\_wp) array *Input/Output*  
**Note:** the second dimension of the array  $A$  must be at least  $N$ .  
*On entry:* the  $n$  by  $n$  upper quasi-triangular matrix  $A$ .

*On exit:* the  $n$  by  $n$  principal matrix square root  $A^{1/2}$ .

3: LDA – INTEGER

*Input*

*On entry:* the first dimension of the array A as declared in the (sub)program from which F01EPF is called.

*Constraint:*  $LDA \geq N$ .

4: IFAIL – INTEGER

*Input/Output*

*On entry:* IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation for details.

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this argument, the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

*On exit:* IFAIL = 0 unless the routine detects an error or a warning has been flagged (see Section 6).

## 6 Error Indicators and Warnings

If on entry IFAIL = 0 or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

A has negative or vanishing eigenvalues. The principal square root is not defined in this case. F01ENF or F01FNF may be able to provide further information.

IFAIL = 2

An internal error occurred. It is likely that the routine was called incorrectly.

IFAIL = -1

*On entry,*  $N = \langle value \rangle$ .  
*Constraint:*  $N \geq 0$ .

IFAIL = -3

*On entry,*  $LDA = \langle value \rangle$  and  $N = \langle value \rangle$ .  
*Constraint:*  $LDA \geq N$ .

IFAIL = -99

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -399

Your licence key may have expired or may not have been installed correctly.

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -999

Dynamic memory allocation failed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

## 7 Accuracy

The computed square root  $\hat{X}$  satisfies  $\hat{X}^2 = A + \Delta A$ , where  $\|\Delta A\|_F \approx O(\epsilon)n\|\hat{X}\|_F^2$ , where  $\epsilon$  is *machine precision*.

## 8 Parallelism and Performance

F01EPF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

F01EPF 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 cost of the algorithm is  $n^3/3$  floating-point operations; see Algorithm 6.7 of Higham (2008).  $O(n)$  of integer allocatable memory is required by the routine.

If  $A$  is a full matrix, then F01ENF should be used to compute the square root. If  $A$  has negative real eigenvalues then F01FNF can be used to return a complex, non-principal square root.

If condition number and residual bound estimates are required, then F01JDF should be used. For further discussion of the condition of the matrix square root see Section 6.1 of Higham (2008).

## 10 Example

This example finds the principal matrix square root of the matrix

$$A = \begin{pmatrix} 6 & 4 & -5 & 15 \\ 8 & 6 & -3 & 10 \\ 0 & 0 & 3 & -4 \\ 0 & 0 & 4 & 3 \end{pmatrix}.$$

### 10.1 Program Text

```

Program f01epfe

!      F01EPF Example Program Text

!      Mark 26 Release. NAG Copyright 2016.

!      .. Use Statements ..
      Use nag_library, Only: f01epf, nag_wp, x04caf
!      .. Implicit None Statement ..
      Implicit None
!      .. Parameters ..
      Integer, Parameter          :: nin = 5, nout = 6
!      .. Local Scalars ..
      Integer                     :: i, ifail, lda, n
!      .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable :: a(:, :)
!      .. Executable Statements ..
      Write (nout,*) 'F01EPF Example Program Results'
      Write (nout,*)
!      Skip heading in data file
      Read (nin,*)
      Read (nin,*) n

      lda = n
      Allocate (a(lda,n))

!      Read A from data file

```

```

      Read (nin,*)(a(i,1:n),i=1,n)

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

!      Find sqrt(A)
      Call f01epf(n,a,lda,ifail)

!      Print solution
      If (ifail==0) Then
        ifail = 0
        Call x04caf('G','N',n,n,a,lda,'sqrt(A)',ifail)
      End If

      End Program f01epfe

```

## 10.2 Program Data

F01EPF Example Program Data

```

4                               :Value of N

6.0      4.0      -5.0      15.0
8.0      6.0      -3.0      10.0
0.0      0.0       3.0      -4.0
0.0      0.0      4.0       3.0  :End of matrix A

```

## 10.3 Program Results

F01EPF Example Program Results

```

sqrt(A)
           1           2           3           4
1      2.0000E+00  1.0000E+00 -2.0000E+00  3.0000E+00
2      2.0000E+00  2.0000E+00  3.1721E-16  1.0000E+00
3      0.0000E+00  0.0000E+00  2.0000E+00 -1.0000E+00
4      0.0000E+00  0.0000E+00  1.0000E+00  2.0000E+00

```

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