# NAG Fortran Library Routine Document

### F04LEF

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

F04LEF solves a system of tridiagonal equations following the factorization by F01LEF. This routine is intended for applications such as inverse iteration as well as straightforward linear equation applications.

# 2 Specification

SUBROUTINE F04LEF (JOB, N, A, B, C, D, IPIV, Y, TOL, IFAIL)

INTEGER

JOB, N, IPIV(N), IFAIL

double precision

A(N), B(N), C(N), D(N), Y(N), TOL

# 3 Description

Following the factorization of the n by n tridiagonal matrix  $(T - \lambda I)$  as

$$T - \lambda I = PLU$$

by F01LEF, F04LEF may be used to solve any of the equations

$$(T - \lambda I)x = y$$
,  $(T - \lambda I)^{\mathrm{T}}x = y$ ,  $Ux = y$ 

for x, the choice of equation being controlled by the parameter JOB. In each case there is an option to perturb zero or very small diagonal elements of U, this option being intended for use in applications such as inverse iteration.

#### 4 References

Wilkinson J H (1965) The Algebraic Eigenvalue Problem Oxford University Press, Oxford

Wilkinson J H and Reinsch C (1971) Handbook for Automatic Computation II, Linear Algebra Springer-Verlag

#### 5 Parameters

1: JOB – INTEGER Input

On entry: must specify the equations to be solved.

$$JOB = 1$$

The equations  $(T - \lambda I)x = y$  are to be solved, but diagonal elements of U are not to be perturbed.

$$JOB = -1$$

The equations  $(T - \lambda I)x = y$  are to be solved and, if overflow would otherwise occur, diagonal elements of U are to be perturbed. See parameter TOL.

JOB = 2

The equations  $(T - \lambda I)^T x = y$  are to be solved, but diagonal elements of U are not to be perturbed.

JOB = -2

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The equations  $(T - \lambda I)^T x = y$  are to be solved and, if overflow would otherwise occur, diagonal elements of U are to be perturbed. See parameter TOL.

JOB = 3

The equations Ux = y are to be solved, but diagonal elements of U are not to be perturbed.

JOB = -3

The equations Ux = y are to be solved and, if overflow would otherwise occur, diagonal elements of U are to be perturbed. See parameter TOL.

2: N – INTEGER Input

On entry: n, the order of the matrix T.

Constraint:  $N \ge 1$ .

#### 3: A(N) – *double precision* array

Input

On entry: the diagonal elements of U as returned by F01LEF.

#### 4: B(N) – *double precision* array

Input

On entry: the elements of the first superdiagonal of U as returned by F01LEF.

#### 5: C(N) – *double precision* array

Input

On entry: the subdiagonal elements of L as returned by F01LEF.

#### 6: D(N) - double precision array

Input

On entry: the elements of the second superdiagonal of U as returned by F01LEF.

# 7: IPIV(N) - INTEGER array

Input

On entry: details of the matrix P as returned by F01LEF.

#### 8: Y(N) – double precision array

Input/Output

On entry: the right-hand side vector y.

On exit: is overwritten by the solution vector x.

#### 9: TOL – double precision

Input/Output

On entry: the minimum perturbation to be made to very small diagonal elements of U. TOL is only referenced when JOB is negative. TOL should normally be chosen as about  $\epsilon ||U||$ , where  $\epsilon$  is the **machine precision**, but if TOL is supplied as non-positive, then it is reset to  $\epsilon \max |u_{ij}|$ .

On exit: if on entry TOL is non-positive, it is reset as just described. Otherwise TOL is unchanged.

#### 10: IFAIL – INTEGER

Input/Output

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Chapter P01 for details.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

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 parameter the recommended value is 0. When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.

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# 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

On entry, N < 1, or 
$$JOB = 0$$
, or  $JOB < -3$  or  $JOB > 3$ .

IFAIL > 1

Overflow would occur when computing the (IFAIL - 1)th element of the solution vector x. This can only occur when JOB is supplied as positive and either means that a diagonal element of U is very small or that elements of the right-hand side vector y are very large.

### 7 Accuracy

The computed solution of the equations  $(T - \lambda I)x = y$ , say  $\bar{x}$ , will satisfy an equation of the form

$$(T - \lambda I + E)\bar{x} = y,$$

where E can be expected to satisfy a bound of the form

$$||E|| \leq \alpha \epsilon ||T - \lambda I||,$$

 $\alpha$  being a modest constant and  $\epsilon$  being the *machine precision*. The computed solution of the equations  $(T - \lambda I)^T x = y$  and Ux = y will satisfy similar results. The above result implies that the relative error in  $\bar{x}$  satisfies

$$\frac{\|\bar{x} - x\|}{\|\bar{x}\|} \le c(T - \lambda I)\alpha\epsilon,$$

where  $c(T - \lambda I)$  is the condition number of  $(T - \lambda I)$  with respect to inversion. Thus if  $(T - \lambda I)$  is nearly singular,  $\bar{x}$  can be expected to have a large relative error. Note that F01LEF incorporates a test for near singularity.

# **8** Further Comments

The time taken by F04LEF is approximately proportional to n.

If you have single systems of tridiagonal equations to solve you are advised that F07CAF (DGTSV) requires less storage and will normally be faster than the combination of F01LEF and F04LEF, but F07CAF (DGTSV) does not incorporate a test for near singularity.

### 9 Example

This example solves the two sets of tridiagonal equations

$$Tx = y$$
 and  $T^{\mathrm{T}}x = y$ 

where

$$T = \begin{pmatrix} 3.0 & 2.1 & 0 & 0 & 0 \\ 3.4 & 2.3 & -1.0 & 0 & 0 \\ 0 & 3.6 & -5.0 & 1.9 & 0 \\ 0 & 0 & 7.0 & -0.9 & 8.0 \\ 0 & 0 & 0 & -6.0 & 7.1 \end{pmatrix} \quad \text{and} \quad y = \begin{pmatrix} 2.7 \\ -0.5 \\ 2.6 \\ 0.6 \\ 2.7 \end{pmatrix}.$$

The example program first calls F01LEF to factorize T and then two calls are made to F04LEF, one to solve Tx = y and the second to solve  $T^{T}x = y$ .

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#### 9.1 Program Text

```
FO4LEF Example Program Text
  Mark 14 Revised. NAG Copyright 1989.
   .. Parameters ..
   INTEGER
                     NMAX
  PARAMETER
                    (NMAX=50)
  INTEGER
                    NIN, NOUT
  PARAMETER
                    (NIN=5, NOUT=6)
   .. Local Scalars ..
  DOUBLE PRECISION LAMBDA, TOL
  INTEGER
                   I, IFAIL, JOB, N
   .. Local Arrays ..
  DOUBLE PRECISION A(NMAX), B(NMAX), C(NMAX), D(NMAX), Y(NMAX),
                    Z(NMAX)
  INTEGER
                    IN(NMAX)
  .. External Subroutines .. EXTERNAL FO1LEF, F04LEF
   .. Executable Statements ..
  WRITE (NOUT,*) 'FO4LEF Example Program Results'
   Skip heading in data file
  READ (NIN,*)
  READ (NIN,*) N
  WRITE (NOUT, *)
   IF (N.LT.1 .OR. N.GT.NMAX) THEN
      WRITE (NOUT, 99999) 'N is out of range. N = ', N
      READ (NIN,*) (A(I),I=1,N)
      IF (N.GT.1) THEN
         READ (NIN,*) (B(I),I=2,N)
         READ (NIN, *) (C(I), I=2, N)
      END IF
      TOL = 5.0D-5
      LAMBDA = 0.0D0
      IFAIL = 1
      CALL FOILEF(N,A,LAMBDA,B,C,TOL,D,IN,IFAIL)
      IF (IFAIL.NE.O) THEN
         WRITE (NOUT, *)
         WRITE (NOUT, 99999) 'FOILEF fails. IFAIL =', IFAIL
      ELSE
         IF (IN(N).NE.O) THEN
            WRITE (NOUT,*) 'Matrix is singular or nearly singular'
            WRITE (NOUT, 99998) 'Diagonal element', IN(N), 'is small'
         ELSE
            READ (NIN, \star) (Y(I), I=1, N)
            DO 20 I = 1, N
               Z(I) = Y(I)
2.0
            CONTINUE
            JOB = 1
            IFAIL = 1
            CALL FO4LEF(JOB, N, A, B, C, D, IN, Y, TOL, IFAIL)
            IF (IFAIL.NE.O) THEN
               WRITE (NOUT, *)
               WRITE (NOUT, 99999) 'FO4LEF fails. IFAIL =', IFAIL
            ELSE
               WRITE (NOUT,*)
               WRITE (NOUT,*) 'Solution vector for T*X = Y'
               WRITE (NOUT, 99997) (Y(I), I=1, N)
            END IF
            JOB = 2
            IFAIL = 1
            CALL FO4LEF(JOB, N, A, B, C, D, IN, Z, TOL, IFAIL)
            IF (IFAIL.NE.O) THEN
               WRITE (NOUT, *)
               WRITE (NOUT, 99999) 'FO4LEF fails. IFAIL =', IFAIL
```

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# 9.2 Program Data

```
F04LEF Example Program Data
5
3.0 2.3 -5.0 -0.9 7.1
2.1 -1.0 1.9 8.0
3.4 3.6 7.0 -6.0
2.7 -0.5 2.6 0.6 2.7
```

#### 9.3 Program Results

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