NAG Library Routine Document

F04AEF

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

F04AEF calculates the accurate solution of a set of real linear equations with multiple right-hand sides using an LU factorization with partial pivoting, and iterative refinement.

2 Specification

```
SUBROUTINE F04AEF(A, LDA, B, LDB, N, M, C, LDC, WKSPCE, AA, LDAA, BB,
1                 LDBB, IFAIL)
INTEGER           LDA, LDB, N, M, LDC, LDAA, LDBB, IFAIL
double precision  A(LDA,*), B(LDB,*), C(LDC,*), WKSPCE(max(1,N)),
1                 AA(LDAA,*), BB(LDBB,*)
```

3 Description

Given a set of real linear equations $AX = B$, the routine first computes an LU factorization of A with partial pivoting, $PA = LU$, where P is a permutation matrix, L is lower triangular and U is unit upper triangular. An approximation to X is found by forward and backward substitution. The residual matrix $R = B - AX$ is then calculated using ***additional precision***, and a correction D to X is found by solving $LUD = PR$. X is replaced by $X + D$ and this iterative refinement of the solution is repeated until full machine accuracy has been obtained.

4 References

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

5 Parameters

1: A(LDA,$*$) – ***double precision*** array *Input*

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

On entry: the n by n matrix A.

2: LDA – INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F04AEF is called.

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

3: B(LDB,$*$) – ***double precision*** array *Input*

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

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

4: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F04AEF is called.

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

5: N – INTEGER *Input*

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

Constraint: N ≥ 0.

6: M – INTEGER *Input*

On entry: m, the number of right-hand sides.

Constraint: M ≥ 0.

7: C(LDC,$*$) – ***double precision*** array *Output*

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

On exit: the n by m solution matrix X.

8: LDC – INTEGER *Input*

On entry: the first dimension of the array C as declared in the (sub)program from which F04AEF is called.

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

9: WKSPCE($\max(1, \mathrm{N})$) – ***double precision*** array *Workspace*

10: AA(LDAA,$*$) – ***double precision*** array *Output*

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

On exit: the triangular factors L and U, except that the unit diagonal elements of U are not stored.

11: LDAA – INTEGER *Input*

On entry: the first dimension of the array AA as declared in the (sub)program from which F04AEF is called.

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

12: BB(LDBB,$*$) – ***double precision*** array *Output*

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

On exit: the final n by m residual matrix $R = B - AX$.

13: LDBB – INTEGER *Input*

On entry: the first dimension of the array BB as declared in the (sub)program from which F04AEF is called.

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

14: 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 Section 3.3 in the Essential Introduction 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.**

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

The matrix A is singular, possibly due to rounding errors.

IFAIL = 2

Iterative refinement fails to improve the solution, i.e., the matrix A is too ill-conditioned.

IFAIL = 3

On entry, N < 0,
or M < 0,
or LDA < max(1, N),
or LDB < max(1, N),
or LDC < max(1, N),
or LDAA < max(1, N),
or LDBB < max(1, N).

7 Accuracy

The computed solutions should be correct to full machine accuracy. For a detailed error analysis see page 107 of Wilkinson and Reinsch (1971).

8 Further Comments

The time taken by F04AEF is approximately proportional to n^3.

If there is only one right-hand side, it is simpler to use F04ATF.

9 Example

This example solves the set of linear equations $AX = B$ where

$$A = \begin{pmatrix} 33 & 16 & 72 \\ -24 & -10 & -57 \\ -8 & -4 & -17 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} -359 \\ 281 \\ 85 \end{pmatrix}.$$

9.1 Program Text

```
*     F04AEF Example Program Text
*     Mark 15 Revised. NAG Copyright 1991.
*     .. Parameters ..
      INTEGER          NMAX, LDA, LDB, LDC, LDAA, LDBB
      PARAMETER        (NMAX=8,LDA=NMAX,LDB=NMAX,LDC=NMAX,LDAA=NMAX,
     +                 LDBB=NMAX)
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, M, N
*     .. Local Arrays ..
      DOUBLE PRECISION A(LDA,NMAX), AA(LDAA,NMAX), B(LDB,1), BB(LDBB,1),
     +                 C(LDC,1), WKSPCE(NMAX)
```

```
*     .. External Subroutines ..
      EXTERNAL         F04AEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F04AEF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      WRITE (NOUT,*)
      M = 1
      IF (N.GE.0 .AND. N.LE.NMAX) THEN
         READ (NIN,*) ((A(I,J),J=1,N),I=1,N), (B(I,1),I=1,N)
         IFAIL = 1
*
         CALL F04AEF(A,LDA,B,LDB,N,M,C,LDC,WKSPCE,AA,LDAA,BB,LDBB,IFAIL)
*
         IF (IFAIL.EQ.0) THEN
            WRITE (NOUT,*) ' Solution'
            WRITE (NOUT,99998) (C(I,1),I=1,N)
         ELSE
            WRITE (NOUT,99997) IFAIL
         END IF
      ELSE
         WRITE (NOUT,99999) 'N is out of range: N = ', N
      END IF
*
99999 FORMAT (1X,A,I5)
99998 FORMAT (1X,F9.4)
99997 FORMAT (1X,' ** F04AEF returned with IFAIL = ',I5)
      END
```

9.2 Program Data

```
F04AEF Example Program Data
  3
   33   16   72
  -24  -10  -57
   -8   -4  -17
 -359  281   85
```

9.3 Program Results

```
 F04AEF Example Program Results

  Solution
    1.0000
   -2.0000
   -5.0000
```