NAG Fortran Library Routine Document

F11MFF

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

F11MFF solves a real sparse system of linear equations with multiple right-hand sides given an LU factorization of the sparse matrix computed by F11MEF.

2 Specification

```
      SUBROUTINE F11MFF (TRANS, N, IPRM, IL, LVAL, IU, UVAL, NRHS, B, LDB,
     1                   IFAIL)
      INTEGER            N, IPRM(7*N), IL(*), IU(*), NRHS, LDB, IFAIL
      double precision   LVAL(*), UVAL(*), B(LDB,*)
      CHARACTER*1        TRANS
```

3 Description

F11MFF solves a real system of linear equations with multiple right-hand sides $AX = B$ or $A^T X = B$, according to the value of the argument TRANS, where the matrix factorization $P_r A P_c = LU$ corresponds to an LU decomposition of a sparse matrix stored in compressed column (Harwell–Boeing) format, as computed by F11MEF.

In the above decomposition L is a lower triangular sparse matrix with unit diagonal elements and U is an upper triangular sparse matrix; P_r and P_c are permutation matrices.

4 References

None.

5 Parameters

1: TRANS – CHARACTER*1 *Input*

On entry: specifies whether $AX = B$ or $A^T X = B$ is solved:

if TRANS $=$ 'N', then $AX = B$ is solved;
if TRANS $=$ 'T', then $A^T X = B$ is solved.

Constraint: TRANS $=$ 'N' or 'T'.

2: N – INTEGER *Input*

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

Constraint: N $\geq$ 0.

3: IPRM$(7 \times \mathrm{N})$ – INTEGER array *Input*

On entry: the column permutation which defines P_c, the row permutation which defines P_r, plus associated data structures as computed by F11MEF.

4: IL$(*)$ – INTEGER array *Input*

On entry: records the sparsity pattern of matrix L as computed by F11MEF.

5: LVAL($*$) – ***double precision*** array *Input*

On entry: records the non-zero values of matrix L and some non-zero values of matrix U as computed by F11MEF.

6: IU($*$) – INTEGER array *Input*

On entry: records the sparsity pattern of matrix U as computed by F11MEF.

7: UVAL($*$) – ***double precision*** array *Input*

On entry: records some non-zero values of matrix U as computed by F11MEF.

8: NRHS – INTEGER *Input*

On entry: $nrhs$, the number of right-hand sides in B.

Constraint: NRHS ≥ 0.

9: B(LDB,$*$) – ***double precision*** array *Input/Output*

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

On entry: the N by NRHS right-hand side matrix B.

On exit: the N by NRHS solution matrix X.

10: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F11MFF is called.

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

11: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter 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, for users 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 $= 1$

On entry, TRANS $\neq$ 'N' or 'T',
or N < 0,
or NRHS < 0,
or LDB $< \max(1, \mathrm{N})$.

IFAIL $= 2$

Ill-defined row permutation in array IPRM. Internal checks have revealed that the IPRM array is corrupted.

IFAIL = 3

Ill-defined column permutations in array IPRM. Internal checks have revealed that the IPRM array is corrupted.

IFAIL = 301

Unable to allocate required internal workspace.

7 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

$$|E| \leq c(n)\epsilon|L||U|,$$

$c(n)$ is a modest linear function of n, and ϵ is the ***machine precision***, when partial pivoting is used.

If $\hat{x}$ is the true solution, then the computed solution x satisfies a forward error bound of the form

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

where $\mathrm{cond}(A, x) = \big\||A^{-1}||A||x|\big\|_\infty / \|x\|_\infty \leq \mathrm{cond}(A) = \big\||A^{-1}||A|\big\|_\infty \leq \kappa_\infty(A)$. Note that $\mathrm{cond}(A, x)$ can be much smaller than $\mathrm{cond}(A)$, and $\mathrm{cond}\big(A^T\big)$ can be much larger (or smaller) than $\mathrm{cond}(A)$.

Forward and backward error bounds can be computed by calling F11MHF, and an estimate for $\kappa_\infty(A)$ can be obtained by calling F11MGF.

8 Further Comments

This routine may be followed by a call to F11MHF to refine the solution and return an error estimate.

9 Example

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

$$A = \begin{pmatrix} 2.00 & 1.00 & 0 & 0 & 0 \\ 0 & 0 & 1.00 & -1.00 & 0 \\ 4.00 & 0 & 1.00 & 0 & 1.00 \\ 0 & 0 & 0 & 1.00 & 2.00 \\ 0 & -2.00 & 0 & 0 & 3.00 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 1.56 & 3.12 \\ -0.25 & -0.50 \\ 3.60 & 7.20 \\ 1.33 & 2.66 \\ 0.52 & 1.04 \end{pmatrix}.$$

Here A is nonsymmetric and must first be factorized by F11MEF.

9.1 Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     F11MFF Example Program Text
*     Mark 21 Release. NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          LA, NMAX, MMAX
      PARAMETER        (LA=10000,NMAX=1000,MMAX=10)
      DOUBLE PRECISION ONE
      PARAMETER        (ONE=1.D0)
*     .. Local Scalars ..
      DOUBLE PRECISION FLOP, THRESH
      INTEGER          I, IFAIL, J, N, NNZ, NNZL, NNZU, NRHS, NZLMX,
     +                 NZLUMX, NZUMX
      CHARACTER        SPEC, TRANS
```

```
*     .. Local Arrays ..
      DOUBLE PRECISION A(LA), LVAL(8*LA), UVAL(8*LA), X(NMAX,MMAX)
      INTEGER          ICOLZP(NMAX+1), IL(7*NMAX+8*LA+4), IPRM(7*NMAX),
     +                 IROWIX(LA), IU(2*NMAX+8*LA+1)
*     .. External Subroutines ..
      EXTERNAL         F11MDF, F11MEF, F11MFF, X04CAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F11MFF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
*
*     Read order of matrix and number of right hand sides
*
      READ (NIN,*) N, NRHS
      IF (N.LE.NMAX .AND. NRHS.LE.MMAX) THEN
*
*        Read the matrix A
*
         DO 20 I = 1, N + 1
            READ (NIN,*) ICOLZP(I)
   20    CONTINUE

         NNZ = ICOLZP(N+1) - 1
         DO 40 I = 1, NNZ
            READ (NIN,*) A(I), IROWIX(I)
   40    CONTINUE
*
*        Read the right hand sides
*
         DO 60 J = 1, NRHS
            READ (NIN,*) (X(I,J),I=1,N)
   60    CONTINUE

*
*        Calculate COLAMD permutation
*
         SPEC = 'M'
         IFAIL = 0
         CALL F11MDF(SPEC,N,ICOLZP,IROWIX,IPRM,IFAIL)
*
*        Factorise
*
         THRESH = ONE
         IFAIL = 0
         NZLMX = 8*NNZ
         NZLUMX = 8*NNZ
         NZUMX = 8*NNZ
         CALL F11MEF(N,IROWIX,A,IPRM,THRESH,NZLMX,NZLUMX,NZUMX,IL,
     +               LVAL,IU,UVAL,NNZL,NNZU,FLOP,IFAIL)
*
*        Solve
*
         TRANS = 'N'
         IFAIL = 0
         CALL F11MFF(TRANS,N,IPRM,IL,LVAL,IU,UVAL,NRHS,X,NMAX,IFAIL)
*
*        Output results
*
         WRITE (NOUT,*)
         CALL X04CAF('G',' ',N,NRHS,X,NMAX,'Solutions',IFAIL)
*
      END IF
      END
```

9.2 Program Data

```
F11MFF Example Program Data
  5 2  N, NRHS
 1
 3
 5
 7
 9
 12   ICOLZP(I) I=1,..,N+1
  2.   1
  4.   3
  1.   1
 -2.   5
  1.   2
  1.   3
 -1.   2
  1.   4
  1.   3
  2.   4
  3.   5    A(I), IROWIX(I) I=1,NNZ
 1.56 -.25 3.6 1.33 .52
 3.12 -.50 7.2 2.66 1.04 X(I,J) J=1,NRHS I=1,N
```

9.3 Program Results

```
 F11MFF Example Program Results

 Solutions
              1          2
 1      0.7000     1.4000
 2      0.1600     0.3200
 3      0.5200     1.0400
 4      0.7700     1.5400
 5      0.2800     0.5600
```