NAG Library Routine Document

F11DRF

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

F11DRF solves a system of linear equations involving the preconditioning matrix corresponding to SSOR applied to a complex sparse non-Hermitian matrix, represented in coordinate storage format.

2 Specification

```
SUBROUTINE F11DRF (TRANS, N, NNZ, A, IROW, ICOL, RDIAG, OMEGA, CHECK, Y, X, IWORK, IFAIL)

INTEGER

N, NNZ, IROW(NNZ), ICOL(NNZ), IWORK(2*N+1), IFAIL

REAL (KIND=nag_wp) OMEGA

COMPLEX (KIND=nag_wp) A(NNZ), RDIAG(N), Y(N), X(N)

CHARACTER(1) TRANS, CHECK
```

3 Description

F11DRF solves a system of linear equations

$$Mx = y$$
, or $M^{\mathrm{H}}x = y$,

according to the value of the parameter TRANS, where the matrix

$$M = \frac{1}{\omega(2-\omega)}(D+\omega L)D^{-1}(D+\omega U)$$

corresponds to symmetric successive-over-relaxation (SSOR) Young (1971) applied to a linear system Ax = b, where A is a complex sparse non-Hermitian matrix stored in coordinate storage (CS) format (see Section 2.1.1 in the F11 Chapter Introduction).

In the definition of M given above D is the diagonal part of A, L is the strictly lower triangular part of A, U is the strictly upper triangular part of A, and ω is a user-defined relaxation parameter.

It is envisaged that a common use of F11DRF will be to carry out the preconditioning step required in the application of F11BSF to sparse linear systems. For an illustration of this use of F11DRF see the example program given in Section 9. F11DRF is also used for this purpose by the Black Box routine F11DSF.

4 References

Young D (1971) Iterative Solution of Large Linear Systems Academic Press, New York

5 Parameters

1: TRANS – CHARACTER(1)

Input

On entry: specifies whether or not the matrix M is transposed.

$$TRANS = 'N'$$
 $Mx = u$ is

$$Mx = y$$
 is solved.

$$TRANS = 'T'$$

$$M^{\mathrm{H}}x = y$$
 is solved.

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

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2: N – INTEGER Input

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

Constraint: $N \ge 1$.

3: NNZ – INTEGER Input

On entry: the number of nonzero elements in the matrix A.

Constraint: $1 \le NNZ \le N^2$.

4: A(NNZ) - COMPLEX (KIND=nag wp) array

Input

On entry: the nonzero elements in the matrix A, ordered by increasing row index, and by increasing column index within each row. Multiple entries for the same row and column indices are not permitted. The routine F11ZNF may be used to order the elements in this way.

5: IROW(NNZ) – INTEGER array

Input

6: ICOL(NNZ) – INTEGER array

Input

On entry: the row and column indices of the nonzero elements supplied in A.

Constraints

IROW and ICOL must satisfy the following constraints (which may be imposed by a call to F11ZNF):

$$1 \leq \operatorname{IROW}(i) \leq \operatorname{N}$$
 and $1 \leq \operatorname{ICOL}(i) \leq \operatorname{N}$, for $i = 1, 2, \dots, \operatorname{NNZ}$; either $\operatorname{IROW}(i-1) < \operatorname{IROW}(i)$ or both $\operatorname{IROW}(i-1) = \operatorname{IROW}(i)$ and $\operatorname{ICOL}(i-1) < \operatorname{ICOL}(i)$, for $i = 2, 3, \dots, \operatorname{NNZ}$.

7: RDIAG(N) – COMPLEX (KIND=nag wp) array

Input

On entry: the elements of the diagonal matrix D^{-1} , where D is the diagonal part of A.

8: OMEGA – REAL (KIND=nag wp)

Input

On entry: the relaxation parameter ω .

Constraint: 0.0 < OMEGA < 2.0.

9: CHECK – CHARACTER(1)

Input

On entry: specifies whether or not the CS representation of the matrix M should be checked.

CHECK = 'C'

Checks are carried on the values of N, NNZ, IROW, ICOL and OMEGA.

CHECK = 'N'

None of these checks are carried out.

See also Section 8.2.

Constraint: CHECK = 'C' or 'N'.

10: Y(N) - COMPLEX (KIND=nag wp) array

Input

On entry: the right-hand side vector y.

11: X(N) - COMPLEX (KIND=nag wp) array

Output

On exit: the solution vector x.

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12: $IWORK(2 \times N + 1) - INTEGER$ array

Workspace

13: 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.

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.

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
```

```
On entry, TRANS \neq 'N' or 'T', or CHECK \neq 'C' or 'N'.
```

IFAIL = 2

```
On entry, N < 1,
or NNZ < 1,
or NNZ > N^2,
or OMEGA lies outside the interval (0.0, 2.0),
```

IFAIL = 3

On entry, the arrays IROW and ICOL fail to satisfy the following constraints:

```
1 \leq \text{IROW}(i) \leq \text{N} and 1 \leq \text{ICOL}(i) \leq \text{N}, for i = 1, 2, \dots, \text{NNZ}; \text{IROW}(i-1) < \text{IROW}(i) or \text{IROW}(i-1) = \text{IROW}(i) and \text{ICOL}(i-1) < \text{ICOL}(i), for i = 2, 3, \dots, \text{NNZ}.
```

Therefore a nonzero element has been supplied which does not lie in the matrix A, is out of order, or has duplicate row and column indices. Call F11ZNF to reorder and sum or remove duplicates.

IFAIL = 4

On entry, the matrix A has a zero diagonal element. The SSOR preconditioner is not appropriate for this problem.

7 Accuracy

If TRANS = 'N' the computed solution x is the exact solution of a perturbed system of equations $(M + \delta M)x = y$, where

$$|\delta M| \le c(n)\epsilon |D + \omega L| |D^{-1}| |D + \omega U|,$$

c(n) is a modest linear function of n, and ϵ is the **machine precision**. An equivalent result holds when TRANS = 'T'.

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8 Further Comments

8.1 Timing

The time taken for a call to F11DRF is proportional to NNZ.

8.2 Use of CHECK

It is expected that a common use of F11DRF will be to carry out the preconditioning step required in the application of F11BSF to sparse linear systems. In this situation F11DRF is likely to be called many times with the same matrix M. In the interests of both reliability and efficiency, you are recommended to set CHECK = 'C' for the first of such calls, and CHECK = 'N' for all subsequent calls.

9 Example

This example solves a complex sparse linear system of equations

$$Ax = b$$

using RGMRES with SSOR preconditioning.

The RGMRES algorithm itself is implemented by the reverse communication routine F11BSF, which returns repeatedly to the calling program with various values of the parameter IREVCM. This parameter indicates the action to be taken by the calling program.

If IREVCM = 1, a matrix-vector product v = Au is required. This is implemented by a call to F11XNF.

If IREVCM = -1, a conjugate transposed matrix-vector product $v = A^{H}u$ is required in the estimation of the norm of A. This is implemented by a call to F11XNF.

If IREVCM = 2, a solution of the preconditioning equation Mv = u is required. This is achieved by a call to F11DRF.

If IREVCM = 4, F11BSF has completed its tasks. Either the iteration has terminated, or an error condition has arisen.

For further details see the routine document for F11BSF.

9.1 Program Text

```
Program f11drfe
     F11DRF Example Program Text
     Mark 24 Release. NAG Copyright 2012.
      .. Use Statements ..
     Use nag_library, Only: f11brf, f11bsf, f11btf, f11drf, f11xnf, nag_wp
!
      .. Implicit None Statement ..
     Implicit None
      .. Parameters ..
!
                                        :: nin = 5, nout = 6
     Integer, Parameter
      .. Local Scalars ..
!
     Real (Kind=nag_wp)
                                        :: anorm, omega, sigmax, stplhs,
                                           stprhs, tol
                                        :: i, ifail, ifaill, irevcm, iterm,
     Integer
                                           itn, liwork, lwneed, lwork, m,
                                          maxitn, monit, n, nnz
     Character (1)
                                        :: ckdrf, ckxnf, norm, precon, trans,
                                           weight
     Character (8)
                                        :: method
!
      .. Local Arrays ..
      Complex (Kind=nag_wp), Allocatable :: a(:), b(:), rdiag(:), work(:), x(:)
     Real (Kind=nag_wp), Allocatable :: wgt(:)
     Integer, Allocatable
                                        :: icol(:), irow(:), iwork(:)
      .. Intrinsic Procedures ..
      Intrinsic
                                        :: max
```

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```
!
      .. Executable Statements ..
     Write (nout,*) 'F11DRF Example Program Results'
     Write (nout,*)
     Skip heading in data file
     Read (nin,*)
     Read algorithmic parameters
     Read (nin,*) n, m
     Read (nin.*) nnz
     lwork = \max(121+n*(3+m)+m*(m+5),120+7*n,120+(2*n+m)*(m+2)+2*n,120+10*n)
     liwork = 2*n + 1
     Allocate (a(nnz),b(n),rdiag(n),work(lwork),x(n),wgt(n),icol(nnz), &
       irow(nnz),iwork(liwork))
     Read (nin,*) method
     Read (nin, \star) precon, norm, iterm
     Read (nin,*) tol, maxitn
     Read (nin,*) anorm, sigmax
     Read (nin,*) omega
     Read the matrix A
     Do i = 1, nnz
       Read (nin,*) a(i), irow(i), icol(i)
     End Do
     Read rhs vector b and initial approximate solution x
1
     Read (nin,*) b(1:n)
     Read (nin,*) x(1:n)
     Call F11BRF to initialize solver
     weight = 'N'
     monit = 0
      ifail: behaviour on error exit
              =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
!
      Call f11brf(method,precon,norm,weight,iterm,n,m,tol,maxitn,anorm,sigmax, &
       monit,lwneed,work,lwork,ifail)
     Calculate reciprocal diagonal matrix elements if necessary
     If (precon=='P' .Or. precon=='p') Then
       iwork(1:n) = 0
       Do i = 1, nnz
          If (irow(i)==icol(i)) Then
            iwork(irow(i)) = iwork(irow(i)) + 1
            If (a(i)/=(0.0E0\_nag\_wp,0.0E0\_nag\_wp)) Then
              rdiag(irow(i)) = (1.0E0_nag_wp, 0.0E0_nag_wp)/a(i)
           Else
              Write (nout,*) 'Matrix has a zero diagonal element'
              Go To 100
           End If
         End If
       End Do
       Do i = 1, n
          If (iwork(i)==0) Then
           Write (nout,*) 'Matrix has a missing diagonal element'
           Go To 100
          End If
          If (iwork(i) >= 2) Then
           Write (nout,*) 'Matrix has a multiple diagonal element'
           Go To 100
         End If
       End Do
```

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```
End If
      Call F11BSF to solve the linear system
      irevcm = 0
      ckxnf = 'C'
      ckdrf = 'C'
      ifail = 1
loop: Do
        Call f11bsf(irevcm,x,b,wgt,work,lwork,ifail)
        If (irevcm/=4) Then
          ifail1 = 1
          Select Case (irevcm)
          Case (1)
            Compute matrix-vector product
            trans = 'N'
            Call f11xnf(trans,n,nnz,a,irow,icol,ckxnf,x,b,ifail1)
            ckxnf = 'N'
          Case (-1)
!
            Compute conjugate transposed matrix-vector product
            trans = 'T'
            Call f11xnf(trans,n,nnz,a,irow,icol,ckxnf,x,b,ifail1)
            ckxnf = 'N'
          Case (2)
!
            SSOR preconditioning
            trans = 'N'
            Call f11drf(trans,n,nnz,a,irow,icol,rdiag,omega,ckdrf,x,b,iwork, &
               ifail1)
            ckdrf = 'N'
          End Select
          If (ifail1/=0) irevcm = 6
        Else If (ifail==0) Then
          Termination
          ifail = 0
          Call f11btf(itn,stplhs,stprhs,anorm,sigmax,work,lwork,ifail)
          Write (nout,99996) itn
          Write (nout,99997) 'Matrix norm =', anorm
          Write (nout,99997) 'Final residual norm =', stplhs
          Write (nout,*)
!
          Output x
          Write (nout,*) '
                                                X'
          Write (nout, 99998) x(1:n)
          Exit loop
        Else
          Write (nout, 99999) ifail
          Exit loop
        End If
      End Do loop
100
     Continue
99999 Format (1X/1X,' ** F11BSF returned with IFAIL = ',I5) 99998 Format (1X,'(',1P,E16.4,',',1P,E16.4,')')
99997 Format (1X,A,1P,E16.3)
99996 Format (1X, 'Converged in', I10, ' iterations')
    End Program flldrfe
```

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9.2 **Program Data**

```
F11DRF Example Program Data
 5
                               NNZ
 16
 'CGS'
                                METHOD
 'P' 'I' 1
                                PRECON, NORM, ITERM
 1.D-10 1000
                               TOL, MAXITN
 0.D0 0.D0
                               ANORM, SIGMAX
 1.4D0
                               OMEGA
 ( 2., 3.)
( 1.,-1.)
(-1., 0.)
              1
                      1
                1
                      2
                1
                      4
 (0., 2.)
                2
                      2
 (-2., 1.)
 ( 1., 0.)
( 0.,-1.)
( 5., 4.)
                2
                      5
                      1
                3
                      3
 ( 3.,-1.)
                3
 (1., 0.)
(-2., 2.)
(-3., 1.)
                      5
                3
                4
                      1
                      4
                4
 (0., 3.)
                4
                      5
 (4.,-2.)
              5
                      2
 (-2., 0.)
(-6., 1.)
                5
                      3
                5
                      5
                               A(I), IROW(I), ICOL(I), I=1,...,NNZ
 ( -3., 3.)
 (-11., 5.)
(23.,48.)
 (-41., 2.)
(-28.,-31.)
                               B(I), I=1,...,N
 ( 0., 0.)
 ( 0., 0.)
 ( 0., 0.)
( 0., 0.)
( 0., 0.)
                               X(I), I=1,...,N
```

5 iterations

9.3 Program Results

Converged in

```
F11DRF Example Program Results
```

```
Converged in 5 iterat.
Matrix norm = 1.500E+01
Final residual norm = 1.776E-14
                   Χ
       1.0000E+00,
                         2.0000E+00)
       2.0000E+00,
                         3.0000E+00)
(
       3.0000E+00,
                        4.0000E+00)
       4.0000E+00,
                        5.0000E+00)
(
       5.0000E+00,
                         6.0000E+00)
```

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