NAG Library Routine Document

F11GFF

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

F11GFF is the third in a suite of three routines for the iterative solution of a symmetric system of simultaneous linear equations (see Golub and Van Loan (1996)). F11GFF returns information about the computations during an iteration and/or after this has been completed. The first routine of the suite, F11GDF, is a setup routine, the second routine, F11GEF is the proper iterative solver.

These three routines are suitable for the solution of large sparse symmetric systems of equations.

2 Specification

```
SUBROUTINE F11GFF (ITN, STPLHS, STPRHS, ANORM, SIGMAX, ITS, SIGERR,      &
                   WORK, LWORK, IFAIL)

INTEGER            ITN, ITS, LWORK, IFAIL
REAL (KIND=nag_wp) STPLHS, STPRHS, ANORM, SIGMAX, SIGERR, WORK(LWORK)
```

3 Description

F11GFF returns information about the solution process. It can be called both during a monitoring step of the solver F11GEF, or after this solver has completed its tasks. Calling F11GFF at any other time will result in an error condition being raised.

For further information you should read the documentation for F11GDF and F11GEF.

4 References

Golub G H and Van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

5 Parameters

1:   ITN – INTEGER   *Output*

   On exit: the number of iterations carried out by F11GEF.

2:   STPLHS – REAL (KIND=nag_wp)   *Output*

   On exit: the current value of the left-hand side of the termination criterion used by F11GEF.

3:   STPRHS – REAL (KIND=nag_wp)   *Output*

   On exit: the current value of the right-hand side of the termination criterion used by F11GEF.

4:   ANORM – REAL (KIND=nag_wp)   *Output*

   On exit: for CG and SYMMLQ methods, the norm $\|A\|_1 = \|A\|_\infty$ when either it has been supplied to F11GDF or it has been estimated by F11GEF (see also Sections 3 and 5 in F11GDF). Otherwise, ANORM $= 0.0$ is returned.

   For MINRES method, an estimate of the infinity norm of the preconditioned matrix operator.

5:    SIGMAX – REAL (KIND=nag_wp)   *Output*

On exit: for CG and SYMMLQ methods, the current estimate of the largest singular value $\sigma_1(\bar{A})$ of the preconditioned iteration matrix $\bar{A} = E^{-1}AE^{-T}$, when either it has been supplied to F11GDF or it has been estimated by F11GEF (see also Sections 3 and 5 in F11GDF). Note that if ITS < ITN then SIGMAX contains the final estimate. If, on final exit from F11GEF, ITS = ITN, then the estimation of $\sigma_1(\bar{A})$ may have not converged; in this case you should look at the value returned in SIGERR. Otherwise, SIGMAX = 0.0 is returned.

For MINRES method, an estimate of the final transformed residual.

6:    ITS – INTEGER   *Output*

On exit: for CG and SYMMLQ methods, the number of iterations employed so far in the computation of the estimate of $\sigma_1(\bar{A})$, the largest singular value of the preconditioned matrix $\bar{A} = E^{-1}AE^{-T}$, when $\sigma_1(\bar{A})$ has been estimated by F11GEF using the bisection method (see also Sections 3, 5 and 9 in F11GDF). Otherwise, ITS = 0 is returned.

7:    SIGERR – REAL (KIND=nag_wp)   *Output*

On exit: for CG and SYMMLQ methods, if $\sigma_1(\bar{A})$ has been estimated by F11GEF using bisection,

$$\text{SIGERR} = \max\left(\frac{\left|\sigma_1^{(k)} - \sigma_1^{(k-1)}\right|}{\sigma_1^{(k)}}, \frac{\left|\sigma_1^{(k)} - \sigma_1^{(k-2)}\right|}{\sigma_1^{(k)}}\right),$$

where k = ITS denotes the iteration number. The estimation has converged if SIGERR $\leq$ SIGTOL where SIGTOL is an input parameter to F11GDF. Otherwise, SIGERR = 0.0 is returned.

For MINRES method, an estimate of the condition number of the preconditioned matrix.

8:    WORK(LWORK) – REAL (KIND=nag_wp) array   *Communication Array*

On entry: the array WORK as returned by F11GEF (see also Section 3 in F11GEF).

9:    LWORK – INTEGER   *Input*

On entry: the dimension of the array WORK as declared in the (sub)program from which F11GFF is called (see also Section 5 in F11GDF).

Constraint: LWORK $\geq$ 120.

Note: although the minimum value of LWORK ensures the correct functioning of F11GFF, a larger value is required by the iterative solver F11GEF (see also Section 5 in F11GDF).

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 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 $= -i$

On entry, the ith argument had an illegal value.

IFAIL $= 1$

F11GFF has been called out of sequence. For example, the last call to F11GEF did not return IREVCM $= 3$ or 4.

IFAIL $= -99$

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

See Section 3.8 in the Essential Introduction for further information.

IFAIL $= -399$

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

See Section 3.7 in the Essential Introduction for further information.

IFAIL $= -999$

Dynamic memory allocation failed.

See Section 3.6 in the Essential Introduction for further information.

7 Accuracy

Not applicable.

8 Parallelism and Performance

Not applicable.

9 Further Comments

None.

10 Example

See Section 10 in F11GDF.