F11GCFP

NAG Parallel Library Routine Document

Note: before using this routine, please read the Users' Note for your implementation to check for implementation-dependent details. You are advised to enclose any calls to NAG Parallel Library routines between calls to Z01AAFP and Z01ABFP.

Note: you should read the the F11 Chapter Introduction before using this routine. In particular, some of the notation and terminology used in this document was introduced in Section 2.1 of the F11 Chapter Introduction.

1 Description

F11GCFP is the third in a suite of three routines for the solution of the real symmetric system of simultaneous linear equations, $Ax = b$, using either the conjugate gradient iterative method (CG) or the SYMMLQ iterative method. F11GCFP returns information about the computations carried out by the second routine in the suite, F11GBFP. F11GCFP can be called either during a monitoring step of F11GBFP or after F11GBFP has completed its tasks. The first routine in the suite, F11GAFP, must be used to initialize the computation.

2 Specification

```
      SUBROUTINE F11GCFP(ICNTXT, ITN, STPLHS, STPRHS, ANORM, SIGMAX,
     1                   ITS, SIGERR, IFAIL)
      DOUBLE PRECISION   STPLHS, STPRHS, ANORM, SIGMAX, SIGERR
      INTEGER            ICNTXT, ITN, ITS, IFAIL
```

3 Usage

3.1 Definitions

None.

3.2 Global and Local Arguments

The following global **input** arguments must have the same value on entry to the routine on each processor and the global **output** arguments will have the same value on exit from the routine on each processor:

Global input arguments: IFAIL

Global output arguments: ITN, STPLHS, STPRHS, ANORM, SIGMAX, ITS, SIGERR, IFAIL

The remaining arguments are local.

3.3 Distribution Strategy

Not applicable.

3.4 Related Routines

This is the last in a suite of three routines. The other two routines are:

F11GAFP: to set up the computation

F11GBFP: to carry out the iterations

4 Arguments

1: ICNTXT — INTEGER *Local Input*

On entry: the Library context, usually returned by a call to the Library Grid initialisation routine Z01AAFP.

Note: the value of ICNTXT **must not** be changed.

2: ITN — INTEGER *Global Output*

On exit: the number of iterations carried out by F11GBFP.

3: STPLHS — DOUBLE PRECISION *Global Output*

On exit: the current value of the left-hand side of the termination criterion used by F11GBFP.

4: STPRHS — DOUBLE PRECISION *Global Output*

On exit: the current value of the right-hand side of the termination criterion used by F11GBFP.

5: ANORM — DOUBLE PRECISION *Global Output*

On exit: the norm $\|A\|_1 = \|A\|_\infty$ if it has been used in the termination criterion, irrespective of whether it has been supplied or estimated by F11GBFP (see also Section 4 and Section 6 of the document for F11GAFP). Otherwise, ANORM = 0.0 is returned.

6: SIGMAX — DOUBLE PRECISION *Global Output*

On exit: 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 F11GAFP or it has been estimated by F11GBFP (see also Section 4 and Section 6 of the document for F11GAFP).

Note that if ITS < ITN then SIGMAX contains the final estimate. If, on final exit from F11GBFP, 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 (see below). Otherwise, SIGMAX = 0.0 is returned.

7: ITS — INTEGER *Global Output*

On exit: 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 F11GBFP using the bisection method (see also Section 4 and Section 6 of the document for F11GAFP).

Otherwise, ITS = 0 is returned.

8: SIGERR — DOUBLE PRECISION *Global Output*

On exit: if $\sigma_1(\bar{A})$ has been estimated by F11GBFP using bisection,

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

where k = ITS denotes the iteration number. The estimation has converged if SIGERR $\leq$ SIGTOL where SIGTOL is an input parameter to F11GAFP. Otherwise, SIGERR = 0.0 is returned.

9: IFAIL — INTEGER *Global Input/Global Output*

The NAG Parallel Library provides a mechanism, via the routine Z02EAFP, to reduce the amount of parameter validation performed by this routine. For a full description refer to the Z02 Chapter Introduction.

On entry: IFAIL must be set to 0, -1 or 1. For users not familiar with this argument (described in the Essential Introduction) the recommended values are:

IFAIL = 0, if multigridding is **not** employed;
IFAIL = -1, if multigridding is employed.

On exit: IFAIL = 0 (or -9999 if reduced error checking is enabled) unless the routine detects an error (see Section 5).

5 Errors and Warnings

If on entry IFAIL = 0 or −1, explanatory error messages are output from the root processor (or processor {0,0} when the root processor is not available) on the current error message unit (as defined by X04AAF).

5.1 Full Error Checking Mode Only

IFAIL = −2000

The routine has been called with an invalid value of ICNTXT on one or more processors.

IFAIL = −1000

The logical processor grid and library mechanism (Library Grid) have not been correctly defined, see Z01AAFP.

5.2 Any Error Checking Mode

IFAIL = 1

F11GCFP has been called out of sequence. For example, the last call to F11GBFP did not return the termination code IREVCM = 3 or 4.

6 Further Comments

6.1 Algorithmic Detail

Not applicable.

6.2 Parallelism Detail

Not applicable.

6.3 Accuracy

Not applicable.

6.4 Computational Costs

The computational costs of F11GCFP are negligible compared to the costs of F11GBFP.

7 References

[1] Barrett R, Berry M, Chan T F, Demmel J, Donato J, Dongarra J, Eijkhout V, Pozo R, Romine C and van der Vorst H (1994) *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods* SIAM, Philadelphia

[2] Dias da Cunha R and Hopkins T (1994) PIM 1.1 — the parallel iterative method package for systems of linear equations user's guide — Fortran 77 version *Technical Report* Computing Laboratory, University of Kent at Canterbury, Kent CT2 7NZ, UK

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

[4] Hestenes M and Stiefel E (1952) Methods of conjugate gradients for solving linear systems *J. Res. Nat. Bur. Stand.* **49** 409–436

[5] Paige C C and Saunders M A (1975) Solution of sparse indefinite systems of linear equations *SIAM J. Numer. Anal.* **12** 617–629

8 Example

See Section 8 of the document for F11GAFP.