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.

1 Description

Note: you should read the F11 Chapter Introduction before trying to use this routine. In particular, some of the notation and terminology used in this document was introduced in Section 2.3 of the F11 Chapter Introduction.

F11GCFP is the third in a suite of three routines for the iterative solution of a symmetric system of simultaneous linear equations $Ax = b$ using either the preconditioned Conjugate Gradient method (Hestenes and Stiefel [4], Golub and Van Loan [3], Barrett *et al.* [1], Dias da Cunha and Hopkins [2]) or a preconditioned Lanczos method based upon the algorithm SYMMLQ (Paige and Saunders [5], Barrett *et al.* [1]). F11GCFP returns information about the computations carried out by the second routine in the suite, F11GBFP. F11GBFP **must** have already been called and completed its tasks, returning the parameter IREVCM = 4, prior to calling F11GCFP, otherwise an error condition will be raised. 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 Data Distribution

3.1 Global and Local Arguments

The input argument IFAIL is global and so must have the same value on entry to the routine on each processor. The output arguments ITN, STPLHS, STPRHS, ANORM, SIGMAX, ITS, SIGERR and IFAIL are global and so will return the same value on each processor. The remaining argument is local.

4 Arguments

1: ICNTXT — INTEGER *Local Input*

On entry: the BLACS context used by the communication mechanism, usually returned by a call to Z01AAFP.

2: ITN — INTEGER *Global Output*

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

3: STPLHS — DOUBLE PRECISION *Global Output*

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

4: STPRHS — DOUBLE PRECISION *Global Output*

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

5: ANORM — DOUBLE PRECISION *Global Output*

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

6: SIGMAX — DOUBLE PRECISION *Global Output*

On exit: the largest singular value $\sigma_1(\bar{A})$ of the preconditioned iteration matrix $\bar{A} = E^{-1}AE^{-T}$, either when this is used by the termination criterion or when the Lanczos method (SYMMLQ) is used without user-specified weights, irrespective of whether $\sigma_1(\bar{A})$ has been supplied or estimated by F11GBFP (see also Sections 4 and 6 of the document for F11GAFP)
Otherwise, SIGMAX = 0.0 is returned.

7: ITS — INTEGER *Global Output*

On exit: the number of iterations employed in the computation of the estimate of $\sigma_1(\bar{A})$, the largest singular value of the preconditioned matrix used during the iteration $\bar{A} = E^{-1}AE^{-T}$, when this has been estimated by F11GBFP using the bisection method (see also Sections 4 and 6 of the document for F11GAFP).
Otherwise, ITS = 0 is returned.

8: SIGERR — DOUBLE PRECISION *Global Output*

On exit: when $\sigma_1(\bar{A})$ has been estimated by F11GBFP and the bisection method has been used, SIGERR $= \max\left(\frac{|\sigma_1(T_k) - \sigma_1(T_{k-1})|}{\sigma_1(T_k)}, \frac{|\sigma_1(T_k) - \sigma_1(T_{k-2})|}{\sigma_1(T_k)}\right)$, where the subscript denotes the iteration number, and k = ITS (see also Sections 4 and 6 of the document for F11GAFP).
Otherwise, SIGERR = 0.0 is returned.

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

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (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 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).

Errors detected by the routine:

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.

IFAIL = 1

F11GCFP has been called out of sequence. For example, the last call to F11GBFP did not return the termination code IREVCM = 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 (1989) *Matrix Computations* Johns Hopkins University Press (2nd 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 the Example Program for F11GAFP.