

## NAG Library Function Document

### nag\_sparse\_herm\_basic\_diagnostic (f11gtc)

#### 1 Purpose

nag\_sparse\_herm\_basic\_diagnostic (f11gtc) is the third in a suite of three functions for the iterative solution of a complex Hermitian system of simultaneous linear equations (see Golub and Van Loan (1996)). nag\_sparse\_herm\_basic\_diagnostic (f11gtc) returns information about the computations during an iteration and/or after this has been completed. The first function of the suite, nag\_sparse\_herm\_basic\_setup (f11grc), is a setup function, the second function, nag\_sparse\_herm\_basic\_solver (f11gsc) is the proper iterative solver.

These three functions are suitable for the solution of large sparse complex Hermitian systems of equations.

#### 2 Specification

```
#include <nag.h>
#include <nagf11.h>

void nag_sparse_herm_basic_diagnostic (Integer *itn, double *stplhs,
    double *stprhs, double *anorm, double *sigmax, Integer *its,
    double *sigerr, const Complex work[], Integer lwork, NagError *fail)
```

#### 3 Description

nag\_sparse\_herm\_basic\_diagnostic (f11gtc) returns information about the solution process. It can be called both during a monitoring step of the solver nag\_sparse\_herm\_basic\_solver (f11gsc) or after this solver has completed its tasks. Calling nag\_sparse\_herm\_basic\_diagnostic (f11gtc) at any other time will result in an error condition being raised.

For further information you should read the documentation for nag\_sparse\_herm\_basic\_setup (f11grc) and nag\_sparse\_herm\_basic\_solver (f11gsc).

#### 4 References

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

#### 5 Arguments

- 1: **itn** – Integer \* *Output*  
*On exit:* the number of iterations carried out by nag\_sparse\_herm\_basic\_solver (f11gsc).
- 2: **stplhs** – double \* *Output*  
*On exit:* the current value of the left-hand side of the termination criterion used by nag\_sparse\_herm\_basic\_solver (f11gsc).
- 3: **stprhs** – double \* *Output*  
*On exit:* the current value of the right-hand side of the termination criterion used by nag\_sparse\_herm\_basic\_solver (f11gsc).

- 4: **anorm** – double \* *Output*  
*On exit:* the norm  $\|A\|_1 = \|A\|_\infty$  when either it has been supplied to `nag_sparse_herm_basic_setup (f11grc)` or it has been estimated by `nag_sparse_herm_basic_solver (f11gsc)` (see also Sections 3 and 5 in `nag_sparse_herm_basic_setup (f11grc)`). Otherwise, **anorm** = 0.0 is returned.
- 5: **sigmax** – double \* *Output*  
*On exit:* the current estimate of the largest singular value  $\sigma_1(\bar{A})$  of the preconditioned iteration matrix  $\bar{A} = E^{-1}AE^{-H}$ , when either it has been supplied to `nag_sparse_herm_basic_setup (f11grc)` or it has been estimated by `nag_sparse_herm_basic_solver (f11gsc)` (see also Sections 3 and 5 in `nag_sparse_herm_basic_setup (f11grc)`). Note that if **its** < **itn** then **sigmax** contains the final estimate. If, on final exit from `nag_sparse_herm_basic_solver (f11gsc)`, **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.
- 6: **its** – Integer \* *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  $\bar{A} = E^{-1}AE^{-H}$ , when  $\sigma_1(\bar{A})$  has been estimated by `nag_sparse_herm_basic_solver (f11gsc)` using the bisection method (see also Sections 3, 5 and 9 in `nag_sparse_herm_basic_setup (f11grc)`). Otherwise, **its** = 0 is returned.
- 7: **sigerr** – double \* *Output*  
*On exit:* if  $\sigma_1(\bar{A})$  has been estimated by `nag_sparse_herm_basic_solver (f11gsc)` using bisection,
- $$\mathbf{sigerr} = \max \left( \frac{|\sigma_1^{(k)} - \sigma_1^{(k-1)}|}{\sigma_1^{(k)}}, \frac{|\sigma_1^{(k)} - \sigma_1^{(k-2)}|}{\sigma_1^{(k)}} \right),$$
- where  $k = \mathbf{its}$  denotes the iteration number. The estimation has converged if **sigerr** ≤ **sigtol** where **sigtol** is an input argument to `nag_sparse_herm_basic_setup (f11grc)`. Otherwise, **sigerr** = 0.0 is returned.
- 8: **work[lwork]** – const Complex *Communication Array*  
*On entry:* the array **work** as returned by `nag_sparse_herm_basic_solver (f11gsc)` (see also Section 3 in `nag_sparse_herm_basic_solver (f11gsc)`).
- 9: **lwork** – Integer *Input*  
*On entry:* the dimension of the array **work** (see also Section 5 in `nag_sparse_herm_basic_setup (f11grc)`).  
*Constraint:* **lwork** ≥ 120.  
**Note:** although the minimum value of **lwork** ensures the correct functioning of `nag_sparse_herm_basic_diagnostic (f11gtc)`, a larger value is required by the iterative solver `nag_sparse_herm_basic_solver (f11gsc)` (see also Section 5 in `nag_sparse_herm_basic_setup (f11grc)`).
- 10: **fail** – NagError \* *Input/Output*  
The NAG error argument (see Section 3.6 in the Essential Introduction).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.  
See Section 3.2.1.2 in the Essential Introduction for further information.

### NE\_BAD\_PARAM

On entry, argument  $\langle value \rangle$  had an illegal value.

### NE\_INT

On entry,  $lwork = \langle value \rangle$ .  
Constraint:  $lwork \geq 120$ .

### NE\_INTERNAL\_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

An unexpected error has been triggered by this function. Please contact NAG.  
See Section 3.6.6 in the Essential Introduction for further information.

### NE\_NO\_LICENCE

Your licence key may have expired or may not have been installed correctly.  
See Section 3.6.5 in the Essential Introduction for further information.

### NE\_OUT\_OF\_SEQUENCE

nag\_sparse\_herm\_basic\_diagnostic (f11gtc) has been called out of sequence.

## 7 Accuracy

Not applicable.

## 8 Parallelism and Performance

Not applicable.

## 9 Further Comments

None.

## 10 Example

See Section 10 in nag\_sparse\_herm\_basic\_setup (f11grc).

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