NAG Library Function Document

nag_sparse_nsym_fac_sol (f11dcc)

1 Purpose

nag_sparse_nsym_fac_sol (f11dcc) solves a real sparse nonsymmetric system of linear equations, represented in coordinate storage format, using a restarted generalized minimal residual (RGMRES), conjugate gradient squared (CGS), or stabilized bi-conjugate gradient (Bi-CGSTAB) method, with incomplete LU preconditioning.

2 Specification

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

```
void nag_sparse_nsym_fac_sol (Nag_SparseNsym_Method method, Integer n,
     Integer nnz, const double a[], Integer la, const Integer irow[],
     const Integer icol[], const Integer ipivp[], const Integer ipivq[],
     const Integer istr[], const Integer idiag[], const double b[],
     Integer m, double tol, Integer maxitn, double x[], double *rnorm,
     Integer *itn, Nag_Sparse_Comm *comm, NagError *fail)
```

3 Description

nag_sparse_nsym_fac_sol (f11dcc) solves a real sparse nonsymmetric linear system of equations:

$$Ax = b,$$

using a preconditioned RGMRES (see Saad and Schultz (1986)), CGS (see Sonneveld (1989)), or Bi-CGSTAB(ℓ) method (see Van der Vorst (1989), Sleijpen and Fokkema (1993)).

nag_sparse_nsym_fac_sol (f11dcc) uses the incomplete LU factorization determined by nag_sparse_nsym_fac (f11dac) as the preconditioning matrix. A call to nag_sparse_nsym_fac_sol (f11dcc) must always be preceded by a call to nag_sparse_nsym_fac (f11dac). Alternative preconditioners for the same storage scheme are available by calling nag_sparse_nsym_sol (f11dec).

The matrix A, and the preconditioning matrix M, are represented in coordinate storage (CS) format (see the f11 Chapter Introduction) in the arrays **a**, **irow** and **icol**, as returned from nag_sparse_nsym_fac (f11dac). The array **a** holds the nonzero entries in these matrices, while **irow** and **icol** hold the corresponding row and column indices.

4 References

Saad Y and Schultz M (1986) GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems *SIAM J. Sci. Statist. Comput.* **7** 856–869

Salvini S A and Shaw G J (1996) An evaluation of new NAG Library solvers for large sparse unsymmetric linear systems *NAG Technical Report TR2/96*

Sleijpen G L G and Fokkema D R (1993) BiCGSTAB(ℓ) for linear equations involving matrices with complex spectrum *ETNA* **1** 11–32

Sonneveld P (1989) CGS, a fast Lanczos-type solver for nonsymmetric linear systems *SIAM J. Sci. Statist. Comput.* **10** 36–52

Van der Vorst H (1989) Bi-CGSTAB, a fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems *SIAM J. Sci. Statist. Comput.* **13** 631–644

5 Arguments

1: **method** – Nag_SparseNsym_Method *Input*

On entry: specifies the iterative method to be used.

method = Nag_SparseNsym_RGMRES
The restarted generalized minimum residual method is used.

method = Nag_SparseNsym_CGS
The conjugate gradient squared method is used.

method = Nag_SparseNsym_BiCGSTAB
Then the bi-conjugate gradient stabilised (ℓ) method is used.

Constraint: **method** = Nag_SparseNsym_RGMRES, Nag_SparseNsym_CGS or Nag_SparseNsym_BiCGSTAB.

2: **n** – Integer *Input*

On entry: the order of the matrix A. This **must** be the same value as was supplied in the preceding call to nag_sparse_nsym_fac (f11dac).

Constraint: $\mathbf{n} \geq 1$.

3: **nnz** – Integer *Input*

On entry: the number of nonzero-elements in the matrix A. This **must** be the same value as was supplied in the preceding call to nag_sparse_nsym_fac (f11dac).

Constraint: $1 \leq \mathbf{nnz} \leq \mathbf{n}^2$.

4: **a**[**la**] – const double *Input*

On entry: the values returned in the array **a** by a previous call to nag_sparse_nsym_fac (f11dac).

5: **la** – Integer *Input*

On entry: the second dimension of the arrays **a**, **irow** and **icol**.This must be the same value as returned by a previous call to nag_sparse_nsym_fac (f11dac).

Constraint: $\mathbf{la} \geq 2 \times \mathbf{nnz}$.

6: **irow**[**la**] – const Integer *Input*
7: **icol**[**la**] – const Integer *Input*
8: **ipivp**[**n**] – const Integer *Input*
9: **ipivq**[**n**] – const Integer *Input*
10: **istr**[**n + 1**] – const Integer *Input*
11: **idiag**[**n**] – const Integer *Input*

On entry: the values returned in the arrays **irow**, **icol**, **ipivp**, **ipivq**, **istr** and **idiag** by a previous call to nag_sparse_nsym_fac (f11dac).

12: **b**[**n**] – const double *Input*

On entry: the right-hand side vector b.

13: **m** – Integer *Input*

On entry: if **method** = Nag_SparseNsym_RGMRES, **m** is the dimension of the restart subspace.

If **method** = Nag_SparseNsym_BiCGSTAB, **m** is the order (ℓ) of the polynomial Bi-CGSTAB method otherwise, **m** is not referenced.

Constraints:

if **method** $=$ Nag_SparseNsym_RGMRES, $0 < \mathbf{m} \leq \min(\mathbf{n}, 50)$;
if **method** $=$ Nag_SparseNsym_BiCGSTAB, $0 < \mathbf{m} \leq \min(\mathbf{n}, 10)$.

14: **tol** – double *Input*

On entry: the required tolerance. Let x_k denote the approximate solution at iteration k, and r_k the corresponding residual. The algorithm is considered to have converged at iteration k if:

$$\|r_k\|_\infty \leq \tau \times \left(\|b\|_\infty + \|A\|_\infty \|x_k\|_\infty\right).$$

If $\mathbf{tol} \leq 0.0$, $\tau = \max(\sqrt{\epsilon}, \sqrt{\mathbf{n}}, \epsilon)$ is used, where ϵ is the ***machine precision***. Otherwise $\tau = \max(\mathbf{tol}, 10\epsilon, \sqrt{\mathbf{n}}, \epsilon)$ is used.

Constraint: $\mathbf{tol} < 1.0$.

15: **maxitn** – Integer *Input*

On entry: the maximum number of iterations allowed.

Constraint: $\mathbf{maxitn} \geq 1$.

16: **x**[**n**] – double *Input/Output*

On entry: an initial approximation to the solution vector x.

On exit: an improved approximation to the solution vector x.

17: **rnorm** – double * *Output*

On exit: the final value of the residual norm $\|r_k\|_\infty$, where k is the output value of **itn**.

18: **itn** – Integer * *Output*

On exit: the number of iterations carried out.

19: **comm** – Nag_Sparse_Comm * *Input/Output*

On entry/exit: a pointer to a structure of type Nag_Sparse_Comm whose members are used by the iterative solver.

20: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

NE_2_INT_ARG_LT

On entry, **la** $= \langle value \rangle$ while **nnz** $= \langle value \rangle$. These arguments must satisfy $\mathbf{la} \geq 2 \times \mathbf{nnz}$.

NE_ACC_LIMIT

The required accuracy could not be obtained. However, a reasonable accuracy has been obtained and further iterations cannot improve the result. You should check the output value of **rnorm** for acceptability. This error code usually implies that your problem has been fully and satisfactorily solved to within, or close to, the accuracy available on your system. Further iterations are unlikely to improve on this situation.

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_BAD_PARAM

On entry, argument **method** had an illegal value.

NE_INT_2

On entry, $\mathbf{m} = \langle value \rangle$, $\min(\mathbf{n}, 10) = \langle value \rangle$.
Constraint: $0 < \mathbf{m} \leq \min(\mathbf{n}, 10)$ when $\mathbf{method} =$ Nag_SparseNsym_BiCGSTAB.

On entry, $\mathbf{m} = \langle value \rangle$, $\min(\mathbf{n}, 50) = \langle value \rangle$.
Constraint: $0 < \mathbf{m} \leq \min(\mathbf{n}, 50)$ when $\mathbf{method} =$ Nag_SparseNsym_RGMRES.

On entry, $\mathbf{nnz} = \langle value \rangle$, $\mathbf{n} = \langle value \rangle$.
Constraint: $1 \leq \mathbf{nnz} \leq \mathbf{n}^2$.

NE_INT_ARG_LT

On entry, $\mathbf{maxitn} = \langle value \rangle$.
Constraint: $\mathbf{maxitn} \geq 1$.

On entry, $\mathbf{n} = \langle value \rangle$.
Constraint: $\mathbf{n} \geq 1$.

NE_INVALID_CS

On entry, the CS representation of A is invalid. Check that the call to nag_sparse_nsym_fac_sol (f11dcc) has been preceded by a valid call to nag_sparse_nsym_fac (f11dac), and that the arrays **a**, **irow** and **icol** have not been corrupted between the two calls.

NE_INVALID_CS_PRECOND

On entry, the CS representation of the preconditioning matrix M is invalid. Check that the call to nag_sparse_nsym_fac_sol (f11dcc) has been preceded by a valid call to nag_sparse_nsym_fac (f11dac), and that the arrays **a**, **irow**, **icol**, **ipivp**, **ipivq**, **istr** and **idiag** have not been corrupted between the two calls.

NE_NOT_REQ_ACC

The required accuracy has not been obtained in **maxitn** iterations.

NE_REAL_ARG_GE

On entry, **tol** must not be greater than or equal to 1.0: $\mathbf{tol} = \langle value \rangle$.

7 Accuracy

On successful termination, the final residual $r_k = b - Ax_k$, where $k = \mathbf{itn}$, satisfies the termination criterion

$$\|r_k\|_\infty \leq \tau \times \left(\|b\|_\infty + \|A\|_\infty \|x_k\|_\infty\right).$$

The value of the final residual norm is returned in **rnorm**.

8 Parallelism and Performance

Not applicable.

9 Further Comments

The time taken by nag_sparse_nsym_fac_sol (f11dcc) for each iteration is roughly proportional to the value of **nnzc** returned from the preceding call to nag_sparse_nsym_fac (f11dac).

The number of iterations required to achieve a prescribed accuracy cannot be easily determined a priori, as it can depend dramatically on the conditioning and spectrum of the preconditioned coefficient matrix, $\bar{A} = M^{-1}A$.

Some illustrations of the application of nag_sparse_nsym_fac_sol (f11dcc) to linear systems arising from the discretization of two-dimensional elliptic partial differential equations, and to random-valued randomly structured linear systems, can be found in Salvini and Shaw (1996).

10 Example

This example program solves a sparse linear system of equations using the CGS method, with incomplete LU preconditioning.

10.1 Program Text

```
/* nag_sparse_nsym_fac_solve (f11dcc) Example Program.
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 *
 */

#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nag_string.h>
#include <nagf11.h>

int main(void)
{
  double                dtol;
  double                *a = 0, *b = 0;
  double                *x = 0;
  double                rnorm;
  double                tol;
  Integer               exit_status = 0;
  Integer               *irow, *icol;
  Integer               *istr = 0, *idiag, *ipivp = 0, *ipivq = 0;
  Integer               i, m, n, nnzc;
  Integer               lfill, npivm;
  Integer               maxitn;
  Integer               itn;
  Integer               nnz;
  Integer               num;
  char                  nag_enum_arg[40];
  Nag_SparseNsym_Method method;
  Nag_SparseNsym_Piv    pstrat;
  Nag_SparseNsym_Fact   milu;
  Nag_Sparse_Comm       comm;
  NagError              fail;

  INIT_FAIL(fail);

  printf("nag_sparse_nsym_fac_sol (f11dcc) Example Program Results\n");

  /* Skip heading in data file */
  scanf("%*[^\n]");
  scanf("%ld%*[^\n]", &n);
  scanf("%ld%*[^\n]", &nnz);
  scanf("%39s%*[^\n]", nag_enum_arg);
  /* nag_enum_name_to_value (x04nac).
   * Converts NAG enum member name to value
   */
  method = (Nag_SparseNsym_Method) nag_enum_name_to_value(nag_enum_arg);
  scanf("%ld%lf%*[^\n]", &lfill, &dtol);
  scanf("%39s%*[^\n]", nag_enum_arg);
  pstrat = (Nag_SparseNsym_Piv) nag_enum_name_to_value(nag_enum_arg);
```

```
  scanf("%39s%*[^\n]", nag_enum_arg);
  milu = (Nag_SparseNsym_Fact) nag_enum_name_to_value(nag_enum_arg);
  scanf("%ld%lf%ld%*[^\n]", &m, &tol, &maxitn);

  /* Read the matrix a */

  num = 2*nnz;
  istr = NAG_ALLOC(n+1, Integer);
  idiag = NAG_ALLOC(n, Integer);
  ipivp = NAG_ALLOC(n, Integer);
  ipivq = NAG_ALLOC(n, Integer);
  x = NAG_ALLOC(n, double);
  b = NAG_ALLOC(n, double);
  a = NAG_ALLOC(num, double);
  irow = NAG_ALLOC(num, Integer);
  icol = NAG_ALLOC(num, Integer);
  if (!istr || !idiag || !ipivp || !ipivq || !irow || !icol || !a || !x || !b)
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }


  for (i = 1; i <= nnz; ++i)
    scanf("%lf%ld%ld%*[^\n]", &a[i-1], &irow[i-1], &icol[i-1]);

  /* Read right-hand side vector b and initial approximate solution x */

  for (i = 1; i <= n; ++i)
    scanf("%lf", &b[i-1]);
  scanf("%*[^\n]");

  for (i = 1; i <= n; ++i)
    scanf("%lf", &x[i-1]);
  scanf("%*[^\n]");

  /* Calculate incomplete LU factorization */

  /* nag_sparse_nsym_fac (f11dac).
   * Incomplete LU factorization (nonsymmetric)
   */
  nag_sparse_nsym_fac(n, nnz, &a, &num, &irow, &icol, lfill, dtol, pstrat,
                      milu, ipivp, ipivq, istr, idiag, &nnzc, &npivm, &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_sparse_nsym_fac (f11dac).\n%s\n",
             fail.message);
      exit_status = 1;
      goto END;
    }

  /* nag_sparse_nsym_fac_sol (f11dcc).
   * Solver with incomplete LU preconditioning (nonsymmetric)
   */
  /* Solve Ax = b using nag_sparse_nsym_fac_sol (f11dcc) */
  nag_sparse_nsym_fac_sol(method, n, nnz, a, num, irow, icol, ipivp, ipivq,
                          istr, idiag, b, m, tol, maxitn, x, &rnorm, &itn,
                          &comm, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_sparse_nsym_fac_sol (f11dcc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }

  printf("%s%10ld%s\n", "Converged in", itn, " iterations");
  printf("%s%16.3e\n", "Final residual norm =", rnorm);

  /* Output x */
```

```
  printf("           x\n");
  for (i = 1; i <= n; ++i)
    printf(" %16.6e\n", x[i-1]);

 END:
  NAG_FREE(istr);
  NAG_FREE(idiag);
  NAG_FREE(ipivp);
  NAG_FREE(ipivq);
  NAG_FREE(irow);
  NAG_FREE(icol);
  NAG_FREE(a);
  NAG_FREE(x);
  NAG_FREE(b);

  return exit_status;
}
```

10.2 Program Data

```
nag_sparse_nsym_fac_sol (f11dcc) Example Program Data
  8                             n
  24                            nnz
  Nag_SparseNsym_CGS            method
  0  0.0                        lfill, dtol
  Nag_SparseNsym_CompletePiv    pstrat
  Nag_SparseNsym_UnModFact      milu
  4  1.0e-10   100              m, tol, maxitn
  2.   1    1
 -1.   1    4
  1.   1    8
  4.   2    1
 -3.   2    2
  2.   2    5
 -7.   3    3
  2.   3    6
  3.   4    1
 -4.   4    3
  5.   4    4
  5.   4    7
 -1.   5    2
  8.   5    5
 -3.   5    7
 -6.   6    1
  5.   6    3
  2.   6    6
 -5.   7    3
 -1.   7    5
  6.   7    7
 -1.   8    2
  2.   8    6
  3.   8    8          a[i-1], irow[i-1], icol[i-1], i=1,...,nnz
  6.   8.  -9.  46.
 17.  21.  22.  34.   b[i-1], i=1,...,n
  0.   0.   0.   0.
  0.   0.   0.   0.   x[i-1], i=1,...,n
```

10.3 Program Results

```
nag_sparse_nsym_fac_sol (f11dcc) Example Program Results
Converged in         4 iterations
Final residual norm =       2.132e-14
           x
     1.000000e-00
     2.000000e+00
     3.000000e+00
     4.000000e+00
     5.000000e+00
     6.000000e+00
     7.000000e+00
```

```
8.000000e+00
```