NAG Library Function Document

nag_complex_sparse_eigensystem_monit (f12asc)

Note: *this function uses* **optional parameters** *to define choices in the problem specification. If you wish to use* default *settings for all of the optional parameters, then the option setting function nag_complex_sparse_eigensystem_option (f12arc) need not be called. If, however, you wish to reset some or all of the settings please refer to Section 11 in nag_complex_sparse_eigensystem_option (f12arc) for a detailed description of the specification of the optional parameters.*

1 Purpose

nag_complex_sparse_eigensystem_monit (f12asc) can be used to return additional monitoring information during computation. It is in a suite of functions consisting of nag_complex_sparse_eigen system_init (f12anc), nag_complex_sparse_eigensystem_iter (f12apc), nag_complex_sparse_eigensys tem_sol (f12aqc), nag_complex_sparse_eigensystem_option (f12arc) and nag_complex_sparse_eigensys tem_monit (f12asc).

2 Specification

```
#include <nag.h>
#include <nagf12.h>
```

```
void nag_complex_sparse_eigensystem_monit (Integer *niter, Integer *nconv,
     Complex ritz[], Complex rzest[], const Integer icomm[],
     const Complex comm[])
```

3 Description

The suite of functions is designed to calculate some of the eigenvalues, λ, (and optionally the corresponding eigenvectors, x) of a standard complex eigenvalue problem $Ax = \lambda x$, or of a generalized complex eigenvalue problem $Ax = \lambda Bx$ of order n, where n is large and the coefficient matrices A and B are sparse and complex. The suite can also be used to find selected eigenvalues/eigenvectors of smaller scale dense complex problems.

On an intermediate exit from nag_complex_sparse_eigensystem_iter (f12apc) with **irevcm** $= 4$, nag_complex_sparse_eigensystem_monit (f12asc) may be called to return monitoring information on the progress of the Arnoldi iterative process. The information returned by nag_complex_sparse_eigen system_monit (f12asc) is:

– the number of the current Arnoldi iteration;

– the number of converged eigenvalues at this point;

– the converged eigenvalues;

– the error bounds on the converged eigenvalues.

nag_complex_sparse_eigensystem_monit (f12asc) does not have an equivalent function from the ARPACK package which prints various levels of detail of monitoring information through an output channel controlled via an argument value (see Lehoucq *et al.* (1998) for details of ARPACK routines). nag_complex_sparse_eigensystem_monit (f12asc) should not be called at any time other than immediately following an **irevcm** $= 4$ return from nag_complex_sparse_eigensystem_iter (f12apc).

4 References

Lehoucq R B (2001) Implicitly restarted Arnoldi methods and subspace iteration *SIAM Journal on Matrix Analysis and Applications* **23** 551–562

Lehoucq R B and Scott J A (1996) An evaluation of software for computing eigenvalues of sparse nonsymmetric matrices *Preprint MCS-P547-1195* Argonne National Laboratory

Lehoucq R B and Sorensen D C (1996) Deflation techniques for an implicitly restarted Arnoldi iteration *SIAM Journal on Matrix Analysis and Applications* **17** 789–821

Lehoucq R B, Sorensen D C and Yang C (1998) *ARPACK Users' Guide: Solution of Large-scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods* SIAM, Philidelphia

5 Arguments

1: **niter** – Integer * *Output*

On exit: the number of the current Arnoldi iteration.

2: **nconv** – Integer * *Output*

On exit: the number of converged eigenvalues so far.

3: **ritz**[*dim*] – Complex *Output*

Note: the dimension, *dim*, of the array **ritz** must be at least **ncv** (see nag_complex_sparse_ei gensystem_init (f12anc)).

On exit: the first **nconv** locations of the array **ritz** contain the converged approximate eigenvalues.

4: **rzest**[*dim*] – Complex *Output*

Note: the dimension, *dim*, of the array **rzest** must be at least **ncv** (see nag_complex_sparse_ei gensystem_init (f12anc)).

On exit: the first **nconv** locations of the array **rzest** contain the complex Ritz estimates on the converged approximate eigenvalues.

5: **icomm**[*dim*] – const Integer *Communication Array*

Note: the dimension, *dim*, of the array **icomm** must be at least max(1, **licomm**), where **licomm** is passed to the setup function (see nag_complex_sparse_eigensystem_init (f12anc)).

On entry: the array **icomm** output by the preceding call to nag_complex_sparse_eigensystem_iter (f12apc).

6: **comm**[*dim*] – const Complex *Communication Array*

Note: the dimension, *dim*, of the array **comm** must be at least max(1, **lcomm**), where **lcomm** is passed to the setup function (see nag_complex_sparse_eigensystem_init (f12anc)).

On entry: the array **comm** output by the preceding call to nag_complex_sparse_eigensystem_iter (f12apc).

6 Error Indicators and Warnings

None.

7 Accuracy

A Ritz value, λ, is deemed to have converged if the magnitude of its Ritz estimate $\leq$ **Tolerance** $\times |\lambda|$. The default **Tolerance** used is the ***machine precision*** given by nag_machine_precision (X02AJC).

8 Parallelism and Performance

nag_complex_sparse_eigensystem_monit (f12asc) is not threaded in any implementation.

9 Further Comments

None.

10 Example

This example solves $Ax = \lambda Bx$ in shifted-inverse mode, where A and B are obtained from the standard central difference discretization of the one-dimensional convection-diffusion operator $\frac{d^2u}{dx^2} + \rho\frac{du}{dx}$ on $[0, 1]$, with zero Dirichlet boundary conditions. The shift, σ, is a complex number, and the operator used in the shifted-inverse iterative process is $\mathrm{OP} = \mathrm{inv}(A - \sigma B) \times B$.

10.1 Program Text

```
/* nag_complex_sparse_eigensystem_monit (f12asc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nag_string.h>
#include <stdio.h>
#include <naga02.h>
#include <nagf12.h>
#include <nagf16.h>

/* Table of constant values */
static Complex four = { 4., 0. };

static void mv(Integer, Complex *, Complex *);
static void my_zgttrf(Integer, Complex *, Complex *, Complex *,
                      Complex *, Integer *, Integer *);
static void my_zgttrs(Integer, Complex *, Complex *, Complex *,
                      Complex *, Integer *, Complex *);

int main(void)
{
  /* Constants */
  Integer licomm = 140, imon = 1;

  /* Scalars */
  Complex rho, s1, s2, s3, sigma;
  double estnrm, hr, hr1, sr, shs;
  Integer exit_status, info, irevcm, j, lcomm, n, nconv, ncv;
  Integer nev, niter, nshift, nx;
  /* Nag types */
  NagError fail;
  /* Arrays */
  Complex *comm = 0, *eigv = 0, *eigest = 0, *dd = 0, *dl = 0, *du = 0;
  Complex *du2 = 0, *resid = 0, *v = 0;
  Integer *icomm = 0, *ipiv = 0;
  /* Ponters */
  Complex *mx = 0, *x = 0, *y = 0;

  exit_status = 0;
  INIT_FAIL(fail);

  printf("nag_complex_sparse_eigensystem_monit (f12asc) Example "
         "Program Results\n");
  /* Skip heading in data file */
#ifdef _WIN32
  scanf_s("%*[^\n] ");
#else
  scanf("%*[^\n] ");
#endif

#ifdef _WIN32
  scanf_s("%" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "%*[^\n] ", &nx, &nev, &ncv);
#else
  scanf("%" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "%*[^\n] ", &nx, &nev, &ncv);
#endif
  n = nx * nx;
  lcomm = 3 * n + 3 * ncv * ncv + 5 * ncv + 60;
  /* Allocate memory */
  if (!(comm = NAG_ALLOC(lcomm, Complex)) ||
      !(eigv = NAG_ALLOC(ncv, Complex)) ||
      !(eigest = NAG_ALLOC(ncv, Complex)) ||
      !(dd = NAG_ALLOC(n, Complex)) ||
      !(dl = NAG_ALLOC(n, Complex)) ||
      !(du = NAG_ALLOC(n, Complex)) ||
      !(du2 = NAG_ALLOC(n, Complex)) ||
      !(resid = NAG_ALLOC(n, Complex)) ||
      !(v = NAG_ALLOC(n * ncv, Complex)) ||
      !(icomm = NAG_ALLOC(licomm, Integer)) ||
      !(ipiv = NAG_ALLOC(n, Integer)))
  {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }
  /* Initialize communication arrays for problem using
     nag_complex_sparse_eigensystem_init (f12anc). */
  nag_complex_sparse_eigensystem_init(n, nev, ncv, icomm, licomm, comm, lcomm,
                                      &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_complex_sparse_eigensystem_init (f12anc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }
  /* Select the required mode using
     nag_complex_sparse_eigensystem_option (f12adc). */
  nag_complex_sparse_eigensystem_option("SHIFTED INVERSE", icomm, comm,
                                        &fail);
  /* Select the  problem type using
     nag_complex_sparse_eigensystem_option (f12adc). */
  nag_complex_sparse_eigensystem_option("GENERALIZED", icomm, comm, &fail);
  /* Set values for sigma and rho */
  /* Assign to Complex type using nag_complex (a02bac) */
  sigma = nag_complex(5000.0, 0.0);
  rho = nag_complex(10.0, 0.0);
  hr1 = (double) (n + 1);
  hr = 1.0 / hr1;
  sr = 0.5 * rho.re;
  shs = sigma.re * hr / 6.0;
  /* Assign to Complex type using nag_complex (a02bac) */
  s1 = nag_complex(-hr1 - sr - shs, 0.0);
  s3 = nag_complex(-hr1 + sr - shs, 0.0);
  s2 = nag_complex(2.0 * hr1 - 4.0 * shs, 0.0);

  for (j = 0; j <= n - 2; ++j) {
    dl[j] = s1;
    dd[j] = s2;
    du[j] = s3;
  }
  dd[n - 1] = s2;

  my_zgttrf(n, dl, dd, du, du2, ipiv, &info);
  irevcm = 0;
```

```
REVCOMLOOP:
  /* repeated calls to reverse communication routine
     nag_complex_sparse_eigensystem_iter (f12apc). */
  nag_complex_sparse_eigensystem_iter(&irevcm, resid, v, &x, &y, &mx, &nshift,
                                      comm, icomm, &fail);
  if (irevcm != 5) {
    if (irevcm == -1) {
      /* Perform  x <--- OP*x = inv[A-SIGMA*M]*M*x */
      mv(nx, x, y);
      my_zgttrs(n, dl, dd, du, du2, ipiv, y);
    }
    else if (irevcm == 1) {
      /* Perform  x <--- OP*x = inv[A-SIGMA*M]*M*x, */
      /* MX stored in mx */
      for (j = 0; j < n; ++j) {
        y[j] = mx[j];
      }
      my_zgttrs(n, dl, dd, du, du2, ipiv, y);
    }
    else if (irevcm == 2) {
      /* Perform  y <--- M*x */
      mv(nx, x, y);
    }
    else if (irevcm == 4 && imon == 1) {
      /* If imon=1, get monitoring information using
         nag_complex_sparse_eigensystem_monit (f12asc). */
      nag_complex_sparse_eigensystem_monit(&niter, &nconv, eigv,
                                           eigest, icomm, comm);
      /* Compute 2-norm of Ritz estimates using
         nag_zge_norm (f16uac). */
      nag_zge_norm(Nag_ColMajor, Nag_FrobeniusNorm, nev, 1,
                   eigest, nev, &estnrm, &fail);
      printf("Iteration %3" NAG_IFMT ", ", niter);
      printf(" No. converged = %3" NAG_IFMT ",", nconv);
      printf(" norm of estimates = %17.8e\n", estnrm);
    }
    goto REVCOMLOOP;
  }
  if (fail.code == NE_NOERROR) {
    /* Post-Process using nag_complex_sparse_eigensystem_sol
       (f12aqc) to compute eigenvalues/vectors. */
    nag_complex_sparse_eigensystem_sol(&nconv, eigv, v, sigma,
                                       resid, v, comm, icomm, &fail);
    printf("\n");
    printf(" The %4" NAG_IFMT " generalized Ritz values closest", nconv);
    printf(" to ( %7.3f , %7.3f ) are:\n\n", sigma.re, sigma.im);
    for (j = 0; j <= nconv - 1; ++j) {
      printf("%8" NAG_IFMT "%5s( %12.4f , %12.4f )\n", j + 1, "",
             eigv[j].re, eigv[j].im);
    }
  }
  else {
    printf(" Error from nag_complex_sparse_eigensystem_iter "
           "(f12apc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }
END:
  NAG_FREE(comm);
  NAG_FREE(eigv);
  NAG_FREE(eigest);
  NAG_FREE(dd);
  NAG_FREE(dl);
  NAG_FREE(du);
  NAG_FREE(du2);
  NAG_FREE(resid);
  NAG_FREE(v);
  NAG_FREE(icomm);
  NAG_FREE(ipiv);

  return exit_status;
```

```
}

static void mv(Integer nx, Complex *v, Complex *y)
{
  /* Compute the out-of--place matrix vector multiplication Y<---M*X, */
  /* where M is mass matrix formed by using piecewise linear elements */
  /* on [0,1]. */

  /* Scalars */
  Complex hsix, z1;
  Integer j, n;
  /* Function Body */
  n = nx * nx;
  /* Assign to Complex type using nag_complex (a02bac) */
  hsix = nag_complex(1.0 / (6.0 * (double) (n + 1)), 0.0);
  /* y[0] = (four*v[0]+v[1])*(h/six) */
  /* Compute Complex multiply using nag_complex_multiply (a02ccc). */
  z1 = nag_complex_multiply(four, v[0]);
  /* Compute Complex addition using nag_complex_add (a02cac). */
  z1 = nag_complex_add(z1, v[1]);
  y[0] = nag_complex_multiply(z1, hsix);
  for (j = 1; j <= n - 2; ++j) {
    /* y[j] = (v[j-1] + four*v[j] + V[j+1])*(h/six) */
    /* Compute Complex multiply using nag_complex_multiply
       (a02ccc). */
    z1 = nag_complex_multiply(four, v[j]);
    /* Compute Complex addition using nag_complex_add (a02cac). */
    z1 = nag_complex_add(v[j - 1], z1);
    z1 = nag_complex_add(z1, v[j + 1]);
    y[j] = nag_complex_multiply(z1, hsix);
  }
  /* y[n-1] = (v[n-2] + four*v[n-1])*(h/six) */
  /* Compute Complex multiply using nag_complex_multiply (a02ccc). */
  z1 = nag_complex_multiply(four, v[n - 1]);
  /* Compute Complex addition using nag_complex_add (a02cac). */
  z1 = nag_complex_add(v[n - 2], z1);
  y[n - 1] = nag_complex_multiply(z1, hsix);
  return;
} /* mv */

static void my_zgttrf(Integer n, Complex dl[], Complex d[],
                      Complex du[], Complex du2[], Integer ipiv[],
                      Integer *info)
{
  /* A simple C version of the Lapack routine zgttrf with argument
     checking removed */
  /* Scalars */
  Complex temp, fact, z1;
  Integer i;
  /* Function Body */
  *info = 0;
  for (i = 0; i < n; ++i) {
    ipiv[i] = i;
  }
  for (i = 0; i < n - 2; ++i) {
    du2[i] = nag_complex(0.0, 0.0);
  }
  for (i = 0; i < n - 2; ++i) {
    if (fabs(d[i].re) + fabs(d[i].im) >= fabs(dl[i].re) + fabs(dl[i].im)) {
      /* No row interchange required, eliminate dl[i]. */
      if (fabs(d[i].re) + fabs(d[i].im) != 0.0) {
        /* Compute Complex division using nag_complex_divide
           (a02cdc). */
        fact = nag_complex_divide(dl[i], d[i]);
        dl[i] = fact;
        /* Compute Complex multiply using nag_complex_multiply
           (a02ccc). */
        fact = nag_complex_multiply(fact, du[i]);
        /* Compute Complex subtraction using
           nag_complex_subtract (a02cbc). */
        d[i + 1] = nag_complex_subtract(d[i + 1], fact);
      }
    }
    else {
      /* Interchange rows I and I+1, eliminate dl[I] */
      /* Compute Complex division using nag_complex_divide
         (a02cdc). */
      fact = nag_complex_divide(d[i], dl[i]);
      d[i] = dl[i];
      dl[i] = fact;
      temp = du[i];
      du[i] = d[i + 1];
      /* Compute Complex multiply using nag_complex_multiply
         (a02ccc). */
      z1 = nag_complex_multiply(fact, d[i + 1]);
      /* Compute Complex subtraction using nag_complex_subtract
         (a02cbc). */
      d[i + 1] = nag_complex_subtract(temp, z1);
      du2[i] = du[i + 1];
      /* Compute Complex multiply using nag_complex_multiply
         (a02ccc). */
      du[i + 1] = nag_complex_multiply(fact, du[i + 1]);
      /* Perform Complex negation using nag_complex_negate
         (a02cec). */
      du[i + 1] = nag_complex_negate(du[i + 1]);
      ipiv[i] = i + 1;
    }
  }
  if (n > 1) {
    i = n - 2;
    if (fabs(d[i].re) + fabs(d[i].im) >= fabs(dl[i].re) + fabs(dl[i].im)) {
      if (fabs(d[i].re) + fabs(d[i].im) != 0.0) {
        /* Compute Complex division using nag_complex_divide
           (a02cdc). */
        fact = nag_complex_divide(dl[i], d[i]);
        dl[i] = fact;
        /* Compute Complex multiply using nag_complex_multiply
           (a02ccc). */
        fact = nag_complex_multiply(fact, du[i]);
        /* Compute Complex subtraction using
           nag_complex_subtract (a02cbc). */
        d[i + 1] = nag_complex_subtract(d[i + 1], fact);
      }
    }
    else {
      /* Compute Complex division using nag_complex_divide
         (a02cdc). */
      fact = nag_complex_divide(d[i], dl[i]);
      d[i] = dl[i];
      dl[i] = fact;
      temp = du[i];
      du[i] = d[i + 1];
      /* Compute Complex multiply using nag_complex_multiply
         (a02ccc). */
      z1 = nag_complex_multiply(fact, d[i + 1]);
      /* Compute Complex subtraction using nag_complex_subtract
         (a02cbc). */
      d[i + 1] = nag_complex_subtract(temp, z1);
      ipiv[i] = i + 1;
    }
  }
  /* Check for a zero on the diagonal of U. */
  for (i = 0; i < n; ++i) {
    if (fabs(d[i].re) + fabs(d[i].im) == 0.0) {
      *info = i;
      goto END;
    }
  }
END:
  return;
}
```

```
static void my_zgttrs(Integer n, Complex dl[], Complex d[],
                      Complex du[], Complex du2[], Integer ipiv[],
                      Complex b[])
{
  /* A simple C version of the Lapack routine zgttrs with argument
     checking removed, the number of right-hand-sides=1, Trans='N' */
  /* Scalars */
  Complex temp, z1;
  Integer i;
  /* Solve L*x = b. */
  for (i = 0; i < n - 1; ++i) {
    if (ipiv[i] == i) {
      /* b[i+1] = b[i+1] - dl[i]*b[i] */
      /* Compute Complex multiply using nag_complex_multiply
         (a02ccc). */
      temp = nag_complex_multiply(dl[i], b[i]);
      /* Compute Complex subtraction using nag_complex_subtract
         (a02cbc). */
      b[i + 1] = nag_complex_subtract(b[i + 1], temp);
    }
    else {
      temp = b[i];
      b[i] = b[i + 1];
      /* Compute Complex multiply using nag_complex_multiply
         (a02ccc). */
      z1 = nag_complex_multiply(dl[i], b[i]);
      /* Compute Complex subtraction using nag_complex_subtract
         (a02cbc). */
      b[i + 1] = nag_complex_subtract(temp, z1);
    }
  }
  /* Solve U*x = b. */
  /* Compute Complex division using nag_complex_divide (a02cdc). */
  b[n - 1] = nag_complex_divide(b[n - 1], d[n - 1]);
  if (n > 1) {
    /* Compute Complex multiply using nag_complex_multiply
       (a02ccc). */
    temp = nag_complex_multiply(du[n - 2], b[n - 1]);
    /* Compute Complex subtraction using nag_complex_subtract
       (a02cbc). */
    z1 = nag_complex_subtract(b[n - 2], temp);
    /* Compute Complex division using nag_complex_divide (a02cdc). */
    b[n - 2] = nag_complex_divide(z1, d[n - 2]);
  }
  for (i = n - 3; i >= 0; --i) {
    /* b[i] = (b[i]-du[i]*b[i+1]-du2[i]*b[i+2])/d[i]; */
    /* Compute Complex multiply using nag_complex_multiply
       (a02ccc). */
    temp = nag_complex_multiply(du[i], b[i + 1]);
    z1 = nag_complex_multiply(du2[i], b[i + 2]);
    /* Compute Complex addition using nag_complex_add
       (a02cac). */
    temp = nag_complex_add(temp, z1);
    /* Compute Complex subtraction using nag_complex_subtract
       (a02cbc). */
    z1 = nag_complex_subtract(b[i], temp);
    /* Compute Complex division using nag_complex_divide
       (a02cdc). */
    b[i] = nag_complex_divide(z1, d[i]);
  }
  return;
}
```

10.2 Program Data

```
nag_complex_sparse_eigensystem_monit (f12asc) Example Program Data
 16  4  10 : Vaues for nx, nev and ncv
```

10.3 Program Results

```
nag_complex_sparse_eigensystem_monit (f12asc) Example Program Results
Iteration   1,  No. converged =   0, norm of estimates =    5.94672394e-07
Iteration   2,  No. converged =   1, norm of estimates =    1.47822750e-09
Iteration   3,  No. converged =   2, norm of estimates =    3.29270191e-11
Iteration   4,  No. converged =   2, norm of estimates =    5.94072850e-14
Iteration   5,  No. converged =   2, norm of estimates =    8.40812032e-16
Iteration   6,  No. converged =   3, norm of estimates =    8.13435708e-18

 The    4 generalized Ritz values closest to ( 5000.000 ,   0.000 ) are:

       1     (    4829.8497 ,      -0.0000 )
       2     (    5279.5223 ,      -0.0000 )
       3     (    4400.6310 ,       0.0000 )
       4     (    5749.7160 ,      -0.0000 )
```