NAG Library Function Document

nag_complex_sym_packed_lin_solve (f04djc)

1 Purpose

nag_complex_sym_packed_lin_solve (f04djc) computes the solution to a complex system of linear equations $AX = B$, where A is an n by n complex symmetric matrix, stored in packed format and X and B are n by r matrices. An estimate of the condition number of A and an error bound for the computed solution are also returned.

2 Specification

```
#include <nag.h>
#include <nagf04.h>

void nag_complex_sym_packed_lin_solve (Nag_OrderType order,
    Nag_UploType uplo, Integer n, Integer nrhs, Complex ap[],
    Integer ipiv[], Complex b[], Integer pdb, double *rcond, double *errbnd,
    NagError *fail)
```

3 Description

The diagonal pivoting method is used to factor A as $A = UDU^{\mathrm{T}}$, if **uplo** = Nag_Upper, or $A = LDL^{\mathrm{T}}$, if **uplo** = Nag_Lower, where U (or L) is a product of permutation and unit upper (lower) triangular matrices, and D is symmetric and block diagonal with 1 by 1 and 2 by 2 diagonal blocks. The factored form of A is then used to solve the system of equations $AX = B$.

4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia http://www.netlib.org/lapack/lug

Higham N J (2002) *Accuracy and Stability of Numerical Algorithms* (2nd Edition) SIAM, Philadelphia

5 Arguments

1:    **order** – Nag_OrderType   *Input*

On entry: the **order** argument specifies the two-dimensional storage scheme being used, i.e., row-major ordering or column-major ordering. C language defined storage is specified by **order** = Nag_RowMajor. See Section 3.2.1.3 in the Essential Introduction for a more detailed explanation of the use of this argument.

Constraint: **order** = Nag_RowMajor or Nag_ColMajor.

2:    **uplo** – Nag_UploType   *Input*

On entry: if **uplo** = Nag_Upper, the upper triangle of the matrix A is stored.

If **uplo** = Nag_Lower, the lower triangle of the matrix A is stored.

Constraint: **uplo** = Nag_Upper or Nag_Lower.

3:    **n** – Integer   *Input*

On entry: the number of linear equations n, i.e., the order of the matrix A.

Constraint: **n** ≥ 0.

4: **nrhs** – Integer   *Input*

On entry: the number of right-hand sides r, i.e., the number of columns of the matrix B.

Constraint: **nrhs** ≥ 0.

5: **ap**[dim] – Complex   *Input/Output*

Note: the dimension, *dim*, of the array **ap** must be at least $\max(1, \mathbf{n} \times (\mathbf{n} + 1)/2)$.

On entry: the n by n symmetric matrix A, packed column-wise in a linear array. The jth column of the matrix A is stored in the array **ap** as follows:

The storage of elements A_{ij} depends on the **order** and **uplo** arguments as follows:

> if **order** = Nag_ColMajor and **uplo** = Nag_Upper,
> A_{ij} is stored in $\mathbf{ap}[(j-1) \times j/2 + i - 1]$, for $i \leq j$;
> if **order** = Nag_ColMajor and **uplo** = Nag_Lower,
> A_{ij} is stored in $\mathbf{ap}[(2n-j) \times (j-1)/2 + i - 1]$, for $i \geq j$;
> if **order** = Nag_RowMajor and **uplo** = Nag_Upper,
> A_{ij} is stored in $\mathbf{ap}[(2n-i) \times (i-1)/2 + j - 1]$, for $i \leq j$;
> if **order** = Nag_RowMajor and **uplo** = Nag_Lower,
> A_{ij} is stored in $\mathbf{ap}[(i-1) \times i/2 + j - 1]$, for $i \geq j$.

On exit: if **fail.code** = NE_NOERROR, the block diagonal matrix D and the multipliers used to obtain the factor U or L from the factorization $A = UDU^{\mathrm{T}}$ or $A = LDL^{\mathrm{T}}$ as computed by nag_zsptrf (f07qrc), stored as a packed triangular matrix in the same storage format as A.

6: **ipiv**[**n**] – Integer   *Output*

On exit: if no constraints are violated, details of the interchanges and the block structure of D, as determined by nag_zsptrf (f07qrc).

> If $\mathbf{ipiv}[k-1] > 0$, then rows and columns k and $\mathbf{ipiv}[k-1]$ were interchanged, and d_{kk} is a 1 by 1 diagonal block;
>
> if **uplo** = Nag_Upper and $\mathbf{ipiv}[k-1] = \mathbf{ipiv}[k-2] < 0$, then rows and columns $k-1$ and $-\mathbf{ipiv}[k-1]$ were interchanged and $d_{k-1:k,k-1:k}$ is a 2 by 2 diagonal block;
>
> if **uplo** = Nag_Lower and $\mathbf{ipiv}[k-1] = \mathbf{ipiv}[k] < 0$, then rows and columns $k+1$ and $-\mathbf{ipiv}[k-1]$ were interchanged and $d_{k:k+1,k:k+1}$ is a 2 by 2 diagonal block.

7: **b**[dim] – Complex   *Input/Output*

Note: the dimension, *dim*, of the array **b** must be at least

> $\max(1, \mathbf{pdb} \times \mathbf{nrhs})$ when **order** = Nag_ColMajor;
> $\max(1, \mathbf{n} \times \mathbf{pdb})$ when **order** = Nag_RowMajor.

The (i, j)th element of the matrix B is stored in

> $\mathbf{b}[(j-1) \times \mathbf{pdb} + i - 1]$ when **order** = Nag_ColMajor;
> $\mathbf{b}[(i-1) \times \mathbf{pdb} + j - 1]$ when **order** = Nag_RowMajor.

On entry: the n by r matrix of right-hand sides B.

On exit: if **fail.code** = NE_NOERROR or NE_RCOND, the n by r solution matrix X.

8: **pdb** – Integer   *Input*

On entry: the stride separating row or column elements (depending on the value of **order**) in the array **b**.

Constraints:

> if **order** = Nag_ColMajor, **pdb** $\geq \max(1, \mathbf{n})$;
> if **order** = Nag_RowMajor, **pdb** $\geq \max(1, \mathbf{nrhs})$.

9:     **rcond** – double *   *Output*

On exit: if no constraints are violated, an estimate of the reciprocal of the condition number of the matrix A, computed as $\mathbf{rcond} = 1/\left(\|A\|_1 \|A^{-1}\|_1\right)$.

10:    **errbnd** – double *   *Output*

On exit: if **fail**.**code** = NE_NOERROR or NE_RCOND, an estimate of the forward error bound for a computed solution $\hat{x}$, such that $\|\hat{x} - x\|_1/\|x\|_1 \leq \mathbf{errbnd}$, where $\hat{x}$ is a column of the computed solution returned in the array **b** and x is the corresponding column of the exact solution X. If **rcond** is less than *machine precision*, then **errbnd** is returned as unity.

11:    **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, $\mathbf{n} = \langle value \rangle$.
Constraint: $\mathbf{n} \geq 0$.

On entry, $\mathbf{nrhs} = \langle value \rangle$.
Constraint: $\mathbf{nrhs} \geq 0$.

On entry, $\mathbf{pdb} = \langle value \rangle$.
Constraint: $\mathbf{pdb} > 0$.

NE_INT_2

On entry, $\mathbf{pdb} = \langle value \rangle$ and $\mathbf{n} = \langle value \rangle$.
Constraint: $\mathbf{pdb} \geq \max(1, \mathbf{n})$.

On entry, $\mathbf{pdb} = \langle value \rangle$ and $\mathbf{nrhs} = \langle value \rangle$.
Constraint: $\mathbf{pdb} \geq \max(1, \mathbf{nrhs})$.

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_RCOND

A solution has been computed, but **rcond** is less than *machine precision* so that the matrix A is numerically singular.

NE_SINGULAR

Diagonal block $\langle value \rangle$ of the block diagonal matrix is zero. The factorization has been completed, but the solution could not be computed.

7   Accuracy

The computed solution for a single right-hand side, $\hat{x}$, satisfies an equation of the form

$$(A + E)\hat{x} = b,$$

where

$$\|E\|_1 = O(\epsilon)\|A\|_1$$

and ϵ is the *machine precision*. An approximate error bound for the computed solution is given by

$$\frac{\|\hat{x} - x\|_1}{\|x\|_1} \leq \kappa(A)\frac{\|E\|_1}{\|A\|_1},$$

where $\kappa(A) = \|A^{-1}\|_1\|A\|_1$, the condition number of A with respect to the solution of the linear equations. nag_complex_sym_packed_lin_solve (f04djc) uses the approximation $\|E\|_1 = \epsilon\|A\|_1$ to estimate **errbnd**. See Section 4.4 of Anderson *et al.* (1999) for further details.

8   Parallelism and Performance

nag_complex_sym_packed_lin_solve (f04djc) is not threaded by NAG in any implementation.

nag_complex_sym_packed_lin_solve (f04djc) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this function. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9   Further Comments

The packed storage scheme is illustrated by the following example when $n = 4$ and **uplo** = Nag_Upper. Two-dimensional storage of the symmetric matrix A:

$$
\begin{matrix}
a_{11} & a_{12} & a_{13} & a_{14} \\
 & a_{22} & a_{23} & a_{24} \\
 & & a_{33} & a_{34} \\
 & & & a_{44}
\end{matrix}
\quad \left(a_{ij} = a_{ji}\right)
$$

Packed storage of the upper triangle of A:

$$\mathbf{ap} = \begin{bmatrix} a_{11}, & a_{12}, & a_{22}, & a_{13}, & a_{23}, & a_{33}, & a_{14}, & a_{24}, & a_{34}, & a_{44} \end{bmatrix}$$

The total number of floating-point operations required to solve the equations $AX = B$ is proportional to $\left(\frac{1}{3}n^3 + 2n^2 r\right)$. The condition number estimation typically requires between four and five solves and never more than eleven solves, following the factorization.

In practice the condition number estimator is very reliable, but it can underestimate the true condition number; see Section 15.3 of Higham (2002) for further details.

Function nag_herm_packed_lin_solve (f04cjc) is for complex Hermitian matrices, and the real analogue of nag_complex_sym_packed_lin_solve (f04djc) is nag_real_sym_packed_lin_solve (f04bjc).

10 Example

This example solves the equations

$$AX = B,$$

where A is the symmetric indefinite matrix

$$A = \begin{pmatrix} -0.56 + 0.12i & -1.54 - 2.86i & 5.32 - 1.59i & 3.80 + 0.92i \\ -1.54 - 2.86i & -2.83 - 0.03i & -3.52 + 0.58i & -7.86 - 2.96i \\ 5.32 - 1.59i & -3.52 + 0.58i & 8.86 + 1.81i & 5.14 - 0.64i \\ 3.80 + 0.92i & -7.86 - 2.96i & 5.14 - 0.64i & -0.39 - 0.71i \end{pmatrix}$$

and

$$B = \begin{pmatrix} -6.43 + 19.24i & -4.59 - 35.53i \\ -0.49 - 1.47i & 6.95 + 20.49i \\ -48.18 + 66.00i & -12.08 - 27.02i \\ -55.64 + 41.22i & -19.09 - 35.97i \end{pmatrix}.$$

An estimate of the condition number of A and an approximate error bound for the computed solutions are also printed.

10.1 Program Text

```
/* nag_complex_sym_packed_lin_solve (f04djc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 8, 2004.
 */

#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf04.h>
#include <nagx04.h>

int main(void)
{

  /* Scalars */
  double       errbnd, rcond;
  Integer      exit_status, i, j, n, nrhs, pdb;

  /* Arrays */
  char         nag_enum_arg[40];
  char         *clabs = 0, *rlabs = 0;
  Complex      *ap = 0, *b = 0;
  Integer      *ipiv = 0;

  /* Nag types */
  NagError      fail;
  Nag_OrderType order;
  Nag_UploType  uplo;


#ifdef NAG_COLUMN_MAJOR
  /*#define A(I,J) a[(J-1)*pda + I - 1]*/
#define A_UPPER(I, J) ap[J*(J-1)/2 + I - 1]
#define A_LOWER(I, J) ap[(2*n-J)*(J-1)/2 + I - 1]
#define B(I, J)       b[(J-1)*pdb + I - 1]
  order = Nag_ColMajor;
#else
  /*#define A(I,J) a[(I-1)*pda + J - 1]*/
#define A_LOWER(I, J) ap[I*(I-1)/2 + J - 1]
#define A_UPPER(I, J) ap[(2*n-I)*(I-1)/2 + J - 1]
#define B(I, J)       b[(I-1)*pdb + J - 1]
  order = Nag_RowMajor;
```

```
#endif

  exit_status = 0;
  INIT_FAIL(fail);

  printf("nag_complex_sym_packed_lin_solve (f04djc) Example Program"
         " Results\n\n");

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

#ifdef _WIN32
  scanf_s("%"NAG_IFMT"%"NAG_IFMT"%*[^\n] ", &n, &nrhs);
#else
  scanf("%"NAG_IFMT"%"NAG_IFMT"%*[^\n] ", &n, &nrhs);
#endif
  if (n > 0 && nrhs > 0)
    {
      /* Allocate memory */
      if (!(clabs = NAG_ALLOC(2, char)) ||
          !(rlabs = NAG_ALLOC(2, char)) ||
          !(ap = NAG_ALLOC(n*(n+1)/2, Complex)) ||
          !(b = NAG_ALLOC(n*nrhs, Complex)) ||
          !(ipiv = NAG_ALLOC(n, Integer)))
        {
          printf("Allocation failure\n");
          exit_status = -1;
          goto END;
        }
#ifdef NAG_COLUMN_MAJOR
      pdb = n;
#else
      pdb = nrhs;
#endif
    }
  else
    {
      printf("%s\n", "n and/or nrhs too small");
      exit_status = 1;
      return exit_status;
    }

  /* Read A from data file */
#ifdef _WIN32
  scanf_s("%39s%*[^\n] ", nag_enum_arg, _countof(nag_enum_arg));
#else
  scanf("%39s%*[^\n] ", nag_enum_arg);
#endif
  /* nag_enum_name_to_value (x04nac).
   * Converts NAG enum member name to value
   */
  uplo = (Nag_UploType) nag_enum_name_to_value(nag_enum_arg);

  /* Read the upper or lower triangular part of the matrix A from */
  /* data file */

  if (uplo == Nag_Upper)
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = i; j <= n; ++j)
            {
#ifdef _WIN32
              scanf_s(" ( %lf , %lf )", &A_UPPER(i, j).re,
                      &A_UPPER(i, j).im);
#else
              scanf(" ( %lf , %lf )", &A_UPPER(i, j).re,
```

```
                                   &A_UPPER(i, j).im);
#endif
            }
         }
#ifdef _WIN32
      scanf_s("%*[^\n] ");
#else
      scanf("%*[^\n] ");
#endif
    }
  else
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = 1; j <= i; ++j)
            {
#ifdef _WIN32
              scanf_s(" ( %lf , %lf )", &A_LOWER(i, j).re,
                      &A_LOWER(i, j).im);
#else
              scanf(" ( %lf , %lf )", &A_LOWER(i, j).re,
                      &A_LOWER(i, j).im);
#endif
            }
        }
#ifdef _WIN32
      scanf_s("%*[^\n] ");
#else
      scanf("%*[^\n] ");
#endif
    }

  /* Read B from data file */
  for (i = 1; i <= n; ++i)
    {
      for (j = 1; j <= nrhs; ++j)
        {
#ifdef _WIN32
          scanf_s(" ( %lf , %lf )", &B(i, j).re, &B(i, j).im);
#else
          scanf(" ( %lf , %lf )", &B(i, j).re, &B(i, j).im);
#endif
        }
    }
#ifdef _WIN32
  scanf_s("%*[^\n] ");
#else
  scanf("%*[^\n] ");
#endif

  /* Solve the equations AX = B for X */
  /* nag_complex_sym_packed_lin_solve (f04djc).
   * Computes the solution and error-bound to a complex
   * symmetric system of linear equations, packed storage.
   */
  nag_complex_sym_packed_lin_solve(order, uplo, n, nrhs, ap, ipiv, b, pdb,
                                   &rcond, &errbnd, &fail);
  if (fail.code == NE_NOERROR)
    {
      /* Print solution, estimate of condition number and approximate */
      /* error bound */

      /* nag_gen_complx_mat_print_comp (x04dbc).
       * Print complex general matrix (comprehensive)
       */
      fflush(stdout);
      nag_gen_complx_mat_print_comp(order, Nag_GeneralMatrix, Nag_NonUnitDiag,
                                    n, nrhs, b, pdb, Nag_BracketForm, 0,
                                    "Solution", Nag_IntegerLabels, 0,
                                    Nag_IntegerLabels, 0, 80, 0, 0,
                                    &fail);
```

```
        if (fail.code != NE_NOERROR)
          {
            printf(
                    "Error from nag_gen_complx_mat_print_comp (x04dbc).\n%s\n",
                    fail.message);
            exit_status = 1;
            goto END;
          }

        printf("\n");

        printf("%s\n%8s%10.1e\n", "Estimate of condition number", "",
               1.0/rcond);
        printf("\n\n");
        printf("%s\n%8s%10.1e\n\n",
               "Estimate of error bound for computed solutions", "", errbnd);
      }
    else if (fail.code == NE_RCOND)
      {
        /* Matrix A is numerically singular.  Print estimate of */
        /* reciprocal of condition number and solution */

        printf("\n");
        printf("%s\n%8s%10.1e\n\n\n",
               "Estimate of reciprocal of condition number", "", rcond);
        /* nag_gen_complx_mat_print_comp (x04dbc), see above. */
        fflush(stdout);
        nag_gen_complx_mat_print_comp(order, Nag_GeneralMatrix, Nag_NonUnitDiag,
                                      n, nrhs, b, pdb, Nag_BracketForm, 0,
                                      "Solution", Nag_IntegerLabels, 0,
                                      Nag_IntegerLabels, 0, 80, 0, 0,
                                      &fail);
        if (fail.code != NE_NOERROR)
          {
            printf(
                    "Error from nag_gen_complx_mat_print_comp (x04dbc).\n%s\n",
                    fail.message);
            exit_status = 1;
            goto END;
          }
      }
    else if (fail.code == NE_SINGULAR)
      {
        /* The upper triangular matrix U is exactly singular.  Print */
        /* details of factorization */

        printf("\n");
        /* nag_pack_complx_mat_print_comp (x04ddc).
         * Print complex packed triangular matrix (comprehensive)
         */
        fflush(stdout);
        nag_pack_complx_mat_print_comp(order, Nag_Upper, Nag_NonUnitDiag, n, ap,
                                       Nag_BracketForm, 0,
                                       "Details of factorization",
                                       Nag_IntegerLabels, 0, Nag_IntegerLabels,
                                       0, 80, 0, 0, &fail);
        if (fail.code != NE_NOERROR)
          {
            printf(
                    "Error from nag_pack_complx_mat_print_comp (x04ddc).\n%s\n",
                    fail.message);
            exit_status = 1;
            goto END;
          }

        /* Print pivot indices */
        printf("\n");
        printf("%s\n", "Pivot indices");

        for (i = 1; i <= n; ++i)
          {
```

```
            printf("%11"NAG_IFMT"%s", ipiv[i - 1], i%7 == 0 || i == n?"\n":" ");
          }
        printf("\n");
      }
    else
      {
        printf(
                "Error from nag_complex_sym_packed_lin_solve (f04djc).\n%s\n",
                fail.message);
        exit_status = 1;
        goto END;
      }
 END:
  NAG_FREE(clabs);
  NAG_FREE(rlabs);
  NAG_FREE(ap);
  NAG_FREE(b);
  NAG_FREE(ipiv);

  return exit_status;
}

#undef B
```

10.2 Program Data

```
nag_complex_sym_packed_lin_solve (f04djc) Example Program Data

    4                 2                                        :N and NRHS
    Nag_Upper                                                 :UPLO
 ( -0.56,  0.12) ( -1.54, -2.86) (  5.32, -1.59) (  3.80,  0.92)
                 ( -2.83 ,-0.03) ( -3.52,  0.58) ( -7.86, -2.96)
                                 (  8.86,  1.81) (  5.14, -0.64)
                                                 ( -0.39 ,-0.71) :End matrix A

 ( -6.43, 19.24) ( -4.59,-35.53)
 ( -0.49, -1.47) (  6.95, 20.49)
 (-48.18, 66.00) (-12.08,-27.02)
 (-55.64, 41.22) (-19.09,-35.97)                               :End matrix B
```

10.3 Program Results

```
nag_complex_sym_packed_lin_solve (f04djc) Example Program Results

 Solution
                           1                            2
 1 (     -4.0000,     3.0000) (     -1.0000,     1.0000)
 2 (      3.0000,    -2.0000) (      3.0000,     2.0000)
 3 (     -2.0000,     5.0000) (      1.0000,    -3.0000)
 4 (      1.0000,    -1.0000) (     -2.0000,    -1.0000)

Estimate of condition number
         2.1e+01


Estimate of error bound for computed solutions
         2.3e-15
```