NAG C Library Function Document

nag_zpptrf (f07grc)

1 Purpose

nag_zpptrf (f07grc) computes the Cholesky factorization of a complex Hermitian positive-definite matrix, using packed storage.

2 Specification

```
void nag_zpptrf (Nag_OrderType order, Nag_UploType uplo, Integer n, Complex ap[],
     NagError *fail)
```

3 Description

nag_zpptrf (f07grc) forms the Cholesky factorization of a complex Hermitian positive-definite matrix A either as $A = U^H U$ if **uplo** = **Nag_Upper**, or $A = LL^H$ if **uplo** = **Nag_Lower**, where U is an upper triangular matrix and L is lower triangular, using packed storage.

4 References

Demmel J W (1989) On floating-point errors in Cholesky *LAPACK Working Note No. 14* University of Tennessee, Knoxville

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

5 Parameters

1: **order** – Nag_OrderType *Input*

On entry: the **order** parameter 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 2.2.1.4 of the Essential Introduction for a more detailed explanation of the use of this parameter.

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

2: **uplo** – Nag_UploType *Input*

On entry: indicates whether the upper or lower triangular part of A is stored and how A is factorized, as follows:

if **uplo** = **Nag_Upper**, then the upper triangular part of A is stored and A is factorized as $U^H U$, where U is upper triangular;

if **uplo** = **Nag_Lower**, then the lower triangular part of A is stored and A is factorized as LL^H, where L is lower triangular.

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

3: **n** – Integer *Input*

On entry: n, the order of the matrix A.

Constraint: **n** ≥ 0.

4: **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 Hermitian positive-definite matrix A, packed by rows or columns. The storage of elements a_{ij} depends on the **order** and **uplo** parameters 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: the upper or lower triangle of A is overwritten by the Cholesky factor U or L as specified by **uplo**, using the same packed storage format as described above.

5: **fail** – NagError * *Output*

The NAG error parameter (see the Essential Introduction).

6 Error Indicators and Warnings

NE_INT

On entry, **n** = ⟨*value*⟩.
Constraint: **n** ≥ 0.

NE_POS_DEF

The leading minor of order ⟨*value*⟩ is not positive-definite and the factorization could not be completed. Hence A itself is not positive-definite. This may indicate an error in forming the matrix A. To factorize a Hermitian matrix which is not positive-definite, call nag_zhptrf (f07prc) instead.

NE_ALLOC_FAIL

Memory allocation failed.

NE_BAD_PARAM

On entry, parameter ⟨*value*⟩ had an illegal value.

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 consult NAG for assistance.

7 Accuracy

If **uplo** = **Nag_Upper**, the computed factor U is the exact factor of a perturbed matrix $A + E$, where

$$|E| \leq c(n)\epsilon|U^H|\,|U|,$$

$c(n)$ is a modest linear function of n, and ϵ is the ***machine precision***.

If **uplo** = **Nag_Lower**, a similar statement holds for the computed factor L. It follows that $|e_{ij}| \leq c(n)\epsilon\sqrt{a_{ii}a_{jj}}$.

8 Further Comments

The total number of real floating-point operations is approximately $\frac{4}{3}n^3$.

A call to this function may be followed by calls to the functions:

nag_zpptrs (f07gsc) to solve $AX = B$;

nag_zppcon (f07guc) to estimate the condition number of A;

nag_zpptri (f07gwc) to compute the inverse of A.

The real analogue of this function is nag_dpptrf (f07gdc).

9 Example

To compute the Cholesky factorization of the matrix A, where

$$A = \begin{pmatrix} 3.23 + 0.00i & 1.51 - 1.92i & 1.90 + 0.84i & 0.42 + 2.50i \\ 1.51 + 1.92i & 3.58 + 0.00i & -0.23 + 1.11i & -1.18 + 1.37i \\ 1.90 - 0.84i & -0.23 - 1.11i & 4.09 + 0.00i & 2.33 - 0.14i \\ 0.42 - 2.50i & -1.18 - 1.37i & 2.33 + 0.14i & 4.29 + 0.00i \end{pmatrix}.$$

using packed storage.

9.1 Program Text

```
/* nag_zpptrf (f07grc) Example Program.
 *
 * Copyright 2001 Numerical Algorithms Group.
 *
 * Mark 7, 2001.
 */

#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf07.h>
#include <nagx04.h>

int main(void)
{
  /* Scalars */
  Integer  ap_len, i, j, n;
  Integer  exit_status=0;
  NagError fail;
  Nag_UploType  uplo_enum;
  Nag_OrderType order;

  /* Arrays */
  char    uplo[2];
  Complex *ap=0;

#ifdef NAG_COLUMN_MAJOR
#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]
  order = Nag_ColMajor;
#else
#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]
  order = Nag_RowMajor;
#endif

  INIT_FAIL(fail);
  Vprintf("f07grc Example Program Results\n\n");

  /* Skip heading in data file */
  Vscanf("%*[^\n] ");
  Vscanf("%ld%*[^\n] ", &n);
  ap_len = n * (n + 1)/2;

  /* Allocate memory */
  if ( !(ap = NAG_ALLOC(ap_len, Complex)) )
    {
      Vprintf("Allocation failure\n");
```

```
      exit_status = -1;
      goto END;
    }

  /* Read A from data file */
  Vscanf(" ' %1s '%*[^\n] ", uplo);
  if (*(unsigned char *)uplo == 'L')
    uplo_enum = Nag_Lower;
  else if (*(unsigned char *)uplo == 'U')
    uplo_enum = Nag_Upper;
  else
    {
      Vprintf("Unrecognised character for Nag_UploType type\n");
      exit_status = -1;
      goto END;
    }
  if (uplo_enum == Nag_Upper)
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = i; j <= n; ++j)
            Vscanf(" ( %lf , %lf )", &A_UPPER(i,j).re, &A_UPPER(i,j).im);
        }
      Vscanf("%*[^\n] ");
    }
  else
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = 1; j <= i; ++j)
            Vscanf(" ( %lf , %lf )", &A_LOWER(i,j).re, &A_LOWER(i,j).im);
        }
      Vscanf("%*[^\n] ");
    }
  /* Factorize A */
  f07grc(order, uplo_enum, n, ap, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from f07grc.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Print details of factorization */
  x04ddc(order, uplo_enum, Nag_NonUnitDiag, n, ap,
         Nag_BracketForm, "%7.4f", "Factor", Nag_IntegerLabels,
         0, Nag_IntegerLabels, 0, 80, 0, 0, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from x04ddc.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }

 END:
  if (ap) NAG_FREE(ap);
  return exit_status;
}
```

9.2 Program Data

```
f07grc Example Program Data
  4                                                        :Value of N
  'L'                                                      :Value of UPLO
 (3.23, 0.00)
 (1.51, 1.92) ( 3.58, 0.00)
 (1.90,-0.84) (-0.23,-1.11) ( 4.09, 0.00)
 (0.42,-2.50) (-1.18,-1.37) ( 2.33, 0.14) ( 4.29, 0.00)  :End of matrix A
```

9.3 Program Results

```
f07grc Example Program Results

 Factor
                    1                  2                  3                  4
 1  ( 1.7972, 0.0000)
 2  ( 0.8402, 1.0683)  ( 1.3164, 0.0000)
 3  ( 1.0572,-0.4674)  (-0.4702, 0.3131)  ( 1.5604, 0.0000)
 4  ( 0.2337,-1.3910)  ( 0.0834, 0.0368)  ( 0.9360, 0.9900)  ( 0.6603, 0.0000)
```