NAG 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

```
#include <nag.h>
#include <nagf07.h>
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 $A = U^{\mathrm{H}}U$ if **uplo** = Nag_Upper or $A = LL^{\mathrm{H}}$ 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 http://www.netlib.org/lapack/lawnspdf/lawn14.pdf

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

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 2.3.1.3 in How to Use the NAG Library and its Documentation 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: specifies whether the upper or lower triangular part of A is stored and how A is to be factorized.

uplo = Nag_Upper
The upper triangular part of A is stored and A is factorized as $U^{\mathrm{H}}U$, where U is upper triangular.

uplo = Nag_Lower
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: $\mathbf{n} \geq 0$.

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 n by n Hermitian matrix A, packed by rows or columns.

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 **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 **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 **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 **ap**$[(i-1) \times i/2 + j - 1]$, for $i \geq j$.

On exit: if **fail.code** = NE_NOERROR, the factor U or L from the Cholesky factorization $A = U^{\mathrm{H}}U$ or $A = LL^{\mathrm{H}}$, in the same storage format as A.

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

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.
See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

NE_BAD_PARAM

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

NE_INT

On entry, **n** = ⟨*value*⟩.
Constraint: $\mathbf{n} \geq 0$.

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 2.7.6 in How to Use the NAG Library and its Documentation for further information.

NE_NO_LICENCE

Your licence key may have expired or may not have been installed correctly.
See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

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.

7 Accuracy

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

$$|E| \leq c(n)\epsilon\left|U^{\mathrm{H}}\right||U|,$$

$c(n)$ 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 $\left|e_{ij}\right| \leq c(n)\epsilon\sqrt{a_{ii}a_{jj}}$.

8 Parallelism and Performance

nag_zpptrf (f07grc) 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 total number of real floating-point operations is approximately $\frac{4}{3}n^3$.

A call to nag_zpptrf (f07grc) 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).

10 Example

This example computes 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.

10.1 Program Text

```
/* nag_zpptrf (f07grc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#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;
  Nag_OrderType order;
  /* Arrays */
  char nag_enum_arg[40];
  Complex *ap = 0;
#ifdef NAG_LOAD_FP
  /* The following line is needed to force the Microsoft linker
     to load floating point support */
  float force_loading_of_ms_float_support = 0;
#endif /* NAG_LOAD_FP */

#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);

  printf("nag_zpptrf (f07grc) 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 "%*[^\n] ", &n);
#else
  scanf("%" NAG_IFMT "%*[^\n] ", &n);
#endif
  ap_len = n * (n + 1) / 2;

  /* Allocate memory */
  if (!(ap = NAG_ALLOC(ap_len, Complex)))
  {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }

  /* Read A from data file */
#ifdef _WIN32
  scanf_s(" %39s%*[^\n] ", nag_enum_arg, (unsigned)_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);

  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
  }
  /* Factorize A */
  /* nag_zpptrf (f07grc).
   * Cholesky factorization of complex Hermitian
   * positive-definite matrix, packed storage
   */
  nag_zpptrf(order, uplo, n, ap, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_zpptrf (f07grc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }
  /* Print details of factorization */
  /* nag_pack_complx_mat_print_comp (x04ddc).
   * Print complex packed triangular matrix (comprehensive)
   */
  fflush(stdout);
  nag_pack_complx_mat_print_comp(order, uplo, Nag_NonUnitDiag, n, ap,
                                 Nag_BracketForm, "%7.4f", "Factor",
                                 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;
  }

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

10.2 Program Data

```
nag_zpptrf (f07grc) Example Program Data
  4                                                       :Value of n
  Nag_Lower                                               :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
```

10.3 Program Results

```
nag_zpptrf (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)
```