

NAG Library Function Document

nag_zpotrf (f07frc)

1 Purpose

nag_zpotrf (f07frc) computes the Cholesky factorization of a complex Hermitian positive definite matrix.

2 Specification

```
#include <nag.h>
#include <nagf07.h>
void nag_zpotrf (Nag_OrderType order, Nag_UptoType uplo, Integer n,
                 Complex a[], Integer pda, NagError *fail)
```

3 Description

nag_zpotrf (f07frc) 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.

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 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_UptoType *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 $U^H U$, 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	<i>Input</i>
<i>On entry:</i> n , the order of the matrix A .		
<i>Constraint:</i> $n \geq 0$.		
4:	a [<i>dim</i>] – Complex	<i>Input/Output</i>
Note: the dimension, <i>dim</i> , of the array a must be at least $\max(1, \mathbf{pda} \times n)$.		
<i>On entry:</i> the n by n Hermitian positive definite matrix A .		
If order = 'Nag_ColMajor', A_{ij} is stored in a [(<i>j</i> – 1) × pda + <i>i</i> – 1].		
If order = 'Nag_RowMajor', A_{ij} is stored in a [(<i>i</i> – 1) × pda + <i>j</i> – 1].		
If uplo = 'Nag_Upper', the upper triangular part of A must be stored and the elements of the array below the diagonal are not referenced.		
If uplo = 'Nag_Lower', the lower triangular part of A must be stored and the elements of the array above the diagonal are not referenced.		
<i>On exit:</i> the upper or lower triangle of A is overwritten by the Cholesky factor U or L as specified by uplo .		
5:	pda – Integer	<i>Input</i>
<i>On entry:</i> the stride separating row or column elements (depending on the value of order) of the matrix A in the array a .		
<i>Constraint:</i> pda ≥ $\max(1, n)$.		
6:	fail – NagError *	<i>Input/Output</i>
The NAG error argument (see Section 3.6 in the Essential Introduction).		

6 Error Indicators and Warnings

NE_BAD_PARAM

On entry, argument $\langle value \rangle$ had an illegal value.

NE_INT

On entry, **n** = $\langle value \rangle$.
Constraint: **n** ≥ 0.

On entry, **pda** = $\langle value \rangle$.
Constraint: **pda** > 0.

NE_INT_2

On entry, **pda** = $\langle value \rangle$ and **n** = $\langle value \rangle$.
Constraint: **pda** ≥ $\max(1, n)$.

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.

NE_POS_DEF

The leading minor of order $\langle value \rangle$ 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_zhetrf (f07mrc) instead.

7 Accuracy

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

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

$c(n)$ 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 Parallelism and Performance

`nag_zpotrf` (f07frc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

`nag_zpotrf` (f07frc) 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 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_zpotrf` (f07frc) may be followed by calls to the functions:

- `nag_zpotrs` (f07fsc) to solve $AX = B$;
- `nag_zpocon` (f07fuc) to estimate the condition number of A ;
- `nag_zpotri` (f07fwc) to compute the inverse of A .

The real analogue of this function is `nag_dpotrf` (f07fdc).

10 Example

This example computes the Cholesky factorization of the matrix A , where

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

10.1 Program Text

```
/* nag_zpotrf (f07frc) Example Program.
*
* Copyright 2001 Numerical Algorithms Group.
*
* Mark 7, 2001.
*/
#include <stdio.h>
#include <nag.h>
#include <nag_stdl�.h>
#include <nagf07.h>
#include <nagx04.h>

int main(void)
{
    /* Scalars */
    Integer i, j, n, pda;
    Integer exit_status = 0;
    Nag_UptoType uplo;
    Nag_MatrixType matrix;
```

```

NagError      fail;
Nag_OrderType order;
/* Arrays */
char          nag_enum_arg[40];
Complex       *a = 0;

#ifndef NAG_COLUMN_MAJOR
#define A(I, J) a[(J-1)*pda + I - 1]
    order = Nag_ColMajor;
#else
#define A(I, J) a[(I-1)*pda + J - 1]
    order = Nag_RowMajor;
#endif

INIT_FAIL(fail);

printf("nag_zpotrf (f07frc) Example Program Results\n\n");

/* Skip heading in data file */
scanf("%*[^\n] ");
scanf("%ld%*[^\n] ", &n);
#ifndef NAG_COLUMN_MAJOR
pda = n;
#else
pda = n;
#endif

/* Allocate memory */
if (!(a = NAG_ALLOC(n* n, Complex)))
{
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
}
/* Read A from data file */
scanf(" %9s%*[^\n] ", nag_enum_arg);
/* nag_enum_name_to_value (x04nac).
 * Converts NAG enum member name to value
 */
uplo = (Nag_UptoType) nag_enum_name_to_value(nag_enum_arg);

if (uplo == Nag_Upper)
{
    matrix = Nag_UpperMatrix;
    for (i = 1; i <= n; ++i)
    {
        for (j = i; j <= n; ++j)
            scanf("( %lf , %lf )", &A(i, j).re, &A(i, j).im);
    }
    scanf("%*[^\n] ");
}
else
{
    matrix = Nag_LowerMatrix;
    for (i = 1; i <= n; ++i)
    {
        for (j = 1; j <= i; ++j)
            scanf("( %lf , %lf )", &A(i, j).re, &A(i, j).im);
    }
    scanf("%*[^\n] ");
}

/* Factorize A */
/* nag_zpotrf (f07frc).
 * Cholesky factorization of complex Hermitian
 * positive-definite matrix
 */
nag_zpotrf(order, uplo, n, a, pda, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_zpotrf (f07frc).\n%s\n", fail.message);
}

```

```

    exit_status = 1;
    goto END;
}
/* Print factor */
/* nag_gen_complx_mat_print_comp (x04dbc).
 * Print complex general matrix (comprehensive)
 */
fflush(stdout);
nag_gen_complx_mat_print_comp(order, matrix, Nag_NonUnitDiag, n, n, a, pda,
                               Nag_BracketForm, "%7.4f", "Factor",
                               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;
}
END:
NAG_FREE(a);
return exit_status;
}

```

10.2 Program Data

```
nag_zpotrf (f07frc) 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_zpotrf (f07frc) 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)	
