NAG C Library Function Document

nag_zhetrf (f07mrc)

1 Purpose

nag_zhetrf (f07mrc) computes the Bunch–Kaufman factorization of a complex Hermitian indefinite matrix.

2 Specification

```
void nag_zhetrf (Nag_OrderType order, Nag_UploType uplo, Integer n, Complex a[],
     Integer pda, Integer ipiv[], NagError *fail)
```

3 Description

nag_zhetrf (f07mrc) factorizes a complex Hermitian matrix A, using the Bunch–Kaufman diagonal pivoting method. A is factorized as either $A = PUDU^HP^T$ if **uplo** = **Nag_Upper**, or $A = PLDL^HP^T$ if **uplo** = **Nag_Lower**, where P is a permutation matrix, U (or L) is a unit upper (or lower) triangular matrix and D is an Hermitian block diagonal matrix with 1 by 1 and 2 by 2 diagonal blocks; U (or L) has 2 by 2 unit diagonal blocks corresponding to the 2 by 2 blocks of D. Row and column interchanges are performed to ensure numerical stability while keeping the matrix Hermitian.

This method is suitable for Hermitian matrices which are not known to be positive-definite. If A is in fact positive-definite, no interchanges are performed and no 2 by 2 blocks occur in D.

4 References

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 has been factorized, as follows:

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

if **uplo** = **Nag_Lower**, the lower triangular part of A is stored and A is factorized as $PLDL^HP^T$, 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: **a**[dim] – Complex *Input/Output*

Note: the dimension, dim, of the array **a** must be at least $\max(1, \textbf{pda} \times \textbf{n})$.

If **order** = **Nag_ColMajor**, the (i,j)th element of the matrix A is stored in **a**$[(j-1) \times \textbf{pda} + i - 1]$ and if **order** = **Nag_RowMajor**, the (i,j)th element of the matrix A is stored in **a**$[(i-1) \times \textbf{pda} + j - 1]$.

On entry: the n by n Hermitian matrix A. If **uplo** = **Nag_Upper**, the upper triangle of A must be stored and the elements of the array below the diagonal are not referenced; if **uplo** = **Nag_Lower**, the lower triangle of A must be stored and the elements of the array above the diagonal are not referenced.

On exit: the upper or lower triangle of A is overwritten by details of the block diagonal matrix D and the multipliers used to obtain the factor U or L as specified by **uplo**.

5: **pda** – Integer *Input*

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

Constraint: **pda** $\geq \max(1, \textbf{n})$.

6: **ipiv**[dim] – Integer *Output*

Note: the dimension, dim, of the array **ipiv** must be at least $\max(1, \textbf{n})$.

On exit: details of the interchanges and the block structure of D.

More precisely, if **ipiv**$[i-1] = k > 0$, d_{ii} is a 1 by 1 pivot block and the ith row and column of A were interchanged with the kth row and column.

If **uplo** = **Nag_Upper** and **ipiv**$[i-2]$ = **ipiv**$[i-1] = -l < 0$, $\begin{pmatrix} d_{i-1,i-1} & d_{i,i-1} \\ d_{i,i-1} & d_{ii} \end{pmatrix}$ is a 2 by 2 pivot block and the $(i-1)$th row and column of A were interchanged with the lth row and column.

If **uplo** = **Nag_Lower** and **ipiv**$[i-1]$ = **ipiv**$[i] = -m < 0$, $\begin{pmatrix} d_{ii} & d_{i+1,i} \\ d_{i+1,i} & d_{i+1,i+1} \end{pmatrix}$ is a 2 by 2 pivot block and the $(i+1)$th row and column of A were interchanged with the mth row and column.

7: **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.

On entry, **pda** = ⟨*value*⟩.
Constraint: **pda** > 0.

NE_INT_2

On entry, **pda** = ⟨*value*⟩, **n** = ⟨*value*⟩.
Constraint: **pda** $\geq \max(1, \textbf{n})$.

NE_SINGULAR

The block diagonal matrix D is exactly singular.

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 factors U and D are the exact factors of a perturbed matrix $A + E$, where

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

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

If **uplo** $=$ **Nag_Lower**, a similar statement holds for the computed factors L and D.

8 Further Comments

The elements of D overwrite the corresponding elements of A; if D has 2 by 2 blocks, only the upper or lower triangle is stored, as specified by **uplo**.

The unit diagonal elements of U or L and the 2 by 2 unit diagonal blocks are not stored. The remaining elements of U or L are stored in the corresponding columns of the array **a**, but additional row interchanges must be applied to recover U or L explicitly (this is seldom necessary). If **ipiv**$[i-1] = i$, for $i = 1, 2, \ldots, n$ (as is the case when A is positive-definite), then U or L is stored explicitly (except for its unit diagonal elements which are equal to 1).

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_zhetrs (f07msc) to solve $AX = B$;

nag_zhecon (f07muc) to estimate the condition number of A;

nag_zhetri (f07mwc) to compute the inverse of A.

The real analogue of this function is nag_dsytrf (f07mdc).

9 Example

To compute the Bunch–Kaufman factorization of the matrix A, where

$$A = \begin{pmatrix} -1.36 + 0.00i & 1.58 + 0.90i & 2.21 - 0.21i & 3.91 + 1.50i \\ 1.58 - 0.90i & -8.87 + 0.00i & -1.84 - 0.03i & -1.78 + 1.18i \\ 2.21 + 0.21i & -1.84 + 0.03i & -4.63 + 0.00i & 0.11 + 0.11i \\ 3.91 - 1.50i & -1.78 - 1.18i & 0.11 - 0.11i & -1.84 + 0.00i \end{pmatrix}.$$

9.1 Program Text

```
/* nag_zhetrf (f07mrc) 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 i, j, n, pda;
  Integer exit_status=0;
  Nag_UploType uplo_enum;
  Nag_MatrixType matrix;

  NagError fail;
  Nag_OrderType order;
  /* Arrays */
  Integer *ipiv=0;
  char    uplo[2];
  Complex *a=0;

#ifdef 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);
  Vprintf("f07mrc Example Program Results\n\n");

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

  /* Allocate memory */
  if ( !(ipiv = NAG_ALLOC(n, Integer)) ||
       !(a = NAG_ALLOC(n* n, 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;
      matrix = Nag_LowerMatrix;
    }
  else if (*(unsigned char *)uplo == 'U')
    {
      uplo_enum = Nag_Upper;
      matrix = Nag_UpperMatrix;
    }
  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(i,j).re, &A(i,j).im);
        }
      Vscanf("%*[^\n] ");
    }
  else
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = 1; j <= i; ++j)
            Vscanf(" ( %lf , %lf )", &A(i,j).re, &A(i,j).im);
        }
      Vscanf("%*[^\n] ");
    }

  /* Factorize A */
  f07mrc(order, uplo_enum, n, a, pda, ipiv, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from f07mrc.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Print factor */
  x04dbc(order, matrix, Nag_NonUnitDiag, n, n, a, pda, Nag_BracketForm,
         "%7.4f", "Details of Factorixation", Nag_IntegerLabels, 0,
         Nag_IntegerLabels, 0, 80, 0, 0, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from x04dbc.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Print pivot indices */
  Vprintf("\nIPIV\n");
  for (i = 1; i <= n; ++i)
    Vprintf("%31d%s", ipiv[i-1], i%7==0 ?"\n":"               ");
  Vprintf("\n");
 END:
  if (ipiv) NAG_FREE(ipiv);
  if (a) NAG_FREE(a);
  return exit_status;
}
```

9.2 Program Data

```
f07mrc Example Program Data
  4                                                        :Value of N
  'U'                                                      :Value of UPLO
 (-1.36, 0.00) ( 1.58, 0.90) ( 2.21,-0.21) ( 3.91, 1.50)
               (-8.87, 0.00) (-1.84,-0.03) (-1.78, 1.18)
                             (-4.63, 0.00) ( 0.11, 0.11)
                                           (-1.84, 0.00)  :End of matrix A
```

9.3 Program Results

```
f07mrc Example Program Results

 Details of Factorixation
                    1                  2                  3                  4
 1  (-1.3600, 0.0000)  ( 3.9100, 1.5000)  ( 0.3100,-0.0433)  (-0.1518,-0.3743)
 2                     (-1.8400, 0.0000)  ( 0.5637,-0.2850)  ( 0.3397,-0.0303)
 3                                        (-5.4176, 0.0000)  ( 0.2997,-0.1578)
 4                                                           (-7.1028, 0.0000)

IPIV
 -4                 -4                 3                  4
```