NAG Library Function Document

nag_zupmtr (f08guc)

1 Purpose

nag_zupmtr (f08guc) multiplies an arbitrary complex matrix $C$ by the complex unitary matrix $Q$ which was determined by nag_zhptrd (f08gsc) when reducing a complex Hermitian matrix to tridiagonal form.

2 Specification

```c
#include <nag.h>
#include <nagf08.h>
void nag_zupmtr (Nag_OrderType order, Nag_SideType side, Nag_UploType uplo,
                 Nag_TransType trans, Integer m, Integer n, Complex ap[],
                 const Complex tau[], Complex c[], Integer pdc, NagError *fail)
```

3 Description

nag_zupmtr (f08guc) is intended to be used after a call to nag_zhptrd (f08gsc), which reduces a complex Hermitian matrix $A$ to real symmetric tridiagonal form $T$ by a unitary similarity transformation: $A = QTQ^H$. nag_zhptrd (f08gsc) represents the unitary matrix $Q$ as a product of elementary reflectors.

This function may be used to form one of the matrix products

$$QC, Q^HC, CQ$$

overwriting the result on $C$ (which may be any complex rectangular matrix).

A common application of this function is to transform a matrix $Z$ of eigenvectors of $T$ to the matrix $QZ$ of eigenvectors of $A$.

4 References


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:  
`sxide` – Nag_SideType

*Input*

On entry: indicates how $Q$ or $Q^H$ is to be applied to $C$.

$sxide = Nag_LeftSide$

$Q$ or $Q^H$ is applied to $C$ from the left.

$sxide = Nag_RightSide$

$Q$ or $Q^H$ is applied to $C$ from the right.

Constraint: `side = Nag_LeftSide` or `Nag_RightSide`.

Mark 25
3:  **uplo** – Nag_UploType  
*Input*
*On entry:* this must be the same argument **uplo** as supplied to nag_zhptrd (f08gsc).
*Constraint:* **uplo** = Nag_Upper or Nag_Lower.

4:  **trans** – Nag_TransType  
*Input*
*On entry:* indicates whether \( Q \) or \( Q^H \) is to be applied to \( C \).
\[ \text{trans} = \text{Nag\_NoTrans} \quad Q \text{ is applied to } C. \]
\[ \text{trans} = \text{Nag\_ConjTrans} \quad Q^H \text{ is applied to } C. \]
*Constraint:* **trans** = Nag_NoTrans or Nag_ConjTrans.

5:  **m** – Integer  
*Input*
*On entry:* \( m \), the number of rows of the matrix \( C \); \( m \) is also the order of \( Q \) if \( \text{side} = \text{Nag\_LeftSide} \).
*Constraint:* \( m \geq 0 \).

6:  **n** – Integer  
*Input*
*On entry:* \( n \), the number of columns of the matrix \( C \); \( n \) is also the order of \( Q \) if \( \text{side} = \text{Nag\_RightSide} \).
*Constraint:* \( n \geq 0 \).

7:  **ap[dim]** – Complex  
*Input/Output*
*Note:* the dimension, \( dim \), of the array \( \text{ap} \) must be at least
\[ \max(1, m \times (m + 1)/2) \text{ when } \text{side} = \text{Nag\_LeftSide}; \]
\[ \max(1, n \times (n + 1)/2) \text{ when } \text{side} = \text{Nag\_RightSide}. \]
*On entry:* details of the vectors which define the elementary reflectors, as returned by nag_zhptrd (f08gsc).
*On exit:* is used as internal workspace prior to being restored and hence is unchanged.

8:  **tau[dim]** – const Complex  
*Input*
*Note:* the dimension, \( dim \), of the array \( \text{tau} \) must be at least
\[ \max(1, m - 1) \text{ when } \text{side} = \text{Nag\_LeftSide}; \]
\[ \max(1, n - 1) \text{ when } \text{side} = \text{Nag\_RightSide}. \]
*On entry:* further details of the elementary reflectors, as returned by nag_zhptrd (f08gsc).

9:  **c[dim]** – Complex  
*Input/Output*
*Note:* the dimension, \( dim \), of the array \( \text{c} \) must be at least
\[ \max(1, \text{pdc} \times n) \text{ when } \text{order} = \text{Nag\_ColMajor}; \]
\[ \max(1, m \times \text{pdc}) \text{ when } \text{order} = \text{Nag\_RowMajor}. \]
The \( (i, j) \)th element of the matrix \( C \) is stored in
\[ c[(j - 1) \times \text{pdc} + i - 1] \text{ when } \text{order} = \text{Nag\_ColMajor}; \]
\[ c[(i - 1) \times \text{pdc} + j - 1] \text{ when } \text{order} = \text{Nag\_RowMajor}. \]
*On entry:* the \( m \) by \( n \) matrix \( C \).
*On exit:* \( \text{c} \) is overwritten by \( QC \) or \( Q^H C \) or \( CQ \) or \( CQ^H \) as specified by \( \text{side} \) and \( \text{trans} \).
10: pdc – Integer

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

Constraints:
- if order = Nag_ColMajor, pdc ≥ max(1, m);
- if order = Nag_RowMajor, pdc ≥ max(1, n).

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 ⟨value⟩ had an illegal value.

NE_INT

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

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

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

NE_INT_2

On entry, pdc = ⟨value⟩ and m = ⟨value⟩.
Constraint: pdc ≥ max(1, m).

On entry, pdc = ⟨value⟩ and n = ⟨value⟩.
Constraint: pdc ≥ 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.

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.

7 Accuracy

The computed result differs from the exact result by a matrix E such that

\[ ||E||_2 = O(\epsilon) ||C||_2, \]

where \( \epsilon \) is the machine precision.
8 Parallelism and Performance

nag_zupmtr (f08guc) is not threaded by NAG in any implementation.

nag_zupmtr (f08guc) 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 $8m^2n$ if $\text{side} = \text{Nag LeftSide}$ and $8mn^2$ if $\text{side} = \text{Nag RightSide}$.

The real analogue of this function is nag_dopmtr (f08ggc).

10 Example

This example computes the two smallest eigenvalues, and the associated eigenvectors, of the matrix $A$, where

$$ A = \begin{pmatrix}
-2.28 + 0.00i & 1.78 - 2.03i & 2.26 + 0.10i & -0.12 + 2.53i \\
1.78 + 2.03i & -1.12 + 0.00i & 0.01 + 0.43i & -1.07 + 0.86i \\
2.26 - 1.01i & 0.01 - 0.43i & -0.37 + 0.00i & 2.31 - 0.92i \\
-0.12 - 2.53i & -1.07 - 0.86i & 2.31 + 0.92i & -0.73 + 0.00i
\end{pmatrix}, $$

using packed storage. Here $A$ is Hermitian and must first be reduced to tridiagonal form $T$ by nag_zhptrd (f08gsc). The program then calls nag_dstebz (f08jjc) to compute the requested eigenvalues and nag_zstein (f08jxc) to compute the associated eigenvectors of $T$. Finally nag_zupmtr (f08guc) is called to transform the eigenvectors to those of $A$.

10.1 Program Text

/* nag_zupmtr (f08guc) Example Program. */
* Copyright 2014 Numerical Algorithms Group.
*/
#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf08.h>
#include <naga02.h>

int main(void)
{
    /* Scalars */
    Integer ap_len, i, j, m, n, nsplit, pdz, d_len, e_len;
    Integer tau_len;
    Integer exit_status = 0;
    double vl = 0.0, vu = 0.0;
    NagError fail;
    Nag_UploType uplo;
    Nag_OrderType order;
    /* Arrays */
    char nag_enum_arg[40];
    Integer *iblock = 0, *ifailv = 0, *isplit = 0;
    Complex *ap = 0, *tau = 0, *z = 0;
    double *d = 0, *e = 0, *w = 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]
#define Z(I, J) z[(J - 1) * pdz + I - 1]
#else
#define A_UPPER(I, J) ap[I * (I - 1) / 2 + J - 1]
#define A_LOWER(I, J) ap[(2 * n - I) * (I - 1) / 2 + J - 1]
#define Z(I, J) z[(I - 1) * pdz + J - 1]
#endif

order = Nag_ColMajor;
#else
order = Nag_RowMajor;
#endif

INIT_FAIL(fail);

printf("nag_zupmtr (f08guc) Example Program Results\n\n");

/* Skip heading in data file */
#ifdef _WIN32
#define _countof(x) sizeof(x)/sizeof(x[0])

#define _NAG_IFMT "%d"
#endif

/* Read A from data file */
#ifdef _WIN32
scanf_s(_NAG_IFMT _countof(nag_enum_arg), &n);
#else
scanf(_NAG_IFMT _countof(nag_enum_arg), &n);
#endif

pdz = n;
ap_len = n*(n+1)/2;
tau_len = n-1;
d_len = n;
e_len = n-1;

/* Allocate memory */
if (!(ap = NAG_ALLOC(ap_len, Complex)) ||
! (d = NAG_ALLOC(d_len, double)) ||
! (e = NAG_ALLOC(e_len, double)) ||
! (iblock = NAG_ALLOC(n, Integer)) ||
! (ifailv = NAG_ALLOC(n, Integer)) ||
! (isplit = NAG_ALLOC(n, Integer)) ||
! (w = NAG_ALLOC(n, double)) ||
! (tau = NAG_ALLOC(tau_len, Complex)) ||
! (z = NAG_ALLOC(n * n, Complex)))
{
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
}

/* Read A from data file */
#ifdef _WIN32
scanf_s(_NAG_IFMT _countof(nag_enum_arg), _countof(nag_enum_arg), &uplo);
#else
scanf(_NAG_IFMT _countof(nag_enum_arg), &uplo);
#endif

/* nag_enum_name_to_value (x04nac). */
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);
            
Mark 25 f08guc.5

f08 – Least-squares and Eigenvalue Problems (LAPACK) f08guc
#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
    }
  }
#endif
/* Reduce A to tridiagonal form T = (Q**H)*A*Q */
/* nag_zhptrd (f08gsc). */
/* Unitary reduction of complex Hermitian matrix to real */
/* symmetric tridiagonal form, packed storage */
/* nag_zhptrd(order, uplo, n, ap, d, e, tau, &fail); */
if (fail.code != NE_NOERROR)
{
  printf("Error from nag_zhptrd (f08gsc).\n%s\n", fail.message);
  exit_status = 1;
  goto END;
}
/* Calculate the two smallest eigenvalues of T (same as A) */
/* nag_dstebz (f08jjc). */
/* Selected eigenvalues of real symmetric tridiagonal matrix */
/* by bisection */
/* nag_dstebz(Nag_Indices, Nag_ByBlock, n, vl, vu, l, 2, 0.0, */
  d, e, &m, &nsplit, w, iblock, isplit, &fail);
if (fail.code != NE_NOERROR)
{
  printf("Error from nag_dstebz (f08jjc).\n%s\n", fail.message);
  exit_status = 1;
  goto END;
}
/* Print eigenvalues */
printf("Eigenvalues\n");
for (i = 0; i < m; ++i)
  printf("%8.4f%s", w[i], (i+1)%8 == 0?"\n":"");
printf("\n\n");
/* Calculate the eigenvectors of T storing the result in Z */
/* nag_zstein (f08jxc). */
/* Selected eigenvectors of real symmetric tridiagonal */
/* matrix by inverse iteration, storing eigenvectors in */
/* complex array */
/* nag_zstein(order, n, d, e, m, w, iblock, isplit, z, pdz, ifailv, */
  &fail);
if (fail.code != NE_NOERROR)
{ 
    printf("Error from nag_zstein (f08jxc).\n\"s
", fail.message); 
    exit_status = 1; 
    goto END; 
} /* Calculate all the eigenvectors of A = Q*(eigenvectors of T) */ /* nag_zupmtr (f08guc). */ 
* Apply unitary transformation matrix determined by * nag_zhptrd (f08gsc) */ 
    nag_zupmtr(order, Nag_LeftSide, uplo, Nag_NoTrans, n, m, ap, 
    tau, z, pdz, &fail); 
    if (fail.code != NE_NOERROR) 
    { 
        printf("Error from nag_zupmtr (f08guc).\n\"s
", fail.message); 
        exit_status = 1; 
        goto END; 
    } /* Normalize the eigenvectors */ 
    for(j=1; j<=m; j++) 
    { 
        for(i=n; i>=1; i--) 
        { 
            z(i, j) = nag_complex_divide(z(i, j),z(1, j)); 
        } 
    } /* Print eigenvectors */ /* nag_gen_complex_mat_print_comp (x04dbc). */ 
* Print complex general matrix (comprehensive) */ 
    fflush(stdout); 
    nag_gen_complex_mat_print_comp(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, 
    m, z, pdz, Nag_BracketForm, "%7.4f", 
    "Eigenvectors", Nag_IntegerLabels, 0, 
    Nag_IntegerLabels, 0, 80, 0, 0, &fail); 
    if (fail.code != NE_NOERROR) 
    { 
        printf( 
            "Error from nag_gen_complex_mat_print_comp (x04dbc).\n\"s
", 
            fail.message); 
        exit_status = 1; 
        goto END; 
    } 
} 
END: 
NAG_FREE(ap); 
NAG_FREE(d); 
NAG_FREE(e); 
NAG_FREE(iblock); 
NAG_FREE(ifailv); 
NAG_FREE(isplit); 
NAG_FREE(tau); 
NAG_FREE(w); 
NAG_FREE(z); 
return exit_status; 
} 

10.2 Program Data 

nag_zupmtr (f08guc) Example Program Data 

<table>
<thead>
<tr>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
</tr>
<tr>
<td>Nag_Upper</td>
</tr>
<tr>
<td>(-2.28, 0.00) (-1.78, -2.03) (2.26, 0.10) (-0.12, 2.53)</td>
</tr>
<tr>
<td>(-1.12, 0.00) (0.01, 0.43) (-1.07, 0.86)</td>
</tr>
<tr>
<td>(-0.37, 0.00) (2.31, -0.92)</td>
</tr>
<tr>
<td>(-0.73, 0.00)</td>
</tr>
</tbody>
</table>

:Value of n
:Value of uplo
:End of matrix A
10.3 Program Results

nag_zupmtr (f08guc) Example Program Results

Eigenvalues
-6.0002       -3.0030

Eigenvectors

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( 1.0000, 0.0000)</td>
<td>( 1.0000, -0.0000)</td>
</tr>
<tr>
<td>2</td>
<td>(-0.2278, -0.2824)</td>
<td>(-2.2999, -1.6237)</td>
</tr>
<tr>
<td>3</td>
<td>(-0.5706, -0.1941)</td>
<td>( 1.1424, 0.5807)</td>
</tr>
<tr>
<td>4</td>
<td>( 0.2388, 0.5702)</td>
<td>(-1.3415, -1.5739)</td>
</tr>
</tbody>
</table>