NAG Library Routine Document

F08GTF (ZUPGTR)

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details.

1 Purpose

F08GTF (ZUPGTR) generates the complex unitary matrix Q, which was determined by F08GSF (ZHPTRD) when reducing a Hermitian matrix to tridiagonal form.

2 Specification

```
SUBROUTINE F08GTF(UPLO, N, AP, TAU, Q, LDQ, WORK, INFO)
INTEGER           N, LDQ, INFO
complex*16        AP(*), TAU(*), Q(LDQ,*), WORK(N-1)
CHARACTER*1       UPLO
```

The routine may be called by its LAPACK name ***zupgtr***.

3 Description

F08GTF (ZUPGTR) is intended to be used after a call to F08GSF (ZHPTRD), which reduces a complex Hermitian matrix A to real symmetric tridiagonal form T by a unitary similarity transformation: $A = QTQ^{\mathrm{H}}$. F08GSF (ZHPTRD) represents the unitary matrix Q as a product of $n-1$ elementary reflectors.

This routine may be used to generate Q explicitly as a square matrix.

4 References

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

5 Parameters

1: UPLO – CHARACTER*1 *Input*

On entry: this **must** be the same parameter UPLO as supplied to F08GSF (ZHPTRD).

Constraint: UPLO = 'U' or 'L'.

2: N – INTEGER *Input*

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

Constraint: $\mathrm{N} \geq 0$.

3: AP$(*)$ – ***complex*16*** array *Input*

Note: the dimension of the array AP must be at least $\max(1, \mathrm{N} \times (\mathrm{N}+1)/2)$.

On entry: details of the vectors which define the elementary reflectors, as returned by F08GSF (ZHPTRD).

4: TAU$(*)$ – ***complex*16*** array *Input*

Note: the dimension of the array TAU must be at least $\max(1, \mathrm{N}-1)$.

On entry: further details of the elementary reflectors, as returned by F08GSF (ZHPTRD).

5: Q(LDQ,$*$) – ***complex*16*** array *Output*

Note: the second dimension of the array Q must be at least $\max(1, \mathrm{N})$.

On exit: the n by n unitary matrix Q.

6: LDQ – INTEGER *Input*

On entry: the first dimension of the array Q as declared in the (sub)program from which F08GTF (ZUPGTR) is called.

Constraint: LDQ $\geq \max(1, \mathrm{N})$.

7: WORK(N $-$ 1) – ***complex*16*** array *Workspace*

8: INFO – INTEGER *Output*

On exit: INFO $= 0$ unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the routine:

INFO < 0

If INFO $= -i$, argument i had an illegal value. An explanatory message is output, and execution of the program is terminated.

7 Accuracy

The computed matrix Q differs from an exactly unitary matrix by a matrix E such that

$$\|E\|_2 = O(\epsilon),$$

where ϵ is the ***machine precision***.

8 Further Comments

The total number of real floating-point operations is approximately $\frac{16}{3}n^3$.

The real analogue of this routine is F08GFF (DOPGTR).

9 Example

This example computes all the eigenvalues and eigenvectors of the matrix A, where

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

using packed storage. Here A is Hermitian and must first be reduced to tridiagonal form by F08GSF (ZHPTRD). The program then calls F08GTF (ZUPGTR) to form Q, and passes this matrix to F08JSF (ZSTEQR) which computes the eigenvalues and eigenvectors of A.

9.1 Program Text

```
*     F08GTF Example Program Text
*     Mark 16 Release. NAG Copyright 1992.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, LDQ
      PARAMETER        (NMAX=8,LDQ=NMAX)
```

```
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INFO, J, N
      CHARACTER        UPLO
*     .. Local Arrays ..
      COMPLEX *16      AP(NMAX*(NMAX+1)/2), Q(LDQ,NMAX), TAU(NMAX),
     +                 WORK(NMAX-1)
      DOUBLE PRECISION D(NMAX), E(NMAX), RWORK(2*NMAX-2)
      CHARACTER        CLABS(1), RLABS(1)
*     .. External Subroutines ..
      EXTERNAL         X04DBF, ZHPTRD, ZSTEQR, ZUPGTR
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F08GTF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*        Read A from data file
*
         READ (NIN,*) UPLO
         IF (UPLO.EQ.'U') THEN
            READ (NIN,*) ((AP(I+J*(J-1)/2),J=I,N),I=1,N)
         ELSE IF (UPLO.EQ.'L') THEN
            READ (NIN,*) ((AP(I+(2*N-J)*(J-1)/2),J=1,I),I=1,N)
         END IF
*
*        Reduce A to tridiagonal form T = (Q**H)*A*Q
*
         CALL ZHPTRD(UPLO,N,AP,D,E,TAU,INFO)
*
*        Form Q explicitly, storing the result in Q
*
         CALL ZUPGTR(UPLO,N,AP,TAU,Q,LDQ,WORK,INFO)
*
*        Calculate all the eigenvalues and eigenvectors of A
*
         CALL ZSTEQR('V',N,D,E,Q,LDQ,RWORK,INFO)
*
         WRITE (NOUT,*)
         IF (INFO.GT.0) THEN
            WRITE (NOUT,*) 'Failure to converge.'
         ELSE
*
*           Print eigenvalues and eigenvectors
*
            WRITE (NOUT,*) 'Eigenvalues'
            WRITE (NOUT,99999) (D(I),I=1,N)
            WRITE (NOUT,*)
            IFAIL = 0
*
            CALL X04DBF('General',' ',N,N,Q,LDQ,'Bracketed','F7.4',
     +                  'Eigenvectors','Integer',RLABS,'Integer',CLABS,
     +                  80,0,IFAIL)
*
         END IF
      END IF
*
99999 FORMAT (8X,4(F7.4,11X,:))
      END
```

9.2 Program Data

```
F08GTF Example Program Data
  4                                                          :Value of N
  'L'                                                        :Value of UPLO
 (-2.28, 0.00)
 ( 1.78, 2.03) (-1.12, 0.00)
 ( 2.26,-0.10) ( 0.01,-0.43) (-0.37, 0.00)
 (-0.12,-2.53) (-1.07,-0.86) ( 2.31, 0.92) (-0.73, 0.00)   :End of matrix A
```

9.3 Program Results

```
 F08GTF Example Program Results

 Eigenvalues
       -6.0002           -3.0030            0.5036            3.9996

 Eigenvectors
                     1                 2                 3                 4
 1  ( 0.7299, 0.0000) (-0.2120, 0.1497) ( 0.1000,-0.3570) ( 0.1991, 0.4720)
 2  (-0.1663,-0.2061) ( 0.7307, 0.0000) ( 0.2863,-0.3353) (-0.2467, 0.3751)
 3  (-0.4165,-0.1417) (-0.3291, 0.0479) ( 0.6890, 0.0000) ( 0.4468, 0.1466)
 4  ( 0.1743, 0.4162) ( 0.5200, 0.1329) ( 0.0662, 0.4347) ( 0.5612, 0.0000)
```