F08GTF (CUPGTR/ZUPGTR) – NAG Fortran Library Routine Document

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

2 Specification

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

The ENTRY statement enables the routine to be called by its LAPACK name.

3 Description

This routine is intended to be used after a call to F08GSF (CHPTRD/ZHPTRD), which reduces a complex Hermitian matrix A to real symmetric tridiagonal form T by a unitary similarity transformation: $A = QTQ^H$. F08GSF 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

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

5 Parameters

1: UPLO — CHARACTER*1 *Input*

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

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

2: N — INTEGER *Input*

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

Constraint: N $\geq$ 0.

3: AP(∗) — ***complex*** array *Input*

Note: the dimension of the array AP must be at least max(1,N∗(N+1)/2).

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

4: TAU(∗) — ***complex*** array *Input*

Note: the dimension of the array TAU must be at least max(1,N−1).

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

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

Note: the second dimension of the array Q must be at least max(1,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 (CUPGTR/ZUPGTR) is called.

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

7: WORK($*$) — ***complex*** array *Workspace*

Note: the dimension of the array WORK must be at least max(1,N−1).

8: INFO — INTEGER *Output*

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

6 Error Indicators and Warnings

INFO < 0

If INFO $= -i$, the ith parameter 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 $\frac{16n^3}{3}$.

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

9 Example

To compute 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 (CHPTRD/ZHPTRD). The program then calls F08GTF (CUPGTR/ZUPGTR) to form Q, and passes this matrix to F08JSF (CSTEQR/ZSTEQR) which computes the eigenvalues and eigenvectors of A.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     F08GTF Example Program Text
*     Mark 16 Release. NAG Copyright 1992.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, LDZ
      PARAMETER        (NMAX=8,LDZ=NMAX)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, INFO, J, N
      CHARACTER        UPLO
*     .. Local Arrays ..
      complex          AP(NMAX*(NMAX+1)/2), TAU(NMAX), WORK(NMAX-1),
     +                 Z(LDZ,NMAX)
      real             D(NMAX), E(NMAX), RWORK(2*NMAX-2)
      CHARACTER        CLABS(1), RLABS(1)
*     .. External Subroutines ..
      EXTERNAL         X04DBF, chptrd, csteqr, cupgtr
*     .. 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 chptrd(UPLO,N,AP,D,E,TAU,INFO)
*
*        Form Q explicitly, storing the result in Z
*
         CALL cupgtr(UPLO,N,AP,TAU,Z,LDZ,WORK,INFO)
*
*        Calculate all the eigenvalues and eigenvectors of A
*
         CALL csteqr('V',N,D,E,Z,LDZ,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,Z,LDZ,'Bracketed','F7.4',
     +                  'Eigenvectors','Integer',RLABS,'Integer',CLABS,
     +                  80,0,IFAIL)
*
         END IF
      END IF
      STOP
*
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)
```
