NAG Library Routine Document

F08CTF (ZUNGQL)

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

F08CTF (ZUNGQL) generates all or part of the complex m by m unitary matrix Q from a QL factorization computed by F08CSF (ZGEQLF).

2 Specification

```
SUBROUTINE F08CTF (M, N, K, A, LDA, TAU, WORK, LWORK, INFO)
INTEGER                M, N, K, LDA, LWORK, INFO
COMPLEX (KIND=nag_wp) A(LDA,*), TAU(*), WORK(max(1,LWORK))
```

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

3 Description

F08CTF (ZUNGQL) is intended to be used after a call to F08CSF (ZGEQLF), which performs a QL factorization of a complex matrix A. The unitary matrix Q is represented as a product of elementary reflectors.

This routine may be used to generate Q explicitly as a square matrix, or to form only its trailing columns.

Usually Q is determined from the QL factorization of an m by p matrix A with $m \geq p$. The whole of Q may be computed by:

```
CALL ZUNGQL(M,M,P,A,LDA,TAU,WORK,LWORK,INFO)
```

(note that the array A must have at least m columns) or its trailing p columns by:

```
CALL ZUNGQL(M,P,P,A,LDA,TAU,WORK,LWORK,INFO)
```

The columns of Q returned by the last call form an orthonormal basis for the space spanned by the columns of A; thus F08CSF (ZGEQLF) followed by F08CTF (ZUNGQL) can be used to orthogonalize the columns of A.

The information returned by F08CSF (ZGEQLF) also yields the QL factorization of the trailing k columns of A, where $k < p$. The unitary matrix arising from this factorization can be computed by:

```
CALL ZUNGQL(M,M,K,A,LDA,TAU,WORK,LWORK,INFO)
```

or its trailing k columns by:

```
CALL ZUNGQL(M,K,K,A,LDA,TAU,WORK,LWORK,INFO)
```

4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia http://www.netlib.org/lapack/lug

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

5 Parameters

1: M – INTEGER *Input*

On entry: m, the number of rows of the matrix Q.

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

2: N – INTEGER *Input*

On entry: n, the number of columns of the matrix Q.

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

3: K – INTEGER *Input*

On entry: k, the number of elementary reflectors whose product defines the matrix Q.

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

4: $\mathrm{A}(\mathrm{LDA},*)$ – COMPLEX (KIND=nag_wp) array *Input/Output*

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

On entry: details of the vectors which define the elementary reflectors, as returned by F08CSF (ZGEQLF).

On exit: the m by n matrix Q.

5: LDA – INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F08CTF (ZUNGQL) is called.

Constraint: $\mathrm{LDA} \geq \max(1,\mathrm{M})$.

6: $\mathrm{TAU}(*)$ – COMPLEX (KIND=nag_wp) array *Input*

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

On entry: further details of the elementary reflectors, as returned by F08CSF (ZGEQLF).

7: $\mathrm{WORK}(\max(1,\mathrm{LWORK}))$ – COMPLEX (KIND=nag_wp) array *Workspace*

On exit: if $\mathrm{INFO} = 0$, the real part of $\mathrm{WORK}(1)$ contains the minimum value of LWORK required for optimal performance.

8: LWORK – INTEGER *Input*

On entry: the dimension of the array WORK as declared in the (sub)program from which F08CTF (ZUNGQL) is called.

If $\mathrm{LWORK} = -1$, a workspace query is assumed; the routine only calculates the optimal size of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued.

Suggested value: for optimal performance, $\mathrm{LWORK} \geq \mathrm{N} \times nb$, where nb is the optimal ***block size***.

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

9: INFO – INTEGER *Output*

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

6 Error Indicators and Warnings

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 Parallelism and Performance

F08CTF (ZUNGQL) is not threaded by NAG in any implementation.

F08CTF (ZUNGQL) 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 routine. 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 $16mnk - 8(m+n)k^2 + \frac{16}{3}k^3$; when $n = k$, the number is approximately $\frac{8}{3}n^2(3m-n)$.

The real analogue of this routine is F08CFF (DORGQL).

10 Example

This example generates the first four columns of the matrix Q of the QL factorization of A as returned by F08CSF (ZGEQLF), where

$$A = \begin{pmatrix} 0.96 - 0.81i & -0.03 + 0.96i & -0.91 + 2.06i & -0.05 + 0.41i \\ -0.98 + 1.98i & -1.20 + 0.19i & -0.66 + 0.42i & -0.81 + 0.56i \\ 0.62 - 0.46i & 1.01 + 0.02i & 0.63 - 0.17i & -1.11 + 0.60i \\ -0.37 + 0.38i & 0.19 - 0.54i & -0.98 - 0.36i & 0.22 - 0.20i \\ 0.83 + 0.51i & 0.20 + 0.01i & -0.17 - 0.46i & 1.47 + 1.59i \\ 1.08 - 0.28i & 0.20 - 0.12i & -0.07 + 1.23i & 0.26 + 0.26i \end{pmatrix}.$$

Note that the block size (NB) of 64 assumed in this example is not realistic for such a small problem, but should be suitable for large problems.

10.1 Program Text

```
    Program f08ctfe

!     F08CTF Example Program Text

!     Mark 25 Release. NAG Copyright 2014.

!     .. Use Statements ..
      Use nag_library, Only: nag_wp, x04dbf, zgeqlf, zungql
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nb = 64, nin = 5, nout = 6
```

```
!     .. Local Scalars ..
      Integer                          :: i, ifail, info, lda, lwork, m, n
      Character (30)                   :: title
!     .. Local Arrays ..
      Complex (Kind=nag_wp), Allocatable :: a(:,:), tau(:), work(:)
      Character (1)                    :: clabs(1), rlabs(1)
!     .. Executable Statements ..
      Write (nout,*) 'F08CTF Example Program Results'
      Write (nout,*)
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) m, n
      lda = m
      lwork = nb*n
      Allocate (a(lda,n),tau(n),work(lwork))

!     Read A from data file

      Read (nin,*)(a(i,1:n),i=1,m)

!     Compute the QL factorization of A
!     The NAG name equivalent of zgeqlf is f08csf
      Call zgeqlf(m,n,a,lda,tau,work,lwork,info)

!     Form the leading N columns of Q explicitly
!     The NAG name equivalent of zungql is f08ctf
      Call zungql(m,n,n,a,lda,tau,work,lwork,info)

!     Form the heading for X04DBF

      Write (title,99999) n
      Flush (nout)

!     Print the leading N columns of Q

!     ifail: behaviour on error exit
!             =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
      ifail = 0
      Call x04dbf('General',' ',m,n,a,lda,'Bracketed','F7.4',title,'Integer', &
        rlabs,'Integer',clabs,80,0,ifail)

99999 Format ('The leading ',I4,' columns of Q')
    End Program f08ctfe
```

10.2 Program Data

```
F08CTF Example Program Data

   6            4                                        :Values of M and N

 ( 0.96,-0.81) (-0.03, 0.96) (-0.91, 2.06) (-0.05, 0.41)
 (-0.98, 1.98) (-1.20, 0.19) (-0.66, 0.42) (-0.81, 0.56)
 ( 0.62,-0.46) ( 1.01, 0.02) ( 0.63,-0.17) (-1.11, 0.60)
 (-0.37, 0.38) ( 0.19,-0.54) (-0.98,-0.36) ( 0.22,-0.20)
 ( 0.83, 0.51) ( 0.20, 0.01) (-0.17,-0.46) ( 1.47, 1.59)
 ( 1.08,-0.28) ( 0.20,-0.12) (-0.07, 1.23) ( 0.26, 0.26) :End of matrix A
```

10.3 Program Results

```
 F08CTF Example Program Results

 The leading    4 columns of Q
                  1                 2                 3                 4
 1  ( 0.2810, 0.5020) (-0.2051,-0.1092) ( 0.3083,-0.6874) ( 0.0181,-0.1483)
 2  ( 0.2707,-0.3296) ( 0.5711, 0.0432) ( 0.2251,-0.1313) ( 0.2930,-0.2025)
 3  (-0.2864,-0.0094) (-0.5416, 0.0454) (-0.2062, 0.0691) ( 0.4015,-0.2170)
 4  ( 0.2262,-0.3854) (-0.3387, 0.2228) ( 0.3259, 0.1178) (-0.0796, 0.0723)
 5  ( 0.0341,-0.0760) ( 0.0098,-0.0712) ( 0.0753, 0.1412) (-0.5317,-0.5751)
 6  (-0.3936,-0.2083) (-0.1296, 0.3691) ( 0.0264,-0.4134) (-0.0940,-0.0940)
```