NAG Fortran Library Routine Document F08CTF (ZUNGOL)

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 FO8CTF (M, N, K, A, LDA, TAU, WORK, LWORK, INFO)

INTEGER

M, N, K, LDA, LWORK, INFO

complex*16

A(LDA,*), TAU(*), WORK(*)
```

The routine may be called by its LAPACK name zungal.

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 $m \ge p$. 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 orthogonalise 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 URL: 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: $M \ge 0$.

2: N – INTEGER Input

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

Constraint: $M \ge N \ge 0$.

3: K – INTEGER Input

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

Constraint: $N \ge K \ge 0$.

4: A(LDA,*) - complex*16 array

Input/Output

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

On entry: details of the vectors which define the elementary reflectors as returned by F08CSF (ZGEQLF) and stored in the (n - k + i)th columns of A, for i = 1, 2, ..., k.

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: LDA $\geq \max(1, M)$.

6: TAU(*) - complex*16 array

Input

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

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

7: WORK(*) - complex*16 array

Workspace

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

On exit: if INFO = 0, the real part of 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 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, LWORK $\geq N \times nb$, where nb is the optimal **block size**. Constraint: LWORK $\geq \max(1, N)$.

9: INFO – INTEGER

Output

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

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6 Error Indicators and Warnings

Errors or warnings detected by the routine:

INFO < 0

If INFO = -i, the *i*th 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 $16mnk - 8(m+n)k^2 + \frac{16}{3}k^3$; when n = k, the number is approximately $\frac{8}{3}n^2(3m-n)$.

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

9 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.

9.1 Program Text

```
FO8CTF Example Program Text
Mark 21 Release. NAG Copyright 2004.
.. Parameters ..
INTEGER
               NIN, NOUT
PARAMETER
                (NIN=5,NOUT=6)
INTEGER
                MMAX, NB, NMAX
PARAMETER
                 (MMAX=8,NB=64,NMAX=8)
               LDA, LWORK
TNTEGER
PARAMETER (LDA=MMAX,LWORK=NB*NMAX)
.. Local Scalars ..
INTEGER I, IFAIL, INFO, J, M, N CHARACTER*30 TITLE
.. Local Arrays ..
COMPLEX *16 A(LDA,NMAX), TAU(NMAX), WORK(LWORK)
CHARACTER CLABS(1), RLABS(1)
.. External Subroutines ..
EXTERNAL XO4DBF, ZGEQLF, ZUNGQL
.. Executable Statements ..
WRITE (NOUT, *) 'F08CTF Example Program Results'
WRITE (NOUT, *)
Skip heading in data file
READ (NIN, *)
READ (NIN,*) M, N
```

```
IF (M.LE.MMAX .AND. N.LE.NMAX .AND. M.GE.N) THEN
         Read A from data file
         READ (NIN, *) ((A(I,J), J=1,N), I=1,M)
         Compute the QL factorization of A
         CALL ZGEQLF(M,N,A,LDA,TAU,WORK,LWORK,INFO)
         Form the leading N columns of Q explicitly
         CALL ZUNGQL(M,N,N,A,LDA,TAU,WORK,LWORK,INFO)
        Form the heading for XO4DBF
        WRITE (TITLE, 99999) N
        Print the leading N columns of Q
         IFAIL = 0
         CALL XO4DBF('General',' ',M,N,A,LDA,'Bracketed','F7.4',TITLE,
                     'Integer', RLABS, 'Integer', CLABS, 80,0, IFAIL)
     ELSE
         WRITE (NOUT,*) 'MMAX and/or NMAX is too small, and/or M.LT.N'
     END IF
      STOP
99999 FORMAT ('The leading ', I4,' columns of Q')
```

9.2 Program Data

```
FO8CTF 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
```

9.3 Program Results

```
FO8CTF 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)
```