NAG Library Routine Document

F08FSF (ZHETRD)

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

F08FSF (ZHETRD) reduces a complex Hermitian matrix to tridiagonal form.

2 Specification

```
SUBROUTINE F08FSF(UPLO, N, A, LDA, D, E, TAU, WORK, LWORK, INFO)
INTEGER              N, LDA, LWORK, INFO
double precision     D(*), E(*)
complex*16           A(LDA,*), TAU(*), WORK(max(1,LWORK))
CHARACTER*1          UPLO
```

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

3 Description

F08FSF (ZHETRD) reduces a complex Hermitian matrix A to real symmetric tridiagonal form T by a unitary similarity transformation: $A = QTQ^{\mathrm{H}}$.

The matrix Q is not formed explicitly but is represented as a product of $n-1$ elementary reflectors (see the F08 Chapter Introduction for details). Routines are provided to work with Q in this representation (see Section 8).

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: indicates whether the upper or lower triangular part of A is stored.

UPLO = 'U'
The upper triangular part of A is stored.

UPLO = 'L'
The lower triangular part of A is stored.

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

2: N – INTEGER *Input*

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

Constraint: N ≥ 0.

3: A(LDA,$*$) – ***complex*16*** array *Input/Output*

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

On entry: the n by n Hermitian matrix A.

If UPLO = 'U', the upper triangular part of A must be stored and the elements of the array below the diagonal are not referenced.

If UPLO = 'L', the lower triangular part of A must be stored and the elements of the array above the diagonal are not referenced.

On exit: A is overwritten by the tridiagonal matrix T and details of the unitary matrix Q as specified by UPLO.

4: LDA – INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F08FSF (ZHETRD) is called.

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

5: D$(*)$ – ***double precision*** array *Output*

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

On exit: the diagonal elements of the tridiagonal matrix T.

6: E$(*)$ – ***double precision*** array *Output*

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

On exit: the off-diagonal elements of the tridiagonal matrix T.

7: TAU$(*)$ – ***complex*16*** array *Output*

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

On exit: further details of the unitary matrix Q.

8: WORK$(\max(1, \mathrm{LWORK}))$ – ***complex*16*** array *Workspace*

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

9: LWORK – INTEGER *Input*

On entry: the dimension of the array WORK as declared in the (sub)program from which F08FSF (ZHETRD) 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 $\geq \mathrm{N} \times nb$, where nb is the optimal ***block size***.

Constraint: LWORK ≥ 1 or LWORK $= -1$.

10: 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 tridiagonal matrix T is exactly similar to a nearby matrix $(A + E)$, where

$$\|E\|_2 \leq c(n)\epsilon\|A\|_2,$$

$c(n)$ is a modestly increasing function of n, and ϵ is the ***machine precision***.

The elements of T themselves may be sensitive to small perturbations in A or to rounding errors in the computation, but this does not affect the stability of the eigenvalues and eigenvectors.

8 Further Comments

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

To form the unitary matrix Q F08FSF (ZHETRD) may be followed by a call to F08FTF (ZUNGTR):

```
CALL ZUNGTR(UPLO,N,A,LDA,TAU,WORK,LWORK,INFO)
```

To apply Q to an n by p complex matrix C F08FSF (ZHETRD) may be followed by a call to F08FUF (ZUNMTR). For example,

```
CALL ZUNMTR('Left',UPLO,'No Transpose',N,P,A,LDA,TAU,C,LDC,
+            WORK,LWORK,INFO)
```

forms the matrix product QC.

The real analogue of this routine is F08FEF (DSYTRD).

9 Example

This example reduces the matrix A to tridiagonal form, where

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

9.1 Program Text

```
*     F08FSF Example Program Text
*     Mark 16 Release. NAG Copyright 1992.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, LDA, LWORK
      PARAMETER        (NMAX=8,LDA=NMAX,LWORK=64*NMAX)
*     .. Local Scalars ..
      INTEGER          I, INFO, J, N
      CHARACTER        UPLO
*     .. Local Arrays ..
      COMPLEX *16      A(LDA,NMAX), TAU(NMAX-1), WORK(LWORK)
      DOUBLE PRECISION D(NMAX), E(NMAX-1)
*     .. External Subroutines ..
      EXTERNAL         ZHETRD
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F08FSF 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,*) ((A(I,J),J=I,N),I=1,N)
         ELSE IF (UPLO.EQ.'L') THEN
            READ (NIN,*) ((A(I,J),J=1,I),I=1,N)
```

```
         END IF
*
*        Reduce A to tridiagonal form
*
         CALL ZHETRD(UPLO,N,A,LDA,D,E,TAU,WORK,LWORK,INFO)
*
*        Print tridiagonal form
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Diagonal'
         WRITE (NOUT,99999) (D(I),I=1,N)
         WRITE (NOUT,*) 'Off-diagonal'
         WRITE (NOUT,99999) (E(I),I=1,N-1)
      END IF
*
99999 FORMAT (1X,8F9.4)
      END
```

9.2 Program Data

```
F08FSF 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

```
 F08FSF Example Program Results

 Diagonal
   -2.2800  -0.1285  -0.1666  -1.9249
 Off-diagonal
   -4.3385  -2.0226  -1.8023
```