

NAG Fortran Library Routine Document

F08FQF (CHEEVD/ZHEEVD)

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.

Warning. The specification of the parameters LRWORK and LIWORK changed at Mark 20 in the case where JOB = 'V' and N > 1: the minimum dimension of the array RWORK has been reduced whereas the minimum dimension of the array IWORK has been increased.

1 Purpose

F08FQF (CHEEVD/ZHEEVD) computes all the eigenvalues, and optionally all the eigenvectors, of a complex Hermitian matrix. If the eigenvectors are requested, then it uses a divide and conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal-Walker-Kahan variant of the QL or QR algorithm.

2 Specification

```

SUBROUTINE F08FQF(JOB, UPLO, N, A, LDA, W, WORK, LWORK, RWORK, LRWORK,
1                IWORK, LIWORK, INFO)
ENTRY          cheevd (JOB, UPLO, N, A, LDA, W, WORK, LWORK, RWORK, LRWORK,
1                IWORK, LIWORK, INFO)
INTEGER        N, LDA, LWORK, LRWORK, IWORK(*), LIWORK, INFO
real          W(*), RWORK(*)
complex      A(LDA,*), WORK(*)
CHARACTER*1    JOB, UPLO

```

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

3 Description

This routine computes all the eigenvalues, and optionally all the eigenvectors, of a complex Hermitian matrix A . In other words, it can compute the spectral factorization of A as

$$A = Z\Lambda Z^H,$$

where Λ is a real diagonal matrix whose diagonal elements are the eigenvalues λ_i , and Z is the (complex) unitary matrix whose columns are the eigenvectors z_i . Thus

$$Az_i = \lambda_i z_i, \quad i = 1, 2, \dots, n.$$

4 References

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

5 Parameters

1: JOB – CHARACTER*1

Input

On entry: indicates whether eigenvectors are computed as follows:

if JOB = 'N', only eigenvalues are computed;

if JOB = 'V', eigenvalues and eigenvectors are computed.

Constraint: JOB = 'N' or 'V'.

- 2: UPLO – CHARACTER*1 *Input*
On entry: indicates whether the upper or lower triangular part of A is stored as follows:
if UPLO = 'U', the upper triangular part of A is stored;
if UPLO = 'L', the lower triangular part of A is stored.
Constraint: UPLO = 'U' or 'L'.
- 3: N – INTEGER *Input*
On entry: n , the order of the matrix A .
Constraint: $N \geq 0$.
- 4: A(LDA,*) – **complex** 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: if JOB = 'V', this is overwritten by the unitary matrix Z which contains the eigenvectors of A .
- 5: LDA – INTEGER *Input*
On entry: the first dimension of the array A as declared in the (sub)program from which F08FQF (CHEEVD/ZHEEVD) is called.
Constraint: $LDA \geq \max(1, N)$.
- 6: W(*) – **real** array *Output*
Note: the dimension of the array W must be at least $\max(1, N)$.
On exit: the eigenvalues of the matrix A in ascending order.
- 7: WORK(*) – **complex** 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 required minimal size of LWORK.
- 8: LWORK – INTEGER *Input*
On entry: the dimension of the array WORK as declared in the (sub)program from which F08FQF (CHEEVD/ZHEEVD) is called, unless LWORK = -1, in which case a workspace query is assumed and the routine only calculates the minimum dimension of WORK.
Constraints:
if $N \leq 1$, $LWORK \geq 1$ or $LWORK = -1$,
if JOB = 'N' and $N > 1$, $LWORK \geq N + 1$ or $LWORK = -1$,
if JOB = 'V' and $N > 1$, $LWORK \geq N \times (N + 2)$ or $LWORK = -1$.
- 9: RWORK(*) – **real** array *Workspace*
Note: the dimension of the array RWORK must be at least $\max(1, LRWORK)$.
On exit: if INFO = 0, RWORK(1) contains the required minimal size of LRWORK.

10: LRWORK – INTEGER

Input

On entry: the dimension of the array RWORK as declared in the (sub)program from which F08FQF (CHEEVD/ZHEEVD) is called, unless LRWORK = -1, in which case a workspace query is assumed and the routine only calculates the minimum dimension of RWORK.

Constraints:

if $N \leq 1$, LRWORK ≥ 1 or LRWORK = -1,
 if JOB = 'N' and $N > 1$, LRWORK $\geq N$ or LRWORK = -1,
 if JOB = 'V' and $N > 1$, LRWORK $\geq 2 \times N^2 + 5 \times N + 1$ or LRWORK = -1.

11: IWORK(*) – INTEGER array

Workspace

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

On exit: if INFO = 0, IWORK(1) contains the required minimal size of LIWORK.

12: LIWORK – INTEGER

Input

On entry: the dimension of the array IWORK as declared in the (sub)program from which F08FQF (CHEEVD/ZHEEVD) is called, unless LIWORK = -1, in which case a workspace query is assumed and the routine only calculates the minimum dimension of IWORK.

Constraints:

if $N \leq 1$, LIWORK ≥ 1 or LIWORK = -1,
 if JOB = 'N' and $N > 1$, LIWORK ≥ 1 or LIWORK = -1,
 if JOB = 'V' and $N > 1$, LIWORK $\geq 5 \times N + 3$ or LIWORK = -1.

13: 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 , the i th parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO = i , the algorithm failed to converge; i indicates the number of elements of an intermediate tridiagonal form which did not converge to zero.

7 Accuracy

The computed eigenvalues and eigenvectors are exact for a nearby matrix $A + E$, where

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

and ϵ is the *machine precision*.

8 Further Comments

The real analogue of this routine is F08FCF (SSYEVD/DSYEVD).

9 Example

To compute all the eigenvalues and eigenvectors of the Hermitian matrix A , where

$$A = \begin{pmatrix} 1.0 + 0.0i & 2.0 + 1.0i & 3.0 + 1.0i & 4.0 + 1.0i \\ 2.0 - 1.0i & 2.0 + 0.0i & 3.0 + 2.0i & 4.0 + 2.0i \\ 3.0 - 1.0i & 3.0 - 2.0i & 3.0 + 0.0i & 4.0 + 3.0i \\ 4.0 - 1.0i & 4.0 - 2.0i & 4.0 - 3.0i & 4.0 + 0.0i \end{pmatrix}.$$

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.

```
*      F08FQF Example Program Text.
*      Mark 20 Revised. NAG Copyright 2001.
*      .. Parameters ..
      INTEGER                NIN, NOUT
      PARAMETER              (NIN=5,NOUT=6)
      INTEGER                NMAX, LDA
      PARAMETER              (NMAX=8,LDA=NMAX)
      INTEGER                LWORK, LIWORK, LRWORK
      PARAMETER              (LWORK=NMAX*(NMAX+2),LIWORK=5*NMAX+3,
+                             LRWORK=2*NMAX*NMAX+5*NMAX+1)
*      .. Local Scalars ..
      INTEGER                I, IFAIL, INFO, J, N
      CHARACTER              JOB, UPLO
*      .. Local Arrays ..
      complex                A(LDA,NMAX), WORK(LWORK)
      real                  RWORK(LRWORK), W(NMAX)
      INTEGER                IWORK(LIWORK)
*      .. External Subroutines ..
      EXTERNAL              X04DAF, cheevd
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F08FQF Example Program Results'
*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
        READ (NIN,*) UPLO
*
*      Read A from data file
*
      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
*
      READ (NIN,*) JOB
*
*      Calculate all the eigenvalues and eigenvectors of A
*
      CALL cheevd(JOB,UPLO,N,A,LDA,W,WORK,LWORK,RWORK,LRWORK,IWORK,
+               LIWORK,INFO)
*
      WRITE (NOUT,*)
      IF (INFO.GT.0) THEN
        WRITE (NOUT,*) 'Failure to converge.'
      ELSE
*
*      Print eigenvalues and eigenvectors
*
        WRITE (NOUT,*) 'Eigenvalues'
        DO 20 I = 1, N
          WRITE (NOUT,99999) I, W(I)
20      CONTINUE
        WRITE (NOUT,*)
```

```

      IFAIL = 0
*
      CALL X04DAF('General',' ',N,N,A,LDA,'Eigenvectors',IFAIL)
*
      END IF
      END IF
      STOP
*
99999 FORMAT (3X,I5,5X,2F8.4)
      END

```

9.2 Program Data

F08FQF Example Program Data

4	:Value of N
'L'	:Value of UPLO
(1.0, 0.0)	
(2.0, 1.0) (2.0, 0.0)	
(3.0, 1.0) (3.0, 2.0) (3.0, 0.0)	
(4.0, 1.0) (4.0, 2.0) (4.0, 3.0) (4.0, 0.0)	:End of matrix A
'V'	:Value of JOB

9.3 Program Results

F08FQF Example Program Results

Eigenvalues

1	-4.2443
2	-0.6886
3	1.1412
4	13.7916

Eigenvectors

	1	2	3	4
1	0.4836	0.6470	-0.4456	-0.3859
	0.0000	0.0000	0.0000	-0.0000
2	0.2912	-0.4984	-0.0230	-0.4441
	-0.3618	-0.1130	-0.5702	0.0156
3	-0.3163	0.2949	0.5331	-0.5173
	-0.3696	0.3165	0.1317	-0.0844
4	-0.4447	-0.2241	-0.3510	-0.5277
	0.3406	-0.2878	0.2261	-0.3168
