

NAG Fortran Library Routine Document

F02GAF

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

F02GAF computes all the eigenvalues, and optionally the Schur factorization, of a complex general matrix.

2 Specification

```
SUBROUTINE F02GAF(JOB, N, A, LDA, W, Z, LDZ, RWORK, WORK, LWORK, IFAIL)
INTEGER          N, LDA, LDZ, LWORK, IFAIL
real           RWORK(*)
complex       A(LDA,*), W(*), Z(LDZ,*), WORK(LWORK)
CHARACTER*1      JOB
```

3 Description

This routine computes all the eigenvalues, and optionally the Schur form or the complete Schur factorization, of a complex general matrix A :

$$A = ZTZ^H,$$

where T is an upper triangular matrix, and Z is a unitary matrix. T is called the *Schur form* of A , and the columns of Z are called the *Schur vectors*.

If it is desired to order the Schur factorization so that specified eigenvalues occur in the leading positions on the diagonal of T , then this routine may be followed by a call of F08QUF (CTRSEN/ZTRSEN). Other reorderings may be achieved by calls to F08QTF (CTREXC/ZTREXC).

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 the Schur form and Schur vectors are to be computed as follows:

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

if JOB = 'S', then eigenvalues and the Schur form T are computed;

if JOB = 'V', then eigenvalues, the Schur form and the Schur vectors are computed.

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

2: N – INTEGER *Input*

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

Constraint: $N \geq 0$.

- 3: 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 general matrix A.
On exit: if JOB = 'S' or 'V', A contains the upper triangular matrix T , the Schur form of A. If JOB = 'N', the contents of A are overwritten.
- 4: LDA – INTEGER Input
On entry: the first dimension of the array A as declared in the (sub)program from which F02GAF is called.
Constraint: $LDA \geq \max(1, N)$.
- 5: W(*) – **complex** array Output
Note: the dimension of the array W must be at least $\max(1, N)$.
On exit: the computed eigenvalues. If JOB = 'S' or 'V', the eigenvalues occur in the same order as on the diagonal of T .
- 6: Z(LDZ,*) – **complex** array Output
Note: the second dimension of the array Z must be at least $\max(1, N)$ if JOB = 'V' and at least 1 otherwise.
On exit: if JOB = 'V', Z contains the unitary matrix Z of Schur vectors.
Z is not referenced if JOB = 'N' or 'S'.
- 7: LDZ – INTEGER Input
On entry: the first dimension of the array Z as declared in the (sub)program from which F02GAF is called.
Constraints:
 $LDZ \geq 1$, if JOB = 'N' or 'S',
 $LDZ \geq \max(1, N)$, if JOB = 'V'.
- 8: RWORK(*) – **real** array Workspace
Note: the dimension of the array RWORK must be at least $\max(1, N)$.
- 9: WORK(LWORK) – **complex** array Workspace
10: LWORK – INTEGER Input
On entry: the dimension of the array WORK as declared in the (sub)program from which F02GAF is called. On some high-performance computers, increasing the dimension of WORK will enable the routine to run faster; a value of $64 \times N$ should allow near-optimal performance on almost all machines.
Constraint: $LWORK \geq \max(1, 2 \times N)$.
- 11: IFAIL – INTEGER Input/Output
On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.
On exit: IFAIL = 0 unless the routine detects an error (see Section 6).
For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, for users not familiar with this parameter the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

6 Error Indicators and Warnings

If on entry IFAIL = 0 or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

On entry, JOB $\neq$ 'N', 'S' or 'V',
 or N < 0,
 or LDA < max(1, N),
 or LDZ < 1, or LDZ < N and JOB = 'V',
 or LWORK < max(1, 2 $\times$ N).

IFAIL = 2

The *QR* algorithm failed to compute all the eigenvalues.

7 Accuracy

The computed Schur factorization is the exact factorization of a nearby matrix $A + E$, where

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

and ϵ is the *machine precision*.

If λ_i is an exact eigenvalue, and $\tilde{\lambda}_i$ is the corresponding computed value, then

$$|\tilde{\lambda}_i - \lambda_i| \leq \frac{c(n)\epsilon\|A\|_2}{s_i},$$

where $c(n)$ is a modestly increasing function of n , and s_i is the reciprocal condition number of λ_i . The condition numbers s_i may be computed by calling F08QYF (CTRSNA/ZTRSNA).

8 Further Comments

The routine calls routines from LAPACK in Chapter F08. It first reduces A to upper Hessenberg form H , using a unitary similarity transformation: $A = QHQ^H$. If only eigenvalues or the Schur form are required, the routine uses the upper Hessenberg *QR* algorithm to compute the eigenvalues or Schur form of H . If the Schur vectors are required, the routine first forms the unitary matrix Q that was used in the reduction to Hessenberg form; it then uses the *QR* algorithm to reduce H to T , using further unitary transformations: $H = STS^H$; and at the same time it accumulates the matrix of Schur vectors $Z = QS$.

Each Schur vector z is normalized so that $\|z\|_2 = 1$, and the element of largest absolute value is real and positive.

The time taken by the routine is approximately proportional to n^3 .

9 Example

To compute the Schur factorization of the matrix A , where

$$A = \begin{pmatrix} -3.97 - 5.04i & -4.11 + 3.70i & -0.34 + 1.01i & 1.29 - 0.86i \\ 0.34 - 1.50i & 1.52 - 0.43i & 1.88 - 5.38i & 3.36 + 0.65i \\ 3.31 - 3.85i & 2.50 + 3.45i & 0.88 - 1.08i & 0.64 - 1.48i \\ -1.10 + 0.82i & 1.81 - 1.59i & 3.25 + 1.33i & 1.57 - 3.44i \end{pmatrix}.$$

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.

```
*      F02GAF Example Program Text
*      Mark 16 Release. NAG Copyright 1992.
*      .. Parameters ..
INTEGER          NIN, NOUT
PARAMETER        (NIN=5,NOUT=6)
INTEGER          NMAX, LDA, LDZ, LWORK
PARAMETER        (NMAX=8,LDA=NMAX,LDZ=NMAX,LWORK=64*NMAX)
*      .. Local Scalars ..
INTEGER          I, IFAIL, J, N
*      .. Local Arrays ..
complex         A(LDA,NMAX), W(NMAX), WORK(LWORK), Z(LDZ,NMAX)
real           RWORK(NMAX)
CHARACTER        CLABS(1), RLABS(1)
*      .. External Subroutines ..
EXTERNAL         F02GAF, X04DBF
*      .. Intrinsic Functions ..
INTRINSIC        imag, real
*      .. Executable Statements ..
WRITE (NOUT,*) 'F02GAF 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,*) ((A(I,J),J=1,N),I=1,N)
*
*      Compute Schur factorization of A
*
IFAIL = 0
*
CALL F02GAF('Vectors',N,A,LDA,W,Z,LDZ,RWORK,WORK,LWORK,IFAIL)
*
WRITE (NOUT,*)
WRITE (NOUT,*) 'Eigenvalues'
WRITE (NOUT,99999) (' (' ,real(W(I)) , ' , ' , imag(W(I)) , ') ' , I=1,N)
WRITE (NOUT,*)
*
CALL X04DBF('General', ' ' ,N,N,A,LDA,'Bracketed','F7.4',
+          'Schur form','Integer',RLABS,'Integer',CLABS,80,0,
+          IFAIL)
*
WRITE (NOUT,*)
*
CALL X04DBF('General', ' ' ,N,N,Z,LDZ,'Bracketed','F7.4',
+          'Schur vectors','Integer',RLABS,'Integer',CLABS,80,
+          0,IFAIL)
*
END IF
STOP
*
99999 FORMAT (3X,4(A,F7.4,A,F7.4,A,:))
END
```

9.2 Program Data

F02GAF Example Program Data

```
4                                     :Value of N
(-3.97,-5.04) (-4.11, 3.70) (-0.34, 1.01) ( 1.29,-0.86)
( 0.34,-1.50) ( 1.52,-0.43) ( 1.88,-5.38) ( 3.36, 0.65)
( 3.31,-3.85) ( 2.50, 3.45) ( 0.88,-1.08) ( 0.64,-1.48)
(-1.10, 0.82) ( 1.81,-1.59) ( 3.25, 1.33) ( 1.57,-3.44) :End of matrix A
```

9.3 Program Results

F02GAF Example Program Results

Eigenvalues

(-6.0004,-6.9998) (-5.0000, 2.0060) (7.9982,-0.9964) (3.0023,-3.9998)

Schur form

	1	2	3	4
1	(-6.0004,-6.9998)	(-0.4701,-0.2119)	(0.0438, 0.5124)	(-0.9097,-0.0925)
2	(0.0000, 0.0000)	(-5.0000, 2.0060)	(0.7150,-0.1028)	(-0.0580, 0.2575)
3	(0.0000, 0.0000)	(0.0000, 0.0000)	(7.9982,-0.9964)	(-0.2232,-1.0549)
4	(0.0000, 0.0000)	(0.0000, 0.0000)	(0.0000, 0.0000)	(3.0023,-3.9998)

Schur vectors

	1	2	3	4
1	(0.8457, 0.0000)	(-0.3613, 0.1351)	(-0.1755, 0.2297)	(0.1099,-0.2007)
2	(-0.0177, 0.3036)	(-0.3366, 0.4660)	(0.7228, 0.0000)	(0.0336, 0.2312)
3	(0.0875, 0.3115)	(0.6311, 0.0000)	(0.2871, 0.4999)	(0.0944,-0.3947)
4	(-0.0561,-0.2906)	(-0.1045,-0.3339)	(0.2476, 0.0195)	(0.8534, 0.0000)
