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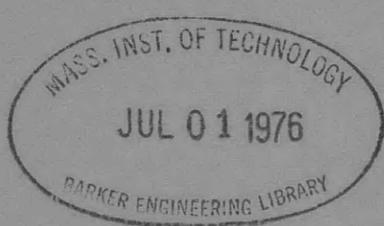
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SOLUTION OF A COMPLEX QUADRATIC EIGENVALUE PROBLEM RELATED TO PIPE FLOW



Donald A. Gignac

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COMPUTATION AND MATHEMATICS DEPARTMENT
RESEARCH AND DEVELOPMENT REPORT

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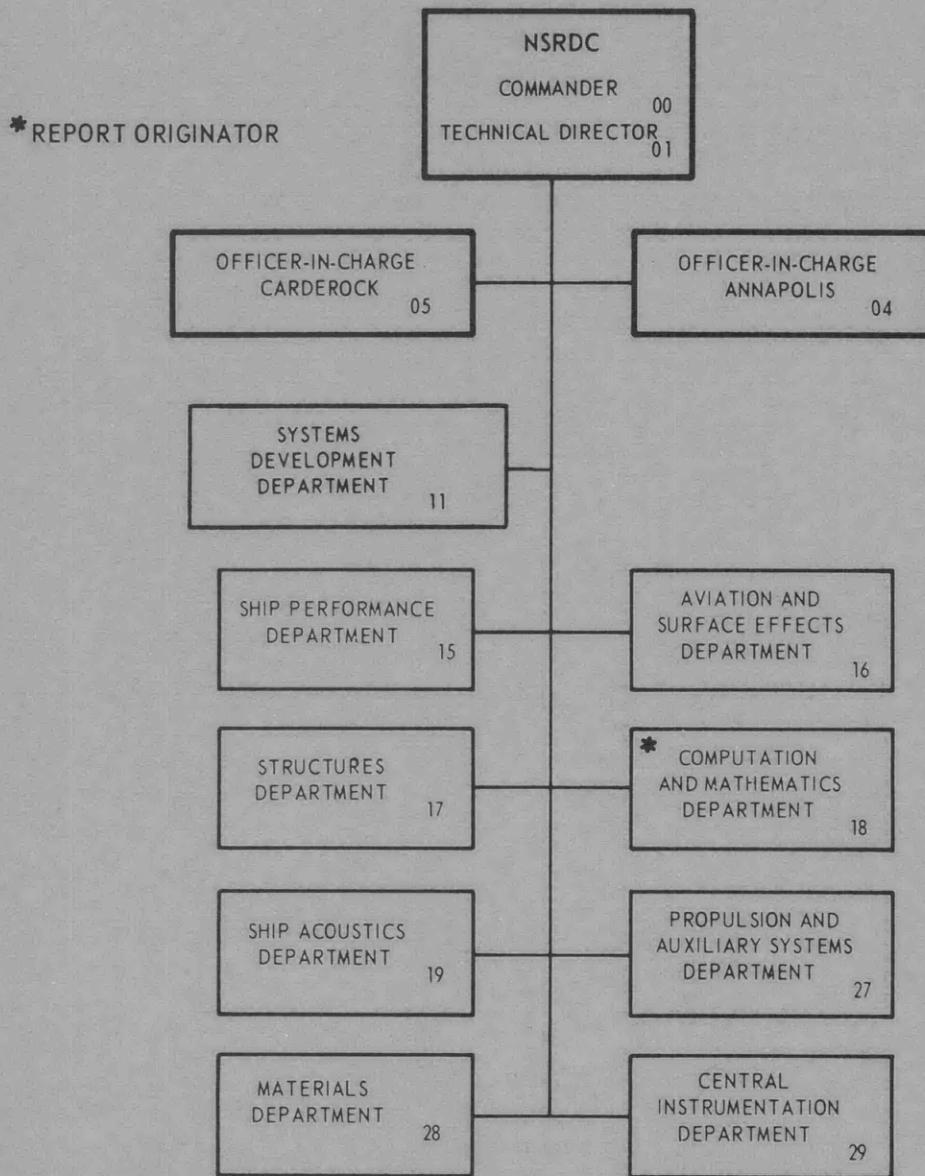
Report 4503

SOLUTION OF A COMPLEX QUADRATIC EIGENVALUE PROBLEM RELATED TO PIPE FLOW

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| 20. ABSTRACT (Continue on reverse side if necessary and identify by block number) A complex quadratic eigenvalue problem of order n ($n = 20, 30, 40, \dots$) encountered in an investigation of pipe flow was reduced to that of computing the eigenvalues of either a real or a complex matrix of order $2n$, depending on the linearization technique used. To get satisfactory results using the CDC 6000 series computer, double precision versions of the appropriate EISPACK subroutines were required. Although the modified subroutines used for the real matrix computations required less core than those used for the | | |

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20. continued:

complex matrix, the calculation time was not significantly faster than that for the complex matrix. The use of "balancing" subroutines merits further investigation.

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INTRODUCTION

The work described in this report was undertaken in response to a request by Dr. R.J. Hansen of the Naval Research Laboratory who was investigating a pipe flow problem in fluid mechanics¹ using a computer program containing an eigenvalue subroutine for complex matrices. The unsatisfactory results previously obtained with this computer program were thought to be due to the complex eigenvalue subroutine then being used, and it was thought that substituting an appropriate sequence of subroutines from the EISPACK subroutine library² might solve the problem. However, for certain matrices generated by the program, the EISPACK subroutines did not produce satisfactory results either.

At first it was felt that the matrices had not been generated with sufficient accuracy, but when further effort in that direction proved unproductive, it was conjectured that the source of the difficulty might lie in the fact that the matrix was generated in double precision while its eigenvalues were computed in single precision. At this point the question arises: If it is desirable or necessary to generate these matrices in double precision,* then should not their eigenvalues be computed in double precision also?

This question should be considered in light of the following observations.

¹ Hansen, R.J., Little, R.C., Reischman, M.M., and Kelleher, M.D., "Stability and the Laminar-to-Turbulent Transition in Pipe Flows of Drag-Reducing Polymer Solutions," a paper to be presented in the Fall of 1974 at the British Hydromechanics Research Association International Congress on Drag Reduction.

² Smith, B.T., Boyle, J.M., Garlow, B.S., Skele, Y., Klema, V.C., and Moler, C.B., "Matrix Eigensystem Subroutines - EISPACK Guide," Vol. 6, "Lecture Notes in Computer Science," New York, Springer-Verlag (1974).

* To accumulate dot products in double precision on the CDC 6400 so as to minimize roundoff error, the whole dot product procedure must be done in double precision, costly though that may be.

First, under certain circumstances even the 48-bit mantissa of the single-precision word of the CDC 6400 may not be sufficient to withstand the accumulation of round-off error in the course of computing the eigenvalues of a complex matrix of rather low order.

Second, if A is the complex matrix generated in double precision and B is the complex matrix obtained by truncating A to single precision, the respective elements of A and B differ by increments of order 10^{-16} . Clearly either matrix can be regarded as having been obtained by perturbing the elements of the other. The crucial question is whether this perturbation significantly changes the eigenvalues, or even alters their very nature?

This report documents an investigation of these difficulties for Hansen's complex eigenvalue problem as well as for an associated real eigenvalue problem.

THE PROBLEM

If A, B, and C are complex matrices of order n, we may define the matrix equation

$$(\lambda^2 A + \lambda B + C)X = 0 \quad (1)$$

as the quadratic eigenvalue problem of order n. If A is invertible, the solution of this problem is equivalent to computing the eigenvalues and eigenvectors of a complex matrix of order 2n.

Two methods can be used to reduce this quadratic eigenvalue problem to a matrix eigenvalue problem. First the substitution of $Y = \lambda X$ into the above equation results in the linear eigenvalue problem of order 2n.

$$\begin{pmatrix} 0 & -I \\ -A^{-1}C & -A^{-1}B \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \lambda \begin{pmatrix} X \\ Y \end{pmatrix} \quad . \quad (2)$$

The second method involves multiplying the quadratic problem by A^{-1} and completing the square to obtain

$$[(\lambda I + \frac{1}{2} A^{-1}B)^2 - (\frac{1}{2} A^{-1}B)^2 + A^{-1}C]X = 0 \quad . \quad (3)$$

Next Y is implicitly defined by the relationship

$$(\lambda I + \frac{1}{2} A^{-1} B)X = A^{-1}Y . \quad (4)$$

Then this relationship is substituted in Equation (3) and multiplication by A and simplification gives the linear eigenvalue problem

$$\begin{pmatrix} -\frac{1}{2} A^{-1} B & | & A^{-1} \\ \hline \frac{1}{4} BA^{-1} B - C & | & -\frac{1}{2} BA^{-1} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \lambda \begin{pmatrix} X \\ Y \end{pmatrix} .$$

The problem at hand is of the form

$$[\lambda^2 P + \lambda(2\theta E + \frac{1}{\theta} Pi) + (-J + Ei)] X = 0$$

where P, E, and J are real matrices of order 20 or more, θ is a real parameter, and i is the square root of -1. The first linearization procedure results in the complex eigenvalue problem

$$\begin{pmatrix} 0 & | & I \\ \hline P^{-1}J - P^{-1}Ei & | & 2\theta P^{-1}E + \frac{1}{\theta} Ii \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \lambda \begin{pmatrix} X \\ Y \end{pmatrix}$$

However, the second linearization procedure produces the complex eigenvalue problem

$$\begin{pmatrix} -\theta P^{-1}E - \frac{1}{2\theta} Ii & | & P^{-1} \\ \hline \theta^2 EP^{-1}E - \frac{1}{4\theta^2} P + J & | & -\theta EP^{-1} - \frac{1}{2\theta} Ii \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \lambda \begin{pmatrix} X \\ Y \end{pmatrix}$$

In this instance the coefficient matrix is the difference of a real non-symmetric matrix and a complex scalar multiple of the identity matrix. This coefficient matrix C is similar to a matrix of simpler form. If we let D be the matrix

$$\left(\begin{array}{c|c} -\frac{I}{\theta E} & \frac{0}{I} \\ \hline & \end{array} \right)$$

then the inverse of D is

$$\left(\begin{array}{c|c} -\frac{I}{\theta E} & \frac{0}{I} \\ \hline & \end{array} \right)$$

and $D^{-1}CD$ is

$$\left(\begin{array}{c|c} -2\theta P^{-1}E & \frac{P^{-1}}{I} \\ \hline -\frac{1}{4\theta^2} P + J & 0 \end{array} \right) - \frac{1}{2\theta} I i$$

Thus we may obtain the eigenvalues of the complex matrix C by computing the eigenvalues of the real non-symmetric matrix

$$\left(\begin{array}{c|c} -2\theta P^{-1}E & \frac{P^{-1}}{I} \\ \hline -\frac{1}{4\theta^2} P + J & 0 \end{array} \right)$$

and subtracting the quantity $\frac{1}{2\theta}$ from their imaginary parts.

THE SUBROUTINES

All the single-precision subroutines (CBAL, COMHES, COMLR, BALANC, ELMHES, ORTHES, HQR) are the standard EISPACK subroutines. They contain instructions pertaining to their calling sequence. The double-precision subroutines (DBAL, DOMHES, DOMLR, DALANC, DLMHES, DRTHES, DQR) were obtained from the corresponding EISPACK subroutines by making the following changes:

- All single-precision variables were changed to double precision.
- The single-precision criterion for the CDC 6400, 2^{-47} , was changed to the double-precision criterion, 2^{-95} .

- The various library subroutines (ABS, SQRT, etc.) were changed to their double-precision counterparts. In the case of DOMLR, it was necessary to supply double-precision subroutines for complex division and complex square-root, since these operations are not available on the CDC 6400. The subroutines provided (CLXDVDE and CLXSQRT) are merely FORTRAN translations of the ALGOL procedures CABS, CDIV, and CSQRT of Martin and Wilkinson.³

- The argument lists for these double-precision subroutines differ from the calling sequences for their EISPACK counterparts only in that all non-integer arrays were double precision instead of single precision.

THE RESULTS

The eigenvalues of the complex matrix provided by the first linearization technique were obtained using the following procedure*:

- The complex matrix was balanced.
- The balanced matrix was reduced to Hessenberg form by stabilized elementary similarity transformations.
- The eigenvalues of the Hessenberg matrix were computed using the LR algorithm for complex matrices.

This procedure was carried out in three different ways:

- 1) The complex matrix generated in double precision was truncated to single precision and the single-precision EISPACK subroutines CBAL, COMHES, COMLR were used (Table 1a).
- 2) The complex matrix generated in double precision was truncated to single precision and the double-precision versions DBAL, DOMHES, DOMLR

³ Martin, R.S. and J.H. Wilkinson, "Similarity Reduction of a General Matrix to Hessenberg Form," Contribution II/13 in Wilkinson, J.H. and C. Reinsch, editors "Handbook for Automatic Computation," Vol. II, "Linear Algebra," New York, 1971, Springer-Verlag.

* For information concerning the Hessenberg reduction and the QR and LR algorithms the reader is referred to Wilkinson, J.H., "The Algebraic Eigenvalue Problem," Clarendon Press, Oxford (1965).

of the EISPACK subroutines were used (Table 1b).

3) DBAL, DOMHES, DOMLR were used on the complex matrix generated in double precision (Table 1c).

The considerable simplification of the eigenvalue problem achieved by using the second linearization technique was not anticipated at the outset of this investigation. When a detailed examination of the eigenvalues computed from the matrix of the first linearization technique suggested that a different linearization technique might yield a matrix more amenable to computation, other linearization techniques were investigated.

The eigenvalues of the real matrix provided by the second linearization technique were obtained using the following procedure:

- The real non-symmetric matrix was balanced.
- The balanced matrix was reduced to Hessenberg form using either stabilized elementary similarity transformations or orthogonal transformations.
- The eigenvalues of the Hessenberg matrix were computed using the QR algorithm.

This procedure was carried out in four different ways.

1) The real matrix generated in double precision was truncated to single precision and the single precision EISPACK subroutines BALANC, ORTHES, and HQR were used (Table 2a).

2) The real matrix generated in double precision was truncated to single precision and the double precision versions DALANC, DRTHES, and DQR of the EISPACK subroutines were used (Table 2b).

3) DALANCE, DRTHES, and DQR were used on the real matrix generated in double precision (Table 2c).

4) DRTHES and DQR were used on the real matrix generated in double precision (Table 2d).

Of the 60 eigenvalues computed, only those that fall in the second and third quadrants are presented in the tables that follow. However, their behavior is representative of the eigenvalues as a whole. The computation times shown are those required to compute all 60 of the eigenvalues.

TABLE 1 - SECOND AND THIRD QUADRANT EIGENVALUES
OBTAINED FROM COMPLEX MATRIX APPROACH

Table 1a
CBAL, COMHES, COMLR Subroutines 21.77 Seconds

| | | |
|----|-----------------------|-----------------------|
| 1 | -.166895348951915E+02 | .453962332056731E+02 |
| 2 | -.316749508523681E+02 | .248351140020612E+00 |
| 3 | -.348884093302488E+02 | .221199870220845E+02 |
| 1 | -.816293526043538E+00 | -.135811109722657E+03 |
| 2 | -.816359999160820E+00 | -.704598564725760E+01 |
| 3 | -.262510336877122E+01 | -.134477603349308E+03 |
| 4 | -.262511208539763E+01 | -.837954278608919E+01 |
| 5 | -.570546363332099E+01 | -.132807670304536E+03 |
| 6 | -.570548098766807E+01 | -.100494914773950E+02 |
| 7 | -.112270549054325E+02 | -.131454972874669E+03 |
| 8 | -.112270792516163E+02 | -.114021920263506E+02 |
| 9 | -.166894713808424E+02 | -.188253246825858E+03 |
| 10 | -.205377373992610E+02 | -.133027945252527E+03 |
| 11 | -.205377768261726E+02 | -.982922388380672E+01 |
| 12 | -.316748791446516E+02 | -.143105511121843E+03 |
| 13 | -.348883045381867E+02 | -.164977092569118E+03 |

Table 1b
DBAL, DOMHES, DOMLR Subroutines 96.19 Seconds
(Matrix has been truncated to single precision significance)

| | | |
|----|-----------------------|-----------------------|
| 1 | -.164163526301686D+02 | .444157924738040D+02 |
| 2 | -.309194743856593D+02 | .795111187632182D-01 |
| 3 | -.342104294907155D+02 | .214986849517767D+02 |
| 1 | -.491817227667278D+00 | -.136123802804776D+03 |
| 2 | -.491817235024852D+00 | -.673334031666884D+01 |
| 3 | -.236178882980058D+01 | -.817847614309992D+01 |
| 4 | -.236178886587554D+01 | -.134678666891774D+03 |
| 5 | -.544207538548246D+01 | -.983990980218899D+01 |
| 6 | -.544207544558938D+01 | -.133017233233870D+03 |
| 7 | -.108592821202510D+02 | -.111690142642918D+02 |
| 8 | -.108592821807477D+02 | -.131688128825279D+03 |
| 9 | -.164163521583046D+02 | -.187272935438159D+03 |
| 10 | -.199544704290707D+02 | -.133174702838537D+03 |
| 11 | -.199544704372173D+02 | -.968244033591238D+01 |
| 12 | -.309194742220807D+02 | -.142936654328604D+03 |
| 13 | -.342104291482651D+02 | -.164355828892842D+03 |

TABLE 1 (CONTINUED)

Table 1c

DBAL, DOMHES, DOMLR Subroutines 94.82 Seconds

| | | |
|----|-----------------------|-----------------------|
| 1 | -.161635728329553D+02 | .432950045889481D+02 |
| 2 | -.335577057717484D+02 | .207044804956883D+02 |
| 1 | -.204921408502598D+00 | -.685273791773558D+01 |
| 2 | -.204921408502598D+00 | -.136004404939408D+03 |
| 3 | -.208873186667484D+01 | -.134653761423907D+03 |
| 4 | -.208873186667484D+01 | -.820338143323628D+01 |
| 5 | -.512410079791166D+01 | -.133057379553590D+03 |
| 6 | -.512410079791166D+01 | -.979976330355343D+01 |
| 7 | -.104158704992893D+02 | -.131751724309115D+03 |
| 8 | -.104158704992893D+02 | -.111054185480280D+02 |
| 9 | -.161635728329553D+02 | -.186152147446091D+03 |
| 10 | -.193106276285779D+02 | -.133126188924393D+03 |
| 11 | -.193106276285779D+02 | -.9730953932749970+01 |
| 12 | -.301520647479031D+02 | -.142565668129680D+03 |
| 13 | -.301520647479031D+02 | -.291474727463061D+00 |
| 14 | -.335577057717484D+02 | -.163561623352832D+03 |

TABLE 2 - SECOND AND THIRD QUADRANT EIGENVALUES
OBTAINED FROM REAL MATRIX APPROACH

Table 2a

| | BALANC, ORTHES, HQR Subroutines | 24.23 Seconds |
|----|---------------------------------|-----------------------|
| 1 | -.160756150689513E+02 | .432634403473735E+02 |
| 2 | -.335103274930459E+02 | .206970748379899E+02 |
| 1 | -.174021213374999E+00 | -.687248959254430E+01 |
| 2 | -.174021213374999E+00 | -.135984653264599E+03 |
| 3 | -.205661137487414E+01 | -.822366618893329E+01 |
| 4 | -.205661137487414E+01 | -.134633476668209E+03 |
| 5 | -.508934051840720E+01 | -.982017385793188E+01 |
| 6 | -.508934051840720E+01 | -.133036968999211E+03 |
| 7 | -.103794737355472E+02 | -.111287013092983E+02 |
| 8 | -.103794737355472E+02 | -.131728441547844E+03 |
| 9 | -.160756150689513E+02 | -.186120583204516E+03 |
| 10 | -.192775922492228E+02 | -.975794068556252E+01 |
| 11 | -.192775922492228E+02 | -.133099202171580E+03 |
| 12 | -.301234424853915E+02 | -.311546785438622E+00 |
| 13 | -.301234424853915E+02 | -.142545596071704E+03 |
| 14 | -.335103274930459E+02 | -.163554217695133E+03 |

Table 2b

| | DALANC, DRTHES, DQR Subroutines (Matrix has been truncated to single precision significance) | 84.58 Seconds |
|----|---|-----------------------|
| 1 | -.161637993977430D+02 | .433345157057497D+02 |
| 2 | -.335630201800936D+02 | .207449518517321D+02 |
| 1 | -.221363489782061D+00 | -.683859559232783D+01 |
| 2 | -.221363489782061D+00 | -.136018547264815D+03 |
| 3 | -.210845322414368D+01 | -.818837272783772D+01 |
| 4 | -.210845322414368D+01 | -.134668770129306D+03 |
| 5 | -.514736174758617D+01 | -.978220853335398D+01 |
| 6 | -.514736174758617D+01 | -.133074934323789D+03 |
| 7 | -.104416528784868D+02 | -.110816366201131D+02 |
| 8 | -.104416528784868D+02 | -.131775506237030D+03 |
| 9 | -.161637993977430D+02 | -.186191658562893D+03 |
| 10 | -.193337651348488D+02 | -.969755942685737D+01 |
| 11 | -.193337651348488D+02 | -.133159583430286D+03 |
| 12 | -.301660899657195D+02 | -.251656928888859D+00 |
| 13 | -.301660899657195D+02 | -.142605485928254D+03 |
| 14 | -.335630201800936D+02 | -.163602094708875D+03 |

TABLE 2 (CONTINUED)

Table 2c

DALANCE, DRTHES, DQR Subroutines 81.25 Seconds

| | | |
|----|-----------------------|-----------------------|
| 1 | -.161635728329553D+02 | .432950045889481D+02 |
| 2 | -.335577057717484D+02 | .207044804956883D+02 |
| 1 | -.204921408502594D+00 | -.685273791773559D+01 |
| 2 | -.204921408502594D+00 | -.136004404939408D+03 |
| 3 | -.208873186667484D+01 | -.820338143323628D+01 |
| 4 | -.208873186667484D+01 | -.134653761423907D+03 |
| 5 | -.512410079791165D+01 | -.979976330355343D+01 |
| 6 | -.512410079791165D+01 | -.133057379553590D+03 |
| 7 | -.104158704992893D+02 | -.111054185480280D+02 |
| 8 | -.104158704992893D+02 | -.131751724309115D+03 |
| 9 | -.161635728329553D+02 | -.186152147446091D+03 |
| 10 | -.193106276285779D+02 | -.973095393274997D+01 |
| 11 | -.193106276285779D+02 | -.133126188924393D+03 |
| 12 | -.301520647479031D+02 | -.291474727463069D+00 |
| 13 | -.301520647479031D+02 | -.142565668129680D+03 |
| 14 | -.335577057717484D+02 | -.163561623352832D+03 |

Table 2d

DRTHES, DQR Subroutines 76.27 Seconds
(No balancing)

| | | |
|----|-----------------------|-----------------------|
| 1 | -.161635728329026D+02 | .43295004588919D+02 |
| 2 | -.335577057717281D+02 | .207044804957628D+02 |
| 1 | -.204921408518517D+00 | -.685273791773917D+01 |
| 2 | -.204921408518517D+00 | -.136004404939404D+03 |
| 3 | -.208873186669188D+01 | -.820338143324120D+01 |
| 4 | -.208873186669188D+01 | -.134653761423902D+03 |
| 5 | -.512410079793201D+01 | -.979976330356033D+01 |
| 6 | -.512410079793201D+01 | -.133057379553583D+03 |
| 7 | -.104158704993175D+02 | -.111054185480356D+02 |
| 8 | -.104158704993175D+02 | -.131751724309108D+03 |
| 9 | -.161635728329026D+02 | -.186152147446035D+03 |
| 10 | -.193106276286219D+02 | -.973095393274980D+01 |
| 11 | -.193106276286219D+02 | -.133126188924393D+03 |
| 12 | -.301520647479561D+02 | -.291474727423287D+00 |
| 13 | -.301520647479561D+02 | -.142565668129720D+03 |
| 14 | -.335577057717281D+02 | -.163561623352906D+03 |

OBSERVATIONS AND CONCLUSIONS

Study of the preceding tables led to the following observations:

- 1) The situation as regards the complex matrix requires double-precision eigenvalue computation on the CDC 6400 computer, as indicated by a comparison of the eigenvalues in Tables 1a and 1c, realizing that
 - i) the real parts of the eigenvalues must be equal in pairs, and
 - ii) the sequence of double-precision subroutines for the complex LR algorithm obtains eigenvalues satisfying i) by iterating directly for each root and not by some deflation procedure which involves solving a quadratic equation, a procedure which could provide equal real parts.The situation for the real matrix is similar. The eigenvalues in Tables 2a and 2c agree to only a few decimal places at best, but the eigenvalues in Tables 1c and 2c are virtually identical. However, the eigenvalues in Table 2c, unlike those in Table 1c, appear to be the result of a series of quadratic deflations. Unfortunately, the double-precision computations take more than four times the time required for the single-precision computations.
- 2) Since the double-precision subroutines are assumed to be more accurate than the corresponding single-precision subroutines, Tables 1b and 1c and Tables 2b and 2c indicate that the original matrix should be generated and input to the eigenvalue subroutines in double precision. Since the 'b' and 'c' eigenvalues are computed using the same double-precision subroutines, the substantial discrepancies between the 'b' and 'c' results can only be explained by the sensitivity of the eigenvalues. Since the 'c' eigenvalues meet the pairwise equality condition on their real parts, the double-precision matrix is the preferred input.
- 3) The situation with respect to the use of balancing subroutines is not clear. Comparison of Tables 2c and 2d indicates that the use of DALANC, the double-precision balancing subroutine for real matrices, is desirable. However, in one instance the use of DBAL, the double-precision balancing matrix for complex matrices, made no appreciable difference. The use of

balancing subroutines is therefore recommended as a matter of policy, although the value of DBAL appears open to question and to merit further investigation.

4) ELMHES and ORTHES, the Hessenberg reduction subroutines for real matrices, and their double precision counterparts DLMHES and DRTHES give comparable accuracy and require similar computation times respectively.

ACKNOWLEDGMENTS

The author wishes to thank Dr. Elizabeth H. Cuthill (1805) for her invaluable assistance and Dr. R.J. Hansen of the Naval Research Laboratory and Professor Matthew Kelleher of the Naval Postgraduate School for their interest and encouragement.

APPENDIX A

PROGRAM LISTINGS

NOTE: It is to be emphasized that the subroutines listed herein are solely the present author's responsibility and were obtained by the modifications described in this report. The comment cards are those of the original single-precision EISPACK subroutines.

```

3          71215001
3          -----
3          SUBROUTINE DBAL(NM,N,AR,AI,LOW,IGH,SCALE)    71215002
3          71215003
3          INTEGER I,J,K,L,M,N, JJ,NM,IGH,LOW,IEXC    71215004
3          REAL AR(NM,N),AI(NM,N),SCALE(N)           71215005
3          REAL C,F,G,R,S,B2,RADIX                   71215006
3          DOUBLE PRECISION AR(NM,N),AI(NM,N),SCALE(N),C,F,G,R,S,B2,RADIX 71215007
3          REAL ABS                                71215008
3          LOGICAL NOCONV                           71215009
3          THIS SUBROUTINE IS A TRANSLATION OF THE ALGOL PROCEDURE      71215010
3          CBALANCE, WHICH IS A COMPLEX VERSION OF BALANCE,             71215011
3          NUM. MATH. 13, 293-304(1969) BY PARLETT AND REINSCH.        71215012
3          HANDBOOK FOR AUTO. COMP., VOL.II-LINEAR ALGEBRA, 315-326(1971). 71215013
3          71215014
3          THIS SUBROUTINE BALANCES A COMPLEX MATRIX AND ISOLATES      71215015
3          EIGENVALUES WHENEVER POSSIBLE.                            71215016
3          ON INPUT-                                         71215017
3          NM MUST BE SET TO THE ROW DIMENSION OF TWO-DIMENSIONAL      71215018
3          ARRAY PARAMETERS AS DECLARED IN THE CALLING PROGRAM       71215019
3          DIMENSION STATEMENT,                               71215020
3          N IS THE ORDER OF THE MATRIX,                         71215021
3          AR AND AI CONTAIN THE REAL AND IMAGINARY PARTS,          71215022
3          RESPECTIVELY, OF THE COMPLEX MATRIX TO BE BALANCED.      71215023
3          ON OUTPUT-                                         71215024
3          AR AND AI CONTAIN THE REAL AND IMAGINARY PARTS,          71215025
3          RESPECTIVELY, OF THE BALANCED MATRIX,                  71215026
3          LOW AND IGH ARE TWO INTEGERS SUCH THAT AR(I,J) AND AI(I,J) 71215027
3          ARE EQUAL TO ZERO IF
3          (1) I IS GREATER THAN J AND                          71215028
3          (2) J=1,...,LOW-1 OR I=IGH+1,...,N,                 71215029
3          SCALE CONTAINS INFORMATION DETERMINING THE          71215030
3          PERMUTATIONS AND SCALING FACTORS USED.                71215031
3          SUPPOSE THAT THE PRINCIPAL SUBMATRIX IN ROWS LOW THROUGH IGH   71215032
3          HAS BEEN BALANCED, THAT P(J) DENOTES THE INDEX INTERCHANGED 71215033
3          WITH J DURING THE PERMUTATION STEP, AND THAT THE ELEMENTS   71215034
3          OF THE DIAGONAL MATRIX USED ARE DENOTED BY D(I,J). THEN     71215035
3          SCALE(J) = P(J),      FOR J = 1,...,LOW-1               71215036
3          = D(J,J)          J = LOW,...,IGH                     71215037
3          = P(J)            J = IGH+1,...,N.                  71215038
3          THE ORDER IN WHICH THE INTERCHANGES ARE MADE IS N TO IGH+1, 71215039
3          THEN 1 TO LOW-1.                                     71215040
3          NOTE THAT 1 IS RETURNED FOR IGH IF IGH IS ZERO FORMALLY. 71215041

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C THE ALGOL PROCEDURE EXC CONTAINED IN CBALANCE APPEARS IN      71215055
C CBAL IN LINE. (NOTE THAT THE ALGOL ROLES OF IDENTIFIERS      71215056
C K,L HAVE BEEN REVERSED.)      71215057
C ARITHMETIC IS REAL THROUGHOUT.      71215058
C QUESTIONS AND COMMENTS SHOULD BE DIRECTED TO B. S. GARBOW,      71215059
C APPLIED MATHEMATICS DIVISION, ARGONNE NATIONAL LABORATORY      71215060
C -----
C ***** RADIX IS A MACHINE DEPENDENT PARAMETER SPECIFYING      71215061
C THE BASE OF THE MACHINE FLOATING POINT REPRESENTATION.      71215062
C *****      71215063
C *****      71215064
C -----      71215065
C ***** RADIX = 2.      71215066
C *****      71215067
C *****      71215068
C *****      71215069
C *****      71215070
C *****      71215071
C *****      71215072
C *****      71215073
C *****      71215074
C *****      71215075
C *****      71215076
C *****      71215077
C *****      71215078
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C *****      71215101
C *****      71215102
C *****      71215103
C *****      71215104
C *****      71215105
C *****      71215106
C *****      71215107
C *****      71215108
C *****      71215109

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      IF (I .EQ. J) GO TO 110          71215110
      IF (AR(J,I) .NE. 0.0 .OR. AI(J,I) .NE. 0.0) GO TO 120 71215111
110    CONTINUE                         71215112
C
      M = L                            71215113
      IEXC = 1                          71215114
      GO TO 20                          71215115
120    CONTINUE                         71215116
C
      GO TO 140                         71215117
C      ***** SEARCH FOR COLUMNS ISOLATING AN EIGENVALUE 71215118
C      AND PUSH THEM LEFT *****           71215119
130    K = K + 1                        71215120
C
140    DO 170 J = K, L                 71215121
C
      DO 150 I = K, L                 71215122
      IF (I .EQ. J) GO TO 150          71215123
      IF (AR(I,J) .NE. 0.0 .OR. AI(I,J) .NE. 0.0) GO TO 170 71215124
150    CONTINUE                         71215125
C
      M = K                            71215126
      IEXC = 2                          71215127
      GO TO 20                          71215128
170    CONTINUE                         71215129
C      ***** NOW BALANCE THE SUBMATRIX IN ROWS K TO L ***** 71215130
      DO 180 I = K, L                 71215131
180    SCALE(I) = 1.0                  71215132
C      ***** ITERATIVE LOOP FOR NORM REDUCTION *****       71215133
190    NOCONV = .FALSE.                71215134
C
      DO 270 I = K, L                 71215135
      C = 0.0                           71215136
      R = 0.0                           71215137
C
      DO 200 J = K, L                 71215138
      IF (J .EQ. I) GO TO 200          71215139
      C = C + ABS(AR(J,I)) + ABS(AI(J,I)) 71215140
      R = R + ABS(AR(I,J)) + ABS(AI(I,J)) 71215141
      C = C +DABS(AR(J,I)) +DABS(AI(J,I)) 71215142
      R = R +DABS(AR(I,J)) +DABS(AI(I,J)) 71215143
200    CONTINUE                         71215144
C
      G = R / RADIX                   71215145
      F = 1.0                          71215146
      S = C + R                        71215147
210    IF (C .GE. G) GO TO 220          71215148
      F = F * RADIX                   71215149
      C = C * B2                      71215150
      GO TO 210                        71215151
220    G = R * RADIX                   71215152
230    IF (C .LT. G) GO TO 240          71215153
      F = F / RADIX                   71215154
      C = C / B2                      71215155
      GO TO 230                        71215156

```

```

C      ***** NOW BALANCE *****
240    IF ((C + R) / F .GE. 0.95 * S) GO TO 270      71215163
      G = 1.0 / F                                     71215164
      SCALE(I) = SCALE(I) * F                         71215165
      NOCONV = .TRUE.                                71215166
C
      DO 250 J = K, N                               71215167
         AR(I,J) = AR(I,J) * G                     71215168
         AI(I,J) = AI(I,J) * G                     71215169
250    CONTINUE                                 71215170
C
      DO 260 J = 1, L                           71215171
         AR(J,I) = AR(J,I) * F                     71215172
         AI(J,I) = AI(J,I) * F                     71215173
260    CONTINUE                                 71215174
C
      270 CONTINUE                                71215175
C
      IF (NOCONV) GO TO 190                      71215176
C
280    LOW = K                                    71215177
      IGH = L                                    71215178
      RETURN                                     71215179
C      ***** LAST CARD OF CBAL *****
      END                                         71215180
                                                71215181
                                                71215182
                                                71215183
                                                71215184
                                                71215185
                                                71215186
                                                71215187

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C                                         82215001
C----- 82215002
C                                         82215003
C SUBROUTINE DOMHES(NM,N,LOW,IGH,AR,AI,INT) 82215004
C                                         82215005
C----- 82215006
C INTEGER I,J,M,N,LA,NM,IGH,KP1,LOW,MM1,MP1 82215007
C REAL AR(NM,N),AI(NM,N) 82215008
C REAL XR,XI,YR,YI
C DOUBLE PRECISION AR(NM,N),AI(NM,N),XR,XI,YR,YI
C REAL ABS 82215009
C INTEGER INT(IGH) 82215010
C COMPLEX X,Y 82215011
C REAL T1(2),T2(2) 82215012
C EQUIVALENCE (X,T1(1),XR),(T1(2),XI),(Y,T2(1),YR),(T2(2),YI) 82215013
C                                         82215014
C THIS SUBROUTINE IS A TRANSLATION OF THE ALGOL PROCEDURE COMHES, 82215015
C NUM. MATH. 12, 349-368(1968) BY MARTIN AND WILKINSON. 82215016
C HANDBOOK FOR AUTO. COMP., VOL.II-LINEAR ALGEBRA, 339-358 (1971). 82215017
C                                         82215018
C GIVEN A COMPLEX GENERAL MATRIX, THIS SUBROUTINE 82215019
C REDUCES A SUBMATRIX SITUATED IN ROWS AND COLUMNS 82215020
C LOW THROUGH IGH TO UPPER HESSENBERG FORM BY 82215021
C STABILIZED ELEMENTARY SIMILARITY TRANSFORMATIONS. 82215022
C                                         82215023
C ON INPUT- 82215024
C                                         82215025
C NM MUST BE SET TO THE ROW DIMENSION OF TWO-DIMENSIONAL 82215026
C ARRAY PARAMETERS AS DECLARED IN THE CALLING PROGRAM 82215027
C DIMENSION STATEMENT, 82215028
C                                         82215029
C N IS THE ORDER OF THE MATRIX, 82215030
C                                         82215031
C LOW AND IGH ARE INTEGERS DETERMINED BY THE BALANCING 82215032
C SUBROUTINE CBAL. IF CBAL HAS NOT BEEN USED, 82215033
C SET LOW=1, IGH=N, 82215034
C                                         82215035
C AR AND AI CONTAIN THE REAL AND IMAGINARY PARTS, 82215036
C RESPECTIVELY, OF THE COMPLEX INPUT MATRIX. 82215037
C                                         82215038
C ON OUTPUT- 82215039
C                                         82215040
C AR AND AI CONTAIN THE REAL AND IMAGINARY PARTS, 82215041
C RESPECTIVELY, OF THE HESSENBERG MATRIX. THE 82215042
C MULTIPLIERS WHICH WERE USED IN THE REDUCTION 82215043
C ARE STORED IN THE REMAINING TRIANGLES UNDER THE 82215044
C HESSENBERG MATRIX, 82215045
C                                         82215046
C INT CONTAINS INFORMATION ON THE ROWS AND COLUMNS 82215047
C INTERCHANGED IN THE REDUCTION. 82215048
C ONLY ELEMENTS LOW THROUGH IGH ARE USED. 82215049
C                                         82215050
C ARITHMETIC IS REAL EXCEPT FOR THE REPLACEMENT OF THE ALGOL 82215051
C PROCEDURE CDIV BY COMPLEX DIVISION. 82215052
C                                         82215053
C QUESTIONS AND COMMENTS SHOULD BE DIRECTED TO B. S. GARROW, 82215054

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C      APPLIED MATHEMATICS DIVISION, ARGONNE NATIONAL LABORATORY      82215055
C-----      82215056
C-----      82215057
C-----      82215058
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C-----      82215060
C-----      82215061
C-----      82215062
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C-----      82215103
C-----      82215104
C-----      82215105
C-----      82215106

```

LA = IGH - 1
 KP1 = LOW + 1
 IF (LA .LT. KP1) GO TO 200
 DO 180 M = KP1, LA
 MM1 = M - 1
 XR = 0.0
 XI = 0.0
 I = M
 DO 100 J = M, IGH
 IF (ABS(AR(J,MM1)) + ABS(AI(J,MM1))
 .LE. ABS(XR) + ABS(XI)) GO TO 100
 X IF(DABS(AR(J,MM1)) +DABS(AI(J,MM1))
 ,LE.DABS(XR) +DABS(XI)) GO TO 100
 XR = AR(J,MM1)
 XI = AI(J,MM1)
 I = J
 100 CONTINUE
 INT(M) = I
 IF (I .EQ. M) GO TO 130
 ***** INTERCHANGE ROWS AND COLUMNS OF AR AND AI ****
 DO 110 J = MM1, N
 YR = AR(I,J)
 AR(I,J) = AR(M,J)
 AR(M,J) = YR
 YI = AI(I,J)
 AI(I,J) = AI(M,J)
 AI(M,J) = YI
 110 CONTINUE
 DO 120 J = 1, IGH
 YR = AR(J,I)
 AR(J,I) = AR(J,M)
 AR(J,M) = YR
 YI = AI(J,I)
 AI(J,I) = AI(J,M)
 AI(J,M) = YI
 120 CONTINUE
 ***** END INTERCHANGE *****
 130 IF (XR .EQ. 0.0 .AND. XI .EQ. 0.0) GO TO 180
 MP1 = M + 1
 DO 160 I = MP1, IGH
 YR = AR(I,MM1)
 YI = AI(I,MM1)
 IF (YR .EQ. 0.0 .AND. YI .EQ. 0.0) GO TO 160
 Y = Y / X
 CALL CLXDVDE(YR,YI,YR,YI,XR,XI)
 AR(I,MM1) = YR

```

      AI(I,MM1) = YI          82215107
C
      DO 140 J = M, N        82215108
        AR(I,J) = AR(I,J) - YR * AR(M,J) + YI * AI(M,J)
        AI(I,J) = AI(I,J) - YR * AI(M,J) - YI * AR(M,J)
140    CONTINUE             82215109
C
      DO 150 J = 1, IGH       82215110
        AR(J,M) = AR(J,M) + YR * AR(J,I) - YI * AI(J,I)
        AI(J,M) = AI(J,M) + YR * AI(J,I) + YI * AR(J,I)
150    CONTINUE             82215111
C
      160    CONTINUE           82215112
C
      180 CONTINUE             82215113
C
      200 RETURN               82215114
C
      ***** LAST CARD OF COMMES *****
      END                      82215115
                                82215116
                                82215117
                                82215118
                                82215119
                                82215120
                                82215121
                                82215122
                                82215123
                                82215124
                                82215125

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C-----95215001
C-----95215002
C-----95215003
C-----95215004
C-----95215005
C-----95215006
C-----95215007
C-----95215008
SUBROUTINE DOMLR(NM,N,LOW,IGH,HR,HI,WR,WI,IERR)95215001
C-----95215002
C-----95215003
C-----95215004
C-----95215005
C-----95215006
C-----95215007
C-----95215008
INTEGER I,J,L,M,N,EN,LL,MM,NM,IGH,IM1,ITS,LOW,MP1,ENM1,IERR95215001
REAL HR(NM,N),HI(NM,N),WR(N),WI(N)95215002
REAL SI,SR,TR,XI,XR,YI,YR,ZZI,ZZR,MACHEP95215003
DOUBLE PRECISION HR(NM,N),HI(NM,N),WR(N),WI(N),SI,SR,TR,XI,XR,95215004
YI,YR,ZZI,ZZR,MACHEP,ZR,ZI95215005
1 EQUIVALENCE (ZR,ZZR),(ZI,ZZI)95215006
C-----95215007
REAL ABS95215008
COMPLEX X,Y,Z95215009
COMPLEX CSQRT,CMPLX95215010
REAL T1(2),T2(2),T3(2)95215011
EQUIVALENCE (X,T1(1),XR),(T1(2),XI),(Y,T2(1),YR),(T2(2),YI),95215012
X (Z,T3(1),ZZR),(T3(2),ZZI)95215013
C-----95215014
THIS SUBROUTINE IS A TRANSLATION OF THE ALGOL PROCEDURE COMLR,95215015
NUM. MATH. 12, 369-376(1968) BY MARTIN AND WILKINSON.95215016
HANDBOOK FOR AUTO. COMP., VOL.II-LINEAR ALGEBRA, 396-403(1971).95215017
C-----95215018
THIS SUBROUTINE FINDS THE EIGENVALUES OF A COMPLEX95215019
UPPER HESSENBERG MATRIX BY THE MODIFIED LR METHOD.95215020
C-----95215021
ON INPUT-95215022
C-----95215023
NM MUST BE SET TO THE ROW DIMENSION OF TWO-DIMENSIONAL95215024
ARRAY PARAMETERS AS DECLARED IN THE CALLING PROGRAM95215025
DIMENSION STATEMENT,95215026
C-----95215027
N IS THE ORDER OF THE MATRIX,95215028
C-----95215029
LOW AND IGH ARE INTEGERS DETERMINED BY THE BALANCING95215030
SUBROUTINE CBAL. IF CBAL HAS NOT BEEN USED,95215031
SET LOW=1, IGH=N,95215032
C-----95215033
HR AND HI CONTAIN THE REAL AND IMAGINARY PARTS,95215034
RESPECTIVELY, OF THE COMPLEX UPPER HESSENBERG MATRIX.95215035
THEIR LOWER TRIANGLES BELOW THE SUBDIAGONAL CONTAIN THE95215036
MULTIPLIERS WHICH WERE USED IN THE REDUCTION BY COMHES,95215037
IF PERFORMED.95215038
C-----95215039
ON OUTPUT-95215040
C-----95215041
THE UPPER HESSENBERG PORTIONS OF HR AND HI HAVE BEEN95215042
DESTROYED. THEREFORE, THEY MUST BE SAVED BEFORE95215043
CALLING COMLR IF SUBSEQUENT CALCULATION OF95215044
EIGENVECTORS IS TO BE PERFORMED,95215045
C-----95215046
WR AND WI CONTAIN THE REAL AND IMAGINARY PARTS,95215047
RESPECTIVELY, OF THE EIGENVALUES. IF AN ERROR95215048
EXIT IS MADE, THE EIGENVALUES SHOULD BE CORRECT95215049
FOR INDICES IERR+1,...,N,95215050
C-----95215051
C-----95215052

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C     IERR IS SET TO          95215053
      ZERO      FOR NORMAL RETURN,
      J        IF THE J-TH EIGENVALUE HAS NOT BEEN
                  DETERMINED AFTER 30 ITERATIONS.          95215054
                                                               95215055
                                                               95215056
                                                               95215057
                                                               95215058
ARITHMETIC IS REAL EXCEPT FOR THE REPLACEMENT OF THE ALGOL          95215059
PROCEDURE CDIV BY COMPLEX DIVISION AND USE OF THE SUBROUTINES          95215060
CSQRT AND CMPLX IN COMPUTING COMPLEX SQUARE ROOTS.          95215061
                                                               95215062
QUESTIONS AND COMMENTS SHOULD BE DIRECTED TO B. S. GARBOV,          95215063
APPLIED MATHEMATICS DIVISION, ARGONNE NATIONAL LABORATORY          95215064
-----          95215065
                                                               95215066
***** MACHEP IS A MACHINE DEPENDENT PARAMETER SPECIFYING          95215067
THE RELATIVE PRECISION OF FLOATING POINT ARITHMETIC.          95215068
                                                               95215069
*****          95215070
MACHEP = 2.**(-95)          95215072
C
C     IERR = 0          95215073
C     ***** STORE ROOTS ISOLATED BY CBAL *****
180 DO 200 I = 1, N          95215074
    IF (I .GE. LOW .AND. I .LE. IGH) GO TO 200          95215075
    WR(I) = HR(I,I)          95215076
    WI(I) = HI(I,I)          95215077
200 CONTINUE          95215078
          95215079
C
C     EN = IGH          95215080
C     TR = 0.0          95215081
C     TI = 0.0          95215082
C     ***** SEARCH FOR NEXT EIGENVALUE *****
C220 IF (EN .LT. LOW) GO TO 1001          95215083
    ITS = 0          95215084
    ENM1 = EN - 1          95215085
    ***** LOOK FOR SINGLE SMALL SUB-DIAGONAL ELEMENT          95215086
    FOR L=EN STEP -1 UNTIL LOW -- *****
240 DO 260 LL = LOW, EN          95215087
    L = EN + LOW - LL          95215088
    IF (L .EQ. LOW) GO TO 300          95215089
    *     IF (ABS(HR(L,L-1)) + ABS(HI(L,L-1)) .LE.
    *     X     MACHEP * (ABS(HR(L-1,L-1)) + ABS(HI(L-1,L-1))
    *     X     + ABS(HR(L,L)) + ABS(HI(L,L)))) GO TO 300          95215090
    *     IF (DABS(HR(L,L-1)) +DABS(HI(L,L-1)) .LE.
    X     MACHEP *(DABS(HR(L-1,L-1)) +DABS(HI(L-1,L-1))
    X     +DABS(HR(L,L)) +DABS(HI(L,L)))) GO TO 300          95215091
260 CONTINUE          95215092
    ***** FORM SHIFT *****
300 IF (L .EQ. EN) GO TO 660          95215093
    IF (ITS .EQ. 30) GO TO 1000          95215094
    IF (ITS .EQ. 10 .OR. ITS .EQ. 20) GO TO 320          95215095
    SR = HR(EN,EN)          95215096
    SI = HI(EN,EN)          95215097
    XR = HR(ENM1,EN) * HR(EN,ENM1) - HI(ENM1,EN) * HI(EN,ENM1)          95215098
    XI = HR(ENM1,EN) * HI(EN,ENM1) + HI(ENM1,EN) * HR(EN,ENM1)          95215099

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IF (XR .EQ. 0.0 .AND. XI .EQ. 0.0) GO TO 340 95215105
YR = (HR(ENM1,ENM1) - SR) / 2.0 95215106
YI = (HI(ENM1,ENM1) - SI) / 2.0 95215107
* Z = CSQRT(CMPLX(YR**2-YI**2+XR,2.0*YR*YI+XI)) 95215108
CALL CLXSQRT(ZR,ZI,YR*YR-YI*YI+XR,2.0*YR*YI+XI)
* IF (YR * ZZR + YI * ZZI .LT. 0.0) Z = -Z 95215109
IF (YR * ZZR + YI * ZZI .GE. 0.0) GO TO 301
ZR=-ZR
ZI=-ZI
* X = X / (Y + Z) 95215110
301 CALL CLXDVDE(XR,XI,XR,XI,YR+ZR,YI+ZI)
SR = SR - XR
SI = SI - XI
GO TO 340
***** FORM EXCEPTIONAL SHIFT *****
* 320 SR = ABS(HR(EN,ENM1)) + ABS(HR(ENM1,EN-2)) 95215115
* 320 SR =DABS(HR(EN,ENM1)) +DABS(HR(ENM1,EN-2))
* SI = ABS(HI(EN,ENM1)) + ABS(HI(ENM1,EN-2)) 95215116
* SI =DABS(HI(EN,ENM1)) +DABS(HI(ENM1,EN-2))
C
340 DO 360 I = LOW, EN
    HR(I,I) = HR(I,I) - SR
    HI(I,I) = HI(I,I) - SI
360 CONTINUE
C
    TR = TR + SR
    TI = TI + SI
    ITS = ITS + 1
C
***** LOOK FOR TWO CONSECUTIVE SMALL
***** SUB-DIAGONAL ELEMENTS *****
* XR = ABS(HR(ENM1,ENM1)) + ABS(HI(ENM1,ENM1)) 95215126
* XR =DABS(HR(ENM1,ENM1)) +DABS(HI(ENM1,ENM1)) 95215127
* YR = ABS(HR(EN,ENM1)) + ABS(HI(EN,ENM1)) 95215128
* YR =DABS(HR(EN,ENM1)) +DABS(HI(EN,ENM1))
ZZR =DABS(HR(EN,EN)) +DABS(HI(EN,EN))
C
***** FOR M=EN-1 STEP -1 UNTIL L DO -- *****
DO 380 MM = L, ENM1 95215131
    M = ENM1 + L - MM 95215132
    IF (M .EQ. L) GO TO 420 95215133
    YI = YR 95215134
* YR = ABS(HR(M,M-1)) + ABS(HI(M,M-1)) 95215135
* YR =DABS(HR(M,M-1)) +DABS(HI(M,M-1))
    XI = ZZR 95215137
    ZZR = XR 95215138
* XR = ABS(HR(M-1,M-1)) + ABS(HI(M-1,M-1)) 95215139
* XR =DABS(HR(M-1,M-1)) +DABS(HI(M-1,M-1))
    IF (YR .LE. MACHEP * ZZR / YI * (ZZR + XR + XI)) GO TO 420 95215140
380 CONTINUE
C
***** TRIANGULAR DECOMPOSITION M=L*R *****
420 MP1 = M + 1 95215141
C
DO 520 I = MP1, EN 95215142
    IM1 = I - 1 95215143
    XR = HR(IM1,IM1) 95215144
    XI = HI(IM1,IM1) 95215145
    95215146
    95215147
    95215148

```

```

      YR = HR(I,IM1)                                95215149
      YI = HI(I,IM1)                                95215150
*     IF (ABS(XR) + ABS(XI) .GE. ABS(YR) + ABS(YI)) GO TO 460 95215151
*     IF (DABS(XR) + DABS(XI) .GE. DABS(YR) + DABS(YI)) GO TO 460
C     ***** INTERCHANGE ROWS OF HR AND HI *****
      DO 440 J = IM1, N                            95215152
      ZZR = HR(IM1,J)                             95215153
      HR(IM1,J) = HR(I,J)                           95215154
      HR(I,J) = ZZR                               95215155
      ZZI = HI(IM1,J)                            95215156
      HI(IM1,J) = HI(I,J)                           95215157
      HI(I,J) = ZZI                               95215158
  440  CONTINUE                                     95215159
C
*     Z = X / Y
      CALL CLXDVDE(ZR,ZI,XR,XI,YR,YI)           95215160
      WR(I) = 1.0                                 95215161
      GO TO 480                                     95215162
* 460  Z = Y / X
  460  CALL CLXDVDE(ZR,ZI,YR,YI,XR,XI)           95215163
      WR(I) = -1.0                               95215164
  480  HR(I,IM1) = ZZR                          95215165
      HI(I,IM1) = ZZI                           95215166
C
      DO 500 J = I, EN                           95215167
      HR(I,J) = HR(I,J) - ZZR * HR(IM1,J) + ZZI * HI(IM1,J) 95215168
      HI(I,J) = HI(I,J) - ZZR * HI(IM1,J) - ZZI * HR(IM1,J) 95215169
  500  CONTINUE                                     95215170
C
  520  CONTINUE                                     95215171
C     ***** COMPOSITION R*L=H *****
      DO 640 J = MP1, EN                         95215172
      XR = HR(J,J-1)                            95215173
      XI = HI(J,J-1)                            95215174
      HR(J,J-1) = 0.0                            95215175
      HI(J,J-1) = 0.0                            95215176
C     ***** INTERCHANGE COLUMNS OF HR AND HI,
C     IF NECESSARY *****
      IF (WR(J) .LE. 0.0) GO TO 580             95215177
C
      DO 540 I = L, J                           95215178
      ZZR = HR(I,J-1)                            95215179
      HR(I,J-1) = HR(I,J)                           95215180
      HR(I,J) = ZZR                               95215181
      ZZI = HI(I,J-1)                            95215182
      HI(I,J-1) = HI(I,J)                           95215183
      HI(I,J) = ZZI                               95215184
  540  CONTINUE                                     95215185
C
  580  DO 600 I = L, J                           95215186
      HR(I,J-1) = HR(I,J-1) + XR * HR(I,J) - XI * HI(I,J) 95215187
      HI(I,J-1) = HI(I,J-1) + XR * HI(I,J) + XI * HR(I,J) 95215188
  600  CONTINUE                                     95215189
C
  640  CONTINUE                                     95215190
C

```

```

C          GO TO 240                                95215201
C          ***** A ROOT FOUND *****
660  WR(EN) = HR(EN,EN) + TR                      95215202
      WI(EN) = HI(EN,EN) + TI                      95215203
      EN = ENM1                                     95215204
      GO TO 220                                     95215205
C          ***** SET ERROR -- NO CONVERGENCE TO AN   95215206
C          EIGENVALUE AFTER 30 ITERATIONS *****       95215207
1000 IERR = EN                                     95215208
1001 RETURN                                       95215209
C          ***** LAST CARD OF COMLR *****           95215210
      END                                         95215211
                                                 95215212
                                                 95215213

```

```

C SUBROUTINE CLXDVDE(ZR,ZI,XR,XI,YR,YI)
C DOUBLE PRECISION ZR,ZI,XR,XI,YR,YI,H,QR,QI,HH
C IF (DABS(YR)+DABS(YI)) 3,1,3
C
1 WRITE(6,2)
2 FORMAT(1H1/14(1H0/),30X,*CLXDVDE MESSAGE - YOU HAVE JUST ATTEMPTED
1 TO DIVIDE BY ZERO.*)
STOP
C
3 IF (DABS(YR)-DABS(YI)) 5,5,4
C
4 H=YI/YR
HH=H*YI+YR
QR=(XR+H*XI)/HH
QI=(XI-H*XR)/HH
ZR=QR
ZI=QI
RETURN
C
5 H=YR/YI
HH=H*YR+YI
QR=(H*XR+XI)/HH
QI=(H*XI-XR)/HH
ZR=QR
ZI=QI
RETURN -
END

```

4

```

      SUBROUTINE CLKSQRT(YR,YI,XR,XI)
C
C      DOUBLE PRECISION YR,YI,XR,XI,XR1,XI1,H,DPCABS
C
C      FIRST COMPUTE DPCABS, THE ABSOLUTE VALUE OF THE RADICAND.
C
C      XR1=DABS(XR)
C      XI1=DABS(XI)
C
C      IF (XI1-XR1) 2,2,1
C
C      1 H=XR1
C          XR1=XI1
C          XI1=H
C
C      2 IF (XI1) 4,3,4
C
C      3 DPCABS=XR1
C          GO TO 5
C
C      4 DPCABS=XR1*DSQRT(1.00+(XI1/XR1)*(XI1/XR1))
C
C
C      5 H=DSQRT((DABS(XR)+DPCABS)/2.00)
C
C          IF,(XI) 6,7,6
C
C          6 XI=XI/(2.00*H)
C
C          7 IF (XR) 9,8,8
C
C          8 YR=H
C              YI=XI
C              RETURN
C
C          9 IF (XI) 11,10,10
C
C          10 YR=XI
C              YI=-1
C              RETURN
C
C          11 YR=-XI
C              YI=-H
C              RETURN
C              END

```

```

C                                         69215001
C                                         69215002
C                                         69215003
* SUBROUTINE BALANC(NM,N,A,LOW,IGH,SCALE) 69215004
SUBROUTINE DALANC(NM,N,A,LOW,IGH,SCALE)   69215005
C                                         69215006
C                                         69215007
* INTEGER I,J,K,L,M,N,JJ,NM,IGH,LOW,IEXC 69215008
* REAL A(NM,N),SCALE(N)                   69215009
* REAL C,F,G,R,S,B2,RADIX                69215010
DOUBLE PRECISION A(NM,N),SCALE(N),C,F,G,R,S,B2,RADIX 69215011
C                                         69215012
REAL ABS                                69215013
LOGICAL NOCONV                           69215014
C                                         69215015
THIS SUBROUTINE IS A TRANSLATION OF THE ALGOL PROCEDURE BALANCE, 69215016
NUM. MATH. 13, 293-304(1969) BY PARLETT AND REINSCH.          69215017
HANDBOOK FOR AUTO. COMP., VOL.II-LINEAR ALGEBRA, 315-326(1971). 69215018
C                                         69215019
THIS SUBROUTINE BALANCES A REAL MATRIX AND ISOLATES           69215020
EIGENVALUES WHENEVER POSSIBLE.                            69215021
C                                         69215022
ON INPUT -                                         69215023
NM MUST BE SET TO THE ROW DIMENSION OF TWO-DIMENSIONAL      69215024
ARRAY PARAMETERS AS DECLARED IN THE CALLING PROGRAM        69215025
DIMENSION STATEMENT,                                     69215026
N IS THE ORDER OF THE MATRIX,                         69215027
A CONTAINS THE INPUT MATRIX TO BE BALANCED.            69215028
C                                         69215029
ON OUTPUT-
A CONTAINS THE BALANCED MATRIX,                      69215030
C                                         69215031
LOW AND IGH ARE TWO INTEGERS SUCH THAT A(I,J)           69215032
IS EQUAL TO ZERO IF                                     69215033
(1) I IS GREATER THAN J AND                          69215034
(2) J=1,...,LOW-1 OR I=IGH+1,...,N,                  69215035
C                                         69215036
SCALE CONTAINS INFORMATION DETERMINING THE             69215037
PERMUTATIONS AND SCALING FACTORS USED.                 69215038
C                                         69215039
SUPPOSE THAT THE PRINCIPAL SUBMATRIX IN ROWS LOW THROUGH IGH    69215040
HAS BEEN BALANCED, THAT P(J) DENOTES THE INDEX INTERCHANGED    69215041
WITH J DURING THE PERMUTATION STEP, AND THAT THE ELEMENTS     69215042
OF THE DIAGONAL MATRIX USED ARE DENOTED BY D(I,J). THEN       69215043
SCALE(J) = P(J), FOR J = 1,...,LOW-1                      69215044
= D(J,J),          J = LOW,...,IGH                     69215045
= P(J)           J = IGH+1,...,N.                      69215046
C                                         69215047
THE ORDER IN WHICH THE INTERCHANGES ARE MADE IS N TO IGH+1,    69215048
THEN 1 TO LOW-1.                                         69215049
C                                         69215050
NOTE THAT 1 IS RETURNED FOR IGH IF IGH IS ZERO FORMALLY.      69215051
C                                         69215052
THE ALGOL PROCEDURE EXC CONTAINED IN BALANCE APPEARS IN      69215053

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C      BALANC IN LINE. (NOTE THAT THE ALGOL ROLES OF IDENTIFIERS      69215054
C      K,L HAVE BEEN REVERSED.)                                     69215055
C
C      QUESTIONS AND COMMENTS SHOULD BE DIRECTED TO B. S. GARBOH,      69215056
C      APPLIED MATHEMATICS DIVISION, ARGONNE NATIONAL LABORATORY      69215057
C
C      -----
C      ***** RADIX IS A MACHINE DEPENDENT PARAMETER SPECIFYING      69215062
C          THE BASE OF THE MACHINE FLOATING POINT REPRESENTATION.      69215063
C
C          ****
C      RADIX = 2.                                                 69215064
C
C      B2 = RADIX * RADIX                                         69215065
C      K = 1                                                       69215066
C      L = N                                                       69215067
C      GO TO 100
C      ***** IN-LINE PROCEDURE FOR ROW AND                      69215071
C          COLUMN EXCHANGE ****
C      20 SCALE(M) = J                                         69215074
C          IF (J .EQ. M) GO TO 50                                69215075
C
C          DO 30 I = 1, L                                         69215076
C              F = A(I,J)
C              A(I,J) = A(I,M)
C              A(I,M) = F
C      30 CONTINUE
C
C          DO 40 I = K, N                                         69215082
C              F = A(J,I)
C              A(J,I) = A(M,I)
C              A(M,I) = F
C      40 CONTINUE
C
C      50 GO TO (90,130), IEXC
C          ***** SEARCH FOR ROWS ISOLATING AN EIGENVALUE        69215089
C          AND PUSH THEM DOWN ****
C      80 IF (L .EQ. 1) GO TO 280
C          L = L - 1
C          ***** FOR J=L STEP -1 UNTIL 1 DO -- *****
C      100 DO 120 JJ = 1, L
C              J = L + 1 - JJ
C
C          DO 110 I = 1, L
C              IF (I .EQ. J) GO TO 110
C                  IF (A(J,I) .NE. 0.0) GO TO 120
C      110 CONTINUE
C
C          M = L
C          IEXC = 1
C          GO TO 20
C      120 CONTINUE
C
C          GO TO 140

```

```

C      ***** SEARCH FOR COLUMNS ISOLATING AN EIGENVALUE          69215109
C      AND PUSH THEM LEFT ****
C      130 K = K + 1                                              69215110
C
C      140 DO 170 J = K, L                                         69215111
C
C          DO 150 I = K, L                                         69215112
C              IF (I .EQ. J) GO TO 150
C              IF (A(I,J) .NE. 0.0) GO TO 170
C 150      CONTINUE
C
C          M = K
C          IEXC = 2
C          GO TO 20
C 170      CONTINUE
C      ***** NOW BALANCE THE SUBMATRIX IN ROWS K TO L ****       69215123
C      DO 180 I = K, L                                         69215124
C
C 180      SCALE(I) = 1.0                                         69215125
C      ***** ITERATIVE LOOP FOR NORM REDUCTION ****             69215126
C 190      NOCONV = .FALSE.                                     69215127
C
C      DO 270 I = K, L                                         69215128
C          C = 0.0
C          R = 0.0
C
C          DO 200 J = K, L                                         69215129
C              IF (J .EQ. I) GO TO 200
C              C = C + ABS(A(J,I))
C              C = C + DABS(A(J,I))
C              R = R + ABS(A(I,J))
C              R = R + DABS(A(I,J))
C 200      CONTINUE
C
C          G = R / RADIX                                         69215130
C          F = 1.0
C          S = C + R                                         69215131
C
C 210      IF (C .GE. G) GO TO 220
C          F = F * RADIX                                         69215132
C          C = C * B2
C          GO TO 210
C 220      G = R * RADIX                                         69215133
C
C 230      IF (C .LT. G) GO TO 240
C          F = F / RADIX                                         69215134
C          C = C / B2
C          GO TO 230
C
C      ***** NOW BALANCE ****                                     69215135
C 240      IF ((C + R) / F .GE. 0.95 * S) GO TO 270
C          G = 1.0 / F                                         69215136
C          SCALE(I) = SCALE(I) * F
C          NOCONV = .TRUE.
C
C          DO 250 J = K, N                                         69215137
C          A(I,J) = A(I,J) * G
C
C          DO 250 J = 1, L                                         69215138

```

| | | |
|-----|---------------------------------|----------|
| 260 | A(J,I) = A(J,I) * F | 69215162 |
| C | 270 CONTINUE | 69215163 |
| C | IF (NOCONV) GO TO 190 | 69215164 |
| C | 280 LOW = K | 69215165 |
| | IGH = L | 69215166 |
| | RETJ FN | 69215167 |
| C | ***** LAST CARD OF BALANC ***** | 69215168 |
| | END | 69215169 |
| | | 69215170 |
| | | 69215171 |
| | | 69215172 |

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C                                         73215001
C----- 73215002
C                                         73215003
* SUBROUTINE ELMHES(NM,N,LOW,IGH,A,INT) 73215004
* SUBROUTINE DLMHES(NM,N,LOW,IGH,A,INT) 73215005
C                                         73215006
* INTEGER I,J,M,N,LA,NM,IGH,KP1,LOW,MM1,MP1 73215007
* REAL A(NM,N) 73215008
* REAL X,Y
* DOUBLE PRECISION A(NM,N),X,Y
C                                         73215009
REAL ABS 73215010
INTEGER INT(IGH) 73215011
C THIS SUBROUTINE IS A TRANSLATION OF THE ALGOL PROCEDURE ELMHES, 73215012
C NUM. MATH. 12, 349-368(1968) BY MARTIN AND WILKINSON. 73215013
C HANDBOOK FOR AUTO. COMP., VOL.II-LINEAR ALGEBRA, 339-358(1971). 73215014
C 73215015
C GIVEN A REAL GENERAL MATRIX, THIS SUBROUTINE
C REDUCES A SUBMATRIX SITUATED IN ROWS AND COLUMNS
C LOW THROUGH IGH TO HESSENBERG FORM BY
C STABILIZED ELEMENTARY SIMILARITY TRANSFORMATIONS. 73215016
C 73215017
C 73215018
C 73215019
C 73215020
C ON INPUT- 73215021
C 73215022
C NM MUST BE SET TO THE ROW DIMENSION OF TWO-DIMENSIONAL 73215023
C ARRAY PARAMETERS AS DECLARED IN THE CALLING PROGRAM 73215024
C DIMENSION STATEMENT, 73215025
C 73215026
C N IS THE ORDER OF THE MATRIX, 73215027
C 73215028
C LOW AND IGH ARE INTEGERS DETERMINED BY THE BALANCING 73215029
C SUBROUTINE BALANC. IF BALANC HAS NOT BEEN USED, 73215030
C SET LOW=1, IGH=N, 73215031
C 73215032
C A CONTAINS THE INPUT MATRIX. 73215033
C 73215034
C ON OUTPUT- 73215035
C 73215036
C A CONTAINS THE HESSENBERG MATRIX. THE MULTIPLIERS 73215037
C WHICH WERE USED IN THE REDUCTION ARE STORED IN THE 73215038
C REMAINING TRIANGLE UNDER THE HESSENBERG MATRIX, 73215039
C 73215040
C INT CONTAINS INFORMATION ON THE ROWS AND COLUMNS 73215041
C INTERCHANGED IN THE REDUCTION. 73215042
C ONLY ELEMENTS LOW THROUGH IGH ARE USED. 73215043
C 73215044
C QUESTIONS AND COMMENTS SHOULD BE DIRECTED TO B. S. GARBOV, 73215045
C APPLIED MATHEMATICS DIVISION, ARGONNE NATIONAL LABORATORY 73215046
C 73215047
C----- 73215048
C LA = IGH - 1 73215049
C KP1 = LOW + 1 73215050
C IF (LA .LT. KP1) GO TO 200 73215051
C 73215052
C 73215053

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```

      DO 180 M = KP1, LA          73215054
      MM1 = M - 1                73215055
      X = 0.0                     73215056
      I = M                      73215057
C
      DO 100 J = M, IGH          73215058
*       IF (ABS(A(J,MM1)) .LE. ABS(X)) GO TO 100
*       IF (DABS(A(J,MM1)) .LE. DABS(X)) GO TO 100
*       X = A(J,MM1)
*       I = J
100    CONTINUE
C
      INT(M) = I                 73215061
      IF (I .EQ. M) GO TO 130    73215062
C     ***** INTERCHANGE ROWS AND COLUMNS OF A *****
      DO 110 J = MM1, N          73215063
      Y = A(I,J)
      A(I,J) = A(M,J)
      A(M,J) = Y
110    CONTINUE
C
      DO 120 J = 1, IGH          73215064
      Y = A(J,I)
      A(J,I) = A(J,M)
      A(J,M) = Y
120    CONTINUE
C     ***** END INTERCHANGE *****
130    IF (X .EQ. 0.0) GO TO 180
      MP1 = M + 1
C
      DO 150 I = MP1, IGH        73215065
      Y = A(I,MM1)
      IF (Y .EQ. 0.0) GO TO 160
      Y = Y / X
      A(I,MM1) = Y
C
      DO 140 J = M, N          73215066
      A(I,J) = A(I,J) - Y * A(M,J)
C
      DO 150 J = 1, IGH          73215067
      A(J,M) = A(J,M) + Y * A(J,I)
C
      160    CONTINUE
C
      180 CONTINUE
C
      200 RETURN
C     ***** LAST CARD OF ELMHES *****
      END                         73215099
                                         73215100
                                         73215101

```

```

C                                         75215001
C                                         -----
C                                         75215002
C                                         75215003
* SUBROUTINE ORTHES(NM,N,LOW,IGH,A,ORT) 75215004
* SUBROUTINE ORTHES(NM,N,LOW,IGH,A,ORT)
C                                         75215005
C                                         -----
C                                         75215006
* INTEGER I,J,M,N,II,JJ,LA,MP,NM,IGH,KP1,LOW 75215007
* REAL A(NM,N),ORT(IGH) 75215008
* REAL F,G,H,SCALE
C                                         75215009
C                                         -----
C                                         75215010
REAL SQRT,ABS,SIGN
C                                         75215011
C                                         -----
C                                         75215012
THIS SUBROUTINE IS A TRANSLATION OF THE ALGOL PROCEDURE ORTHES, 75215013
NUM. MATH. 12, 349-368(1968) BY MARTIN AND WILKINSON.
C                                         75215014
HANDBOOK FOR AUTO. COMP., VOL.II-LINEAR ALG IBRA, 339-358(1971).
C                                         75215015
C                                         -----
C                                         75215016
GIVEN A REAL GENERAL MATRIX, THIS SUBROUTINE 75215017
REDUCES A SUBMATRIX SITUATED IN ROWS AND COLUMNS 75215018
LOW THROUGH IGH TO UPPER HESSENBERG FORM BY 75215019
ORTHOGONAL SIMILARITY TRANSFORMATIONS.
C                                         75215020
C                                         -----
C                                         75215021
ON INPUT- 75215022
C                                         -----
C                                         75215023
NM MUST BE SET TO THE ROW DIMENSION OF TWO-DIMENSIONAL 75215024
ARRAY PARAMETERS AS DECLARED IN THE CALLING PROGRAM 75215025
DIMENSION STATEMENT,
C                                         75215026
C                                         -----
C                                         75215027
N IS THE ORDER OF THE MATRIX,
C                                         75215028
C                                         -----
C                                         75215029
LOW AND IGH ARE INTEGERS DETERMINED BY THE BALANCING 75215030
SUBROUTINE BALANC. IF BALANC HAS NOT BEEN USED, 75215031
SET LOW=1, IGH=N,
C                                         75215032
C                                         -----
C                                         75215033
A CONTAINS THE INPUT MATRIX.
C                                         75215034
C                                         -----
C                                         75215035
ON OUTPUT-
C                                         -----
C                                         75215036
A CONTAINS THE HESSENBERG MATRIX. INFORMATION ABOUT 75215037
THE ORTHOGONAL TRANSFORMATIONS USED IN THE REDUCTION 75215038
IS STORED IN THE REMAINING TRIANGLE UNDER THE 75215039
HESSENBERG MATRIX,
C                                         75215040
C                                         -----
C                                         75215041
ORT CONTAINS FURTHER INFORMATION ABOUT THE TRANSFORMATIONS. 75215042
ONLY ELEMENTS LOW THROUGH IGH ARE USED.
C                                         75215043
C                                         -----
C                                         75215044
QUESTIONS AND COMMENTS SHOULD BE DIRECTED TO B. S. GARBOV, 75215045
APPLIED MATHEMATICS DIVISION, ARGONNE NATIONAL LABORATORY 75215046
C                                         -----
C                                         75215047
C                                         -----
C                                         75215048
LA = IGH - 1 75215049
KP1 = LOW + 1 75215050
IF ( LA .LT. KP1) GO TO 200 75215051
C                                         75215052
DO 180 M = KP1, LA 75215053

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```

H = 0.0          75215054
ORT(M) = 0.0    75215055
SCALE = 0.0     75215056
C     ***** SCALE COLUMN (ALGOL TOL THEN NOT NEEDED) *****
      DO 90 I = M, IGH 75215057
+ 90  SCALE = SCALE + ABS(A(I,M-1)) 75215058
      90  SCALE = SCALE +DABS(A(I,M-1)) 75215059
C
      IF (SCALE .EQ. 0.0) GO TO 180 75215060
      MP = M + IGH 75215061
C     ***** FOR I=IGH STEP -1 UNTIL M DO -- *****
      DO 130 II = M, IGH 75215062
      I = MP - II 75215063
      ORT(I) = A(I,M-1) / SCALE 75215064
      H = H + ORT(I) * ORT(I) 75215065
100    CONTINUE 75215066
C
*      G = -SIGN(SQRT(H),ORT(M)) 75215067
*      G = -DSIGN(DSQRT(H),ORT(M)) 75215068
      H = H - ORT(M) * G 75215069
      ORT(M) = ORT(M) - G 75215070
C     ***** FORM (I-(U*UT)/H) * A *****
      DO 130 J = M, N 75215071
      F = 0.0 75215072
C     ***** FOR I=IGH STEP -1 UNTIL M DO -- *****
      DO 110 II = M, IGH 75215073
      I = MP - II 75215074
      F = F + ORT(I) * A(I,J) 75215075
110    CONTINUE 75215076
C
      F = F / H 75215077
C
      DO 120 I = M, IGH 75215078
120    A(I,J) = A(I,J) - F * ORT(I) 75215079
C
130    CONTINUE 75215080
C
      ***** FORM (I-(U*UT)/H)*A*(I-(U*UT)/H) *****
      DO 160 I = 1, IGH 75215081
      F = 0.0 75215082
C     ***** FOR J=IGH STEP -1 UNTIL M DO -- *****
      DO 140 JJ = M, IGH 75215083
      J = MP - JJ 75215084
      F = F + ORT(J) * A(I,J) 75215085
140    CONTINUE 75215086
C
      F = F / H 75215087
C
      DO 150 J = M, IGH 75215088
150    A(I,J) = A(I,J) - F * ORT(J) 75215089
C
160    CONTINUE 75215090
C
      ORT(M) = SCALE * ORT(M) 75215091
      A(M,M-1) = SCALE * G 75215092
180    CONTINUE 75215093

```

200 RETURN
***** LAST CARD OF ORTHES *****
END

75215107
75215108
75215109
75215110

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C          86215001
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C          86215050
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C          86215051
C          -----
C          86215052
C          -----
C          86215053

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* SUBROUTINE HQR(NM,N,LOW,IGH,H,WR,WI,IERR) 86215001
* SUBROUTINE DQP(NM,N,LOW,IGH,H,WR,WI,IERR) 86215002
* INTEGER I,J,K,L,M,N,EN,LL,MM,NA,NM,IGH,ITS,LOW,MP2,ENM2,IERR 86215003
* REAL H(NM,N),WR(N),WI(N) 86215004
* REAL P,Q,R,S,T,W,X,Y,ZZ,MACHEP 86215005
* DOUBLE PRECISION H(NM,N),WR(N),WI(N),P,Q,R,S,T,W,X,Y,ZZ,MACHEP 86215006
* REAL SQRT,ABS,SIGN 86215007
* INTEGER MIN0 86215008
* LOGICAL NOTLAS 86215009
* THIS SUBROUTINE IS A TRANSLATION OF THE ALGOL PROCEDURE HQR, 86215010
* NUM. MATH. 14, 219-231(1970) BY MARTIN, PETERS, AND WILKINSON. 86215011
* HANDBOOK FOR AUTO. COMP., VOL.II-LINEAR ALGEBRA, 359-371(1971). 86215012
* THIS SUBROUTINE FINDS THE EIGENVALUES OF A REAL 86215013
* UPPER HESSENBERG MATRIX BY THE QR METHOD. 86215014
* ON INPUT- 86215015
* NM MUST BE SET TO THE ROW DIMENSION OF TWO-DIMENSIONAL 86215016
* ARRAY PARAMETERS AS DECLARED IN THE CALLING PROGRAM 86215017
* DIMENSION STATEMENT, 86215018
* N IS THE ORDER OF THE MATRIX, 86215019
* LOW AND IGH ARE INTEGERS DETERMINED BY THE BALANCING 86215020
* SUBROUTINE BALANC. IF BALANC HAS NOT BEEN USED, 86215021
* SET LOW=1, IGH=N, 86215022
* H CONTAINS THE UPPER HESSENBERG MATRIX. INFORMATION ABOUT 86215023
* THE TRANSFORMATIONS USED IN THE REDUCTION TO HESSENBERG 86215024
* FORM BY ELMHFS OR ORTHES, IF PERFORMED, IS STORED 86215025
* IN THE REMAINING TRIANGLE UNDER THE HESSENBERG MATRIX. 86215026
* ON OUTPUT- 86215027
* H HAS BEEN DESTROYED. THEREFORE, IT MUST BE SAVED 86215028
* BEFORE CALLING HQR IF SUBSEQUENT CALCULATION AND 86215029
* BACK TRANSFORMATION OF EIGENVECTORS IS TO BE PERFORMED, 86215030
* WR AND WI CONTAIN THE REAL AND IMAGINARY PARTS, 86215031
* RESPECTIVELY, OF THE EIGENVALUES. THE EIGENVALUES 86215032
* ARE UNORDERED EXCEPT THAT COMPLEX CONJUGATE PAIRS 86215033
* OF VALUES APPEAR CONSECUTIVELY WITH THE EIGENVALUE 86215034
* HAVING THE POSITIVE IMAGINARY PART FIRST. IF AN 86215035
* ERROR EXIT IS MADE, THE EIGENVALUES SHOULD BE CORRECT 86215036
* FOR INDICES IERR+1,...,N, 86215037
* IERR IS SET TO 86215038
* ZERO FOR NORMAL RETURN, 86215039
* J IF THE J-TH EIGENVALUE HAS NOT BEEN 86215040

```

C DETERMINED AFTER 30 ITERATIONS. 86215054
C QUESTIONS AND COMMENTS SHOULD BE DIRECTED TO B. S. GARBOB, 86215055
C APPLIED MATHEMATICS DIVISION, ARGONNE NATIONAL LABORATORY 86215056
C ----- 86215057
C 86215058
C ----- 86215059
C 86215060
C ***** * MACHEP IS A MACHINE DEPENDENT PARAMETER SPECIFYING 86215061
C THE RELATIVE PRECISION OF FLOATING POINT ARITHMETIC. 86215062
C 86215063
C ***** * 86215064
* MACHEP = 2.**(-47) 86215065
* MACHEP = 2. DO**(-95)
C
IERR = J 86215066
C ***** * STORE ROOTS ISOLATED BY BALANC *****
DO 50 I = 1, N 86215067
IF (I .GE. LOW .AND. I .LE. IGH) GO TO 50 86215068
WR(I) = H(I,I) 86215069
WI(I) = 0.0 86215070
50 CONTINUE 86215071
EN = IGH 86215072
T = 0.0 86215073
C ***** * SEARCH FOR NEXT EIGENVALUES *****
60 IF (EN .LT. LOW) GO TO 1001 86215074
ITS = J 86215075
NA = EN - 1 86215076
ENM2 = NA - 1 86215077
C ***** * LOOK FOR SINGLE SMALL SUB-DIAGONAL ELEMENT 86215078
C FOR L=FN STEP -1 UNTIL LOW DO -- *****
70 DO 80 LL = LOW, EN 86215079
L = EN + LOW - L 86215080
IF (L .EQ. LOW) GO TO 100 86215081
* IF (ABS(H(L,L-1)) .LE. MACHEP * (ABS(H(L-1,L-1)) 86215082
* X + ABS(H(L,L)))) GO TO 100 86215083
* IF (DABS(H(L,L-1)) .LE. MACHEP * (DABS(H(L-1,L-1)) 86215084
X + DABS(H(L,L)))) GO TO 100 86215085
80 CONTINUE 86215086
C ***** * FORM SHIFT *****
100 X = H(EN,EN) 86215087
IF (L .EQ. EN) GO TO 270 86215088
Y = H(NA,NA) 86215089
W = H(EN,NA) * H(NA,EN) 86215090
IF (L .EQ. NA) GO TO 280 86215091
IF (ITS .EQ. 30) GO TO 1000 86215092
IF (ITS .NE. 10 .AND. ITS .NE. 20) GO TO 130 86215093
C ***** * FORM EXCEPTIONAL SHIFT *****
T = T + X 86215094
C
DO 120 I = LOW, EN 86215095
120 H(I,I) = H(I,I) - X 86215096
C
* S = AES(H(EN,NA)) + ABS(H(NA,ENM2)) 86215097
* S = DABS(H(EN,NA)) + DABS(H(NA,ENM2)) 86215098

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X = 0.75 * S          86215105
Y = X                 86215106
W = -0.4375 * S * S   86215107
130 ITS = ITS + 1     86215108
C      **** * LOOK FOR TWO CONSECUTIVE SMALL    86215109
C      SUB-DIAGONAL ELEMENTS.                   86215110
C      FOR M=EN-2 STEP -1 UNTIL L DO -- *****    86215111
C
DO 140 MM = L, ENM2   86215112
  M = ENM2 + L - MM   86215113
  ZZ = H(M,M)          86215114
  R = X - ZZ           86215115
  S = Y - ZZ           86215116
  P = (R * S - W) / H(M+1,M) + H(M,M+1)       86215117
  Q = H(M+1,M+1) - ZZ - R - S                  86215118
  R = H(M+2,M+1)          86215119
*   S = ABS(P) + ABS(Q) + ABS(R)                86215120
*   S = DABS(P) + DABS(Q) + DABS(R)
  P = P / S
  Q = Q / S
  R = R / S
  IF (M .EQ. L) GO TO 150
*   IF (ABS(H(M,M-1)) * (ABS(Q) + ABS(R)) .LE. MACHEP * ABS(P) 86215121
*   * (ABS(H(M-1,M-1)) + ABS(ZZ) + ABS(H(M+1,M+1))) GO TO 150 86215122
*   IF (DABS(H(M,M-1)) * (DABS(Q) + DABS(R)) .LE. MACHEP * DABS(P) 86215123
*   * (DABS(H(M-1,M-1)) + DABS(ZZ) + DABS(H(M+1,M+1))) GO TO 150 86215124
140 CONTINUE
C
150 MP2 = M + 2        86215125
C
DO 160 I = MP2, EN    86215126
  H(I,I-2) = 0.0
  IF (I .EQ. MP2) GO TO 160
  H(I,I-3) = 0.0
160 CONTINUE
C      **** * DOUBLE QR STEP INVOLVING ROWS L TO EN AND    86215127
C      COLUMNS M TO EN ****
DO 260 K = M, NA        86215128
  NOTLAS = K .NE. NA
  IF (K .EQ. M) GO TO 170
  P = H(K,K-1)
  Q = H(K+1,K-1)
  R = 0.0
  IF (NOTLAS) R = H(K+2,K-1)
*   X = ABS(P) + ABS(Q) + ABS(R)                      86215129
*   X = DABS(P) + DABS(Q) + DABS(R)                  86215130
  IF (X .EQ. 0.0) GO TO 260
  P = P / X
  Q = Q / X
  R = R / X
*   170 S = SIGN(SQRT(P*P+Q*Q+R*R),P)            86215131
*   170 S = DSIGN(DSQRT(P*P+Q*Q+R*R),P)          86215132
  IF (K .EQ. M) GO TO 180
  H(K,K-1) = -S * X
  GO TO 190
180 IF (L .NE. M) H(L,K-1) = -H(K,K-1)          86215133

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190      P = P + S          86215155
        X = P / S          86215156
        Y = Q / S          86215157
        ZZ = R / S         86215158
        Q = Q / P          86215159
        R = R / P          86215160
C      ***** ROW MODIFICATION *****
        DO 210 J = K, EN    86215161
          P = H(K,J) + Q * H(K+1,J)
          IF (.NOT. NOTLAS) GO TO 200
          P = P + R * H(K+2,J)
          H(K+2,J) = H(K+2,J) - P * ZZ
200      H(K+1,J) = H(K+1,J) - P * Y
        H(K,J) = H(K,J) - P * X
210      CONTINUE
C
        J = 1+NO(EN,<+3)    86215170
C      ***** COLUMN MODIFICATION *****
        DO 230 I = L, J    86215171
          P = X * H(I,K) + Y * H(I,K+1)
          IF (.NOT. NOT_AS) GO TO 220
          P = P + ZZ * H(I,K+2)
          H(I,K+2) = H(I,K+2) - P * R
220      H(I,K+1) = H(I,K+1) - P * Q
          H(I,K) = H(I,K) - P
230      CONTINUE
C
        260 CONTINUE
C
        GO TO 70
C      ***** ONE ROOT FOUND *****
270      WR(EN) = X + T          86215182
        WI(EN) = C.0            86215183
        EN = NA                86215184
        GO TO 60
C      ***** TWO ROOTS FOUND *****
280      P = (Y - X) / 2.0      86215185
        Q = P * P + W          86215186
*       ZZ = SQRT(ABS(Q))      86215187
*       ZZ = DSQRT(DABS(Q))    86215188
        X = X + T              86215189
        IF (Q .LT. 0.0) GO TO 320
C      ***** REAL PAIR *****
*       ZZ = P + SIGN(ZZ,F)    86215190
*       ZZ = P + DSIGN(ZZ,F)   86215191
        WR(NA) = X + ZZ         86215192
        WR(EN) = WR(NA)         86215193
        IF (ZZ .NE. C.0) WR(EN) = X - W / ZZ
        WI(NA) = C.0            86215194
        WI(EN) = C.0            86215195
        GO TO 330
C      ***** COMPLEX PAIR *****
320      WR(NA) = X + P          86215196
        WR(EN) = X + P          86215197
        WI(NA) = ZZ             86215198

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```
      WI(EN) = -ZZ          86215208
330  EN = EN/2          86215209
      GO TO 63          86215210
C      ***** SET ERROR -- NO CONVERGENCE TO AN          86215211
C          EIGENVALJE AFTER 30 ITERATIONS *****          86215212
1000 IERR = EN          86215213
1001 RETURN          86215214
C      ***** LAST CARD OF HQR *****          86215215
      END          86215216
```

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