

> diagonalization of a 3x3 matrix
>

> | 0 T01 T02 |
> | | | |
> H= | T01 DELTA1 T12 |
> | | | |
> | T02 T12 DELTA2 |

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C       * TEST WITH DIAGONALIZATION *
C       PARAMETER (D=3)
C       REAL     A(D,D),R(D),E(D)
C       INTEGER IA,N,IV,IFAIL
C       INTEGER I,J,K,L
C       REAL     DELTA1,DELTA2,T01,T02,T12

C       IA       = D
C       N        = D
C       IV       = D
C       IFAIL    = 0

C       PRINT *,'* DIAGONALIZATION OF A 3X3 MATRIX *'

C       WRITE(6,*)
C       WRITE(6,*) 'ENTER DELTA1 AND DELTA2 :'
C       READ(5,*) DELTA1,DELTA2
C       WRITE(6,*) 'ENTER T01, T02, AND T12 :'
C       READ(5,*) T01,T02,T12

C       DO 15 K=1,D
C       R(K) = 0.
C       E(K) = 0.
C       DO 20 L=1,D
C       A(K,L) = 0.
20       CONTINUE
15       CONTINUE
C       A(1,1)    = 0.
C       A(2,2)    = DELTA1
C       A(3,3)    = DELTA2
C       A(2,1)    = T01
C       A(3,1)    = T02
C       A(3,2)    = T12

C       CALL DIAG(IA,N,A,R,E,A,IFAIL)
C       IF (IFAIL.EQ.0) GO TO 30
C       WRITE(6,40) IFAIL
40       FORMAT(' ERROR IN DIAG,   IFAIL =',I2)
C       WRITE(6,*) ' '
C       WRITE(6,*) '*****'
C       WRITE(6,*) '        ERROR IN DIAGONALIZATION'
C       WRITE(6,*) '*****'
C       STOP
30       CONTINUE
C       WRITE(6,*)
C       DO 80 I=1,N
C       WRITE(6,*)
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WRITE(6,*) 'EIGEN VALUE NR: ', I, '          ENERGY :', R(I)
WRITE(6,*) 'EIGEN VECTOR  : '
DO 90 J=1,N
WRITE(6,*) '          ', A(J,I)
90  CONTINUE
80  CONTINUE
C
WRITE(6,*) '*****'
WRITE(6,*) '  DIAGONALIZATION PROGRAM FINISHED'
WRITE(6,*) '*****'
STOP
END
C
C
C
SUBROUTINE DIAG(KMX,NLS,VECT,EIG,FK,C,M)
DIMENSION VECT(KMX,KMX),EIG(KMX),FK(KMX),C(KMX,KMX)
CALL TRED2 (KMX,NLS,C,EIG,FK,VECT)
CALL TQL2 (KMX,NLS,EIG,FK,C,M)
RETURN
END
C*****

SUBROUTINE TRED2(NM, N, A, D, E, Z)
DIMENSION A(NM,N), D(N), E(N), Z(NM,N)
DO 20 I=1,N
C
DO 10 J=1,I
Z(I,J) = A(I,J)
10  CONTINUE
20  CONTINUE
C
IF (N.EQ.1) GO TO 160
***** FOR I=N STEP -1 UNTIL 2 DO -- *****
DO 150 II=2,N
I = N + 2 - II
L = I - 1
H = 0.0
SCALE = 0.0
IF (L.LT.2) GO TO 40
C ***** SCALE ROW (ALGOL TOL THEN NOT NEEDED) *****
DO 30 K=1,L
SCALE = SCALE + ABS(Z(I,K))
30  CONTINUE
C
IF (SCALE.NE.0.0) GO TO 50
40  E(I) = Z(I,L)
GO TO 140
C
50  DO 60 K=1,L
Z(I,K) = Z(I,K)/SCALE
H = H + Z(I,K)*Z(I,K)
60  CONTINUE
C
F = Z(I,L)
G = -SIGN(SQRT(H),F)
E(I) = SCALE*G
H = H - F*G
Z(I,L) = F - G
F = 0.0
C
DO 100 J=1,L

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        Z(J,I) = Z(I,J) / (SCALE*H)
        G = 0.0
C ***** FORM ELEMENT OF A*U *****
        DO 70 K=1,J
            G = G + Z(J,K)*Z(I,K)
70     CONTINUE
C
        JP1 = J + 1
        IF (L.LT.JP1) GO TO 90
C
        DO 80 K=JP1,L
            G = G + Z(K,J)*Z(I,K)
80     CONTINUE
C ***** FORM ELEMENT OF P *****
90     E(J) = G/H
        F = F + E(J)*Z(I,J)
100    CONTINUE
C
        HH = F / (H+H)
C ***** FORM REDUCED A *****
        DO 120 J=1,L
            F = Z(I,J)
            G = E(J) - HH*F
            E(J) = G
C
            DO 110 K=1,J
                Z(J,K) = Z(J,K) - F*E(K) - G*Z(I,K)
110    CONTINUE
120    CONTINUE
C
            DO 130 K=1,L
                Z(I,K) = SCALE*Z(I,K)
130    CONTINUE
C
140    D(I) = H
150    CONTINUE
C
160    D(1) = 0.0
        E(1) = 0.0
C ***** ACCUMULATION OF TRANSFORMATION MATRICES *****
        DO 220 I=1,N
            L = I - 1
            IF (D(I).EQ.0.0) GO TO 200
C
            DO 190 J=1,L
                G = 0.0
C
                DO 170 K=1,L
                    G = G + Z(I,K)*Z(K,J)
170    CONTINUE
C
                DO 180 K=1,L
                    Z(K,J) = Z(K,J) - G*Z(K,I)
180    CONTINUE
190    CONTINUE
C
200    D(I) = Z(I,I)
        Z(I,I) = 1.0
        IF (L.LT.1) GO TO 220
C
        DO 210 J=1,L
            Z(I,J) = 0.0
            Z(J,I) = 0.0

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210     CONTINUE
C
220     CONTINUE
C
      RETURN
      END

C #####

      SUBROUTINE TQL2(NM, N, D, E, Z, IERR)
      DIMENSION D(N), E(N), Z(NM,N)
      REAL MACHEP
C
      *****
      MACHEP = 2.**(-46)
C
      ***** MACHEP IS A MACHINE DEPENDENT PARAMETER SPECIFYING
C
      THE RELATIVE PRECISION OF FLOATING POINT ARITHMETIC.
C
      IERR = 0
      IF (N.EQ.1) GO TO 160
C
      DO 10 I=2,N
         E(I-1) = E(I)
10     CONTINUE
C
      F = 0.0
      B = 0.0
      E(N) = 0.0
C
      DO 110 L=1,N
         J = 0
         H = MACHEP*(ABS(D(L))+ABS(E(L)))
         IF (B.LT.H) B = H
C
      ***** LOOK FOR SMALL SUB-DIAGONAL ELEMENT *****
         DO 20 M=L,N
            IF (ABS(E(M)).LE.B) GO TO 30
C
      ***** E(N) IS ALWAYS ZERO, SO THERE IS NO EXIT
C
      THROUGH THE BOTTOM OF THE LOOP *****
20     CONTINUE
30     IF (M.EQ.L) GO TO 100
40     IF (J.EQ.30) GO TO 150
         J = J + 1
C
      ***** FORM SHIFT *****
         P = (D(L+1)-D(L))/(2.0*E(L))
         R = SQRT(P*P+1.0)
         H = D(L) - E(L)/(P+SIGN(R,P))
C
         DO 50 I=L,N
            D(I) = D(I) - H
50     CONTINUE
C
         F = F + H
C
      ***** QL TRANSFORMATION *****
         P = D(M)
         C = 1.0
         S = 0.0
         MML = M - L
C
      ***** FOR I=M-1 STEP -1 UNTIL L DO -- *****
         DO 90 II=1,MML
            I = M - II
            G = C*E(I)
            H = C*P
            IF (ABS(P).LT.ABS(E(I))) GO TO 60
            C = E(I)/P

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        R = SQRT(C*C+1.0)
        E(I+1) = S*P*R
        S = C/R
        C = 1.0/R
        GO TO 70
60      C = P/E(I)
        R = SQRT(C*C+1.0)
        E(I+1) = S*E(I)*R
        S = 1.0/R
        C = C*S
70      P = C*D(I) - S*G
        D(I+1) = H + S*(C*G+S*D(I))
C      ***** FORM VECTOR *****
        DO 80 K=1,N
            H = Z(K,I+1)
            Z(K,I+1) = S*Z(K,I) + C*H
            Z(K,I) = C*Z(K,I) - S*H
80      CONTINUE
C
90      CONTINUE
C
        E(L) = S*P
        D(L) = C*P
        IF (ABS(E(L)).GT.B) GO TO 40
100     D(L) = D(L) + F
110     CONTINUE
C      ***** ORDER EIGENVALUES AND EIGENVECTORS *****
        DO 140 II=2,N
            I = II - 1
            K = I
            P = D(I)
C
            DO 120 J=II,N
                IF (D(J).GE.P) GO TO 120
                K = J
                P = D(J)
120     CONTINUE
C
            IF (K.EQ.I) GO TO 140
            D(K) = D(I)
            D(I) = P
C
            DO 130 J=1,N
                P = Z(J,I)
                Z(J,I) = Z(J,K)
                Z(J,K) = P
130     CONTINUE
C
140     CONTINUE
C
        GO TO 160
C      ***** SET ERROR -- NO CONVERGENCE TO AN
C      ***** EIGENVALUE AFTER 30 ITERATIONS *****
150     IERR = L
160     RETURN
C      ***** LAST CARD OF TQL2 *****
        END

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