The University of Wisconsin
Computer Sciences Department
1210 West Dayton Street
Madison, Wisconsin 53706

Received: June 20, 1974

An Energy Conserving Modification of Numerical Methods for the Integration of Equations of Motion

by

Robert A. LaBudde
Mathematics Research Center

Donald Greenspan
Computer Sciences Department and
Academic Computing Center

Computer Sciences Technical Report #217
June 1974

ADDENDUM TO APPENDIX OF TR 217

The unmodified third-order Adams' method corresponds to the case METH = 0 replacing line 28 of FDM3 on page 19. The conservative version corresponds to METH = 1 as shown.

The data used to generate the example given is read in at line 7 of DTEST on page 15. The values were

METHOD = 4
IBIT = 0
ISW = 0
B = 0.5
ZO = 0.0
E = 1.32845 (= 2 - 0.67155)
H = 0.050457 68858
HMAX = 4.0366 15087
STEP = 0.0

ABSTRACT

In the integration of the equations of motion of a system of particles, conventional numerical methods generate an error in the total energy of the same order as the truncation error. A simple modification of these methods is described, which results in exact conservation of the energy.

1. Introduction

When applied to the motion of a system of particles, conventional numerical methods for the integration of ordinary differential equations only approximately conserve the total energy of the system. The error in the calculated value of the energy is of the same order as the truncation error in the velocities. In previous work [1]-[5], a new class of methods was described, which maximally conserve the constants of motion. These methods exactly conserve the total energy and linear momentum, and conserve the total angular momentum to at least one higher order than the corresponding conventional methods.

In what follows, our purpose is to show how conventional numerical methods--exemplified by the third-order Taylor series and Adams' formulae--can be modified so that exact conservation of energy occurs. This modification simply involves the introduction of adjustable, multiplicative parameters, whose values are unity for the conventional case.

2. Equations of Motion

The following is a brief description of the equations of motion of a system of n particles, interacting according to a pairwise-additive potential. For more details, see [1] or [5].

Suppose particle i has mass m_i, and position vector

$$\vec{r}_i = \langle x_i, y_i, z_i \rangle \qquad (2.1)$$

velocity vector

$$\vec{v}_i = \left\langle \frac{dx_i}{dt}, \frac{dy_i}{dt}, \frac{dz_i}{dt} \right\rangle \qquad (2.2)$$

and acceleration

$$\vec{a}_i = \left\langle \frac{d^2x_i}{dt^2}, \frac{d^2y_i}{dt^2}, \frac{d^2z_i}{dt^2} \right\rangle \qquad (2.3)$$

Newton's laws of motion

$$m_i\vec{a}_i = \vec{F}_i \qquad (2.4)$$

relate the accelerations $\vec{a}_i$ to the forces $\vec{F}_i$, given by

$$\vec{F}_i = - \frac{\partial \phi}{\partial \vec{r}_i} \qquad (2.5)$$

where ϕ is the potential of interaction. It will be assumed that ϕ has the pairwise-additive form

$$\phi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n) = \sum_{i<j} \phi_{ij}(r_{ij}) \qquad (2.6)$$

where r_{ij} is the magnitude of the vector distance $\vec{r}_{ij}$ between particles i and j :

$$\vec{r}_{ij} = \vec{r}_j - \vec{r}_i \tag{2.7}$$

As a consequence of equation (2.6),

$$\vec{F}_i = \sum_{j=1}^{n} \vec{F}_{ji} \tag{2.8}$$

where

$$\vec{F}_{ji} = - \vec{F}_{ij} \tag{2.9a}$$

$$= - \frac{d\phi_{ji}}{dr_{ji}} \frac{\vec{r}_{ji}}{r_{ji}} \tag{2.9b}$$

$$= \frac{d\phi_{ij}}{dr_{ij}} \frac{\vec{r}_{ij}}{r_{ij}} \tag{2.9c}$$

and $\vec{F}_{ji} = \vec{0}$ if $j = i$. The introduction of equation (2.8) into equation (2.4) gives the equations of motion

$$m_i \vec{a}_i = \sum_{j=1}^{n} \vec{F}_{ji} \tag{2.10a}$$

$$= \sum_{j=1}^{n} \frac{d\phi_{ij}}{dr_{ij}} \frac{\vec{r}_{ij}}{r_{ij}} \tag{2.10b}$$

Equations (2.10) are a system of second-order ordinary differential equations for the $\vec{r}_i$. This system may be used to solve for the $\vec{r}_i{}'$ and $\vec{v}_i{}'$ at any later time $t' = t + \Delta t$, given the $\vec{r}_i$ and $\vec{v}_i$ at time t .

Conservation of the total energy E occurs because of the existence of the potential ϕ . Here,

$$E = \sum_{i=1}^{n} \frac{1}{2}m_i(\vec{v}_i \cdot \vec{v}_i) + \phi \qquad (2.11a)$$

$$= \sum_{i=1}^{n} \frac{1}{2}m_i(\vec{v}_i \cdot \vec{v}_i) + \sum_{i<j} \phi_{ij} \qquad (2.11b)$$

where $\vec{a} \cdot \vec{b}$ denotes the scalar product of two vectors $\vec{a}$ and $\vec{b}$. Conservation of energy is expressed by the equation

$$E(t') = E(t)$$

for any two times t and t', and E evaluated along the trajectory.

3. Conventional Numerical Methods

A simple example of a conventional approximation method for the numerical solution of equations (2.10) is provided by the truncated Taylor-series formulae

$$\vec{r}\,'_{c,i} = \vec{r}_i + \vec{v}_i \Delta t + \frac{1}{m_i} \sum_{j=1}^{n} \left[\vec{F}_{ji} \frac{(\Delta t)^2}{2} + \vec{G}_{ji} \frac{(\Delta t)^3}{6} \right] \tag{3.1a}$$

$$\vec{v}\,'_{c,i} = \vec{v}_i + \frac{1}{m_i} \sum_{j=1}^{n} \left[\vec{F}_{ji} \Delta t + \vec{G}_{ji} \frac{(\Delta t)^2}{2} \right] \tag{3.1b}$$

where the $\vec{r}\,'_{c,i}$ and $\vec{v}\,'_{c,i}$ are the calculated values for the $\vec{r}\,'_i$ and $\vec{v}\,'_i$ at time $t' = t + \Delta t$, and

$$\vec{G}_{ji} = \frac{d\vec{F}_{ji}}{dt} \tag{3.2a}$$

$$= -\frac{d\phi_{ji}}{dr_{ji}} \frac{\vec{v}_{ji}}{r_{ji}} - \left[\frac{d^2\phi_{ji}}{dr_{ji}^{\,2}} - \frac{1}{r_{ji}} \frac{d\phi_{ji}}{dr_{ji}} \right] \frac{\dot{r}_{ji}\vec{r}_{ji}}{r_{ji}} \tag{3.2b}$$

where

$$\dot{r}_{ji} = \frac{dr_{ji}}{dt} \tag{3.3a}$$

$$= \frac{\vec{r}_{ji} \cdot \vec{v}_{ji}}{r_{ji}} \tag{3.3b}$$

and

$$\vec{v}_{ji} = \vec{v}_i - \vec{v}_j \tag{3.4}$$

The method of equations (3.1) is of third-order, since

$$\vec{r}\,'_i = \vec{r}\,'_{c,i} + O[(\Delta t)^4] \tag{3.5a}$$

$$\vec{v}\,'_i = \vec{v}\,'_{c,i} + O[(\Delta t)^3] \tag{3.5b}$$

due to the neglect of the succeeding Taylor-series terms. These errors generate an error of $O[(\Delta t)^3]$ in the value of the energy E'_c calculated using the $\vec{r}'_{c,i}$ and $\vec{v}'_{c,i}$:

$$\Delta E_c = E'_c - E \tag{3.6a}$$

$$= O[(\Delta t)^3] \tag{3.6b}$$

The third-order Adams' method arises via equations (3.1) and the approximation

$$\vec{G}_{ij} = \vec{G}^a_{ij} + O[\Delta t] \tag{3.7}$$

where

$$\vec{G}^a_{ij} = \frac{\vec{F}'_{c,ij} - \vec{F}_{ij}}{\Delta t} \tag{3.8a}$$

In equation (3.8), $\vec{F}'_{c,ij}$ denotes the value of $\vec{F}_{ij}$ obtained from equation (2.9b) using the $r'_{c,ij}$. Equations (3.5) and (3.6) also hold when the $\vec{G}^a_{ij}$ are used for the $\vec{G}_{ij}$.

4. Energy Conserving Modification of Conventional Methods

Consider the third-order methods of Section 3, with $\vec{G}^{*}_{ij}$ replacing either the $\vec{G}_{ij}$ or $\vec{G}^{a}_{ij}$:

$$\vec{r}\,'_{c,i} = \vec{r}_i + \vec{v}_i\Delta t + \frac{1}{m_i}\sum_{j=1}^{n}\left[\vec{F}_{ji}\,\frac{(\Delta t)^2}{2} + \vec{G}_{ji}{}^{*}\,\frac{(\Delta t)^3}{6}\right] \qquad (4.1a)$$

$$v'_{c,i} = \vec{v}_i + \frac{1}{m_i}\sum_{j=1}^{n}\left[\vec{F}_{ji}\Delta t + \vec{G}^{*}_{ji}\,\frac{(\Delta t)^2}{2}\right] \qquad (4.1b)$$

When equations (4.1) are used to obtain estimates for the $\vec{r}\,'_i$ and $\vec{v}\,'_i$, an error ΔE_c is made in the total energy, which is given by

$$\Delta E_c = E'_c - E \qquad (4.2a)$$

$$= \sum_{i=1}^{n} \tfrac{1}{2}m_i(\vec{v}\,'_{c,i}\cdot\vec{v}\,'_{c,i} - \vec{v}_i\cdot\vec{v}_i) + \phi'_c - \phi \qquad (4.2b)$$

$$= \Delta t \sum_{i=1}^{n}\sum_{j=1}^{n}\Big[(\vec{v}_i + \frac{\Delta t}{2m_i}\sum_{k=1}^{n}\vec{F}_{ki})\cdot\vec{F}_{ji}$$

$$+ \frac{\Delta t}{2}(\vec{v}_i + \frac{\Delta t}{m_i}\sum_{k=1}^{n}\Big\{\vec{F}_{ki} + \vec{G}^{*}_{ki}\,\frac{\Delta t}{4}\Big\})\cdot\vec{G}^{*}_{ji}\Big] + \Delta\phi \qquad (4.2c)$$

$$= \Delta t \sum_{i<j}\Big[\Big[\Big\{\vec{v}_{ij} + \vec{a}_{ij}\Delta t + \vec{b}_{ij}\,\frac{(\Delta t)^2}{4}\Big\}\cdot\vec{G}^{*}_{ij}\,\frac{\Delta t}{2}$$

$$+ (\vec{v}_{ij} + \vec{a}_{ij}\,\frac{\Delta t}{2})\cdot\vec{F}_{ij} + \frac{\Delta\phi_{ij}}{\Delta t}\Big] \qquad (4.2d)$$

where

$$\vec{a}_{ij} = \sum_{k=1}^{n} \left[\frac{\vec{F}_{kj}}{m_j} - \frac{\vec{F}_{ki}}{m_i} \right] \tag{4.3a}$$

$$\vec{b}_{ij} = \sum_{k=1}^{n} \left[\frac{\vec{G}^{\,*}_{kj}}{m_j} - \frac{\vec{G}^{*}_{ki}}{m_i} \right] \tag{4.3b}$$

and

$$\Delta\phi_{ij} = \phi'_{c,ij} - \phi_{ij} \tag{4.4a}$$

$$= \phi_{ij}(r'_{c,ij}) - \phi_{ij}(r_{ij}) \tag{4.4b}$$

where

$$\vec{r}\,'_{c,ij} = \vec{r}\,'_{c,j} - \vec{r}\,'_{c,i} \tag{4.5}$$

Suppose now, instead of using $\vec{G}^{\,*}_{ij} = \vec{G}_{ij}$ or $\vec{G}^{a}_{ij}$ in equation (4.2)--which leads to an error ΔE_c of $O[(\Delta t)^3]$--that adjustable $\vec{G}^{*}_{ij}$

$$\vec{G}^{\,*}_{ij} = \epsilon_{ij}\, \vec{G}_{ij} \tag{4.6}$$

or

$$\vec{G}^{*}_{ij} = \epsilon_{ij}\, \vec{G}^{a}_{ij} \tag{4.7}$$

is used. The ϵ_{ij} are to be chosen so that

$$\epsilon_{ij} = 1 + O[\Delta t] \tag{4.8}$$

(preserving the order of the method), and such that exact conservation of energy occurs. Solving

$$\Delta E_c = 0 \tag{4.9}$$

for the ϵ_{ij} gives, for example, for (4.6), the equations (cf. [1] and [5])

$$\left\{\vec{v}_{ij} + \vec{a}_{ij}\Delta t + \vec{b}_{ij}\frac{(\Delta t)^2}{4}\right\} \cdot \vec{G}_{ij}\frac{\Delta t}{2}\epsilon_{ij} + (\vec{v}_{ij} + \vec{a}_{ij}\frac{\Delta t}{2}) \cdot \vec{F}_{ij} + \frac{\Delta\phi_{ij}}{\Delta t} = 0 \qquad (4.10)$$

Equations (4.10) are a set of implicit, coupled equations in the ϵ_{ij}, since the $\vec{b}_{ij}$ and $\phi'_{c,ij}$ depend upon the values of the ϵ_{ij}.

For small Δt, equations (4.10) are strongly linear in the ϵ_{ij}. The only nonlinear dependences on the ϵ_{ij} occur through the $\vec{b}_{ij}$ and $\phi'_{c,ij}$ (through the $r'_{c,ij}$). In both these cases, the terms involving the ϵ_{ij} occur with coefficients proportional to $(\Delta t)^3$. (Compare equations (4.1), (4.5), and (4.10).) In contrast, the coefficients of the linear terms in ϵ_{ij}, namely

$$(\vec{v}_{ij} + \vec{a}_{ij}\Delta t) \cdot \vec{G}_{ij}\frac{\Delta t}{2} \qquad (4.11)$$

are of $O[\Delta t]$.

Because equations (4.10) are linear except for terms of $O[(\Delta t)^3]$, they may be easily solved via the iteration formulae

$$\epsilon_{ij} = -\frac{2}{\Delta t}\frac{\frac{\Delta\phi_{ij}}{\Delta t} + (\vec{v}_{ij}+\vec{a}_{ij}\frac{\Delta t}{2})\cdot\vec{F}_{ij}}{\vec{G}_{ij}\cdot(\vec{v}_{ij}+\vec{a}_{ij}\Delta t+\vec{b}_{ij}\frac{(\Delta t)^2}{4})} \qquad (4.12)$$

For small Δt, equations (4.12) are solved via successive substitutions, starting with

$$\epsilon_{ij} = 1 \qquad (4.13)$$

Iteration to convergence of the ϵ_{ij} guarantees exact conservation of energy in the method.

Higher-order formulae may be obtained directly in the same way as equations (4.10). If the highest-order terms involve

$$\vec{F}_{ij}^{(m)} = \frac{d^m\vec{F}_{ij}}{dt^m} \tag{4.14}$$

then these are replaced by

$$\vec{F}_{ij}^{(m)*} = \epsilon_{ij}\,\vec{F}_{ij}^{(m)} \tag{4.15}$$

where the ϵ_{ij} satisfy equations (4.8). The formulae for the $\vec{v}\,'_{c,i}$ are substituted in equation (4.2b), the sum transformed to $i < j$, and the ij terms set individually to zero. These resulting implicit equations in the ϵ_{ij} are then solved by standard methods, with the first approximations given by equations (4.13) .

For very high order methods, the extra algebra needed to obtain the ϵ_{ij} is considerable, and substantially reduces the relative efficiency of the method. However, it should be noted that conservation of energy guarantees stability in the usual sense (bounded motion), which is always a desirable computational property.

5. Numerical Example

As an illustration of the affect of the modification described in Section 4, the modified and unmodified forms of the third-order Adams' method were compared numerically on a sample two-dimensional problem involving two particles.

Here $n = 2$,

$$m_1 = m_2 = 2 \tag{5.1}$$

and the gravitational interaction

$$\phi_{12}(r_{12}) = -\frac{1}{r_{12}} \tag{5.2}$$

were used. The initial conditions were chosen so that the center-of-mass of the system was at rest and

$$\vec{r}_{12}(0) = \langle\tfrac{1}{2},0\rangle \tag{5.3a}$$

$$\vec{v}_{12}(0) = \langle 0,1.63\rangle \tag{5.3b}$$

The value of the energy is then

$$E = -0.6715500000... \tag{5.4}$$

Because of the form (5.2) of ϕ_{12} , the exact motion that occurs traces out a closed ellipse with major-axis

$$2a = 1.48909\ 23855 \tag{5.5}$$

corresponding to upper and lower bounds on r_{12} of

$$r_> = 0.98909\ 23855 \tag{5.6a}$$

$$r_< = 0.50000\ 00000 \tag{5.6b}$$

The motion repeats itself with period τ equal to

$$\tau = 4.0366\ 15087 \tag{5.7}$$

The implicit equations of the third-order methods were iterated to a relative convergence of 10^{-8} . A constant step-size of

$$\Delta t = \tau/80 \qquad (5.8)$$

was used. In order to focus attention on the errors made in the methods, results were obtained at times t which were multiples of the period τ , where the exact solution returns to the initial conditions. Measures of the error at these points are the error in the calculated value of E and the deviations from zero of dX/dt and Y , and from $\frac{1}{2}$ of r_{12} .

Table I gives these quantities for several times $t' = m\tau$. It can be seen that the unmodified Adams' method makes an error in E as well as larger errors in dX/dt and Y , and compares unfavorably with the modified method. Another simple measure of the error for this problem is the number of steps over which a phase error of 180° is made: i.e., the time at which $r_{12} = 0.985$ instead of 0.5 . For the unmodified methods this was about 2800 steps (35τ). For the modified methods, at 20000 steps (250τ) a phase error of less than 180° had been made.

Programs for the methods are given in the Appendix of [6].

TABLE I.

Comparison of Modified and Unmodified Methods on a Simple Gravitation Problem

At times $t = m\tau$

m	Method	E	r	$\frac{dX}{dt}$	Y
0	Exact[a]	-0.67155	0.50000	0.00000	0.00000
1	U[b]	-0.67140	0.50221	0.20630	-0.08704
	M[c]	-0.67155	0.49997	0.02164	-0.00462
2	U	-0.67099	0.50873	0.40254	-0.17213
	M	-0.67155	0.49997	0.04328	-0.00923
3	U	-0.67040	0.51924	0.58036	-0.25351
	M	-0.67155	0.50001	0.06492	-0.01385
5	U	-0.66905	0.55019	0.86162	-0.39996
	M	-0.67155	0.50017	0.10818	-0.02311
10	U	-0.66679	0.65934	1.15127	-0.64976
	M	-0.67155	0.50116	0.21592	-0.04639
100	U	-0.66561	0.97998	0.82003	-0.97598
	M	-0.67155	0.62554	1.35684	-0.57888

[a] Initial conditions

[b] Unmodified third-order Adams' method

[c] Third-order Adams' method modified to give exact energy conservation.

References

1. R. A. LaBudde and D. Greenspan, "Discrete Mechanics --A General Treatment", to be published in J. Computational Phys.

2. R. A. LaBudde and D. Greenspan, "Discrete Mechanics for Anisotropic Potentials", Univ. of Wis. Computer Sciences Dept. Report WIS-CS-203 (1974) .

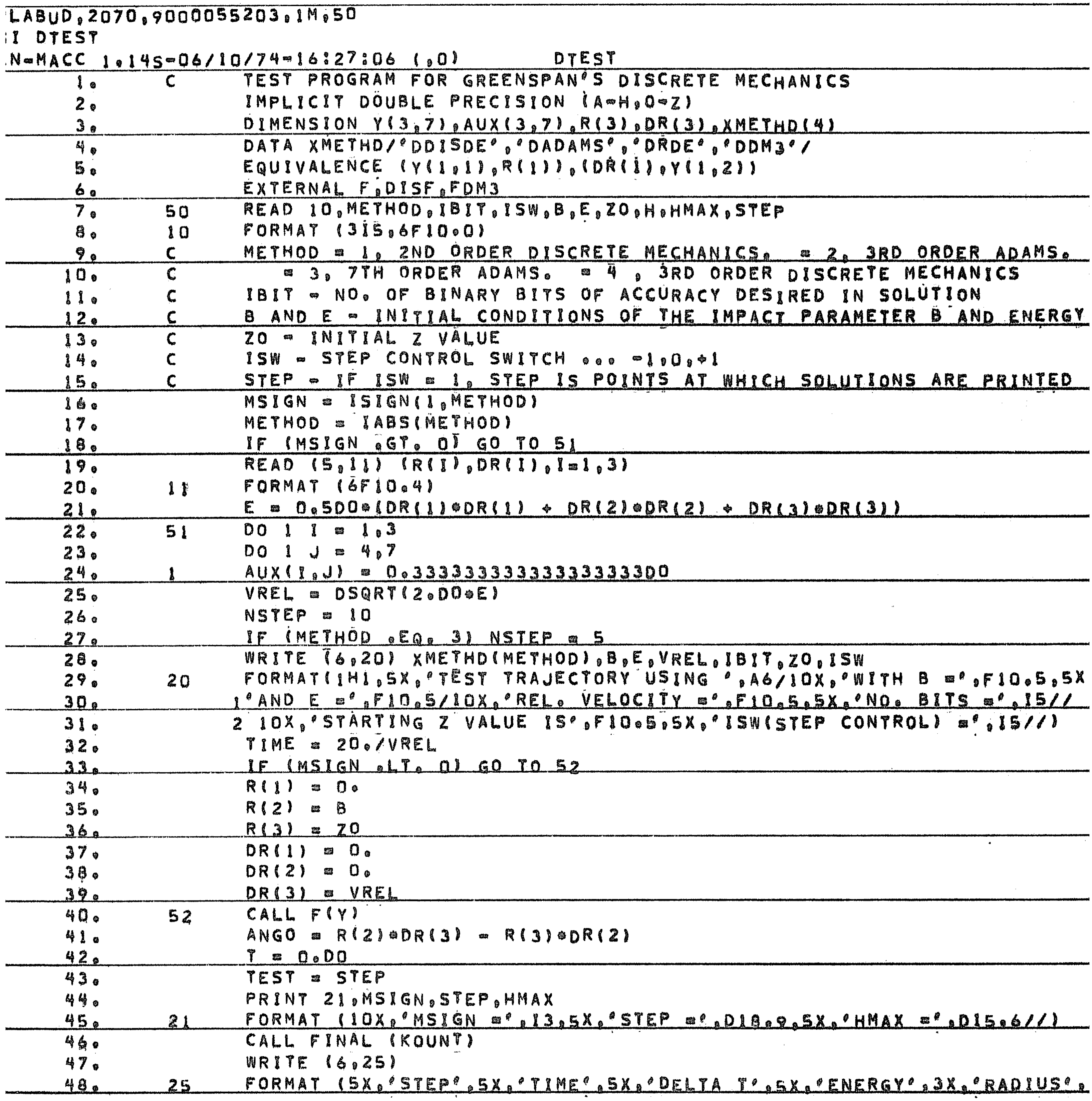
3. R. A. LaBudde and D. Greenspan, "Energy and Momentum Conserving Methods of Arbitrary Order for the Numerical Integration of Equations of Motion. I. Motion of a Single Particle", Univ. of Wis. Computer Sciences Dept. Report WIS-CS-208 (1974).

4. R. A. LaBudde and D. Greenspan, "Discrete Mechanics for Nonseparable Potentials with Application to the LEPS Form", Univ. of Wis. Computer Sciences Dept. Report WIS-CS-210 (1974).

5. R. A. LaBudde and D. Greenspan, "Energy and Momentum Conserving Methods of Arbitrary Order for the Numerical Integration of Equations of Motion. II. Motion of a System of Particles," Univ. of Wis. Computer Sciences Dept. Report WIS-CS-215 (1974).

6. R. A. LaBudde and D. Greenspan, "An Energy Conserving Modification of Numerical Methods for the Integration of Equations of Motion," Univ. of Wis. Computer Sciences Dept. Report WIS-CS-217 (1974) .

APPENDIX



```
LABUD,2070,9000055203,1M,50
I DTEST
N-MACC 1.14S-06/10/74-16:27:06 (,0)          DTEST
      C         TEST PROGRAM FOR GREENSPAN'S DISCRETE MECHANICS
                IMPLICIT DOUBLE PRECISION (A-H,O-Z)
                DIMENSION Y(3,7),AUX(3,7),R(3),DR(3),XMETHD(4)
                DATA XMETHD/'DDISDE','DADAMS','DRDE','DDM3'/
                EQUIVALENCE (Y(1,1),R(1)),(DR(1),Y(1,2))
                EXTERNAL F,DISF,FDM3
      50        READ 10,METHOD,IBIT,ISW,B,E,ZO,H,HMAX,STEP
      10        FORMAT (3I5,6F10.0)
      C         METHOD = 1, 2ND ORDER DISCRETE MECHANICS.  = 2, 3RD ORDER ADAMS.
      C            = 3, 7TH ORDER ADAMS.  = 4 , 3RD ORDER DISCRETE MECHANICS
      C         IBIT - NO. OF BINARY BITS OF ACCURACY DESIRED IN SOLUTION
      C         B AND E - INITIAL CONDITIONS OF THE IMPACT PARAMETER B AND ENERGY
      C         ZO - INITIAL Z VALUE
      C         ISW - STEP CONTROL SWITCH ... -1,0,+1
      C         STEP - IF ISW = 1, STEP IS POINTS AT WHICH SOLUTIONS ARE PRINTED
                MSIGN = ISIGN(1,METHOD)
                METHOD = IABS(METHOD)
                IF (MSIGN .GT. 0) GO TO 51
                READ (5,11) (R(I),DR(I),I=1,3)
      11        FORMAT (6F10.4)
                E = 0.5D0*(DR(1)*DR(1) + DR(2)*DR(2) + DR(3)*DR(3))
      51        DO 1 I = 1,3
                DO 1 J = 4,7
      1         AUX(I,J) = 0.33333333333333333D0
                VREL = DSQRT(2.D0*E)
                NSTEP = 10
                IF (METHOD .EQ. 3) NSTEP = 5
                WRITE (6,20) XMETHD(METHOD),B,E,VREL,IBIT,ZO,ISW
      20        FORMAT(1H1,5X,'TEST TRAJECTORY USING ',A6/10X,'WITH B =',F10.5,5X
               1'AND E =',F10.5/10X,'REL. VELOCITY =',F10.5,5X,'NO. BITS =',I5//
               2 10X,'STARTING Z VALUE IS',F10.5,5X,'ISW(STEP CONTROL) =',I5//)
                TIME = 20./VREL
                IF (MSIGN .LT. 0) GO TO 52
                R(1) = 0.
                R(2) = B
                R(3) = ZO
                DR(1) = 0.
                DR(2) = 0.
                DR(3) = VREL
      52        CALL F(Y)
                ANGO = R(2)*DR(3) - R(3)*DR(2)
                T = 0.D0
                TEST = STEP
                PRINT 21,MSIGN,STEP,HMAX
      21        FORMAT (10X,'MSIGN =',I3,5X,'STEP =',D18.9,5X,'HMAX =',D15.6//)
                CALL FINAL (KOUNT)
                WRITE (6,25)
      25        FORMAT (5X,'STEP',5X,'TIME',5X,'DELTA T',5X,'ENERGY',3X,'RADIUS',
     1 6X,'X',6X,'XDOT',9X,'Y',6X,'YDOT',9X,'Z',6X,'ZDOT',6X,'VREL'/)
      I = 0
      RR =DSQRT(R(1)**2 + R(2)**2 + R(3)**2)
      WRITE (6,30) I,T,H,E,RR,(R(J),DR(J),J=1,3),VREL
   30 FORMAT (4X,I6,F10.5,F10.6,8F10.5,F12.6)
      CALL TIMSET (0.)
      GO TO (60,70,80,85),METHOD
   60 CALL DSTART (HMAX,H,T,Y,AUX,IBIT,3,DISF,ISW,3)
      GO TO 90
   70 CALL ASTART(HMAX,H,T,Y,AUX,IBIT,3,F,ISW,3)
      GO TO 90
   80 CALL RDEO  (HMAX,H,T,Y,AUX,IBIT,3,F,ISW,3)
      GO TO 90
   85 DO 86 I = 1,3
   86 Y(I,4) = 0.
      CALL DM3IN (HMAX,H,T,Y,AUX,IBIT,3,FDM3,ISW,3)
   90 DO 100 I = 1,20001
      RR =DSQRT(R(1)**2 + R(2)**2 + R(3)**2)
      IF (RR . GT. 10. .AND. T .GE. TIME) GO TO 200
      IF (NSTEP*(I/NSTEP) + 1 .NE. I .AND. ISW .LE. 0) GO TO 95
      IF (ISW .EQ. 1 .AND. DABS(T-TEST) .GT. 1.D-5*TEST) GO TO 95
      TEST = TEST + STEP
      VREL = DR(1)*DR(1) + DR(2)*DR(2) + DR(3)*DR(3)
      CALL DFPOT(RR,FORCE,POT)
      EE = 0.5D0*VREL + POT
      VREL = DSQRT(VREL)
      PRINT 30,I,T,H,EE,RR,(R(J),DR(J),J=1,3),VREL
   95 GO TO (96,97,98,99),METHOD
   96 CALL DISDE (H,T,Y,AUX,DISF,3)
      GO TO 100
   97 CALL ADAMS (H,T,Y,AUX,F,3)
      GO TO 100
   98 CALL RDE   (H,T,Y,AUX,F,3)
      GO TO 100
   99 CALL DM3 (H,T,Y,AUX,FDM3,3)
  100 CONTINUE
  200 VREL =DSQRT(DR(1)*DR(1)+DR(2)*DR(2)+DR(3)*DR(3))
      CALL TIMGET('END')
      CALL FINAL (KOUNT)
      CHI = ACOS(DR(3)/VREL)*SIGN(1.,DR(2))
      RR = DSQRT (R(1)*R(1) + R(2)*R(2) + R(3)*R(3) )
      CALL DISPOT (RR,POT)
      EE = 0.5D0*VREL*VREL + POT
      PRINT 30,I,T,H,EE,RR
      ANG = R(2)*DR(3) - R(3)*DR(2)
      EANG = ANG - ANGO
      WRITE (6,40) CHI,KOUNT,ANG,EANG
   40 FORMAT (5X,'ANGLE OF DEFLECTION IS',E15.6,5X,'NO POT. EVAL.',I8/
     1 5X,'FINAL ANG. MOMENTUM =',E15.7,5X,'ERROR =',E15.6)
      GO TO 50
      END

 END OF COMPILATION:          NO  DIAGNOSTICS.
SI DDM3
AN-MACC 1.145-06/10/74-16:27:25 (,0)       DDM3
      SUBROUTINE DM3IN  (HMAX,H,X,Y,AUX,IBIT,N,F,ISW,NDIM)
C     SUBROUTINE WHICH SOLVES SYSTEM OF N 2ND ORDER DIFF. EQTNS. USING
```

```
C        GREENSPAN'S DICRETE MECHANICS (THIRD-ORDER)
C        Y(I,1) = Y(I), Y(I,2) = YP(I)=DY(I)/DX, Y(I,3) =D2Y(I)/DX2
C        Y(I,4) = H*D3Y(I)/DX3
C        NOTE - COLUMN 5 OF AUX SHOULD CONTAIN WEIGHTS OF Y(I) (SUM = 1)
C        NOTE - F(H,YPR,Y,ISW)  SHOULD STORE VALUE IN Y(I,3)
C        ISW = -1,0,+1. IF 0, NO STEP CONTROL. IF -1, NO MOD CONTROL
         IMPLICIT DOUBLE PRECISION (A-H,O-Z)
         DIMENSION Y(NDIM,4), AUX(NDIM,5)
         DATA BETA/2.D0/,BINV/0.5D0/,BETA2/4.D0/
         DATA ITER/4/,FACTOR/1.D-8/
         MODH = ISW
         HMIN = HMAX/1048576.D0
         HUP = 1.00000000001D0*HMAX
         XO = X
         M = N
         EPS = 0.02D0/(DABS(H)*BETA**IBIT)
         ISTEP =0
         IDELAY = 0
         ITOV =0
         IF (ISW .NE. 0) GO TO 400
         EPS = 1.D+100
         HUP = - 1.D0
         GO TO 400
         ENTRY DM3 (H,X,Y,AUX,F,NDIM)
         IF (IDELAY .EQ. 0) GO TO 300
         IDELAY = IDELAY - 1
         GO TO 400
   300   IF (ITOV .EQ. 0) GO TO  400
         HW = BETA*H
         IF (MODH*DABS(DMOD(X-XO,HW)) .GT. HMIN .OR. DABS(HW) .GE. HUP)
        1 GO TO 400
         H = HW
         EPS = BINV*EPS
   400   HW = 0.5D0*H
         TO = 0.
         DO 450 I = 1,M
         AUX(I,1) = Y(I,1)
         AUX(I,2) = Y(I,2)
         AUX(I,3) = Y(I,1) + H*(Y(I,2) + HW*Y(I,3) )
         Y(I,1) = AUX(I,3)
         AUX(I,4) = Y(I,2) + H*Y(I,3)
         Y(I,2) = AUX(I,4)
   450   TO = TO + AUX(I,5)*ABS(Y(I,1))
         TO = TO*FACTOR
         H2 = 0.1666666666666666667D0*H*H
         DO 550 J = 1,ITER
         T = 0.
         DODA =0.
         CALL F (H,AUX,Y,J,ITSW,ETA)
         DO 500 I=1,M
         W = Y(I,1)
         W2 = ETA*Y(I,4)
         Y(I,1) = AUX(I,3) + H2*W2
         Y(I,2) = AUX(I,4) + HW*W2
         T = T + AUX(I,5)*ABS(Y(I,1)-W)
   500   DODA = DODA + AUX(I,5)*ABS(W2)
         IF (ITSW .NE. 0) GO TO 550
```

```
          IF (Y .LT. TO) GO TO 580
    550   CONTINUE
          GO TO 620
    580   IF (DODA .GT. EPS) GO TO 620
          ITOV = 0
          IF (DODA*BETA2 .LT. EPS) ITOV = 1
          GO TO 650
    620   IF (ABS(H) .LT. HMIN) GO TO 1500
          DO 630 I = 1,M
          Y(I,1) = AUX(I,1)
    630   Y(I,2) = AUX(I,2)
          H = BINV*H
          EPS = BETA*EPS
          IDELAY = 1
          GO TO 400
    650   ISTEP = ISTEP +1
          X = X+H
          DO 700 I =1,M
    700   Y(I,3) = Y(I,3) + Y(I,4)
          RETURN
    1500  WRITE (6,10) ISTEP,X,H,EPS,T,DODA
    10    FORMAT ('0*****DDM3 FAILS AT STEP',I6,5X,'AT X =',D20.9,2X,'AND S
         1EP-SIZE',E15.6/5X,'ERROR CRITERION=',E15.6/5X,'STABILITY TEST =',
         2E15.6,5X,'TRUNCATION TEST =',E15.6/)
          WRITE (6,20) ((Y(I,J),J=1,4),I=1,M)
    20    FORMAT (20X,'Y(I,1)',12X,'Y(I,2)',12X,'Y(I,3)',12X,'Y(I,4)'/
         1 (10X,4E18.8))
          WRITE (6,30) ((AUX(I,J),J=1,5),I=1,M)
    30    FORMAT (/10X,'AUXILIARY MATRIX'/(10X,5E18.8))
          STOP
          END

 END OF COMPILATION:          NO  DIAGNOSTICS.
:I DF
N-MACE 1.14S-06/10/74-16:27:41 (,0)         DF
          SUBROUTINE DISF (RP,R,ISW)
    C     NOTE - EACH OF THE FOLLOWING ACCELERATION ROUTINES ASSUMES MASS =
    C     THIS ENTRY (DISF) RETURNS SECOND-ORDER DISCRETE MECHANICS ACCEL.
          IMPLICIT DOUBLE PRECISION (A-H,O-Z)
          DIMENSION RP(1),R(3,1)
          IF (ISW .GT. 1) GO TO 100
          RRP =DSQRT(RP(1)*RP(1) + RP(2)*RP(2)+RP(3)*RP(3))
          CALL DISPOT (RRP,VP)
    100   RR = SQRT(R(1,1)*R(1,1)+R(2,1)*R(2,1)+R(3,1)*R(3,1))
          CALL DISPOT (RR,V)
          DODA = (RR - RRP)*(RR + RRP)
          ACOEF = 0.D0
          IF (DABS(DODA) .GT. 1.D-20) ACOEF = (VP-V)/DODA
          DO 200 I = 1,3
    200   R(I,3) = ACOEF*(R(I,1) + RP(I))
          RETURN
          ENTRY F(R)
    C     ENTRY POINT F RETURNS CLASSICAL EXACT ACCELERATION AS FORCE/MASS
          RR =DSQRT(R(1,1)*R(1,1)+R(2,1)*R(2,1)+R(3,1)*R(3,1))
          CALL DFPOT (RR,V,VP)
          V = -V/RR
          DO 300 I = 1,3
```

```
        300    R(I,3) = V*R(I,1)
               RETURN
               ENTRY FDM3 (H,RB4,R,ISW,ITSW,ETA)
        C      ENTRY POINT FDM3 RETURNS 3RD ORDER DISCRETE MECHANICS ACCELERATIO
               DIMENSION RB4(3,1)
               METH = 1
               ITSW = 0
               ETA = 1.D0
               IF (ISW .GT. 1 .OR. METH .EQ. 0) GO TO 400
               RRP =DSQRT(RB4(1,1)*RB4(1,1) + RB4(2,1)*RB4(2,1)+RB4(3,1)*RB4(3,1
              1 )
               CALL DISPOT (RRP,VP)
        400    RR =DSQRT(R(1,1)*R(1,1) + R(2,1)*R(2,1)+R(3,1)*R(3,1) )
               CALL DFPOT (RR,FN,V)
               FN = -FN/RR
               DENOM = 0.D0
               BNUM = (V-VP)/H
               DO 500 I = 1,3
               WORK = FN*R(I,1) - R(I,3)
               IF (METH .EQ. 0) GO TO 500
               DODA = 0.5D0*(R(I,2) + RB4(I,2))
               DENOM = DENOM + WORK*DODA
               BNUM = BNUM + R(I,3)*DODA
        500    R(I,4) = WORK
               IF (METH .EQ. 0) RETURN
               ETA = -2.D0*BNUM/DENOM
               IF (ETA .GT. 0.6D0 .AND. ETA .LT. 1.4D0) RETURN
               ETA = 1.D0
               RETURN
               END

 END OF COMPILATION:          NO  DIAGNOSTICS.
I GPOT
N-MACC 1.14S-06/10/74-16:27:46 (,0)         GPOT
               SUBROUTINE DISPOT (R,POT)
               IMPLICIT DOUBLE PRECISION (A-H,O-Z)
               ISW = 1
        100    POT = -1.D0/R
               NPOT = NPOT + 1
               GO TO (200,300),ISW
        200    RETURN
               ENTRY DFPOT (R,F,POT)
               ISW = 2
               GO TO 100
        300    F = 1.D0/(R*R)
               RETURN
               ENTRY FINAL (KOUNT)
               KOUNT = NPOT
               NPOT = 0
               RETURN
               END

 END OF COMPILATION:          NO  DIAGNOSTICS.

7M-06/10-16:27
       IS NOT DEFINED - REFERENCED IN ELEMENT    DTEST
       IS NOT DEFINED - REFERENCED IN ELEMENT    DTEST
```