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

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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

\[
\mathbf{r}_i = \langle x_i, y_i, z_i \rangle
\]  

(2.1)

velocity vector

\[
\mathbf{v}_i = \left( \frac{dx_i}{dt}, \frac{dy_i}{dt}, \frac{dz_i}{dt} \right)
\]  

(2.2)

and acceleration

\[
\mathbf{a}_i = \left( \frac{d^2x_i}{dt^2}, \frac{d^2y_i}{dt^2}, \frac{d^2z_i}{dt^2} \right)
\]  

(2.3)

Newton's laws of motion

\[
m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i
\]  

(2.4)

relate the accelerations \( \ddot{\mathbf{r}}_i \) to the forces \( \mathbf{F}_i \), given by

\[
\mathbf{F}_i = -\nabla \phi
\]  

(2.5)

where \( \phi \) is the potential of interaction. It will be assumed that \( \phi \) has the pairwise-additive form

\[
\phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_n) = \sum_{i<j} \phi_{ij}(r_{ij})
\]  

(2.6)

where \( r_{ij} \) is the magnitude of the vector distance \( \mathbf{r}_{ij} \) between particles \( i \) and \( j \).
\[ \dot{r}_{ij} = \ddot{r}_j - \ddot{r}_i \quad (2.7) \]

As a consequence of equation (2.6),

\[ \dot{F}_i = \sum_{j=1}^{n} \dot{F}_{ji} \quad (2.8) \]

where

\[ \dot{F}_{ji} = - \dot{F}_{ij} \quad (2.9a) \]

\[ = - \frac{d\phi_{ji}}{dr_{ji}} \frac{\ddot{r}_{ji}}{r_{ji}} \quad (2.9b) \]

\[ = \frac{d\phi_{ij}}{dr_{ij}} \frac{\ddot{r}_{ij}}{r_{ij}} \quad (2.9c) \]

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

\[ m_i \ddot{a}_i = \sum_{j=1}^{n} \dot{F}_{ji} \quad (2.10a) \]

\[ = \sum_{j=1}^{n} \frac{d\phi_{ij}}{dr_{ij}} \frac{\ddot{r}_{ij}}{r_{ij}} \quad (2.10b) \]

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

Conservation of the total energy \( E \) occurs because of the existence of the potential \( \phi \). Here,
\[ E = \sum_{i=1}^{n} \frac{1}{2} m_i (v_i \cdot \vec{v}_i) + \phi \]  \hfill (2.11a)

\[ = \sum_{i=1}^{n} \frac{1}{2} m_i (v_i \cdot \vec{v}_i) + \sum_{i<j} \phi_{ij} \]  \hfill (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

\[
\dot{\mathbf{r}}_{c,i} = \dot{\mathbf{r}}_i + \dot{\mathbf{v}}_i \Delta t + \frac{1}{m_i} \sum_{j=1}^{n} \left[ \ddot{\mathbf{r}}_{ji} \frac{(\Delta t)^2}{2} + \dddot{\mathbf{r}}_{ji} \frac{(\Delta t)^3}{6} \right]
\]  

(3.1a)

\[
\dot{\mathbf{v}}_{c,i} = \dot{\mathbf{v}}_i + \frac{1}{m_i} \sum_{j=1}^{n} \left[ \ddot{\mathbf{r}}_{ji} \Delta t + \dddot{\mathbf{r}}_{ji} \frac{(\Delta t)^2}{2} \right]
\]  

(3.1b)

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

\[
\dddot{G}_{ji} = \frac{d^2 \phi_{ji}}{dt^2}
\]  

(3.2a)

\[
= - \frac{d \phi_{ji}}{dr_{ji}} \frac{\dot{\mathbf{v}}_{ji}}{r_{ji}} - \left[ \frac{d^2 \phi_{ji}}{dr_{ji}^2} - \frac{1}{r_{ji}} \frac{d \phi_{ji}}{dr_{ji}} \right] \frac{\dot{r}_{ji}}{r_{ji}} \frac{\dot{r}_{ji}}{r_{ji}}
\]  

(3.2b)

where

\[
\dot{r}_{ji} = \frac{dr_{ji}}{dt}
\]  

(3.3a)

\[
= \frac{\dot{r}_{ji} \cdot \dot{v}_{ji}}{r_{ji}}
\]  

(3.3b)

and

\[
\dot{v}_{ji} = \dot{v}_i - \dot{v}_j
\]  

(3.4)

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

\[
\dddot{\mathbf{r}}_i = \dddot{\mathbf{r}}_{c,i} + O[(\Delta t)^4]
\]  

(3.5a)

\[
\dddot{\mathbf{v}}_i = \dddot{\mathbf{v}}_{c,i} + O[(\Delta t)^3]
\]  

(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 \( \hat{r}'_{c,i} \) and \( \hat{v}'_{c,i} \):

\[
\Delta E_c = E'_c - E = O[(\Delta t)^3] \tag{3.6a}
\]

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

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

where

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

In equation (3.8), \( \hat{F}'_{c,ij} \) denotes the value of \( \hat{F}_{ij} \) obtained from equation (2.9b) using the \( r'_{c,ij} \).

Equations (3.5) and (3.6) also hold when the \( \hat{G}^a_{ij} \) are used for the \( \hat{G}_{ij} \).
4. Energy Conserving Modification of Conventional Methods

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

\[ \dot{r}_{c,i} = \dot{r}_i + \dot{v}_i \Delta t + \frac{1}{m_i} \sum_{j=1}^{n} \left[ \dot{F}_{ji} \frac{(\Delta t)^2}{2} + \dot{G}_{ji}^* \frac{(\Delta t)^3}{6} \right] \quad (4.1a) \]

\[ \dot{v}_{c,i} = \dot{v}_i + \frac{1}{m_i} \sum_{j=1}^{n} \left[ \dot{F}_{ji} \Delta t + \dot{G}_{ji}^* \frac{(\Delta t)^2}{2} \right] \quad (4.1b) \]

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

\[ \Delta E_c = E_c' - E \quad (4.2a) \]

\[ = \sum_{i=1}^{n} \frac{1}{2m_i} (\dot{v}_{c,i}'^2 - v_i^2) + \phi_c' - \phi \quad (4.2b) \]

\[ = \Delta t \sum_{i=1}^{n} \sum_{j=1}^{n} \left[ (\dot{v}_i + \frac{\Delta t}{2m_i} \sum_{k=1}^{n} \dot{F}_{ki} \cdot \dot{F}_{ji}) \cdot \dot{G}_{ji}^* \right] \]

\[ + \frac{\Delta t}{2} \left( \dot{v}_i + \frac{\Delta t}{m_i} \sum_{k=1}^{n} \dot{F}_{ki} + \dot{G}_{ki}^* \frac{\Delta t}{4} \right) \cdot \dot{G}_{ji}^* \]

\[ = \Delta t \sum_{i<j} \left[ \left( \dot{v}_{ij} + \dot{a}_{ij} \Delta t + \dot{b}_{ij} \frac{(\Delta t)^2}{4} \right) \cdot \dot{G}_{ij}^* \frac{\Delta t}{2} \right. \]

\[ + (\dot{v}_{ij} + \dot{a}_{ij} \frac{\Delta t}{2}) \cdot \dot{G}_{ij}^* \frac{\Delta \phi_{ij}}{\Delta t} \quad (4.2d) \]
where
\[ \hat{a}_{ij} = \frac{n}{k=1} \left[ \frac{\hat{\mathbf{f}}_{kj}}{m_j} - \frac{\hat{\mathbf{f}}_{ki}}{m_i} \right] \]  
\[ \hat{b}_{ij} = \frac{n}{k=1} \left[ \frac{\hat{\mathbf{g}}_{kj}^*}{m_j} - \frac{\hat{\mathbf{g}}_{ki}^*}{m_i} \right] \]  
\[ (4.3a) \]
\[ (4.3b) \]

and
\[ \Delta \phi_{ij} = \phi_{c,i} - \phi_{ij} \]  
\[ = \phi_{ij}(r_{c,i}) - \phi_{ij}(r_{ij}) \]  
\[ (4.4a) \]
\[ (4.4b) \]

where
\[ \hat{r}_{c,i} = \hat{r}_{c,i} - \hat{r}_{c,i} \]  
\[ (4.5) \]

Suppose now, instead of using \( \hat{\mathbf{g}}_{ij}^* = \hat{\mathbf{g}}_{ij} \) or \( \hat{\mathbf{g}}_{ij}^a \)
in equation (4.2)—which leads to an error \( \Delta E_c \) of \( O[(\Delta t)^3] \)—that adjustable \( \hat{\mathbf{g}}_{ij}^* \)
\[ \hat{\mathbf{g}}_{ij}^* = \epsilon_{ij} \hat{\mathbf{g}}_{ij} \]  
\[ (4.6) \]
or
\[ \hat{\mathbf{g}}_{ij}^* = \epsilon_{ij} \hat{\mathbf{g}}_{ij}^a \]  
\[ (4.7) \]
is used. The \( \epsilon_{ij} \) are to be chosen so that
\[ \epsilon_{ij} = 1 + O[\Delta t] \]  
\[ (4.8) \]
(preserving the order of the method), and such that exact conservation of energy occurs. Solving
\[ \Delta E_c = 0 \]  
\[ (4.9) \]
for the \( \epsilon_{ij} \) gives, for example, for (4.6), the equations (cf. [1] and [5])

\[
\left\{ \hat{v}_{ij} + \hat{a}_{ij} \Delta t + \hat{b}_{ij} \frac{(\Delta t)^2}{4} \right\} \cdot \hat{G}_{ij} \frac{\Delta t}{2} \epsilon_{ij} + (\hat{v}_{ij} + \hat{a}_{ij} \frac{\Delta t}{2}) \cdot \hat{F}_{ij} + \frac{\Delta \phi_{ij}}{\Delta t} = 0
\]

(4.10)

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

For small \( \Delta t \), equations (4.10) are strongly linear in the \( \epsilon_{ij} \). The only nonlinear dependences on the \( \epsilon_{ij} \) occur through the \( \hat{b}_{ij} \) and \( \phi', \epsilon_{ij} \) (through the \( r', \epsilon_{ij} \)). In both these cases, the terms involving the \( \epsilon_{ij} \) 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 \( \epsilon_{ij} \), namely

\[
(\hat{v}_{ij} + \hat{a}_{ij} \Delta t) \cdot \hat{G}_{ij} \frac{\Delta t}{2}
\]

(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

\[
\epsilon_{ij} = \frac{2}{\Delta t} \frac{\Delta \phi_{ij} + (\hat{v}_{ij} + \hat{a}_{ij} \frac{\Delta t}{2}) \cdot \hat{F}_{ij}}{\hat{G}_{ij} \cdot (\hat{v}_{ij} + \hat{a}_{ij} \Delta t + \hat{b}_{ij} \frac{(\Delta t)^2}{4})}
\]

(4.12)

For small \( \Delta t \), equations (4.12) are solved via successive substitutions, starting with

\[
\epsilon_{ij} = 1
\]

(4.13)
Iteration to convergence of the $\epsilon_{ij}$ 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

$$\hat{F}_{ij}^{(m)} = \frac{d^m F_{ij}}{dt^m}$$

(4.14)

then these are replaced by

$$\hat{F}_{ij}^{(m)*} = \epsilon_{ij} \hat{F}_{ij}^{(m)}$$

(4.15)

where the $\epsilon_{ij}$ satisfy equations (4.8). The formulae for the $v_{c,i}$ 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 $\epsilon_{ij}$ 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 $\epsilon_{ij}$ 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 \( n = 2 \),
\[
m_1 = m_2 = 2
\] (5.1)

and the gravitational interaction
\[
\phi_{12}(r_{12}) = -\frac{1}{r_{12}}
\] (5.2)

were used. The initial conditions were chosen so that the center-of-mass of the system was at rest and
\[
\vec{r}_{12}(0) = \left< \frac{1}{2}, 0 \right> \quad \text{(5.3a)}
\]
\[
\vec{v}_{12}(0) = <0, 1.63> \quad \text{(5.3b)}
\]

The value of the energy is then
\[
E = -0.6715500000\ldots
\] (5.4)

Because of the form (5.2) of \( \phi_{12} \), the exact motion that occurs traces out a closed ellipse with major-axis
\[2a = 1.48909 \ 23855 \] (5.5)
corresponding to upper and lower bounds on \( r_{12} \) of
\[
r_+ = 0.98909 \ 23855 \] (5.6a)
\[
r_- = 0.50000 \ 00000 \] (5.6b)
The motion repeats itself with period \( \tau \) equal to
\[\tau = 4.0366 \ 15087 \] (5.7)
The implicit equations of the third-order methods were iterated to a relative convergence of $10^{-8}$. A constant step-size of

$$\Delta t = \tau/80$$  \hspace{1cm} (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 $\tau$, 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 $180^\circ$ 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 (35\tau). For the modified methods, at 20000 steps (250\tau) a phase error of less than $180^\circ$ 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 $t = m t$

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

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a Initial conditions  
b Unmodified third-order Adams' method  
c Third-order Adams' method modified to give exact energy conservation.
References


APPENDIX

LABUD, 2070, 9000055203, 1M, 50
: I DTEST
N=MACC 10 14S-06/10/74=16:27:06 (0) DTEST

1. C TEST PROGRAM FOR GREENSPAN'S DISCRETE MECHANICS

2. IMPLICIT DOUBLE PRECISION (A-H,O-Z)

3. DIMENSION Y(3,7), AUX(3,7), R(3), DR(3), XMETHOD(4)

4. DATA XMETHOD,'DDISDE', 'DADAMS', 'DRDE', 'DDM3' /

5. EQUIVALENCE (Y(1,1), R(1)), (DR(1), Y(1,2))

6. EXTERNAL F, DISF, FDM3

7. 50 C METHOD = 1, 2ND ORDER DISCRETE MECHANICS, = 2, 3RD ORDER ADAMS

8. 10 C = 3, 7TH ORDER ADAMS, = 4, 3RD ORDER DISCRETE MECHANICS

9. C IBIT = NO. OF BINARY BITS OF ACCURACY DESIRED IN SOLUTION

10. C AND E = INITIAL CONDITIONS OF THE IMPACT PARAMETER B AND ENERGY

11. C Z0 = INITIAL Z VALUE

12. C ISW = STEP CONTROL SWITCH ... = 1, 0 = 1

13. C STEP = IF ISW = 1, STEP IS POINTS AT WHICH SOLUTIONS ARE PRINTED

14. C MSIGN = ISIGN (1, METHOD)

15. C METHOD = IABS (METHOD)

16. C IF (MSIGN = 0) GO TO 51

17. C READ (5,1) (R(1), DR(1), I=1,3)

18. C FORMAT (6F10.4)

19. C E = 0.5D0*DR(1)*DR(1) + DR(2)*DR(2) + DR(3)*DR(3)

20. 10 DO I = 1, 3

21. C DO J = 4, 7

22. 51 AUX(I,J) = 0.3333333333333333D0

23. C VREL = DSQRT(2.0*E)

24. C NSTEP = 10

25. C IF (METHOD + Eq. 3) NSTEP = 5

26. C WRITE (6,20) XMETHOD, METHOD, B, E, VREL, IBIT, Z0, ISW

27. C FORMAT (1H1, 5X, 'TEST TRAJECTORY USING ', 'A6/10X, 'WITH B = ', 'F10.5', '5X

28. C AND E = ', 'F10.5', '5X, 'NO. BITS AT', 'ISW (STEP CONTROL) = ', '15//

29. C 2 10X, 'STARTING Z VALUE IS ', 'F10.5', '5X, 'ISW (STEP CONTROL) = ', 'ISW //

30. C TIME = 20.0*VREL

31. C IF (MSIGN = LT. 0) GO TO 52

32. C R(1) = 0

33. C R(2) = B

34. C R(3) = Z0

35. C DR(1) = 0

36. C DR(2) = 0

37. C DR(3) = VREL

38. 52 CALL F(Y)

39. ANGO = R(2)*DR(3) - R(3)*DR(2)

40. T = 0.0*DO

41. TEST = STEP

42. PRINT 21, MSIGN, STEP, HMAX

43. C FORMAT (10X, 'MSIGN = ', 'I3', '5X, 'STEP = ', 'D18.9', '5X, 'HMAX = ', 'D15.6//

44. C CALL FINAL (KOUNT)

45. C WRITE (6,25)


47. C}
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
FORMAT (4X,16,F10.5,F10.6,8F10.5,F12.6)
call timer(0)
go to 60
Call dstart (HMAX,H,T,Y,AUX,IBIT,3,DISF,ISW,3)
go to 90
Call astart (HMAX,H,T,Y,AUX,IBIT,3,F,ISW,3)
go to 90
Call redo (HMAX,H,T,Y,AUX,IBIT,3,F,ISW,3)
go to 90
do 86 i = 1,3
88 y(i) = 0
Call dm3in (HMAX,H,T,Y,AUX,IBIT,3,FDM3,ISW,3)
do 100 i = 1,2000
rr = dsqrt(r(1)*2 + r(2)*2 + r(3)*2)
if (rr > gt)*0.1*and. t.ge. time) go to 200
if (nstep*1/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 dpot(rr,forq,pot)
e = 0.5*dr*vrel + pot
vrel = dsqrt(vrel)
print 30,i,t,h,e,rr,r(j),dr(j),j=1,3,vrel
95 go to (96,97,98,99)*method
call disde (H,T,Y,AUX,DISF,3)
go to 100
97 call adams (H,T,Y,AUX,FDMSF,3)
go to 100
98 call rede (H,T,Y,AUX,FDMSF,3)
go to 100
99 call dm3 (H,T,Y,AUX,FDMSF,3)
100 continue
200 vrel = dsqrt(dr(1)*dr(1) + dr(2)*dr(2) + dr(3)*dr(3))
call timer ("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)
e = 0.5*dr*vrel*vrel + pot
print 30,i,t,h,e,rr
ang = r(2)*dr(3) - r(3)*dr(2)
94 eang = ang - ang
write (6,40) chi,kount,ang,eang
format (5x,"angle of deflection is",f10.6"
95 5x,"final ang. momentum is",e15.6"
96 5x,"error is",e15.6"
97 go to 50
98 end
99 end of compilation; no diagnostics.
51 dmm3
4n-macc 1.145-06/10/74=16:27:25 (0) dmm3
1, sub routine dm3in (hmax,h,x,y,aux,ibit,n,f,sw,ndim)
2, c sub routine which solves system of n 2nd order diff. eqns. using
3. C GREENSPAN'S DISCRETE MECHANICS (THIRD-ORDER)
4. C Y(I,1) = Y(I,0), Y(I,2) = DY(I)/DX, Y(I,3) = D2Y(I)/DX2
5. C Y(I,4) = H*DY(I)/DX
6. C NOTE = COLUMN 5 OF AUX SHOULD CONTAIN WEIGHTS OF Y(I) (SUM = 1)
7. C NOTE = F(H, YPR, Y, ISW) SHOULD STORE VALUE IN Y(I,3)
8. C ISW = -1..0,1, IF 0, NO STEP CONTROL, IF = 0, NO MOD CONTROL
9. C IMPLICIT DOUBLE PRECISION (A=H,O=Z)
10. C DIMENSION Y(NDIM,4), AUX(NDIM,5)
11. C DATA BETA2/2DO,=B/0,5DO/=BETA2/4,DO/
12. C DATA ITER/4.,FACTOR/1.,D=8/
13. C MODH = ISW
14. C HMIN = HMAX/1048576.DO
15. C HUP = 1.000000000.D0*HMAX
16. C XO = X
17. C M = N
18. C EPS = 0.02DO/(DABS(H)BETA4IBIT)
19. C ISTEP = 0
20. C IDELAY = 0
21. C ITOV = 0
22. C IF (ISW = NE.0,0) GO TO 400
23. C EPS = 1.0*100
24. C HUP = -1.0DO
25. C GO TO 400
26. C ENTRY DM3 (H,X,Y,AUX,F,NDIM)
27. C IF (IDelay = Eq. 0) GO TO 300
28. C IDELAY = IDELAY = 1
29. C GO TO 400
30. C 300 IF (ITOV = EQ. 0) GO TO 400
31. C HW = BETA*H
32. C IF (MODH*DABS(DMOD(X-XO,HW)) GT HMIN OR. DABS(HW) GT HUP)
33. C 1 GO TO 400
34. C H = HW
35. C EPS = BINV*EPS
36. C 400 HW = 0.5DO*H
37. C TO = 0.
38. C DO 450 I = 1..M
39. C AUX(I,0) = Y(I,0)
40. C AUX(I,2) = Y(I,2)
41. C AUX(I,3) = Y(I,1) + H*(Y(I,2) + HW*Y(I,3))
42. C Y(I,1) = AUX(I,1)
43. C Y(I,2) = AUX(I,4)
44. C Y(I,3) = AUX(I,4)
45. C 450 TO = TO + AUX(I,5)*ABS(Y(I,1))
46. C TO = TO*FACTOR
47. C H2 = 0.1666666666666667DO*H*H
48. C DO 550 J = 1..ITER
49. C T = 0.
50. C DODA = 0.
51. C CALL F(H,AUX,Y,ITSW,ETA)
52. C DO 500 I=1..M
53. C W = Y(I,1)
54. C W2 = ETA*Y(I,4)
55. C Y(I,1) = AUX(I,3) + H2*W2
56. C Y(I,2) = AUX(I,4) + HW*W2
57. C T = T + AUX(I,5)*ABS(Y(I,1)-W)
58. C 500 DODA = DODA + AUX(I,5)*ABS(W2)
59. C IF (ITSW = NE. 0, 0) GO TO 550
<table>
<thead>
<tr>
<th>Line</th>
<th>Statement</th>
</tr>
</thead>
<tbody>
<tr>
<td>550</td>
<td>CONTINUE</td>
</tr>
<tr>
<td>580</td>
<td>IF (DODA  GT  EPS) GO TO 620</td>
</tr>
<tr>
<td>580</td>
<td>ITOV  = 0</td>
</tr>
<tr>
<td>580</td>
<td>IF (DODA = BETA2  LT  EPS) ITOV  = 1</td>
</tr>
<tr>
<td>620</td>
<td>GO TO 650</td>
</tr>
<tr>
<td>620</td>
<td>IF (ABS(H)  LT  MINH) GO TO 1500</td>
</tr>
<tr>
<td>630</td>
<td>DO 630 I = 1,M</td>
</tr>
<tr>
<td>630</td>
<td>Y(I,K) = AUX(I,K)</td>
</tr>
<tr>
<td>630</td>
<td>Y(I,2) = AUX(I,2)</td>
</tr>
<tr>
<td>630</td>
<td>H = INVH</td>
</tr>
<tr>
<td>650</td>
<td>ISTEP = ISTEP + 1</td>
</tr>
<tr>
<td>670</td>
<td>X = X+H</td>
</tr>
<tr>
<td>700</td>
<td>DO 700 I = 1 M</td>
</tr>
<tr>
<td>770</td>
<td>Y(I,3) = Y(I,3) + Y(I,4)</td>
</tr>
<tr>
<td>800</td>
<td>WRITE (6,10) ISTEP, X, H, EPS,T,DODA</td>
</tr>
<tr>
<td>810</td>
<td>FORMAT ('Qступил', 16, 5X, AT X =', D20, 9, 2X, 'AND S', 1E15, 6, 5X, 'ERROR CRITERION'), E15, 6, 5X, 'STABILITY TEST =', 2E15, 6, 5X, 'TRUNCATION TEST =', E15, 6, 1)</td>
</tr>
<tr>
<td>840</td>
<td>WRITE (6,120) (10, Y(I,J), J=1,5) I=1 M</td>
</tr>
<tr>
<td>850</td>
<td>FORMAT ('/10X,' 'AUXILIARY MATRIX', '/10X, 5E18, 8'))</td>
</tr>
<tr>
<td>870</td>
<td>STOP</td>
</tr>
</tbody>
</table>

END OF COMPILATION: NO DIAGNOSTICS.

I DF
N=MACE 1.145=06/10/74=16:27:41 (0)

DF

SUBROUTINE DISP (RP, R, ISW)

NOTE - EACH OF THE FOLLOWING ACCELERATION ROUTINES ASSUMES MASS =

THIS ENTRY (DISP) RETURNS SECOND-ORDER DISCRETE MECHANICS ACCEL.

IMPLICIT DOUBLE PRECISION (A=H, D=Z)

DIMENSION RP(1), R(3, 1)

IF (ISW = 67, 1) GO TO 100

RRP = DSQRT(RP(1) * RP(1) + RP(2) * RP(2) + RP(3) * RP(3))

CALL DISPOT (RRP, VP)

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 = DODA

IF (DABS(DODA)  GT  1.0 D=20) ACOEF = (VP-V)/DODA

DO 200 I = 1,3

R(I, 3) = ACOEF * (R(I, 1) + RP(I))

RETURN

ENTRY F(R)

ENTRY POINT F RETURMS 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 DFPOF (RR, V, VP)

V = -V/RR

DO 300 I = 1,3
R(I,3) = V*R(I,1)
RETURN
ENTRY FDM3 (H,RB(4),R,ISW,ITSW,ETA)

C ENTRY POINT FDM3 RETURNS 3RD ORDER DISCRETE MECHANICS ACCELERATION
DIMENSION RB(3,1)
METH = 1
ITSW = 0
ETA = 1.0
IF (ISW .GT. 1 .OR. METH .EQ. 0) GO TO 400
RR = DSQRT(R(I,1)*RB(1,1) + RB(2,1)**2 + RB(3,1)**2)
CALL DFPOT(RR,FP)
FN = -FN/RR
DENOM = 0.0
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 = 0.5*DO(I+1)
DENOM = DENOM + WORK*DO(I+1)
BNUM = BNUM + R(I,3)*DO(I+1)
R(I,4) = WORK
IF (METH .EQ. 0) RETURN
ETA = -2.0*DO(I) + BNUM/DENOM
IF (ETA .GT. 0.0) AND ETA .LT. 1.4 DO 1 RETURN
500 ETA = 1.0 DO 500 ETA = 1.0
RETURN
END

END OF COMPILATION: NO DIAGNOSTICS.

N=MACC 14S=06/10/74=16:27:46 (a)
SUBROUTINE DISPOT (R,POT)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
ISW = 1
POT = -1.0/DO(R)
NPOT = NPOT + 1
GO TO (200,300),ISW
RETURN
ENTRY DFPOT (R,F,POT)
ISW = 2
GO TO 100
F = 1.0/DO(R)
RETURN
ENTRY FINAL (KOUNT)
KOUTH = NPOT
NPOT = 0
RETURN
END

END OF COMPILATION: NO DIAGNOSTICS.

7M=06/10-16:27
IS NOT DEFINED - REFERENCED IN ELEMENT DTSG
IS NOT DEFINED - REFERENCED IN ELEMENT DTSG