ENERGY AND MOMENTUM CONSERVING
METHODS OF ARBITRARY ORDER
FOR THE NUMERICAL INTEGRATION
OF EQUATIONS OF MOTION

I. Motion of a Single Particle

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Robert A. LaBudde
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ABSTRACT

Conventional numerical methods, when applied to the ordinary differential equations of motion of classical mechanics, conserve the total energy and angular momentum only to the order of the truncation error. Since these constants of the motion play a central role in mechanics, it is a great advantage to be able to conserve them exactly. A new numerical method is developed, which is a generalization to arbitrary order of the "discrete mechanics" described in earlier work, and which conserves the energy and angular momentum to all orders. This new method can be applied much like a "corrector" as a modification to conventional numerical approximations, such as those obtained via Taylor series, Runge-Kutta, or predictor-corrector formulae. The theory is extended to a system of particles in Part II of this work.

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# TABLE OF CONTENTS

1. Introduction 1  
2. Definitions 3  
3. Conventional Numerical Solutions 5  
4. Conservative Solutions 9  
   A. First Formulation 10  
   B. Second Formulation 16  
5. Related Theory and Remarks 24  
   A. Truncation Error 24  
   B. Propagation of Error 30  
   C. Comparison of the Two Formulations 37  
6. Numerical Examples 39  
7. Conclusion 44  

References 45  
APPENDIX 47
1. Introduction

The theory of the motion of a system of particles is dominated by the concepts of the conservation of the total energy and linear and angular momenta. These quantities are unique in the sense of being the only extensive constants of motion: i.e., simple additive functions of the individual particles [1]. Furthermore, they are directly related to the fundamental transformational invariances of the equations of motion [2].

Because of the importance of these additive constants of motion in mechanics, it is particularly disturbing when their values are changed because of truncation error in conventional numerical solutions. In addition, since the energy and momenta are easily ascertained from the initial conditions, it is reasonable to suppose this information could be used to improve the solution.

In previous work [3]-[4], an unconventional second-order numerical solution to the equations of motion of a system of particles was developed for the case of a separable, radial potential. The method was shown to be of comparable accuracy to the third-order Adams' method, and had the desirable property of exactly conserving the additive constants of motion [4]. The major disadvantage of this new method – denoted "discrete mechanics" – is its low order of approximation: third-order in the coordinates; second-order in the velocities.

In what follows, the "discrete mechanics" presented previously [4] is found to be the lowest-order member of a family of conservative solutions. In addition, the theory to be developed shows it to be actually third-order in the velocities (explaining the comparison in [4] with the third-order Adams' method). The general formula for an arbitrary degree of numerical approximation is developed in Sect. 4 and is compared
with results obtained from conventional Adams' methods of orders 3 through 8 in Section 6. Attention will be directed in the present paper to the motion of a single particle: the theory is extended to a system of particles in Part II, to be presented in [5].

As mentioned previously [4], the only requirement for conservation of the total linear momentum (and consequently the center-of-mass motion) is consistency, which is a property of every numerical method of order 2 or higher. Since all the methods to be mentioned (including the conventional Adams' methods) satisfy this criterion, conservation of the total linear momentum will not receive special attention.
2. Definitions

For simplicity, the problem will be restricted initially to the case of the motion of a single particle in a central field. This case includes most common two-body interactions [6]: e.g., the motion of the earth about the sun.

Suppose the particle has mass $m$ and position vector

$$\mathbf{r} = \langle x, y, z \rangle$$

(2-1)

with respect to the origin of the central field. Let $\mathbf{v}$ denote the velocity of the particle

$$\mathbf{v} = \frac{d\mathbf{r}}{dt} = \langle \frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt} \rangle$$

(2-2)

Newton's second law of motion specifies $\mathbf{r}(t)$ as the solution of the second-order ordinary differential equation

$$m \frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}(\mathbf{r})$$

(2-3)

where the force field $\mathbf{F}(\mathbf{r})$ is given as the negative gradient of a central potential $\phi(r)$:

$$\mathbf{F}(\mathbf{r}) = -\frac{\partial \phi(r)}{\partial \mathbf{r}}$$

(2-4a)

$$= -\left( \frac{d\phi}{dr} \right) \frac{\mathbf{r}}{r}$$

(2-4b)

where

$$\frac{\partial}{\partial \mathbf{r}} = \langle \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \rangle$$

(2-5)
is the gradient with respect to \( \vec{r} \), and

\[
\vec{r} = \left| \vec{r} \right| = \sqrt{X^2 + Y^2 + Z^2}
\]  

(2-6)

Therefore the exact solution for the position \( \vec{r}' \) and velocity \( \vec{v}' \) at any later time \( t' = t + \Delta t \) is given by the solution of the differential equations (2-3) and (2-4) with initial conditions \( \vec{r}(t) \) and \( \vec{v}(t) \).

Since \( \phi \) is differentiable and a function of \( r \) alone, the energy \( E \) and angular momentum \( \vec{L} \) are conserved [2], i.e., are independent of \( t \).

For the present problem,

\[
E = \frac{1}{2} m(\vec{v} \cdot \vec{v}) + \phi(r)
\]  

(2-7a)

\[
\vec{L} = m(r \times \vec{v})
\]  

(2-7b)

where \( \cdot \) and \( \times \) denote the scalar and vector products, respectively.

Central potentials are the most common form of interactions. Typical examples of \( \phi(r) \) that occur in practice are: (a) gravitational,

\[
\phi(r) = -\frac{GMm}{r}
\]  

(2-8)

where \( GM \) is the gravitational constant for, e.g., the sun; and (b) intermolecular interaction in a dilute gas characterized by, e.g., the Lennard-Jones potential [7],

\[
\phi(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]
\]  

(2-9)

where \( \epsilon \) and \( \sigma \) are constants of the gas involved.
3. Conventional Numerical Solutions

Among the most popular techniques for solving the system of differential eqs. (2-3) and (2-4) numerically are truncated Taylor series, predictor-corrector, and Runge-Kutta formulae. The Taylor series solution is constructed by noting that, when no explicit time dependence occurs in the equations of motion,

\[
\frac{d}{dt} = \frac{\vec{r}}{dt} \cdot \frac{\partial}{\partial \vec{r}} + \frac{\vec{v}}{dt} \cdot \frac{\partial}{\partial \vec{v}} \quad (3-1a)
\]

\[
\vec{v} = \vec{v} \cdot \frac{\partial}{\partial \vec{r}} + \frac{\vec{F}}{m} \cdot \frac{\partial}{\partial \vec{v}} \quad (3-1b)
\]

Eqs. (3-1) may be used to obtain all higher time-derivatives of \(\vec{r}\) in terms of the initial conditions \(\vec{r}\) and \(\vec{v}\): e.g.,

\[
m \frac{d^3 \vec{r}}{dt^3} = \frac{d\vec{F}}{dt} \quad (3-2a)
\]

\[
= - \left( \frac{1}{r} \right) \frac{d \Phi}{dr} \vec{v} + \frac{1}{r^2} \frac{d \Phi^2}{dr^2} + \frac{2}{r} \frac{d \Phi}{dr} \vec{v} \times \vec{r} \quad (3-2b)
\]

Further derivatives may be developed recursively using eqs. (3-1).

By writing \(r'\) and \(v'\) in the form of Taylor series, one has

\[
\vec{r}' = \vec{r} + \vec{v} \Delta t + \frac{\vec{F}}{m} (\Delta t)^2 + \frac{d^3 \vec{r}}{dt^3} (\Delta t)^3 + \ldots \quad (3-3a)
\]

\[
\vec{v}' = \vec{v} + \frac{\vec{F}}{m} \Delta t + \frac{d^3 \vec{r}}{dt^3} (\Delta t)^2 + \ldots \quad (3-3b)
\]

Then, because vector dependences only on \(\vec{r}\) and \(\vec{v}\) occur (see (2-4b) and, e.g., eqs. (3-2)), both \(r'\) and \(v'\) can be written in the form...
\[ \vec{r}' = f_1 \vec{r} + f_2 \vec{v} \quad (3-4a) \]
\[ \vec{v}' = f_3 \vec{r} + f_4 \vec{v} \quad (3-4b) \]

where the \( f_i \) are scalar functions. This observation will be used later in Sect. 4.

Predictor-corrector approximations \( \vec{r}'_c \) and \( \vec{v}'_c \) for \( \vec{r}' \) and \( \vec{v}' \), respectively, can be written in the form

\[ \vec{r}'_c = \vec{r}'_p + \delta \vec{r}_c \quad (3-5a) \]
\[ \vec{v}'_c = \vec{v}'_p + \delta \vec{v}_c \quad (3-5b) \]

where

\[ \delta \vec{r}_c = \gamma_0 (\Delta t)^2 (\vec{F}(r'_c) - \vec{F}'_p) / m \quad (3-6a) \]
\[ \delta \vec{v}_c = \gamma_1 \Delta t (\vec{F}(r'_c) - \vec{F}'_p) / m \quad (3-6b) \]

In eqs. (3-5) and (3-6), \( \vec{r}'_c, \vec{v}'_c, \) and \( \vec{F}'_c \) are "predicted" approximate values for \( r'_c, v'_c, \) and \( F'_c = F(r'_c) \), respectively, obtained via interpolation over previous steps. (In the case of an Adams' method, \( \vec{r}'_p, \vec{v}'_p, \) and \( \vec{F}'_p \) are obtained using only \( \vec{r}, \vec{v}, \) and previous values of the forces.) The "corrector" coefficients \( \gamma_0 \) and \( \gamma_1 \) are usually chosen to eliminate the leading terms in the truncation errors of \( \vec{r}'_c \) and \( \vec{v}'_c \).

Since \( \delta \vec{r}_c \) and \( \delta \vec{v}_c \) are implicit in \( \vec{r}'_c \) via \( \vec{F}(r'_c) \), eqs. (3-5) are implicit in \( \vec{r}'_c \) and must be solved by an iterative process. Normally this is done by simple successive substitutions, starting with \( \vec{r}'_c = \vec{r}'_p \).

If this process is to converge rapidly, \( \vec{r}'_p \) must be a good approximation
to $\vec{r}'$. Assuming the method is $n$-th order, i.e.,

$$\vec{r}' = \vec{r}'_C + O[(\Delta t)^{n+1}]$$  \hspace{1cm} (3-7a)

$$\vec{v}' = \vec{v}'_C + O[(\Delta t)^n]$$  \hspace{1cm} (3-7b)

the "predictors" $\vec{r}'_P$ and $\vec{v}'_P$ are usually at least $(n-1)$-st order:

$$\vec{r}' = \vec{r}'_P + O[(\Delta t)^n]$$  \hspace{1cm} (3-8a)

$$\vec{v}' = \vec{v}'_P + O[(\Delta t)^{n-1}]$$  \hspace{1cm} (3-8b)

It should be noted that, if the predictor-corrector system is constructed using only the initial conditions and information (such as the forces) from the differential eqs. (2-3), then $\vec{r}'_P, \vec{v}'_P, \vec{r}'_C, \vec{v}'_C$ are linearly dependent on $\vec{r}$ and $\vec{v}$ in a way similar to eqs. (3-4) for $\vec{r}'$ and $\vec{v}'$.

As an illustration of the predictor-corrector method, the lowest-order Adams' formulae result for the case $n = 3$, where

$$\vec{r}'_P = \vec{r} + \vec{v} \Delta t + \frac{\vec{F}}{m} (\Delta t)^2$$  \hspace{1cm} (3-9a)

$$\vec{v}'_P = \vec{v} + \frac{\vec{F}}{m} \Delta t$$  \hspace{1cm} (3-9b)

$$\vec{F}'_P = \vec{F}(\vec{r})$$  \hspace{1cm} (3-9c)

and $\gamma_0 = 1/6, \gamma_1 = 1/2$, i.e.,

$$\vec{r}'_C = \frac{(\Delta t)^2}{6} (\vec{F}(\vec{r}') - \vec{F})/m$$  \hspace{1cm} (3-10a)
\[ \delta v_c = \frac{\Delta t}{2} (F(r'_c) - F)/m \quad (3-10b) \]

Substitution of eqs. (3-9) and (3-10) into eqs. (3-5) gives the following implicit equations for \( \vec{r}'_c \) and \( \vec{v}'_c \):

\[ \vec{r}'_c = \vec{r} + \vec{v} \Delta t + \frac{F}{m} \left( \frac{\Delta t}{2} + \frac{(\Delta t)^2}{6} (F(r'_c) - F)/m \right) \quad (3-11a) \]

\[ \vec{v}'_c = \vec{v} + \frac{F}{m} \Delta t + \frac{(\Delta t)^2}{2} (F(r'_c) - F)/m \quad (3-11b) \]

The truncation errors in \( \vec{r}'_c \) and \( \vec{v}'_c \) are given by (see, e.g., [8]):

\[ \vec{r}'_c = \vec{r}'_c - \left( \frac{\Delta t}{24} \frac{d^4 r}{dt^4} \right) + \mathcal{O}((\Delta t)^5) \quad (3-12a) \]

\[ \vec{v}'_c = \vec{v}'_c - \left( \frac{\Delta t}{12} \frac{d^4 r}{dt^4} \right) + \mathcal{O}((\Delta t)^4) \quad (3-12b) \]

In general with methods of this type, special starting and step-size changing formulae are necessary, although of course this is not the case for the simple \( n = 3 \) formulae above.

Runge-Kutta formulae for second-order differential equations, although easily applied, are more complicated in form, and will be of little heuristic value in the discussion that follows. For this reason these methods will not be discussed in any detail in the present work.
4. **Conservative Solutions**

Since conventional numerical methods of order \( n \) conserve the values of \( E \) and \( \dot{L} \) only to terms of \( O[(\Delta t)^n] \), it is of interest to find a method which conserves \( E \) and \( \dot{L} \) to **all** orders, i.e., exactly. For these quantities to be maintained at their initial values for all steps, \( \Delta E \) and \( \Delta \dot{L} \) must vanish, where

\[
\Delta E = E' - E \quad (4-1a)
\]
\[
\Delta \dot{L} = \dot{L}' - \dot{L} \quad (4-1b)
\]

and \( E' = E(t') \) and \( \dot{L}' = \dot{L}(t') \). But

\[
\Delta E = \frac{1}{2} m (\mathbf{v}' \cdot \mathbf{v}' - \mathbf{v} \cdot \mathbf{v}) + \Delta \phi \quad (4-2)
\]

where

\[
\Delta \phi = \phi(r') - \phi(r) \quad (4-3)
\]

and

\[
\Delta \dot{L} = m (\mathbf{r}' \times \mathbf{v}' - \mathbf{r} \times \mathbf{v}) \quad (4-4)
\]

For conservation of energy and angular momentum, eqs. (4-2) and (4-4) must vanish for all values of \( \mathbf{r} \), \( \mathbf{v} \), and \( \Delta t \).

The objective in this section is to derive formulae for numerical estimates \( \mathbf{r}' \) and \( \mathbf{v}' \) for \( \mathbf{r} \) and \( \mathbf{v} \) which exactly satisfy the equations \( \Delta E = 0 \) and \( \Delta \dot{L} = 0 \). Suppose that \( \mathbf{r}'_a \) and \( \mathbf{v}'_a \) are approximations to \( \mathbf{r}' \) and \( \mathbf{v}' \), respectively, obtained, e.g., by any of the methods of Sect. 3 above. In analogy with the predictor-corrector methods, define \( \delta \mathbf{r}_e \) and \( \delta \mathbf{v}_e \) by

\[
\mathbf{r}'_e = \mathbf{r}'_a + \delta \mathbf{r}_e \quad (4-5a)
\]
\[ \mathbf{v}'_e = \mathbf{v}'_a + \delta \mathbf{v}_e \]

(4-5b)

In the above equations, as with the "correctors" of Sect. 3, \(\delta \mathbf{v}_a\) and \(\delta \mathbf{v}_e\) are of the same orders in \(\Delta t\) as the truncation errors in \(\mathbf{r}'_a\) and \(\mathbf{v}'_a\), respectively.

Two formulations of conservative numerical methods will be developed. In Sect. 4A below, \(\mathbf{r}'_e = \mathbf{r}'_a\) (i.e., \(\delta \mathbf{r}_e = 0\)) and \(\delta \mathbf{v}_e\) is determined so that conservation of energy and angular momentum results. In Sect. 4B, \(\delta \mathbf{v}_e\) is expressed in terms of \(\delta \mathbf{v}_e\) by assuming a truncated Taylor series for \(\mathbf{r}'\), and \(\delta \mathbf{v}_e\) is determined via conservation of energy and angular momentum.

For the purpose of illustration, the Adams' predictors of eqs. (3-9) will be carried through as examples for \(\mathbf{r}'_a\) and \(\mathbf{v}'_a\), i.e.,

\[ \mathbf{r}'_a = \mathbf{r} + \mathbf{v} \Delta t + \frac{\mathbf{F}}{m} \frac{(\Delta t)^2}{2} \]

(4-6a)

\[ \mathbf{v}'_a = \mathbf{v} + \frac{\mathbf{F}}{m} \Delta t \]

(4-6b)

Of course, the Adams' correctors of eqs. (3-11) would result for \(\mathbf{r}'_e\) and \(\mathbf{v}'_e\) from the choices for \(\delta \mathbf{r}_e\) and \(\delta \mathbf{v}_e\) from eqs. (3-10), but these values would not satisfy the conservation principles exactly. Note that there is no requirement that \(\mathbf{r}'_a\) and \(\mathbf{v}'_a\) be obtained from explicit formulae: only their values are needed.

A. First Formulation

The equations of motion (2-3) and (2-4) are a system of second-order ordinary differential equations with first-derivatives absent. It is therefore possible to obtain an estimate \(\mathbf{r}'_e\) of \(\mathbf{r}'\) independently of that for \(\mathbf{v}'\). (For example, in eq. (3-11a), \(\mathbf{v}'_c\) does not occur). Suppose
\( \hat{r}' \) and \( \hat{v}' \) are approximations to \( r' \) and \( v' \), respectively, and take \( \hat{r}' = \hat{a} \) (i.e., set \( \delta r = 0 \)); \( \hat{v}' \) is then given by eq. (4-5b), and the problem is to determine \( \delta v_e \) so that conservation of energy and angular momentum results.

The calculated change \( \Delta \hat{L}_e \) in \( \hat{L} \) over the time step \( \Delta t \) is given by

\[
\frac{\Delta \hat{L}_e}{m} = \hat{r}'_e \times \hat{v}'_e - \hat{r} \times \hat{v}
\]

\( = [\hat{r}'_e \times \hat{v}'_a - \hat{r} \times \hat{v}] + \hat{r}'_e \times \delta \hat{v}_e \) \hspace{1cm} (4-7b)

with the unknown part \( \delta \hat{v}_e \) of \( \hat{v}'_e \) isolated in the second term of eq. (4-7b).

Taking the cross product with respect to \( \hat{r}'_e \) from the left gives

\[
\hat{r}'_e \times \frac{\Delta \hat{L}_e}{m} = [\hat{r}'_e \times (\hat{r}'_e \times \hat{v}'_e) - \hat{r}'_e \times (\hat{r} \times \hat{v})] \\
+ \hat{r}'_e \times (\hat{r}'_e \times \delta \hat{v}_e)
\]

\( = [\hat{r}'_e \cdot \hat{v}'_e] \hat{r}'_e - (\hat{r}'_e \cdot \hat{v}) \hat{r} \) \hspace{1cm} (4-8)

The vector triple products may be decomposed via the formula

\[
\hat{a} \times (\hat{b} \times \hat{c}) = (\hat{a} \cdot \hat{c}) \hat{b} - (\hat{a} \cdot \hat{b}) \hat{c}
\]

\( \hspace{1cm} (4-9) \)

giving for eq. (4-8)

\[
\hat{r}'_e \times \frac{\Delta \hat{L}_e}{m} = \hat{\beta} - (\hat{r}'_e)^2 \delta \hat{v}_e + \epsilon \hat{r}'_e
\]

\( \hspace{1cm} (4-10) \)

where

\[
\hat{\beta} = \hat{r}_e \times (\hat{r}'_e \times \hat{v}') - \hat{r} \times (\hat{r}_e \times \hat{v})
\]

\( = [(\hat{r}'_e \cdot \hat{v}') \hat{r}'_e - (\hat{r}'_e \cdot \hat{v}) \hat{r}] \)

\( - [(\hat{r}'_e)^2 \hat{v}'_a - (\hat{r}'_e \cdot \hat{r}) \hat{v}] \) \hspace{1cm} (4-11b)
and

$$\epsilon = \hat{r}' \cdot \delta \hat{v}_e$$  \hspace{1cm} (4-12)$$

Eq. (4-10) may now be solved for the value of $\delta \hat{v}_e$ that makes

$$\hat{r}'_e \times \Delta \hat{L}_e / m = 0$$  \hspace{1cm} (4-13)$$

namely

$$\delta \hat{v}_e = \frac{1}{(r'_e)^2} \left[ \epsilon r'_e + \beta \right]$$  \hspace{1cm} (4-14)$$

where $\epsilon$ is arbitrary and $\beta$ is given by eq. (4-11).

For $\delta \hat{v}_e$ given by eq. (4-14), the components of $\Delta \hat{L}_e$ perpendicular to $\hat{r}'_e$ vanish by eq. (4-13), and only

$$\Delta \hat{L}_e / m = (\hat{r}'_e \cdot \Delta \hat{L}_e / m(r'_e)^2) \hat{r}'_e$$  \hspace{1cm} (4-15)$$

remains to be considered.

Since $\delta \hat{v}_e$ enters eq. (4-7b) only via the cross product $\hat{r}'_e \times \delta \hat{v}_e$, this component of $\Delta \hat{L}_e$ in the $\hat{r}'_e$ direction cannot be affected by the choice of $\delta \hat{v}_e$. It will now be shown this component of $\Delta \hat{L}_e$ vanishes from other considerations.

Now,

$$\hat{r}'_e \cdot \Delta \hat{L}_e / m = \hat{r}'_e \cdot [\hat{r}'_e \times \hat{v}_a - \hat{r} \times \hat{v}]$$  \hspace{1cm} (4-16a)$$

$$= - \hat{r}'_e \cdot (\hat{r} \times \hat{v})$$  \hspace{1cm} (4-16b)$$

$$= - [\hat{r}'_e \hat{r} \hat{v}]$$  \hspace{1cm} (4-16c)$$

where $[\hat{r}'_e \hat{r} \hat{v}]$ denotes the scalar triple product of $\hat{r}'_e$, $\hat{r}$, and $\hat{v}$.
This quantity vanishes, and consequently

\[ \hat{r}'_e \cdot \Delta \hat{L}_e / m = 0 \quad (4-17) \]

if and only if \( \hat{r}'_e, \hat{r}, \) and \( \hat{v} \) are linearly dependent. Assuming \( \hat{r}'_e = \hat{r}'_a \) is obtained by using one of the methods mentioned in Sect. 3, it was remarked in Sect. 3 that these estimates of \( \hat{r}' \) preserve the property of the exact solution of being a linear combination of the initial conditions:

\[ \hat{r}'_e = f_1 \hat{r} + f_2 \hat{v} \quad (4-18) \]

Thus, assuming the estimate \( \hat{r}'_e \) of \( \hat{r}' \) has the property given in eq. (4-18), \( \hat{r}'_e, \hat{r}, \) and \( \hat{v} \) are linearly dependent, and eq. (4-17) is satisfied. Coupled with this assumption, the choice of \( \delta v_e \) given by eq. (4-14) leads to

\[ \Delta \hat{L}_e = \hat{0} \quad (4-19) \]

exactly conserving the angular momentum.

In eq. (4-14), only \( \epsilon \) remains unknown. The energy change over the step \( \Delta t \) is given by

\[ \Delta E_e = \frac{1}{2} m ((\hat{v}'_e)^2 - \hat{v}^2) + \Delta \phi_e \quad (4-20) \]

where

\[ \Delta \phi_e = \phi(r'_e) - \phi(r) \quad (4-21) \]

Substitution of eq. (4-14) into eq. (4-5b) and squaring gives

\[ (\hat{v}'_e)^2 = (\hat{v}'_a)^2 + [\epsilon^2 + 2(\hat{r}'_e \cdot \hat{v}'_a)\epsilon + 2(\hat{\beta} \cdot \hat{v}'_a)
\]

\[ + \hat{\beta}^2/r_e^2] / (r'_e)^2 \]

(4-22)
since, by eq. (4-11), \( \mathbf{r}_e' \cdot \mathbf{\beta} = 0 \). Inserting eq. (4-22) into eq. (4-20) gives

\[
\Delta E_e = \frac{m}{2(\mathbf{v}_a')^2} \left[ \epsilon^2 + 2(\mathbf{r}_e' \cdot \mathbf{v}_a') \epsilon + 2(\mathbf{\beta} \cdot \mathbf{v}_a') + \frac{\mathbf{\beta}(r_e')^2}{2(\mathbf{v}_a')^2} \right] \\
+ \frac{1}{2} m ((\mathbf{v}_a')^2 - \mathbf{v}^2) + \Delta\phi_e
\]

(4-23)

Requiring that

\[
\Delta E_e = 0
\]

(4-24)

gives the following quadratic equation for \( \epsilon \):

\[
\epsilon^2 + 2(\mathbf{r}_e' \cdot \mathbf{v}_a') \epsilon + \\
\left[ 2(\mathbf{\beta} \cdot \mathbf{v}_a') + \frac{\mathbf{\beta}(r_e')^2}{2(\mathbf{v}_a')^2} + (\mathbf{v}_a')^2 (\mathbf{v}_a')^2 - \mathbf{v}^2 + \frac{2\Delta\phi_e}{m} \right] = 0
\]

(4-25)

This equation may be solved for \( \epsilon \) by several routes, including the quadratic formula, functional iteration, or Newton's method.

If \( \mathbf{v}_a' \) has an associated error of \( \mathcal{O}([\Delta t]^n) \) and \( \mathbf{r}_e' \) is exact to at least this order, then \( \mathbf{\delta v}_e, \mathbf{\beta}, \) and \( \epsilon \) are all of \( \mathcal{O}([\Delta t]^n) \), and eq. (4-25) is only weakly quadratic for small \( \Delta t \). Solving for \( \epsilon \) via the linear term in eq. (4-25),

\[
\epsilon = -\frac{A + \epsilon^2}{B}
\]

(4-26)

where

\[
A = 2(\mathbf{\beta} \cdot \mathbf{v}_a') + \frac{\mathbf{\beta}(r_e')^2}{2(\mathbf{v}_a')^2} + (r_e')^2 ((\mathbf{v}_a')^2 - \mathbf{v}^2 + \frac{2\Delta\phi_e}{m})
\]

(4-27a)
\[ \mathbf{B} = 2 \frac{\mathbf{r}'}{e} \cdot \frac{\mathbf{v}'}{a} \] 

(4-27b)

Since $A$ and $B$ are independent of $\varepsilon$ and $\varepsilon = O((\Delta t)^n)$, eq. (4-26) may be solved iteratively starting with $\varepsilon = 0$.

When $\frac{\mathbf{r}'}{e} \cdot \frac{\mathbf{v}'}{a} = 0$, eq. (4-26) breaks down, and there are two equal and opposite solutions to eq. (4-25), given by

\[ \varepsilon = \pm \sqrt{-A} \] 

(4-28)

Both solutions are physically meaningful, one corresponding to the forward motion and the other to the backward motion. The correct root can only be determined by consideration of the absolute time scale. This phenomenon occurs because the computed solution contacts a caustic surface of the equations of motion: the exact solution has the same type of ambiguity at the similar point $\mathbf{r}' \cdot \mathbf{v}' = 0$, i.e., a radial turning-point of the motion.

Taken together then, eqs. (4-5b), (4-14), and (4-26) represent a complete system of equations from which $\mathbf{v}'_e$ may be found, given $\mathbf{r}'_e$, which a fortiori conserves energy and angular momentum. Since the exact $\mathbf{r}'$ and $\mathbf{v}'$ also satisfy $\Delta E = 0$ and $\Delta L = 0$, the equations given above also represent a complete system for determining $\mathbf{v}'$ given $\mathbf{r}'$: i.e., if $\mathbf{r}'_e = \mathbf{r}'$ then $\mathbf{v}'_e = \mathbf{v}'$. This absence of truncation error in $\mathbf{v}'_e$ will be discussed more fully in Sect. 5.B.

As an illustration of the use of the above equations, suppose that $\mathbf{r}'_e$ is given by the $n = 3$ Adams' corrector $\mathbf{r}'_c$ of eq. (3-11a), and $\mathbf{v}'_a$ is given by the corresponding Adams' predictor of eq. (3-9b):

\[ \mathbf{r}'_e = \mathbf{r} + \mathbf{v} \Delta t + \frac{F}{m} \frac{(\Delta t)^2}{2} + \frac{(\Delta t)^2}{6} \left( \frac{F(r') - F}{m} \right) / m \] 

(4-29a)
\[ \hat{v}'_a = \hat{v} + \frac{F}{m} \Delta t \]  \hspace{1cm} (4-29b)

The first step in the calculation is the determination of the value for \( \hat{r}'_e \) by iteration of eq. (4-29a), which requires reevaluation of \( F(\hat{r}'_e) \) every iteration. Once \( \hat{r}'_e \) is found, and \( \hat{v}'_a \) formed from eq. (4-29b), \( \hat{\beta} \) is calculated from eq. (4-11). The potential term \( \phi(\hat{r}'_e) \) is then evaluated, and the constants A and B calculated from eqs. (4-27).

After these preliminaries, the quantity \( \epsilon \) is now found by iterating eq. (4-26) to convergence using the starting value \( \epsilon = 0 \). The iteration to convergence is important because energy is conserved (i.e., \( \Delta E = 0 \)) only to the extent \( \epsilon \) is found. The value of \( \hat{v}'_e \) is finally obtained via substitution of \( \epsilon \) and \( \hat{\beta} \) into eqs. (4-5b) and (4-14):

\[ \hat{v}'_e = \hat{v}'_a + \delta v'_e \]  \hspace{1cm} (4-30a)
\[ = \hat{v}'_a + [\epsilon \hat{r}'_e + \hat{\beta}]/(r'_e)^2 \]  \hspace{1cm} (4-30b)

The quantities \( \hat{r}'_e \) and \( \hat{v}'_e \) represent the computed solution at the time \( t' = t + \Delta t \).

B. Second Formulation

In Sect. 4.A above, it was shown that the energy and angular momentum conservation conditions (4-24) and (4-19) were sufficient to determine \( \delta v'_e \) (and hence \( \hat{v}'_e \)) given an estimate \( \hat{r}'_e \) for \( \hat{r}' \). This assumption that \( \hat{r}'_e \) is obtained by some outside numerical approximation, e.g., an Adams' corrector \( \hat{r}'_e \), led to eqs. (4-14) and (4-26) for \( \delta v'_e \). Since, however, \( \delta v'_e \) is an estimate of the error of \( \hat{v}'_a \), it is also an estimate of the next term in the Taylor series of \( \hat{v}' \), i.e., proportional to \( \frac{d^n r}{dt^n} \). This information could have been used to improve the order
of approximation of $\hat{r}'$ as follows.

Suppose that $\hat{r}'_a$ and $\hat{v}'_a$ are approximations to $\hat{r}'$ and $\hat{v}'$ with errors of $O[(\Delta t)^n]$ and $O[(\Delta t)^{n-1}]$, respectively. Let $\delta r_a$ and $\delta v_a$ denote the truncation errors of $\hat{r}'_a$ and $\hat{v}'_a$, respectively:

$$\hat{r}' = \hat{r}'_a + \delta r_a \quad (4-31a)$$

$$\hat{v}' = \hat{v}'_a + \delta v_a \quad (4-31b)$$

Expanding $\delta r_a$ and $\delta v_a$ in powers of $\Delta t$ gives

$$\delta r_a = A_n(\Delta t)^n \frac{d^{n-1}r}{dt^n} + O[(\Delta t)^{n+1}] \quad (4-32a)$$

$$\delta v_a = B_n(\Delta t)^{n-1} \frac{d^{n-1}r}{dt^n} + O[(\Delta t)^n] \quad (4-32b)$$

where $A_n$ and $B_n$ are the truncation error coefficients of $\hat{r}'_a$ and $\hat{v}'_a$, respectively. Examination of eqs. (4-32) shows that, because $\hat{r}'$ and $\hat{v}'$ have related Taylor series expansions,

$$\delta r_a = \gamma(\Delta t)\delta v_a + O[(\Delta t)^{n+1}] \quad (4-33)$$

where

$$\gamma = \frac{A_n}{B_n} \quad (4-34)$$

is the ratio of the truncation error coefficients. (Note that if $\hat{r}'_a = \hat{r}'_p$ and $\hat{v}'_a = \hat{v}'_p$ are a pair of "predictors", $\gamma = \gamma_0/\gamma_1$ is the ratio of the corresponding "corrector" coefficients). Eq. (4-33) thus gives a lowest-
order approximation for $\delta \mathbf{r}_a^*$ given $\delta \mathbf{v}_a^*$.

Suppose $\mathbf{r}'_e$ and $\mathbf{v}'_e$ are to be constructed via

$$\mathbf{r}'_e = \mathbf{r}_a^* + \delta \mathbf{r}_e$$  \hspace{1cm} (4-35a)

$$\mathbf{v}'_e = \mathbf{v}_a^* + \delta \mathbf{v}_e$$  \hspace{1cm} (4-35b)

where $\mathbf{r}_a^*$ and $\mathbf{v}_a^*$ are as above. Clearly if $\delta \mathbf{r}_e = \delta \mathbf{r}_a^*$ and $\delta \mathbf{v}_e = \delta \mathbf{v}_a^*$, eqs. (4-35) correspond to eqs. (4-31), and $\mathbf{r}'_e$ and $\mathbf{v}'_e$ are exact. Suppose $\delta \mathbf{v}_e$ is left undetermined, and $\delta \mathbf{r}_e$ is determined via

$$\delta \mathbf{r}_e = \gamma \Delta t \delta \mathbf{v}_e$$  \hspace{1cm} (4-36)

Comparison of eqs. (4-36) and (4-33) shows that if $\delta \mathbf{r}_e$ approximates $\delta \mathbf{r}_a^*$ correctly except for terms of $O[(\Delta t)^n]$ or higher, satisfying eq. (4-36) exactly generates an error of $O[(\Delta t)^{n+1}]$ in $\mathbf{r}'_e$, since eq. (4-36) corresponds to truncating the error expansion of $\delta \mathbf{r}_a^*$:

$$\mathbf{r}'_e = \mathbf{r}_e + O[(\Delta t)^{n+1}]$$  \hspace{1cm} (4-37)

The use of eq. (4-36) will now allow simultaneous determination of $\mathbf{r}'_e$ and $\mathbf{v}'_e$ via conservation of energy and angular momentum.

Substitution of eqs. (4-35) and (4-36) into eq. (4-4) gives

$$\Delta \mathbf{L}_e/m = \left[ \mathbf{r}_a^* \times \mathbf{v}_a^* - \mathbf{r} \times \mathbf{v} \right] + \alpha \times \delta \mathbf{v}_e$$  \hspace{1cm} (4-38)

where

$$\alpha = \mathbf{r}_a^* + \gamma \Delta t \mathbf{v}_a^*$$  \hspace{1cm} (4-39)
Eq. (4-38) is the analog to eq. (4-7b). Since the form of eq. (4-38)
is identical to that of eq. (4-7b), the same method of solution for \( \delta \varepsilon \)suffices.

Now, since

\[
\overset{\sim}{\alpha} \cdot \Delta \overset{\sim}{L}_{\text{e}} / m = 0
\]  

(4-40)

because \( \overset{\sim}{\alpha}, \overset{\sim}{r}, \) and \( \overset{\sim}{v} \) are all linear combinations of \( \overset{\sim}{r} \) and \( \overset{\sim}{v} \) (see discussion following eq. (4-17)), the value of \( \delta \varepsilon \) which conserves angular momentum is given as the solution to the equation

\[
\overset{\sim}{\alpha} \times \Delta \overset{\sim}{L}_{\text{e}} / m = 0
\]  

(4-41)

Similar to eq. (4-10),

\[
\overset{\sim}{\alpha} \times \Delta \overset{\sim}{L}_{\text{e}} / m = \overset{\sim}{\beta} - \alpha \overset{\sim}{\delta \varepsilon} + \varepsilon \overset{\sim}{\alpha}
\]  

(4-42)

where

\[
\overset{\sim}{\beta} = \overset{\sim}{\alpha} \times \left[ \overset{\sim}{r} \times \overset{\sim}{v} - \overset{\sim}{r} \times \overset{\sim}{v} \right]
\]  

(4-43a)

\[
= \left[ (\overset{\sim}{\alpha} \cdot \overset{\sim}{v}) \overset{\sim}{r} - (\overset{\sim}{\alpha} \cdot \overset{\sim}{r}) \overset{\sim}{v} \right] - \left[ (\overset{\sim}{\alpha} \cdot \overset{\sim}{r}) \overset{\sim}{v} - (\overset{\sim}{\alpha} \cdot \overset{\sim}{r}) \overset{\sim}{v} \right]
\]  

(4-43b)

and

\[
\varepsilon = \overset{\sim}{\alpha} \cdot \overset{\sim}{\delta \varepsilon}
\]  

(4-44)

is unknown. The solution to eq. (4-41) is then given by

\[
\overset{\sim}{\delta \varepsilon} = \frac{1}{\alpha^2} \left[ \varepsilon \overset{\sim}{\alpha} + \overset{\sim}{\beta} \right]
\]  

(4-45)

completely analogous to eq. (4-14).
The unknown part of $\delta \dot{v}_e$ is now localized in the quantity $\varepsilon$, which will be found from the energy condition. Substitution of eqs. (4-35), (4-36), and (4-45) into eq. (4-2) gives (after setting $\Delta E = 0$) the following equation for $\varepsilon$:

$$
\varepsilon^2 + 2(\alpha \cdot \dot{v}'_a)\varepsilon + \left[ 2(\beta \cdot \dot{v}'_a) + \beta^2/\alpha^2 + \frac{2}{\alpha}(v'_a)^2 - v^2 + \frac{2\Delta \phi}{m} \right] = 0 \tag{4-46}
$$

where

$$
\Delta \phi = \phi(r'_e) - \phi(r) \tag{4-47}
$$

Note that $\Delta \phi$ is implicit in $\varepsilon$ through $r'_e$: in contrast to eq. (4-25), eq. (4-46) can be solved only by iterative means. Since $\delta \dot{v}_e$ is $O[(\Delta t)^{n-1}]$ from eq. (4-32b), so are $\varepsilon$ and $\dot{\beta}$. Therefore eq. (4-46) is only weakly implicit in $\varepsilon$ (i.e., to $O[(\Delta t)^{2n-2}]$) and

$$
\varepsilon = -\frac{A + C(\varepsilon)}{B} \tag{4-48}
$$

may be solved via functional iteration starting with $\varepsilon = 0$, where

$$
A = 2(\beta \cdot \dot{v}'_a) + \beta^2/\alpha^2 + \alpha(\dot{v}'_a)^2 - v^2 \tag{4-49a}
$$

$$
B = 2(\alpha \cdot \dot{v}'_a) \tag{4-49b}
$$

$$
C = 2\alpha^2 \Delta \phi/m + \varepsilon^2 \tag{4-49c}
$$

The sequence of steps necessary for computing the conservative solutions $r'_e$ and $v'_e$ are as follows: first the approximate values $r'_e$ and $v'_e$
and $v'$ are calculated, and then $\alpha$ and $\beta$ are evaluated from eqs. (4-39) and (4-43b). The constants $A$ and $B$ are obtained via eqs. (4-49), and $C$ is evaluated using $r'$ for $r_e$ and $\epsilon = 0$. A new approximation is constructed for $\epsilon$ using eq. (4-48), $\delta v_e'$ is formed from eq. (4-45), $\delta r_e$ is calculated from eq. (4-36), and $r_e'$ from eq. (4-35a). Using the new values for $\epsilon$ and $r_e'$, $C$ is reevaluated, and a new iteration of eq. (4-48) started. This process is continued until a convergent value for $\epsilon$ is obtained. The corresponding values of $r_e'$ and $v_e'$ will conserve angular momentum to within round-off error, and energy to within the degree of convergence in $\epsilon$.

For the special case when $n = 2$ and

\[ r' \atop a = r + \dot{r} \Delta t \]  \hspace{1cm} (4-50a)
\[ v' \atop a = v \]  \hspace{1cm} (4-50b)

the truncation errors are given by

\[ r' = r \atop a + \frac{(\Delta t)^2}{2} \frac{d^2 r}{dt^2} + O[(\Delta t)^3] \]  \hspace{1cm} (4-51a)
\[ v' = v \atop a + \Delta t \frac{d \dot{r}}{dt} + O[(\Delta t)^2] \]  \hspace{1cm} (4-51b)

and so $\gamma = 1/2 \cdot \frac{1}{1} = 1/2$, and

\[ \alpha = r + \frac{\Delta t}{2} v \]  \hspace{1cm} (4-52a)
\[ \beta = 0 \]  \hspace{1cm} (4-52b)

These values of $\alpha$ and $\beta$ lead to
\[
\delta v_e = \epsilon^* \alpha
\]  
(4-53)

where

\[
\epsilon^* = \epsilon / \alpha^2
\]  
(4-54)

The value of \(\epsilon^*\) is obtained via iteration of

\[
\epsilon^* = -\frac{2\Delta \phi/m + \alpha^2 (\epsilon^*)^2}{2(\alpha \cdot \nu)}
\]  
(4-55)

This \(n = 2\) conservative method represented by eqs. (4-50), (4-52), (4-53), and (4-55) is equivalent to the "second-order discrete mechanics" of [4], where instead of \(\delta v_e\) the discrete mechanics "force" \(\mathbf{F}^*\) was defined: the transformation is given by

\[
\delta v_e = \Delta t \mathbf{F}^* / m
\]  
(4-56)

As an additional illustration, consider \(\mathbf{r}'_a\) and \(\mathbf{v}'_a\) given by the \(n = 3\) predictors \(\mathbf{r}'_p\) and \(\mathbf{v}'_p\) of eqs. (3-9):

\[
\mathbf{r}'_a = \mathbf{r} + \mathbf{v} \Delta t + \frac{\mathbf{F}}{m} \frac{(\Delta t)^2}{2}
\]  
(4-57a)

\[
\mathbf{v}'_a = \mathbf{v} + \frac{\mathbf{F}}{m} \Delta t
\]  
(4-57b)

For this case, \(\gamma = 1/6 + 1/2 = 1/3\) from eqs. (3-10), and

\[
\alpha = \frac{\mathbf{r}'_a}{\mathbf{v}'_a} - \frac{\Delta t}{3} \mathbf{v}'_a
\]  
(4-58a)

\[
= \mathbf{r} + \frac{2\Delta t}{3} \mathbf{v} + \frac{(\Delta t)^2}{6} \frac{\mathbf{F}}{m}
\]  
(4-58b)
The value of $\vec{\beta}$ is best obtained via substitution of eqs. (4-57) and (4-58) into eq. (4-43b). The values of A and B are obtained from eqs. (4-49), and eq. (4-48) is iterated to find $\varepsilon$. At each stage the iterate for $\varepsilon$ is found, $\vec{\delta}v_e$ formed, and $\vec{r_e'}$ calculated from

$$\frac{\vec{\delta}r_e}{3} = \frac{\Delta t}{3} \vec{\delta}v_e$$  \hspace{1cm} (4-59)$$

and eq. (4-35a). The magnitude $r_e'$ is then found, and $\phi(r_e')$ evaluated. A new iteration is then performed.
5. Related Theory and Remarks

The formulations given in both Sects. 4.A and 4.B conserve the energy and angular momentum at their initial values—an advantage not enjoyed by conventional methods. In addition, these conservative methods enjoy improved truncation error properties, and close ties with the exact solution, which will be discussed in the next sections.

A. Truncation Error

For the first conservative formulation of Sect. 4.A, the value of \( \tilde{r}' \) obtained is of course identical to that of the underlying approximation \( \tilde{r}' \), and has the associated truncation error. For example, if \( \tilde{r}'_a = \tilde{r}'_c \), the \( n = 3 \) corrector of eq. (3-11a), then by eq. (3-12a),

\[
\tilde{r}' = \tilde{r}'_e - \frac{(\Delta t)}{24} \frac{d^4 \tilde{r}}{dt^4} + O[(\Delta t)^5]
\]  

(5-1)

Note, that since no approximations were made in deriving eqs. (4-14) and (4-26) for \( \tilde{v}'_e \), except that the \( \tilde{r}'_e \) used was an inexact estimate of \( \tilde{r}' \), there is no associated truncation error in \( \tilde{v}'_e \). The only error in \( \tilde{v}'_e \) is that propagated from that of the previous steps and the truncation error in \( \tilde{r}'_e \); this will be discussed more fully in Sect. 5.B.

For the case of the second conservative formulation of Sect. 4.B, eq. (4-36) holds for the exact \( \delta \tilde{r}'_a \) and \( \delta \tilde{v}'_a \) only if \( \tilde{r}' \) is a polynomial of degree \( n \) or less in \( \Delta t \) (compare eqs. (4-33) and (4-36)). Therefore the use of eq. (4-36) in general corresponds to truncating the Taylor series expansion of \( \tilde{r}' \) at the \( n \)-th term,
and generates a truncation error of $O((\Delta t)^{n+1})$:

$$\tilde{r}' = \tilde{r}_e' + O((\Delta t)^{n+1}) \quad (5-2)$$

Once eq. (4-36) was assumed, the derivation of $\tilde{v}_e'$ followed just as in Sect. 4.A, with no further approximations; As in Sect. 4.A, there is no associated truncation error in $\tilde{v}_e'$. The only error in $\tilde{v}_e'$ is again that propagated from previous steps or from the error in $\tilde{r}_e'$.

Knowing that $\tilde{r}_e'$ as calculated from the second formulation of Sect. 4.B satisfies eq. (5-2), the corresponding local truncation error coefficient $E_{n+1}$ will now be derived, where

$$\tilde{r}' = \tilde{r}_e' + E_{n+1} (\Delta t)^{n+1} \frac{d^{n+1} r}{dt^{n+1}} + O((\Delta t)^{n+2}) \quad (5-3)$$

Suppose that $\tilde{r}_a'$ and $\tilde{v}_a'$ have truncation errors given by eqs. (4-32), i.e.,

$$\tilde{r}_a = r' - \tilde{r}_a' \quad (5-4a)$$

$$= A_n (\Delta t)^n \frac{d^n r}{dt^n} + A_{n+1} (\Delta t)^{n+1} \frac{d^{n+1} r}{dt^{n+1}} + O((\Delta t)^{n+2}) \quad (5-4b)$$

and

$$\tilde{v}_a = v' - \tilde{v}_a' \quad (5-5a)$$

$$= B_n (\Delta t)^{n-1} \frac{d^{n-1} r}{dt^{n-1}} + B_{n+1} (\Delta t)^n \frac{d^n r}{dt^n} + O((\Delta t)^{n+1}) \quad (5-5b)$$

where $A_n$, $A_{n+1}$ and $B_n$, $B_{n+1}$ are the truncation error coefficients of $\tilde{r}_a'$ and $\tilde{v}_a'$, respectively. Comparison of eqs. (4-31) and (4-35),
together with eqs. (5-4) and (5-5), leads to

\[ \delta \tilde{r}_e = O[(\Delta t)^n] \]  
\[ \delta \tilde{v}_e = O[(\Delta t)^{n-1}] \]  

(5-6a)

(5-6b)

Now suppose further that the only error introduced in the calculation of \( \tilde{v}'_e \) and \( \tilde{v}_e \) in Sect. 4.B was that due to the use of eq. (4-36); i.e., the use of an inexact value for \( \tilde{r}'_e \). Since by eq. (5-2) the error in \( \tilde{r}'_e \) is \( O[(\Delta t)^{n+1}] \), this induces (by expanding \( \phi(\tilde{r}'_e) \) as a Taylor series and by eqs. (4-43), (4-45), and (4-47)) an error of the same order in \( \tilde{v}_e \):

\[ \delta \tilde{v}_a = \delta \tilde{v}_e + O[(\Delta t)^{n+1}] \]  

(5-7)

Comparing eqs. (5-7) and (5-5b) gives

\[ \delta \tilde{v}_e = \frac{B_n}{n} (\Delta t)^{n-1} \frac{d}{dt} \tilde{r} + \frac{B_n}{n+1} (\Delta t)^n \frac{d}{dt} \tilde{r} + O[(\Delta t)^{n+1}] \]  

(5-8)

The form of \( \tilde{r}_e \) may now be obtained through the use of eq. (4-36):

\[ \delta \tilde{r}_e = \gamma(\Delta t) \delta \tilde{v}_e \]  

(5-9a)

\[ = \gamma \frac{B_n}{n} (\Delta t)^n \frac{d}{dt} \tilde{r} + \gamma \frac{B_n}{n+1} (\Delta t)^{n+1} \frac{d}{dt} \tilde{r} + O[(\Delta t)^{n+2}] \]  

(5-9b)

Noting that \( \gamma = \frac{A_n}{B_n} \),

\[ \delta \tilde{r}_e = \frac{A_n}{n} (\Delta t)^n \frac{d}{dt} \tilde{r} + \frac{A_n B_n}{B_n} (\Delta t)^{n+1} \frac{d}{dt} \tilde{r} \]  

\[ + O[(\Delta t)^{n+2}] \]  

(5-10)
Comparing eq. (5-10) with the exact eq. (5-4b) for \( \delta \mathbf{r}_a \), gives

\[
\delta \mathbf{r}_a = \delta \mathbf{r}_e + E_{n+1} (\Delta t)^{n+1} \frac{d^{n+1} \mathbf{r}}{dt^{n+1}} + O[(\Delta t)^{n+2}] \quad (5-11)
\]

where

\[
E_{n+1} = A_{n+1} - \frac{A_n B_{n+1}}{B_n} \quad (5-12)
\]

Finally, eqs. (5-7) and (5-11) may be translated via eqs. (4-35) into error equations in \( \dot{\mathbf{r}}_e \) and \( \dot{\mathbf{v}}_e \):

\[
\dot{\mathbf{r}}_e = \dot{\mathbf{r}}'_e + E_{n+1} (\Delta t)^{n+1} \frac{d^{n+1} \mathbf{r}}{dt^{n+1}} + O[(\Delta t)^{n+2}] \quad (5-13a)
\]

\[
\dot{\mathbf{v}}_e = \dot{\mathbf{v}}'_e + O[(\Delta t)^{n+1}] \quad (5-13b)
\]

where \( E_{n+1} \) is given by eq. (5-12).

As an example of the use of eqs. (5-13), consider the \( n = 2 \) conservative method of eqs. (4-50), (4-51), and following equations of Sect. 4.B. This method, as remarked previously, corresponds to the "discrete mechanics" of [4]. For \( \mathbf{r}_a' \) and \( \mathbf{v}_a' \), given by eqs. (4-51),

\[
\dot{\mathbf{r}}_a' = \dot{\mathbf{r}}_a' + \frac{(\Delta t)^2}{2} \frac{d^2 \mathbf{r}}{dt^2} + \frac{(\Delta t)^3}{6} \frac{d^3 \mathbf{r}}{dt^3} + O[(\Delta t)^4] \quad (5-14a)
\]

\[
\dot{\mathbf{v}}_a' = \dot{\mathbf{v}}_a' + \Delta t \frac{d^2 \mathbf{r}}{dt^2} + \frac{(\Delta t)^2}{2} \frac{d^3 \mathbf{r}}{dt^3} + O[(\Delta t)^3] \quad (5-14b)
\]

or

\[
A_{2*} = \frac{1}{2} \quad (5-15a)
\]
\[ A_3 = 1/6 \]  \hspace{1cm} (5-15b)

\[ B_2 = 1 \]  \hspace{1cm} (5-15c)

\[ B_3 = 1/2 \]  \hspace{1cm} (5-15d)

and

\[ \gamma = \frac{A_2}{B_2} \]  \hspace{1cm} (5-16a)

\[ = \frac{1}{2} \]  \hspace{1cm} (5-16b)

Substitution of eqs. (5-15) into eqs. (5-12) and (5-13) give \((n = 2)\)

\[ \vec{r}' = \vec{r}_e' - \frac{(\Delta t)^3}{12} \frac{d^3 \vec{r}}{dt^3} + O[(\Delta t)^4] \]  \hspace{1cm} (5-17a)

\[ \vec{v}' = \vec{v}_e' + O[(\Delta t)^3] \]  \hspace{1cm} (5-17b)

and so the "discrete mechanics" of [4] is a third-order method. This result explains the effectiveness of "discrete mechanics" when compared to the third-order Adams' method of eqs. (3-11) in [4a].

As a further illustration, consider the \(n = 3\) formulae of eqs. (4-57) for \(\vec{r}'_a\) and \(\vec{v}'_a\). For these predictors

\[ \vec{r}' = \vec{r}'_a + \frac{(\Delta t)^3}{6} \frac{d^3 \vec{r}}{dt^3} + \frac{(\Delta t)^4}{24} \frac{d^4 \vec{r}}{dt^4} + O[(\Delta t)^5] \]  \hspace{1cm} (5-18a)

\[ \vec{v}' = \vec{v}'_a + \frac{(\Delta t)^2}{2} \frac{d^3 \vec{r}}{dt^3} + \frac{(\Delta t)^3}{6} \frac{d^4 \vec{r}}{dt^4} + O[(\Delta t)^4] \]  \hspace{1cm} (5-18b)
or

\[ A_3 = \frac{1}{6} \]  
\[ A_4 = \frac{1}{24} \]  
\[ B_3 = \frac{1}{2} \]  
\[ B_4 = \frac{1}{6} \]  

(5-19a)  
(5-19b)  
(5-19c)  
(5-19d)

Combined with eqs. (5-12) and (5-13), eqs. (5-19) give

\[ \hat{r}' = \hat{r}'_e - \frac{(\Delta t)^4}{72} \frac{d^4}{dt^4} \hat{r} + O[(\Delta t)^5] \]  
\[ \hat{v}' = \hat{v}'_e + O[(\Delta t)^4] \]  

(5-20a)  
(5-20b)

for the errors in the corresponding conservative solutions \( \hat{r}'_e \) and \( \hat{v}'_e \) of Sect. 4.B. Note that the use of the Adams' corrector formula of eq. (3-10a) leads to a truncation error coefficient of \(-1/24\) in eq. (3-12a), while the conservative solution of Sect. 4.B gives a smaller truncation error coefficient of \(-1/72\) in eq. (5-20a). In addition, \( \hat{v}'_e \) is a fourth-order approximation to \( \hat{v}' \), while \( \hat{v}'_c \) of eq. (3-11b) is only a third-order approximation to \( \hat{v}' \). Thus the conservative formulation of Sect. 4.B, when used with the Adams' predictors \( \hat{r}'_p \) and \( \hat{v}'_p \) for \( \hat{r}'_a \) and \( \hat{v}'_a \), is superior to the Adams' correctors from the standpoint of order, truncation error, and conservation of the constants of motion.
B. Propagation of Error

In the case of the predictor-corrector methods of eqs. (3-5), the explicit dependences of $\delta r_c$ and $\delta v_c$ on $\Delta t$ in eqs. (3-6) guarantees that any error (except round-off) made in evaluating these quantities will be unimportant in the limit as $\Delta t \to 0$. Suppose errors $\eta(r') = r' - r_p'$ and $\eta(v') = v' - v_p'$ are introduced (via truncation error, error in the initial conditions, etc.) in $r_p'$ and $v_p'$, respectively. Then the propagated errors in $r_c'$ and $v_c'$, respectively, are given by

$$\eta(r') = \eta(r_p') + O[(\Delta t)^2] \quad (5-21a)$$

$$\eta(v') = \eta(v_p') + O[\Delta t] \quad (5-21b)$$

In the case of an Adams' method

$$r_p' = r + v \Delta t + O[(\Delta t)^2] \quad (5-22a)$$

$$v_p' = v + O[\Delta t] \quad (5-22b)$$

and hence

$$\eta(r_p') = \eta(r) + O[\Delta t] \quad (5-23a)$$

$$\eta(v_p') = \eta(v) + O[\Delta t] \quad (5-23b)$$

so that, from eqs. (5-21),

$$\eta(r_c') = \eta(r) + O[\Delta t] \quad (5-24a)$$

$$\eta(v_c') = \eta(v) + O[\Delta t] \quad (5-24b)$$
giving the errors in \( \dot{r}_c \) and \( \dot{v}_c \) in terms of those in \( \dot{r} \) and \( \dot{v} \), respectively. Therefore, for the case of an Adams' method, in the limit \( \Delta t \to 0 \) the errors in \( \dot{r} \) and \( \dot{v} \) are propagated with unit coefficients in \( \dot{r}_c \) and \( \dot{v}_c \), respectively. This is usually phrased in terms of the statement that for an Adams' method, the principal roots of the asymptotic (\( \Delta t \to 0 \)) stability matrix have value unity.

Because the forms of the Taylor series and Runge-Kutta methods are similar to eqs. (5-22), this property of unit feedback of the errors in \( \dot{r} \) and \( \dot{v} \) into the calculated values for \( \dot{r} \) and \( \dot{v} \) (for small \( \Delta t \)) also holds for these methods.

The question is now whether this desirable property of unit (and no more) propagation of the errors in \( \dot{r} \) and \( \dot{v} \) occurs with the conservative formulations of Sect. 4 for small \( \Delta t \). Suppose, as above, that \( \dot{r}_a \) and \( \dot{v}_a \) satisfy equations similar to (5-22):

\[
\begin{align*}
\dot{r}'_a &= \dot{r} + \dot{v} \Delta t + O[(\Delta t)^2] \quad (5-25a) \\
\dot{v}'_a &= \dot{v} + O[\Delta t] \quad (5-25b)
\end{align*}
\]

and errors \( \hat{\eta}(\dot{r}) \) and \( \hat{\eta}(\dot{v}) \) are introduced into \( \dot{r} \) and \( \dot{v} \), respectively.

Consider first the formulation of Sect. 4.A. Then \( \dot{r}'_e = \dot{r}'_a \), and by expanding in Taylor series,

\[
\begin{align*}
\hat{\eta}(\dot{r}'_e) &= \left( \frac{\partial \dot{r}'_e}{\partial \dot{r}} \right)_e \cdot \hat{\eta}(\dot{r}) + \left( \frac{\partial \dot{r}'_e}{\partial \dot{v}} \right)_e \cdot \hat{\eta}(\dot{v}) + O[\eta^2] \quad (5-26a) \\
&= \left( \frac{\partial \dot{r}'_a}{\partial \dot{r}} \right)_e \cdot \hat{\eta}(\dot{r}) + \left( \frac{\partial \dot{r}'_a}{\partial \dot{v}} \right)_e \cdot \hat{\eta}(\dot{v}) + O[\eta^2] \quad (5-26b)
\end{align*}
\]

where \( \partial a/\partial b \) denotes the Jacobian matrix of \( a \) with respect to \( b \), with elements
\[
\frac{\partial \tilde{a}_i}{\partial \tilde{b}_j} = \frac{\partial a_i}{\partial b_j} \tag{5-27}
\]

and \((\partial \tilde{r}^{i}/\partial \tilde{r})_{\tilde{v}}\) and \((\partial \tilde{r}^{i}/\partial \tilde{v})_{\tilde{r}}\) denote derivatives of \(\tilde{r}^{i}\) with respect to \(\tilde{r}\) and \(\tilde{v}\), respectively, with \(\tilde{r}^{i}\) and \(\tilde{v}^{i}\) treated as functions of \(\tilde{r}\) and \(\tilde{v}\). From eq. (5-25a):

\[
\left(\frac{\partial \tilde{r}^{i}}{\partial \tilde{r}}\right)_{\tilde{v}} = I \tag{5-28a}
\]

\[
\left(\frac{\partial \tilde{r}^{i}}{\partial \tilde{v}}\right)_{\tilde{r}} = (\Delta t) I + O[(\Delta t)^2] \tag{5-28b}
\]

where \(I\) is the identity matrix. Eq. (5-26b) may be written, then,

\[
\tilde{\eta}(\tilde{r}^{i}) = \tilde{\eta}(\tilde{r}) + O[\Delta t + \eta^2] \tag{5-29}
\]

Eq. (5-29) is still satisfied for \(\tilde{r}^{i}\) given by the second conservative formulation of Sect. 4.B, since

\[
\tilde{r}^{i} = \tilde{r}^{i} + O[\Delta t] \tag{5-30}
\]

by virtue of eqs. (4-35a) and (4-36). Therefore both conservative formulations preserve the property of unit propagation of error of \(\tilde{r}\) into \(\tilde{r}^{i}\). The asymptotic \((\Delta t \to 0)\) stability properties of the conservative \(\tilde{r}^{i}\) are thus identical to those of the underlying approximation \(\tilde{r}^{i}\).

For the case of \(\tilde{v}^{i}\) of Sect. 4.A, the error \(\tilde{\eta}(\tilde{v}^{i})\) induced by errors \(\tilde{\eta}(\tilde{r})\) and \(\tilde{\eta}(\tilde{v})\) in \(\tilde{r}\) and \(\tilde{v}\) is given by

\[
\tilde{\eta}(\tilde{v}^{i}) = \left(\frac{\partial \tilde{v}^{i}}{\partial \tilde{r}}\right)_{\tilde{v}} \cdot \tilde{\eta}(\tilde{r}) + \left(\frac{\partial \tilde{v}^{i}}{\partial \tilde{v}}\right)_{\tilde{r}} \cdot \tilde{\eta}(\tilde{v}) + O[\eta^2] \tag{5-31}
\]
Since $\vec{v}_e$ is given by eq. (4-5b),

\[
\frac{\partial \vec{v}_e}{\partial \vec{r}} = \left( \frac{\partial \vec{v}_e}{\partial \vec{r}} \right)_V + \left( \frac{\partial \delta \vec{v}}{\partial \vec{r}} \right)_V
\]

(5-32a)

\[
\frac{\partial \vec{v}_e}{\partial \vec{V}} = \left( \frac{\partial \vec{v}_e}{\partial \vec{V}} \right)_r + \left( \frac{\partial \delta \vec{v}}{\partial \vec{V}} \right)_r
\]

(5-32b)

Because eqs. (5-25) are assumed to hold,

\[
\frac{\partial \vec{a}}{\partial \vec{r}} = O[\Delta t]
\]

(5-33a)

\[
\frac{\partial \vec{a}}{\partial \vec{V}} = I + O[\Delta t]
\]

(5-33b)

and eqs. (5-32) become

\[
\frac{\partial \vec{v}_e}{\partial \vec{r}} = \left( \frac{\partial \delta \vec{v}}{\partial \vec{r}} \right)_V + O[\Delta t]
\]

(5-34a)

\[
\frac{\partial \vec{v}_e}{\partial \vec{V}} = I + \left( \frac{\partial \delta \vec{v}}{\partial \vec{V}} \right)_r + O[\Delta t]
\]

(5-34b)

Relations (5-34), when substituted into eq. (5-31) give

\[
\vec{\eta}(\vec{v}_e) = \vec{\eta}(\vec{v}) + \left( \frac{\partial \delta \vec{r}}{\partial \vec{r}} \right)_V \cdot \vec{\eta}(\vec{r}) + \left( \frac{\partial \delta \vec{v}}{\partial \vec{V}} \right)_r \cdot \vec{\eta}(\vec{v}) + O[\Delta t + \eta^2]
\]

(5-35)
Since the objective is to show

\[ \hat{\eta}(\vec{v}'_e) = \hat{\eta}(\vec{v}) + O[\Delta t + \eta^2] \]  

(5-36)

(preserving the asymptotic stability properties of \( \vec{v}'_a \)), all that remains is to prove

\[ \frac{\partial \hat{\eta}}{\partial \vec{v}} \left( -\frac{\vec{e}}{\partial \vec{r}} \right) \vec{v} = O[\Delta t] \]  

(5-37a)

\[ \frac{\partial \delta \vec{v}}{\partial \vec{r}} \left( -\frac{\vec{e}}{\partial \vec{v}} \right) \vec{r} = O[\Delta t] \]  

(5-37b)

By virtue of the chain-rule and eqs. (5-28),

\[ \frac{\partial \vec{v}}{\partial \vec{r}} = \frac{\partial \vec{v}}{\partial \vec{r}_e} + \frac{\partial \vec{r}'}{\partial \vec{r}_e} \cdot \frac{\partial \vec{e}}{\partial \vec{v}} + \frac{\partial \vec{v}_a}{\partial \vec{r}_a} \cdot \frac{\partial \vec{r}_a'}{\partial \vec{v}} \]  

(5-38a)

\[ = \frac{\partial \vec{v}}{\partial \vec{r}_e} + \frac{\partial \vec{v}_a}{\partial \vec{r}_a} + O[\Delta t] \]  

(5-38b)

(where multiplications occur after differentiations).

Similarly,

\[ \frac{\partial \vec{v}}{\partial \vec{r}} = \frac{\partial \vec{v}}{\partial \vec{v}_a} + \frac{\partial \vec{r}_a'}{\partial \vec{v}_a} \cdot \frac{\partial \vec{v}}{\partial \vec{v}} + \frac{\partial \vec{v}_a}{\partial \vec{v}_a} \cdot \frac{\partial \vec{v}_a'}{\partial \vec{v}} \]  

(5-39a)

\[ = \frac{\partial \vec{v}}{\partial \vec{v}_a} + \frac{\partial \vec{v}_a}{\partial \vec{v}_a} + O[\Delta t] \]  

(5-39b)

Carrying out the differentiations of \( \vec{\beta} \) via eq. (4-11) gives

\[ \frac{\partial \vec{\beta}}{\partial \vec{r}_e} = -\frac{\partial \vec{\phi}}{\partial \vec{r}} + O[\Delta t] \]  

(5-40a)

\[ = \vec{v} \vec{r} - r \vec{I} + O[\Delta t] \]  

(5-40b)
where

\[ \vec{r} \cdot \vec{v} = \vec{r} \cdot \vec{v} \]  (5-41)

and \( \mathbf{a} \cdot \mathbf{b} \) denotes the dyadic matrix with components

\[ (\mathbf{a} \cdot \mathbf{b})_{ij} = a_i b_j \]  (5-42)

Using eqs. (5-38) for \( \left( \frac{\partial \mathbf{B}}{\partial \mathbf{r}} \right) \mathbf{v} \) gives, together with eqs. (5-40),

\[ \left( \frac{\partial \mathbf{B}}{\partial \mathbf{r}} \right)_v = \left( \frac{\partial \mathbf{B}}{\partial \mathbf{r}} \right)_{\mathbf{v}} + \left( \frac{\partial \mathbf{B}}{\partial \mathbf{r}} \right)_{\mathbf{v}'} + O[\Delta t] \]  (5-43a)

\[ = O[\Delta t] \]  (5-43b)

A similar effect occurs for \( \left( \frac{\partial \mathbf{B}}{\partial \mathbf{v}} \right) \mathbf{r} \) because of antisymmetric contributions from terms in \( \mathbf{v} \) and \( \mathbf{v}' \):

\[ \frac{\partial \mathbf{B}}{\partial \mathbf{v}} = - \frac{\partial \mathbf{B}}{\partial \mathbf{v}} + O[\Delta t] \]  (5-44a)

\[ = r \mathbf{r} - r^2 \mathbf{I} + O[\Delta t] \]  (5-44b)

and so

\[ \left( \frac{\partial \mathbf{B}}{\partial \mathbf{v}} \right)_{\mathbf{r}} = \left( \frac{\partial \mathbf{B}}{\partial \mathbf{v}} \right)_{\mathbf{r}} + \left( \frac{\partial \mathbf{B}}{\partial \mathbf{r}} \right)_{\mathbf{v}} + O[\Delta t] \]  (5-45a)

\[ = O[\Delta t] \]  (5-45b)

Implicit differentiation of eq. (4-25) gives for the contributions from \( \epsilon \).
\[ \frac{\partial \epsilon}{\partial \hat{r}} = - \frac{\partial \epsilon}{\partial \hat{r}} + O[\Delta t] \]  
(5-46a)

\[ \frac{\partial \hat{F}}{\partial \hat{m}} = \frac{\hat{r}}{\hat{r}} \cdot \frac{\hat{F}}{\hat{r}} + O[\Delta t] \]  
(5-46b)

and

\[ \frac{\partial \epsilon}{\partial \hat{v}} = - \frac{\partial \epsilon}{\partial \hat{v}} + O[\Delta t] \]  
(5-47a)

\[ \frac{\partial \hat{v}}{\partial \hat{a}} = - \frac{\hat{r}}{\hat{r}} \cdot \hat{v} + O[\Delta t] \]  
(5-47b)

Substitution of eqs. (5-46) and (5-47) into eqs. (5-38) and (5-39) for \( \epsilon \) gives

\[ \frac{\partial \epsilon}{\partial \hat{r}} \hat{v} = \frac{\partial \epsilon}{\partial \hat{r}} + \frac{\partial \epsilon}{\partial \hat{r}} \hat{e} + O[\Delta t] \]  
(5-48a)

\[ = O[\Delta t] \]  
(5-48b)

and

\[ \frac{\partial \epsilon}{\partial \hat{v}} \hat{r} = \frac{\partial \epsilon}{\partial \hat{v}} + \frac{\partial \epsilon}{\partial \hat{v}} \hat{a} + O[\Delta t] \]  
(5-49a)

\[ = O[\Delta t] \]  
(5-49b)

Finally, direct differentiation of eq. (4-14) gives

\[ \frac{\partial \delta \hat{v}}{\partial \hat{r}} \hat{\nu} = \frac{1}{(r_e')^2} \left[ \hat{r}' \hat{e} \left( \frac{\partial \epsilon}{\partial \hat{r}} \hat{\nu} + \frac{\partial \hat{B}}{\partial \hat{r}} \hat{\nu} \right) \right] + O([\Delta t]^n) \]  
(5-50a)

and
\[
\frac{\partial \delta \overset{e}{r}}{\partial \overset{e}{v}} \left( \frac{\partial \overset{e}{v}}{\partial \overset{e}{r}} \right) = \frac{1}{(r'_e)^2} \left[ \overset{e}{r}' \left( \frac{\partial \overset{e}{v}}{\partial \overset{e}{r}} \right) + \left( \frac{\partial \overset{e}{r}}{\partial \overset{e}{v}} \right) \right] + O[(\Delta t)^{n+1}] \]  
(5-50b)

Substitution of eqs. (5-43b), (5-45b), (5-48b) and (5-49b) into eqs. (5-50) give (since \(n \geq 2\))

\[
\frac{\partial \delta \overset{e}{v}}{\partial \overset{e}{r}} \left( \frac{\partial \overset{e}{v}}{\partial \overset{e}{r}} \right) = O[\Delta t] \]  
(5-51a)

\[
\frac{\partial \delta \overset{e}{v}}{\partial \overset{e}{v}} \left( \frac{\partial \overset{e}{r}}{\partial \overset{e}{v}} \right) = O[\Delta t] \]  
(5-51b)

These relations ensure that (via eq. (5-35)), eq. (5-36) holds, and there is only unit reintroduction of the error of \(\overset{e}{v}\) into \(\overset{e}{v}'\).

The development of eqs. (5-26) through (5-51) also holds for the second formulation of Sect. 4.B with substitution of \(\overset{e}{r}'_a\) for \(\overset{e}{r}'_a\). Thus both conservative formulations preserve the desirable asymptotic (\(\Delta t \to 0\)) stability properties of the underlying approximations \(\overset{e}{r}'_a\) and \(\overset{e}{v}'_a\) of only unit propagation of the errors in \(\overset{e}{r}\) and \(\overset{e}{v}\). This occurs because of the antisymmetry with respect to interchange of \(\overset{e}{r}'_e\) and \(\overset{e}{v}'_e\) with \(\overset{e}{r}\) and \(\overset{e}{v}\) in the conservative relations.

C. Comparison of the Two Formulations

Two conservative formulations have been proposed, those of Sects. 4.A and 4.B. The two methods differ in the handling of the estimate \(\overset{e}{r}'_e\) for \(\overset{e}{r}'\), and have correspondingly different characteristics.

The formulation of Sect. 4.A enjoys the advantage of using a conventional method to find an approximation \(\overset{e}{r}'_e = \overset{a}{r}'\) for \(\overset{e}{r}'\),
and is thus "explicit" in \( \tilde{r}_e' \), maintaining the "without first-derivatives present" nature of the equations of motion. As a consequence, eq. (4-25) is a simple, explicit quadratic equation in \( \epsilon \), and is easily solved explicitly by, e.g., the quadratic formula.

On the other hand, the version of Sect. 4.B is implicit in \( \tilde{r}_e' \), and both \( \tilde{r}_e' \) and \( \tilde{v}_e' \) must be determined via joint iteration of the implicit quadratic eq. (4-46). This dual iteration destroys the property of "first-derivatives absent", and requires the extra work of redetermining \( \phi(r'_e) \) at each iteration. On the other hand, when the same approximation \( \tilde{r}_a' \) is used in Sect. 4.B as in Sect. 4.A, the second formulation results in one higher order approximations for both \( \tilde{r}_e' \) and \( \tilde{v}_e' \).

Thus the first formulation, being "explicit" in \( \tilde{r}_e' \), has the advantages and disadvantages of a "predictor": the method is relatively easy to implement, requires only one potential evaluation \( \phi(r'_e) \) per step, and requires no iteration. The second formulation, being "implicit" in \( \tilde{r}_e' \), enjoys the advantages, and suffers from the disadvantages, of a "corrector": an implicit (quadratic) equation must be solved, with the accompanying reevaluation of the potential, but the final results are of higher accuracy.
6. Numerical Examples

In this section, the results of Sect. 4 are compared with conventional procedures, with the underlying approximations \( \hat{r} \) and \( \hat{v} \) being given by Adams' methods. In general with predictor-corrector methods special starting and step-size changing procedures are necessary: in the calculations below the Adams-Nordsieck formulation for second-order differential equations was used [8]-[9], with the control algorithms as given by Nordsieck [9]. (Programs for implementing this method for \( n = 3 \) to \( n = 8 \) are given in the Appendices of [10]).

A comparison between the conventional Adams-Nordsieck methods for \( n = 3 \) to \( n = 8 \) with the corresponding versions of the conservative methods of Sect. 4 are given in Tables I and II, for the example of Sect. 7.a of [4]. Here \( \phi(r) \) is in the Lennard-Jones form of eq. (2-9) with \( \varepsilon = 1 \) and \( \sigma = 1 \). The initial conditions were

\[
\hat{r}(0) = <0, 1, -20> \tag{6-1a}
\]

\[
\hat{v}(0) = <0, 0, \sqrt{2}> \tag{6-1b}
\]

The mass \( m \) was chosen to be unity, giving

\[
E = 1.000000 \tag{6-2a}
\]

\[
\hat{L} = <\sqrt{2}, 0, 0> \tag{6-2b}
\]

The Adams' corrector \( \hat{r}_c \) was used for the approximation \( \hat{r}_a \) of \( r' \) for the method of Sect. 4.A; the Adams' predictor \( \hat{r}_p \) was used for \( \hat{r}_a \) in the method of Sect. 4.B. Thus both conservative
formulations gave errors of $O((\Delta t)^{n+1})$ in $\vec{r}'$ and $\vec{v}'$. Instead of changing the step-control procedure to take advantage of the extra order of accuracy in $\vec{v}'$ in the conservative formulations (which would result in fewer steps), identical step-control procedures were used as in the Adams' methods to control truncation error. (Programs are given in the Appendices of [10]). The superiority of the conservative methods is then reflected in the higher accuracy of the results. Occasionally the conservation of $E$ required a slightly smaller value of $\Delta t$ in the version of Sect. 4.B: this is reflected in the variations in the total number of steps in Table II.

For comparison, the calculated values of $E$ and $L$ at the last steps ($r > 20$) of the computation are given, along with the maximum observed derivations in these quantities. Finally, the calculated value of the angle of deflection $\chi$, is defined by

$$\chi = \cos^{-1} \frac{\vec{v} \cdot v(0)}{\|\vec{v}\| \|v(0)\|}$$

(6-3)

where $v(0)$ is given by eq. (6-1a), and for $\vec{v}$ evaluated at the last step. The correct value of $\chi$ is $0.996932$, and is also listed in Tables I and II. For further details of the problem and the evaluation of $\chi$, see [4].

Table I compares the Adams' methods with the corresponding methods of Sect. 4.A., with iteration of the implicit equation in $\vec{r}'$ to a relative convergence in $\|\vec{r}'\|$ of $10^{-3}$. Table II compares the Adams' and Sec. 4.B methods, with iteration of the implicit equations in $\vec{r}'$ and $\vec{v}'$ to a relative convergence in $\|\vec{r}'\|$ and $\|\vec{v}'\|$ of $10^{-10}$. Both Tables I and II show the superior accuracy of the conservative formulations in computing $\chi$ because of the extra order of accuracy in $\vec{v}'$. In addition, of course, the conservative formulations give excellent values for $E$ and $\vec{L}$. 
TABLE I. \(^a\) Comparison of Adams' Methods
vs. First Conservative Formulation
for \( n = 3 \) to \( n = 8 \).

<table>
<thead>
<tr>
<th>Method</th>
<th>Order</th>
<th>No.</th>
<th>Final (^c)</th>
<th>( \max \Delta E \times 10^6 )</th>
<th>( \chi )</th>
<th>Final (^f)</th>
<th>( \Delta L \chi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adams'</td>
<td>( n = 3 )</td>
<td>1895</td>
<td>1.001251</td>
<td>-3346</td>
<td>.996854</td>
<td>.87(-3)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>383</td>
<td>.986616</td>
<td>-293338</td>
<td>.981370</td>
<td>.16(-2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>197</td>
<td>.981625</td>
<td>-29975</td>
<td>.986446</td>
<td>-.21(-2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>190</td>
<td>1.047371</td>
<td>+52422</td>
<td>1.01762</td>
<td>.12(-2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>204</td>
<td>.984948</td>
<td>-18296</td>
<td>.990096</td>
<td>.49(-5)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>235</td>
<td>1.152245</td>
<td>+153832</td>
<td>1.05494</td>
<td>-.81(-5)</td>
<td></td>
</tr>
<tr>
<td>Sect. 4.A (^g)</td>
<td>( n = 3 )</td>
<td>1892</td>
<td>1.000000</td>
<td>0</td>
<td>.996932</td>
<td>.83(-16)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>392</td>
<td>1.000000</td>
<td>0</td>
<td>.996932</td>
<td>-.49(-16)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>196</td>
<td>1.000000</td>
<td>0</td>
<td>.996932</td>
<td>-.42(-16)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>141</td>
<td>1.000000</td>
<td>0</td>
<td>.996931</td>
<td>-.49(-16)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>117</td>
<td>1.000000</td>
<td>0</td>
<td>.996934</td>
<td>-.42(-16)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>106</td>
<td>1.000000</td>
<td>0</td>
<td>.996934</td>
<td>-.21(-16)</td>
<td></td>
</tr>
<tr>
<td>Exact</td>
<td></td>
<td></td>
<td>1.000000</td>
<td>0</td>
<td>.996932</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>
TABLE I - FOOTNOTES

\(^a\) Adams' correctors and implicit equations iterated to a relative convergence of \(10^{-3}\) in \(\|r\|^2\). Numbers in parentheses denote powers of ten.

\(^b\) Total number of steps necessary to reach final state when \(r > 20\).

\(^c\) Calculated using \(r\) and \(v\) at final step.

\(^d\) Maximum observed deviation between calculated value of \(E\) and true value \(E = 1.000000\) during any step of the calculation.

\(^e\) Angle of deflection calculated at final step.

\(^f\) Error in \(X\) component of the angular momentum \(\vec{L}\) at the final step.

\(^g\) First conservative formulation of Section 4.A using the Adams' correctors for \(r_a\)'s. (Same step size control algorithm as in the Adams' methods.)
TABLE II. a Comparison of Adams' Methods vs. Second Conservative Formulation for \( n = 3 \) to \( n = 8 \)

<table>
<thead>
<tr>
<th>Method</th>
<th>Order</th>
<th>No. b</th>
<th>Final c</th>
<th>max d</th>
<th>( \chi^e )</th>
<th>Final f</th>
</tr>
</thead>
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<tr>
<td></td>
<td></td>
<td>Steps</td>
<td>( E )</td>
<td>( \Delta E \times 10^6 )</td>
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<tr>
<td>Adams'</td>
<td>n = 3</td>
<td>1893</td>
<td>1.000003</td>
<td>+26</td>
<td>.996957</td>
<td>-.15(-6)</td>
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<tr>
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<td>393</td>
<td>1.000016</td>
<td>+19</td>
<td>.996957</td>
<td>-.12(-4)</td>
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<td>197</td>
<td>1.000004</td>
<td>+21</td>
<td>.996957</td>
<td>-.55(-5)</td>
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<td>.996993</td>
<td>-.16(-4)</td>
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<td>1.000038</td>
<td>+42</td>
<td>.997001</td>
<td>-.19(-4)</td>
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<td>8</td>
<td>106</td>
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<td>+97</td>
<td>.997102</td>
<td>-.73(-4)</td>
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<td>n = 3</td>
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<td>1.000000</td>
<td>0</td>
<td>.996932</td>
<td>.62(-16)</td>
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<td>0</td>
<td>.996932</td>
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<td>0</td>
<td>.996932</td>
<td>.14(-16)</td>
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<td>.996932</td>
<td>.69(-17)</td>
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<td>0</td>
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</table>

TABLE II - FOOTNOTES

a. Adams' correctors and implicit equations iterated to a relative convergence of \( 10^{-10} \) in \( \| r' \| \). Numbers in parentheses denote powers of ten.

b, c, d, e, f. See Table I.

g. Second conservative formulation of Sect. 4.B using the Adams' predictors for \( \hat{r}_a' \). (Same step-size control as in the Adams' methods.)
7. Conclusion

A numerical method for the solution for the motion of a particle subject to a central potential has been given which conserves exactly the additive constants of motion. Two formulations of the method were given, one "explicit", and the other "implicit", in the final position vector $\mathbf{r}'$. The method can be applied as a modification to conventional approximation schemes, such as truncated Taylor-series, Runge-Kutta formulae, or predictor-corrector methods. In direct numerical comparison with Adams' methods of order $n = 3$ to $n = 8$, the conservative formulations were found to be superior from the standpoint of exact conservation of energy and angular momentum, smaller truncation error in $\mathbf{r}'$, and an extra order of accuracy in $\mathbf{v}'$. 
References


3. D. Greenspan:
   (a) "Topics in the Computer Simulation of Discrete Physics", Univ. of Wis., Computer Sciences Dept., Report WIS-CS-130 (1971);
   (b) "Discrete Newtonian Gravitation and the Three-Body Problem", Univ. of Wis., Computer Sciences Dept., Report WIS-CS-133 (1971), to appear in Foundations of Physics;
   (c) "Discrete Bars, Conductive Heat Transfer, and Elasticity", Univ. of Wis., Computer Sciences Dept., Report WIS-CS-164 (1972), to appear in Computers and Structures;
   (d) "Discrete Newtonian Gravitation and the N-Body Problem", Utilitas Math., 2, 105 (1972);
   (e) "New Forms of Discrete Mechanics", Kybernetes, 1, 87 (1972);
   (f) "An algebraic, energy conserving formulation of classical molecular and Newtonian n-body interaction", Bull. Amer. Math. Soc. 79, 423 (1973);

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


WARNING

ACC 1.1CS-C2/24/74-21:23:31 (.C)

C****************************

C PROGRAM FOR CALCULATING TWO-BODY ORBITS OR ANGLES OF SCATTERING
C USING ADAMS/CONSERVATIVE ADAMS METHODS OF ADJUSTABLE ORDER.
C THE CALCULATIONS ARE CARRIED OUT IN THE XY PLANE IN RELATIVE
C COORDINATES (ORIGIN AT ONE PARTICLE).

C****************************

C IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C DIMENSION Y(N+1),AUX(N+1),E(3),DR(3)
C DATA AUX(1,1)/C+5CD/AUX(2,1)/C-1CD/
C C**** ACTE THE IMPACT OF THIS EQUIVALENCE STATEMENT ...
C EQUIVALENCE (Y(1:1),R(1)),(DR(1),Y(1:2)),(T(3),Y(3:1)),(H,Y(3:2))
C 1 = (MAX,Y(3,4)),EPSIT,AUX(3,1),(Y(2,1)) = (B,Y(1:1))
C EXTERNAL EDOM
C READ (5,11) KSIGN,METHOD,IODR,IPIT,ISW,EPSIT,E,Y,E,YCC,HMAX,STEP
C FORMAT (5,12) BSIGN,MTL,CM,MC,TC
C MSIGN - IF GE 0, INITIAL CONDITIONS ARE OBTAINED FROM B,E, AND YC.
C IF MSIGN .LT. 0, INITIAL CONDITIONS ARE READ IN.
C METHOD = 1, ADAMS TYPE 1. IF = 2, CONSERVATIVE TYPE 1. IF = 3, TYPE2
C METHOD = 4, IF ADAMS TYPE. = 1 IF ENERGY CONSERVING
C IORD - DESIRED ORDER OF METHOD 3 LE IORD LE 9
C ITOL - NC. OF BINARY BITS OF ACCURACY DESIRED IN SOLUTION
C ISW - STEP CONTROL SWITCH ... IF -1, NC MOD CONTROL. IF 0 NC MOD
C OF TOLNATION CONTROL. IF =1 MOD AND TOLNATION CONTROL.
C EPSIT - CONVERGENCE CRITERION FOR CORRECTOR ITERATION
C EPSIT .NE. 0 AND F - INITIAL CONDITIONS OF THE IMPACT PARAMETER E AND ENERGY
C YO - INITIAL Y-COORDINATE WHEN MSIGN .GE. 0
C H - INITIAL STEPSIZE
C HMAX - UPPER BOUND ON STEPSIZE
C STEP - INCREMENT IN T AT WHICH POINTS ARE PRINTED
C****************************
C IF (MSIGN .GE. 0) GO TO 51
C READ (5,11) (R(I),CR(I),I=1,2)
C FORMAT (4F10.4)
C E = 0.5CD*(OR(1)+DR(1) + DR(2)*DR(2))
C VREL = DSQRT(2.0CD*E)
C NSTP = 10
C IF (TCD .GE. E) NSTP = E
C WRITE (6,20) METHD,IODR,B,E,VREL,IBIT,YC,ISW,EPSIT
C FORMAT (1H1,5*1X,METHD,15X,TCD,ECD,15X,IDO,15X,ECD,15X,B,ECD,15X,YC,15X,EPSIT)
C 2 10X**WITH B = **F10.5,5X**E = **F10.5/10X**RELATIVE VELOCITY =
C 3F10.5/10X**NC. OF BINARY BITS = **TF,5X**YC = **F10.5/10X**STEP CONTROL SWT
C 4TCH = **IS,5X**ITERATION CRITERION = **D15.5//
C TYPE = 2C,ECD/PC1X(1,CD,VREL)
C IF (MSIGN .LT. 0) GO TO 52
C DR(1) = 1.0CD
C DR(2) = VREL
C Y(3,1) = HMAX/1.E4B576DE
C ANGO = R(1)*DR(2) - R(2)*DR(1)
C CALL FSTART (METHD,IODR,1.0CD)
C CALL FADAM(Y)
C WRITE (6,17) ((Y(I,J),J=1,4),I=1,3)
C FORMAT (10X,5Y MATPIX ...)//(10X,4D18.8)
56. WRITE (F, 14) (AUX(I, I), I = 1, 3)
57. 14 FORMAT (//ICX,*FIRST COLUMN OF AUX IS*,*3D18.6)//
58. T = 0. DC
59. TEST = STEP
60. WRITE (6, 15) H, HMAX, STEP
61. 15 FORMAT (ICX, *INITIAL STEPSIZE = *3D15.6, 5X,*TIME STEP = *3D23.10)//
62. CALL ETOTAL (KCLNT)
63. WRITE (6, 25)
64. 25 FORMAT (EX,*STEP*,5X,*TIME*,5X,*DELTA T*,5X,*ENERGY*,5X,*RADIUS*,
65. 1 3X,*X*,?X,*XDOT*,3X,*Y*,7X,*YDOT*,7X,*VREL*//)
66. 5 = C
67. RR = DSQRT(R(1)*R(1) + R(2)*R(2))
68. WRITE (6, 30) I, J, H, E, RR, (R(J), J = 1, 2), VREL
69. 30 FORMAT (4X,5I8,10F11.6)
70. CALL HDMIN (Y, AUX, IORD, IBIT, 2, FHODM, ISW, 3)
71. CC ICC I = 1, 2, CCCC
72. RR = DSQRT(R(1)*R(1) + R(2)*R(2))
73. IF (RR .GT. 10. CE. ANG .AND. T .CE. TIME) GO TO 2CC
74. IF (T .LT. TEST - 1.0 - 4) GO TO 100
75. TEST = TEST + STEP
76. IF (T .GT. TEST - 1.0 - 4) GO TO 90
77. VREL = CR(1)*CR(1) + CR(2)*CR(2)
78. CALL DF10(RR, FORCE, POT)
79. E = E .55C * VREL + POT
80. VREL = DSQRT(VREL)
81. WRITE (*,30) T, J, H, E, R, (R(J), J = 1, 2), VREL
82. 30 FORMAT (9E11.6)
83. CALL HODM (Y, AUX, FHODM, 3)
84. 100 WRITE (*, 4C) 1
85. 200 VREL = DSQRT(DR(1)*CR(1) + DR(2)*CR(2))
86. CALL T10C1(*END*)
87. CALL FINAL (KOUNT)
88. CHI = CACCS(CR(2)/VREL)*CISIGN (1. CC*CR(1))
89. RR = DSQRT(R(1)*R(1) + R(2)*R(2))
90. CALL DISFCT (RR, FCT)
91. E = 0.55D0*VREL*VREL + POT
92. WRITE (*,3C) T, J, H, E, RR
93. ANG = R(1)*DR(2) - R(2)*DR(1)
94. EANG = ANG - ANCC
95. WRITE (*,4C) CHI, KOUNT, ANG, EANG
96. 4C FORMAT (EX,*ANGLE OF DEFLECTION IS *3D15.6, 5X,*NO. PCT. *EVAL*/*18/
97. 1 5X,*FINAL ANGULAR MOMENTUM = *3D18.3, 5X,*ERRORR = *3D18.8)
98. CC TO CC
99. END

END OF COMPILATION: NO DIAGNOSTICS.
CFIGM

1.  C
2.  C***** SUBROUTINE WHICH GIVES FORCES FOR DHODM
3.  C
4.  SUBROUTINE FSTART(METHOD,ICRD,FITL)
5.  C***************************************************************************
6.  C IF METHOD = 0, ADAMS-TYPE, IF METHOD = 1, THEN CONSERVATIVE.
7.  C ICRD - ORDER OF METHOD DESIRED... (3 LE IORD LE 6)
8.  C FITL - CONVERGENCE CRITERION IN FUNCTIONAL ITERATION.
9.  C ENERGY WILL BE CONSERVED TO WITHIN ETOL PER STEP
10. C***************************************************************************
11. C
12. C********************************************************************************************************
13. DIMENSION COEF(2,6),AUX(3,11,Q(3,1))
14. DATA CCFC/C.1E66666666666666667DC,C.5C,C.125C,C.416666666666666E
15. 100,C.105555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555555
AV = C * CC
AR = D * DD
AF = C * CC
AS = D * DD
CC 280 I = 1, 2
IF (METH = 3, 3) GO TO 270
BETA(I) = G(I+1)
ALPHA(I) = 3(I+1)
CC TO 275
ALPHA(I) = AUX(I+9) - HGM*AUX(I+9)
EETA(I) = ALY(I+8)
AS = AS + ALPHA(I) * ALPHA(I)
ARP = ARF + ALPHA(I) * BETA(I)
AVP = AVF + ALPHA(I) * AUX(I+3)
AV = AV + ALPHA(I) * AUX(I+6)
AR = AR + ALPHA(I) * AUX(I+5)
TCF = FACTCR(FPHI - PHIF)
DO 100 I = 1, 2
BETA(I) = (((AVF*EETA(I) - AV*AUX(I+6)) - (ARP*ALY(I+9) - AR*AUX(I+6)))
1 / ASQ
WORK = AUX(I+9) + BETA(I)
TOP = TOP + (WORK - AUX(I+6)) * (WORK + AUX(I+6))
KOUNT = C
OLDEPS = EPSLN
EPSLN = -(TCF + EPSLN*EPSLN*ASQ)/(2*CC*AVF)
IF (METH = 3, 3, OR, DABS(EPSLN - OLDEPS) < LT. 1.E-10*DABS(EPSLN))
1 00 GC TO 4CC
KOUNT = KOUNT + 1
IF (KCLN < LT. 1E) GC TO 35C
C CALCULATE ERROR IN ENERGY AND NEW VELOCITIES
DELE = FACTCR(FPHI - PHIF)
DO 450 I = 1, 2
WORK = EPSLN * ALPHA(I) + BETA(I)
Q(I*IND) = WORK/MC
G(I+2) = WORK + AUX(I+6)
DELE = DELE + (Q(I+2) - AUX(I+6)) * (Q(I+2) + AUX(I+6))
IF (DABS(DELE) > T.E. EPSLN ITSH = 1
RETURN
ITSH = C
DO 480 I = 1, 2
G(I+2) = ALY(I+9) + HC*G(I, IND)
RETURN
C C**** FORCE ENTRY FOR CLASSICAL FORCE
ENTRY FADAM (Q)
R = CSQRT(G(I+1) * G(I+1) + Q(2, 1) * Q(2, 1))
CALL DFPOS(R, FN, V)
FA = - FA/R
DO 500 I = 1, 2
G(I+2) = FA*8(I+1)
RETURN
END OF COMPILE: NO DIAGNOSTIC.
**ACC 1 CS=2 2/47 74-21:27:38 (C) DCHFM**

1. **SUBROUTINE HODM2N (Q,AUX,IXD,INIT,N,F,ISW,NDIM)**
2. **C********************************************************************
3. **C VARIABLE ORDER ADAMS METHOD FOR NUMERICAL INTEGRATION**
4. **C SOLVES A SECOND ORDER SYSTEM OF EQUATIONS C2Q(I)/DX2 =**
5. **C F(X, I, DQ/DX), I = 1, 2, ..., N BY 2ND ORDER NORDSTROM METHODS**
6. **C G = A MATRIX OF SIZE AT LEAST Q(N+1,TORD+1) WHICH CONTAINS Q(I) IN**
7. **C Q(I,1), DQ1(I)/DX IN Q(I,2), DQ2(I)/DX2 IN Q(I,3), ETC.**
8. **C AND X1+X2+MAX IN G(N+1,1), N = 1, 4 (WHERE H IS STEPSIZE, AND**
9. **C MIN AND MAX ARE LOWER AND UPPER BOUNDS ON H)**
10. **C ALX - LEAK STORAGE OF SIZE AT LEAST 1C*(N+1)**
11. **C AUX(I,1) SHOULD CONTAIN WEIGHTS ASSIGNED TO EQNKS (SUM = 1)**
12. **C ALX(I,1) = 2 4 WILL CONTAIN A RECORD OF THE INITIAL CONDITIONS**
13. **C AUX(I,J) WHEN J = 5, 7 WILL CONTAIN STARTING CONDITIONS FOR CURRENT**
14. **C STEP, AUX(I,J) WHEN J = 8, 10 WILL CONTAIN PREVIOUSIT CONVERGENCE**
15. **C METHOD ASSUMES THAT AUX(N+1) CONTAINS ITERATION CONVERGENCE**
16. **C CRITERIA FOR FUNCTIONAL ITERATION**
17. **C IORD - ORDER OF METHOD DESIRED (3,LE, IORD .LE. 8)**
18. **C IEINT - NO. OF BITS OF ACCURACY REQUIRED OF CQII/4X. IF LT C,**
19. **C G MATRIX IS ASSUMED ALREADY PREINITIALIZED**
20. **C K = NUMBER OF EQUATIONS TO BE SOLVED**
21. **C CALL F (AUX, J, ITS = 1) SHOULD STORE DQ(I)/DX2 IN Q(I,3) AND ETA**
22. **C (Q(I,3) - AUX(I,1)) IN Q(I,TORD+1). J IS ITERATION NO. AND ITSW**
23. **C SHOULD BE SET TO 1 IF ITERATION CANNOT END THIS TIME**
24. **C ACTF THAT ITSK IS A VECTOR, WHERE ITSW(1) IS SET, ITS*(2) IS**
25. **C IORD + 1, AND ITSW(3) IS NO. OF EQUATIONS**
26. **C ITS = -1.0N+1. IF C, NO STEP CONTROL (OTHER THAN STABILITY)**
27. **C IF = -1, NO STEP CONTROL MOD INITIAL TEST**
28. **C ACTF - DIMENSIONED COLUMN LENGTH OF Q AND AUX**
29. **C********************************************************************
30. **C****************************EFFECTIVE PRECISION (A-H,C-Z)**
31. **C****************************DIMENSION BETAL6(9), SINV7(9), S(NCIM+1), AUX(NCIM+1), COEF(6,8),**
32. **C 1 C(88,6), EFVEC(6), *TVEC(3)**
33. **C====================================================================**
34. **C====================================================================**
35. **C====================================================================**
36. **C====================================================================**
37. **C====================================================================**
38. **C====================================================================**
39. **C====================================================================**
40. **C====================================================================**
41. **C====================================================================**
42. **C====================================================================**
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45. **C====================================================================**
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47. **C====================================================================**
48. **C====================================================================**
49. **C====================================================================**
50. **C====================================================================**
51. **C====================================================================**
52. **C====================================================================**
53. **C====================================================================**
54. **C====================================================================**
55. **C====================================================================**
NORD6 = E* NORD
AFLUS1 = A + 1
HLO = 1.0000000000010D*Q(NPLUS1, 3)
HUP = 1.0000000000010D*Q(NPLUS1, 4)
MODH = ISW
XC = G(AFLUS1, 1)
M = N
CC 1 CC 1 = 1, 2
JJ = J + 1
CC 1 CC I = 1, M
AUX(I, JJ) = G(I, J)
EFS = EREV((NORD)/(DAES(G(NPLUS1, 2))*2**TABST(I, IBIT)))
IF (ISW .NE. G) GO TO 250
EFS = 1.D+2CC
HUP = -1.D0
ISTEP = S
IF (IBIT .LT. 0) ISTEP = NORD6
ITOV = C
IDELAY = NORD
IF (IBIT .LT. C) CC TO 4CC
DO 260 J = 4, NORD3
CC 2 CC I = 1, M
Q(I, J) = 0.D0
CC TO 4CC
C ENTRY POINT FOR REVERSING STEP-SIZE
ENTRY HCRVES (G, AUX, F, NCI)
IDELAY = NORD
ASSIGN 4CC TO ISTAT
GO TO 1000
C ENTRY HCOD (G, AUX, F, NCI)
C NORMAL ENTRY POINT FOR INTEGRATING ONE STEP
IF (IDELAY .LE. 0) GO TO 370
IDELAY = IDelay - 1
GO TO 400
C CHECK IF STEP-SIZE CAN BE DOUBLED
IF (ITOV .EQ. 0) GO TO 400
PH = BETA(1)*G(AFLUS1, 2)
T = 0(NPLUS1, 1) - XO
I = T/PH
IF (MODH*DAEB(T - I*HW) .GT. HLO .OR. DAEB(HW) .GT. HUP) GO TO 400
ASSIGN 4CC TO ISTAT
GO TO 1200
CALL F(AUX, G, C, ITWS)
H = 0(NPLUS1, 2)
TC = C, CC
DO 420 I = 1, M
C STORE STARTING CONDITIONS OF STEP IN AUX(I, J), J = 5, 6, 7
DO 420 J = 1, 3
ALX(I, J) = G(I, J)
C STORE PREDICTORS IN AUX(I, J), J = 8, 9, 10
K = C, CC
DO 410 K = 1, NORD
113. 41C  W = W + COEF(K,J)*X(I,K+2)
114. 42C  ALX(I*,7) = h
115. 45D  AUX(I*,8) = Q(I,1) + H*(Q(I,2) + H*AUX(I,8))
116. 46C  ALX(I*,9) = G(I,2) + H*AUX(I,9)
117. 41D  Q(I,1) = AUX(I,3)
118. 49D  G(I,2) = ALX(I,9)
119. 45D  TO = TO + AUX(I,1)*DABS(Q(I,1))
120. 46C  TC = TC*ALX(NPLUS1,1)
121. 45D  Q(NPLUS1,1) = Q(NPLUS1,1) + H
122. 49D  H2 = C(1,ACRD)*H
123. 46C  HW = C(2,NORD)*H
124.  C  SOLVE CORRECTORS BY FUNCTIONAL ITERATION
125.  DO 550 J = 1,ITEP
126.  I = C,CC
127.  CALL F (AUX*3,J,ITSW)
128.  DC ECG I = 1,9
129.  W = Q(I,1)
130.  C(I,1) = ALX(I,8) + H2*C(I,NORD3)
131. 500  T = T + AUX(I,1)*DABS(Q(I,1) - W)
132.  IF (ITSW .GE. C .AND. T .LT. TC) GC TO EEC
133.  IF (ITSW .GT. 1) GO TO 555
134. 555  CONTINUE
135.  C  ITERATION DID NOT CONVERGE
136.  EEC  ITA = C
137.  GO TO 590
138.  EEC  ITA = 1
139.  CALL F (AUX*3,1,ITSW)
140.  CALL VCALC (ALX*,1,ITSW)
141.  C**** CALCULATE ESTIMATE OF TRUNCATION ERROR
142.  DODA = D*CO
143.  DC ECG I = 1,9
144.  M30  DODA = DODA + AUX(I,1)*DABS(3(I,NORD3))
145.  C  TEST TRUNCATION ERROR
146.  IF (DODA .GT. EPS) GO TO 590
147.  ITE = 1
148.  ITOV = 1
149.  IF (CCCA - BINV(ACRD+1)*EPS) EEC,ECC,E55
150. 597  ITB = 0
151. 595  ITOV = C
152. 560  IF (ITSW .GE. NORD6) GO TO 605
153.  IF (ITSW .GT. C) GO TO 65C
154. 605  IF (ITA .EQ. 0) GO TO 62C
155. 61C  IF (ITSW .LE. 1) GC TO EEC
156.  C  HALVE STEP-SIZE
157.  E2C  IF (DABS(Q(NPLUS1,2)) .LT. HLC) GC TO 15EC
158.  Q(NPLUS1,1) = Q(NPLUS1,1) - Q(NPLUS1,2)
159.  Q(NPLUS1,2) = BINV(1)*Q(NPLUS1,2)
160.  EPS = BETA(1)*EPS
161.  DC E3C I = 1,9
162.  DO 625 J = 1,3
163. 625  G(T,J) = AUX(T,J+4)
164. 62C  DO 630 J = 4,NORD3
165. 630  G(T,J) = BINV(J-3)*G(I,J)
166. 63C  IDelay = NORD
167.  GC TO 4EC
168.  C  UPDATE INTERPOLATED DERIVATIVES
170.  653  ISTEP = ISTEP +1
171.  IF (NORD .EQ. 1) GO TO 755
172.  DO 700 I = 1,M
173.  CCDA = G(I,3) - AUX(I,1)
174.  DO 700 J = 4,MORD
175.  K = CCDA*C(J,NORD)
176.  DO 660 K = J,MORD
177.  EEC  K = K + CCEF(K-2,J)*G(I,K)
178.  700  Q(I,J) = W
179.  7CF  IF (ISTEP .LT. NORD6) RETURN
180.  C  TRANSFER TO SPECIAL ROUTINES FOR STARTING PROCEDURE
181.  IF (ISTEP .NE. (ISTEP/NORD)*NORD) GO TO 4CC
182.  IF (ISTEP .EQ. NORD2) GO TO 710
183.  IF (ISTEP .EQ. NORD4) GO TO 760
184.  IF (ISTEP .EQ. NORD6) GO TO 770
185.  ASSIGN 4CC TO ISTAT
186.  GO TO 1000
187.  C  RESET TC I.C. AND REVERSE STEP DIRECTION
188.  710  DO 750 J = 1,M
189.  J = J + 1
190.  DO 750 I = 1,M
191.  750  G(I,J) = AUX(I,J)
192.  Q(NPLUS1+1) = X0
193.  CC TO 3CC
194.  C  HALVE STEP-SIZE AND REVERSE DIRECTION
195.  76E  G(NPLUS1+2) = BINV1*G(NPLUS1,2)
196.  EPS = BETA1*EPS
197.  DC 755  C = 4,NORD3
198.  DO 765 I = 1,M
199.  765  G(I,J) = BINV(J-3)*G(I,J)
200.  IF (ITB*NE.0) GO TO 710
201.  C  IF TRUNCATION TEST FAILED FOR THIS STEP (ITB = C), THEN RESTART
202.  C  WITH CURRENT SMALLER STEPSIZE AS ESTIMATE
203.  ASSIGN 2CC TO ISTAT
204.  GO TO 1000
205.  C  DOUBLE STEPSIZE
206.  770  ASSIGN 710 TO ISTAT
207.  CC TO 12CC
208.  C  PROCEDURE FOR REVERSING STEP DIRECTION
209.  1CC  G(NPLUS1+2) = -G(NPLUS1,2)
210.  DO 1100 J = 4,NORD3+2
211.  DC 1100 I = 1,M
212.  1100  G(I,J) = -Q(I,J)
213.  CC TO ISTAT*(255,4CC)
214.  C  PROCEDURE FOR DOUBLING STEP-SIZE
215.  12CC  G(NPLUS1+2) = BETA1*G(NPLUS1,2)
216.  EPS = BINV1*EPS
217.  DC 13CC  C = 4,NORD3
218.  DO 1300 I = 1,M
219.  13CC  G(I,J) = BETA(J-3)*G(I,J)
220.  IDELAY = NORD
221.  CC TO ISTAT*(4CC,710)
222.  C  ERROR TERMINATION IF STEPSIZE IS TOO SMALL
223.  15CC  FRINT 1C,ISTEP,(G(NPLUS1,I),I=1,4),CCDA,EPS,T,TO
224.  1C  FORMAT (10******,H5M,F5.0,X=*C19.9/5X,*STEP=*
225.  1,C15.9,5X,*UNITS=*,C21.9/5X,*TRUNCATION TEST=C19.9,5X,*CRITERIA=C19.9/5X
226.  PRION=*C19.9/5X,*ITERATION TEST=C19.9,5X,*CRITERIA=C19.9/5X
3 *SOLUTION MATRIX ...*/

CC 1ECC I = 1*M

1500 PRINT 20, I, {0(I,J), J=1, NORD3}

FFORMAT (EX, IE, 8D15.7)

DO 1700 I = 1*M

17CC PRINT 3C, I, {ALX(I,J), J=1,10}

FORMAT (/5X, IE, 6D17.9/10X, 4D17.9)

STOP

END

ND OF COMPIILATION: NO DIAGNOSTICS.
SUBROUTINE DISFCT (R,POT)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
DATA KCLAT /0/
ISW = 1

1. IC = RE = 1.0E/R**E
2. POT = 4.00*RE*(RE - 1.0E)
3. KCOUNT = KCLAT + 1
4. GO TO (200,300),ISW
5. RETURN
6. ENTRY DFPOI (R*,FN*,POT)
7. ISW = 2
8. GO TO 100
9. FN = 4E.0C*RE*(C.50C - RE)/R
10. RETURN
11. ENTRY FINAL (I)
12. I = KCOUNT
13. KCOUNT = C
14. RETURN
15. END

END OF Compilation: NO Diagnostics.