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Note

The Accuracy and the Preservation Property of the Discrete Mechanics

1. Introduction

LaBudde and Greenspan [1] proposed a scheme for numerical solution of classical equations of motion. They termed it "discrete mechanics," generalizing the previous schemes adopted by Greenspan [2–6]. Its unique property is its preservation of the total energy and the linear and angular momenta just as is required of real solutions. However, their scheme has local accuracy of third order, i.e., it involves errors of order $(\Delta t)^3$ at each incremental step, Δt being the time interval. Although they noted that higher-order schemes were desired, it is impossible to improve the accuracy within their framework. Here, we point out that there exists a scheme of higher-order accuracy which also exhibits the desired preservation property. At the same time, we discuss some of the limitations inherent to those types.

2. Computational Scheme for a Trajectory

The equation we consider here is Newton's equation of motion for a particle

$$m\ddot{\mathbf{r}} = \mathbf{f}, \tag{2.1}$$

where $\mathbf{r} = \mathbf{r}(t)$ is the position of the particle at time t, m the mass of the particle, $\ddot{\mathbf{r}} = \mathrm{d}^2\mathbf{r}/\mathrm{d}t^2$ the acceleration and $\mathbf{f}$ the force acting on it. In this paper, we assume a potential $\phi(\mathbf{r})$, which determines the force $\mathbf{f}$ by

$$\mathbf{f} = -\mathrm{grad}\,\phi(\mathbf{r}). \tag{2.2}$$

We fix an origin in the space for the sake of simplicity. Generalization to the case where many particles are interacting with a potential, say, depending on the distance between each two particle pair, is easy. Equations (2.1) and (2.2) are viewed as giving the acceleration $\ddot{\mathbf{r}}$ at each moment, given the position of the particle at that moment.

Following LaBudde and Greenspan, we try to predict the values at the next step by

$$\mathbf{r}_{i+1} = A\mathbf{r}_i + B\mathbf{v}_i\,\Delta t + a\ddot{\mathbf{r}}_i(\Delta t)^2, \tag{2.3}$$

$$\mathbf{v}_{i+1}\,\Delta t = C\mathbf{r}_i + D\mathbf{v}_i\,\Delta t + b\ddot{\mathbf{r}}_i(\Delta t)^2, \tag{2.4}$$

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where $\mathbf{r}_i$, $\mathbf{v}_i$ and $\ddot{\mathbf{r}}_i$ are the position, the velocity and the acceleration of the particle, respectively, at time t, $\Delta t = t_{i+1} - t_i$ being a fixed time interval, and A, B, C, D, a and b fixed constants. In view of the Taylor expansion

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \dot{\mathbf{r}}(t)\,\Delta t + \ddot{\mathbf{r}}(t)(\Delta t)^2/2! + \dddot{\mathbf{r}}(t)(\Delta t)^2/3! + \cdots, \tag{2.5}$$

$$\mathbf{v}(t+\Delta t) = \mathbf{v}(t) + \dot{\mathbf{v}}(t)\,\Delta t + \ddot{\mathbf{v}}(t)(\Delta t)^2/2! + \cdots, \tag{2.6}$$

it seems that we must necessarily put

$$\begin{aligned} &A = 1, \quad B = 1, \quad a = 1/2, \\ &C = 0, \quad D = 1, \quad b = 1, \end{aligned} \tag{2.7}$$

if we wish to attain the highest order of accuracy, because $\mathbf{v} = \dot{\mathbf{r}}$ and $\dot{\mathbf{v}} = \ddot{\mathbf{r}}$. This is the scheme LaBudde and Greenspan used.

Seemingly, there is no alternative, and the best we can attain is the local truncation error of order $(\Delta t)^3$ for the position and $(\Delta t)^2$ for the velocity. However, if we regard Eqs. (2.3) and (2.4) as a mere scheme to compute $\mathbf{r}$ alone, we do not have to think of $\mathbf{v}$ as the velocity. It is just an auxiliary variable. This policy is a very practical one, because our interest about the motion of a particle is in most cases its exact trajectory, i.e., its position at a given time. In order to distinguish the auxiliary variable from the velocity, wirte $\mathbf{z}_i$ instead of $\mathbf{v}_i$. First eliminate the auxiliary variable $\mathbf{z}_i\,\Delta t$ from Eqs. (2.3) and (2.4) (read $\mathbf{v}_i$ as $\mathbf{z}_i$). From Eq. (2.3) we have

$$\mathbf{z}_i\,\Delta t = (\mathbf{r}_{i+1} - A\mathbf{r}_i - a\ddot{\mathbf{r}}_i(\Delta t)^2)/B. \tag{2.8}$$

Substitution of this in Eq. (2.4) yields

$$\begin{aligned} &\mathbf{r}_{i+2} - (A+D)\,\mathbf{r}_{i+1} + (AD - BC)\,\mathbf{r}_i \\ &\quad = a\ddot{\mathbf{r}}_{i+1}(\Delta t)^2 + (bB - aD)\,\ddot{\mathbf{r}}_i(\Delta t)^2. \end{aligned} \tag{2.9}$$

Next, we try to determine A, B, C, D, a and b so that Eq. (2.9) holds up to the highest possible order of accuracy. It turns out that we can match the terms of up to order $(\Delta t)^3$ but not those of $(\Delta t)^4$ and that the necessary and sufficient condition for that is

$$\begin{aligned} &A + D = 2, \quad AD - BC = 1, \\ &\quad a = 1, \qquad\quad b = D/B. \end{aligned} \tag{2.10}$$

If we put $A = 1$ and $B = 1$ in particular, we get $C = 0$, $D = 1$ and $a = b = 1$ and hence

$$\mathbf{r}_{i+1} = \mathbf{r}_i + \mathbf{z}_i\,\Delta t + \ddot{\mathbf{r}}_i(\Delta t)^2, \tag{2.11}$$

$$\mathbf{z}_{i+1}\,\Delta t = \quad \mathbf{z}_i\,\Delta t + \ddot{\mathbf{r}}_i(\Delta t)^2, \tag{2.12}$$

up to order $(\Delta t)^4$. This coincides with the so-called "summed form of the explicit central difference method," and the auxiliary variable $\mathbf{z}_i$ turns out to be the central

difference approximation of $\mathbf{v}(t_i + \Delta t/2)$ [7]. Hence, the initial value $\mathbf{z}_i$ is given by $\mathbf{v}(0) + \dot{\mathbf{r}}(0)\Delta t/2$. The only difference from (2.7) is that $a = 1$ instead of $\frac{1}{2}$. Yet, as we have shown, this modification increases the order of accuracy for the position.

What we have discussed above is the "local truncation error." The "global accuracy" is $O((\Delta t)^2)$. This is readily seen if we note that the coefficient matrix

$$\mathbf{A} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \tag{2.13}$$

is similar to a 2×2 Jordan cell of eigenvalue 1, for its trace is 2 and its determinant is 1 according to Eqs. (2.10), yet $B \neq 0$. This means that $\mathbf{A}^n$ grows "linearly," not exponentially, in n as $n \to \infty$, no matter how we choose A, B, C and D as long as they satisfy Eqs. (2.10). Hence, $\sum_{i=0}^{n} O((\Delta t)^4)\,\mathbf{A}^i$ is $O((\Delta t)^2)$. It is also easy to check that any scheme satisfying Eqs. (2.10) can be rewritten is the form of Eqs. (2.11) and (2.12) by an appropriate change of variables. Equations (2.11) and (2.12) are also written as

$$\mathbf{r}_{i+1} = \mathbf{r}_i + \mathbf{z}_{i+1}\,\Delta t, \tag{2.14}$$

$$\mathbf{z}_{i+1}\,\Delta t = \mathbf{z}_i\,\Delta t + \ddot{\mathbf{r}}_i(\Delta t)^2. \tag{2.15}$$

3. Kinetic Energy, Work and Potential

As was stated in the previous section, we do not lose generality if we consider Eqs. (2.11) and (2.12). Note that elimination of $\ddot{\mathbf{r}}_i(\Delta t)^2$ from Eqs. (2.11) and (2.12) gives

$$\mathbf{z}_i\,\Delta t = \mathbf{r}_i - \mathbf{r}_{i-1}. \tag{3.1}$$

Now, we turn to the preservation property, following LaBudde and Greenspan [1]. We first consider the "kinetic energy"

$$K_i = m\mathbf{z}_i^2/2, \tag{3.2}$$

which is a discrete approximation of the kinetic energy at $t = t_i + \Delta t/2$. From Eqs. (2.15) and (3.1), we have

$$\begin{aligned} K_{i+1} - K_i &= m(\mathbf{z}_{i+1}^2 - \mathbf{z}_i^2)/2 \\ &= m(\mathbf{z}_{i+1} + \mathbf{z}_i) \cdot (\mathbf{z}_{i+1} - \mathbf{z}_i)/2 \\ &= m(\mathbf{r}_{i+1} - \mathbf{r}_{i-1}) \cdot \ddot{\mathbf{r}}_i/2 \\ &= \mathbf{f}_i \cdot \overline{\Delta \mathbf{r}}_i, \end{aligned} \tag{3.3}$$

where we have defined the "mean increment" by

$$\overline{\Delta \mathbf{r}}_i = (\mathbf{r}_{i+1} - \mathbf{r}_{i-1})/2. \tag{3.4}$$

(In this section, we are considering a part of a computed solution of Eqs. (2.11) and (2.12), assuming that the subscripts are in a defined range.) The "work" $W^n_{i=m}$ done from $t=t_m$ to $t=t_n$ is defined as follows:

$$K_n - K_m = W^n_{i=m}, \tag{3.5}$$

$$W^n_{i=m} = \sum_{i=m}^{n-1} \mathbf{f}_i \cdot \overline{\Delta \mathbf{r}}_i. \tag{3.6}$$

Next, we say that a force $\mathbf{f}_i$ is "conservative" if there exists a scalar function Φ such that

$$\mathbf{f}_i \cdot (\mathbf{r}_{i+1} - \mathbf{r}_{i-1}) = -[\Phi(\mathbf{r}_{i+1}) - \Phi(\mathbf{r}_{i-1})]. \tag{3.7}$$

We call the function $\Phi(\mathbf{r}_i)$ the "potential" for the force $\mathbf{f}_i$. Then,

$$\begin{aligned} W^n_{i=m} &= -\sum_{i=m}^{n-1} [\Phi(\mathbf{r}_{i+1}) - \Phi(\mathbf{r}_{i-1})]/2 \\ &= -[\bar{\Phi}_n - \bar{\Phi}_m], \end{aligned} \tag{3.8}$$

where we have put

$$\bar{\Phi}_i = [\Phi(\mathbf{r}_i) + \Phi(\mathbf{r}_{i-1})]/2. \tag{3.9}$$

Hence, from Eqs. (3.5) and (3.8), we observe the "conservation law of total energy," though its form is slightly different from that of LaBudde and Greenspan, as follows:

$$K_n - K_m = -[\Phi_n - \bar{\Phi}_m] \qquad \text{or} \qquad K_i + \bar{\Phi}_i = \text{const.} \tag{3.10}$$

As was pointed out by LaBudde and Greenspan, this kind of preservation property is desirable, for we can test the correctness of the computation by checking it and it prevents some type of divergence of the solution. We should note, however, that this preservation is assured only when the scheme for values at time t_{i+1} involves the "future" force at time t_{i+1}. This is also true of the scheme of LaBudde and Greenspan. In any case, the prediction of values at time t_{i+1} must be performed by explicitly solving it or by iterative correction of a temporary solution. This is obvious, because this process forces the preservation to be held at the next step. However, besides exceptional cases, it is often difficult to find an appropriate "potential" Φ. If we make an approximation $\Phi(\mathbf{r}) = \phi(\mathbf{r})$ (cf. Eqs. (3.7) and (2.2)), then we are introducing another type of error, which brings into expression (2.11) errors of $O((\Delta t)^3)$. This fact also applies to the scheme of LaBudde and Greenspan, though they did not comment on it. This is one of the major limitations inherent to all formulations of this type.

On the oter hand, the conservation of angular momentum is straightforward. This

is because it is not so much a physical property as a geometrical one. Define the "angular momentum" $\mathbf{L}_i$ by

$$\mathbf{L}_i = m\mathbf{r}_i \times \mathbf{z}_i. \tag{3.11}$$

Then,

$$\begin{aligned}\mathbf{L}_{i+1} &= m[\mathbf{r}_i + \mathbf{z}_i \Delta t + \mathbf{f}_i(\Delta t)^2/m] \times [\mathbf{z}_i + \mathbf{f}_i \Delta t/m] \\ &= \mathbf{L}_i + \mathbf{N}_i \Delta t,\end{aligned} \tag{3.12}$$

where

$$\mathbf{N}_i = \mathbf{r}_i \times \mathbf{f}_i \tag{3.13}$$

is the "torque." (In the formula of LaBudde and Greenspan, $\mathbf{r}_i$ is replaced by $(\mathbf{r}_{i+1} + \mathbf{r}_i)/2$.) This result does not depend on what kind of force $\mathbf{f}_i$ is used. In particular, if the force is "central," i.e.,

$$\mathbf{r}_i \times \mathbf{f}_i = 0, \tag{3.14}$$

then the "angular momentum" (or the "areal velocity") is conserved:

$$\mathbf{L}_i = \text{const.} \tag{3.15}$$

EXAMPLE 1 (LINEAR OSCILLATION). Consider a quadratic "potential"

$$\Phi(\mathbf{r}_i) = k\mathbf{r}_i^2/2. \tag{3.16}$$

Then

$$\begin{aligned}-[\Phi(\mathbf{r}_{i+1}) - \Phi(\mathbf{r}_{i-1})] &= -k(\mathbf{r}_{i+1}^2 - \mathbf{r}_{i-1}^2)/2 \\ &= -k(\mathbf{r}_{i+1} + \mathbf{r}_{i-1}) \cdot (\mathbf{r}_{i+1} - \mathbf{r}_{i-1})/2.\end{aligned} \tag{3.17}$$

Thus, we can see that the "linear" force

$$\mathbf{f}_i = -k\bar{\mathbf{r}}_i \tag{3.18}$$

has this "potential," where

$$\bar{\mathbf{r}}_i = (\mathbf{r}_{i+1} + \mathbf{r}_{i-1})/2 \tag{3.19}$$

is the "mean displacement." The scheme is rearranged into the following explicit form:

$$\mathbf{r}_{i+1} = [\mathbf{r}_i - k\mathbf{r}_{i-1}(\Delta t)^2/2m + \mathbf{z}_i \Delta t]/[1 + k(\Delta t)^2/2m], \tag{3.20}$$

$$\mathbf{z}_{i+1} = [\mathbf{z}_i - k(\mathbf{r}_i + \mathbf{r}_{i-1})\Delta t/2m]/[1 + k(\Delta t)^2/2m]. \tag{3.21}$$

Then, we always have

$$m\mathbf{z}_i^2/2 + k(\mathbf{r}_i^2 + \mathbf{r}_{i-1}^2)/4 = \text{const.} \tag{3.22}$$

EXAMPLE 2 (INVERSE SQUARE LAW). If we put

$$\Phi(\mathbf{r}_i) = -k/\|\mathbf{r}_i\|, \tag{3.23}$$

$\|\ \|$ denoting the Euclidean norm (or L^2 norm), we have

$$\begin{aligned}
&-[\Phi(\mathbf{r}_{i+1}) - \Phi(\mathbf{r}_{i-1})] \\
&\quad = k(1/\|\mathbf{r}_{i+1}\| - 1/\|\mathbf{r}_{i-1}\|) \\
&\quad = -k(\|\mathbf{r}_{i+1}\| - \|\mathbf{r}_{i-1}\|)/\|\mathbf{r}_{i+1}\|\,\|\mathbf{r}_{i-1}\| \\
&\quad = -k\,\frac{\mathbf{r}_{i+1}^2 - \mathbf{r}_{i-1}^2}{\|\mathbf{r}_{i+1}\|\,\|\mathbf{r}_{i-1}\|(\|\mathbf{r}_{i+1}\| + \|\mathbf{r}_{i-1}\|)} \\
&\quad = -k\,\frac{1}{\|\mathbf{r}_{i+1}\|\,\|\mathbf{r}_{i-1}\|}\,\frac{\mathbf{r}_{i+1} + \mathbf{r}_{i-1}}{\|\mathbf{r}_{i+1}\| + \|\mathbf{r}_{i-1}\|} \cdot (\mathbf{r}_{i+1} - \mathbf{r}_{i-1}).
\end{aligned} \tag{3.24}$$

Thus, we can see that the force of the "inverse square law"

$$\mathbf{f}_i = -k\bar{\mathbf{n}}_i/\bar{r}_i^2 \tag{3.25}$$

has this "potential," where

$$\bar{r}_i = \sqrt{\|\mathbf{r}_{i+1}\|\,\|\mathbf{r}_{i-1}\|}, \tag{3.26}$$

$$\bar{\mathbf{n}}_i = (\mathbf{r}_{i+1} + \mathbf{r}_{i-1})/(\|\mathbf{r}_{i+1}\| + \|\mathbf{r}_{i-1}\|) \tag{3.27}$$

are the "mean distance" and the "mean direction," respectively. Then, we always have

$$m\mathbf{z}_i^2/2 - k(1/\|\mathbf{r}_i\| + 1/\|\mathbf{r}_{i-1}\|)/4 = \text{const.} \tag{3.28}$$

4. CONCLUSION

Within the framework of Eqs. (2.3) and (2.4), the fourth-order local accuracy for the position is the highest attainable. Of course, there are many higher accuracy numerical schemes for differential equations available [8–9], but then we can no longer obtain simple laws of preservation.

On the other hand, the scheme presented here is by no means always the best recommendable one for practical use. In fact, the choice of a suitable one is a difficult problem, largely depending on the physical properties of the problem under consideration. Our purpose here is to point out that the idea of LaBudde and

Greenspan, i.e., the conservation properties, can actually be extended to a scheme with higher accuracy. That possibility has been exhausted here, and we have also shown its limitations.

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