Verletアルゴリズムにおける積分誤差について〔英文〕

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Evaluation of integration error on the Verlet algorithm

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Abstract

Accuracy of the Verlet algorithm is evaluated for the original and the revised formulas by integrating the equation of motion for a harmonic oscillator. The drift behavior, which is the deviation of the total energy with time, is attributed to the cancelling error during iteration. The energy is inefficient in detecting the integration error on the algorithm.

1. Introduction

The Verlet algorithm[1] is one of the useful methods in dynamic simulations with numerical integration of the equation of motion. The algorithm is derived from finite differences and solves the equation step by step in time. The feature of this algorithm is to require only one calculation of force acting on dynamic points per one step, indicating reduction of computing time.

In real simulations no method has been proposed in evaluating accuracy of integration of the equation. The total energy has been monitored as a measure of accuracy for the conserved system of the energy. For instance the value of time mesh for the integration has been chosen by monitoring the energy[2][3]. The validity, however, has not been examined for the simulations. The drift of the energy, which is

deviation from the initial energy with time, has been found in the simulation of a harmonic oscillator[4]. However we have not examined the relation between the extent of the drift of the energy and the accuracy on the position and velocity of dynamic points during long-time integration.

This paper clarifies the relation between the extent of the drift and the accuracy of the integration. The equation of motion for a harmonic oscillator has been integrated for this purpose. In Sec. 2 we will derive the Verlet algorithm. The integration error with the algorithm will be examined in Sec. 3. Concluding remarks will be given in Sec. 4.

2. Derivation of the Verlet algorithm

The Verlet algorithm[1] is derived from the Taylor expansions around time t as follows:[5]

$$x(t+h)=x(t)+h\frac{dx(t)}{dt}+\frac{h^2}{2!}\frac{d^2x(t)}{dt^2}+\frac{h^3}{3!}\frac{d^3x(t)}{dt^3}+\frac{h^4}{4!}\frac{d^4x(t)}{dt^4}+\cdots\cdots \quad (1)$$

$$x(t-h)=x(t)-h\frac{dx(t)}{dt}+\frac{h^2}{2!}\frac{d^2x(t)}{dt^2}-\frac{h^3}{3!}\frac{d^3x(t)}{dt^3}+\frac{h^4}{4!}\frac{d^4x(t)}{dt^4}-\cdots\cdots \quad (2)$$

where $x(t)$ is the position vector of a dynamic point in three dimensions at time t and h is a mesh of time. Adding them we obtain

$$x(t+h)=2x(t)-x(t-h)+h^2\frac{d^2x(t)}{dt^2}+O(h^4), \quad (3)$$

where $O(h^4)$ is the local truncation error on the order of h^4. This gives the time development of position of the point, i.e., the position at time $t+h$ is developped from the positions at t and $t-h$, and from a acceleration $d^2x(t)/dt^2$ acting on the point at t.

The time deveropment of velocity of the point is derived from subtracting (2) from (1):

$$\frac{dx(t)}{dt}=v(t)=\frac{x(t+h)-x(t-h)}{2h}+O(h^2), \quad (4)$$

where $O(h^2)$ is the local truncation error on the order of h^2. The velocity vector $v(t)$ with three dimensions at time t is calculated from the

positions at $t+h$ and $t-h$.

The formula (3) containes addition of h^0 and h^2 terms indicating appearance of a cancelling error during long-time integration. In order to avoid the error, a revised formulas have been proposed in real calculations[5]. First we define $\Delta x(t+h)$ as

$$\Delta x(t+h)=x(t+h)-x(t). \tag{5}$$

Then the formula (3) is rewritten as

$$\Delta x(t+h)=\Delta x(t)+h^2\frac{d^2x(t)}{dt^2}. \tag{6}$$

The position at time t_m ($t_m=m\times h$, $m=1, 2, \cdots\cdots$) is calculated with

$$x(t_m)=x(0)+\sum_{i=1}^{m}\Delta x(t_i). \tag{7}$$

The time development of velocity is calculated with

$$\frac{dx(t)}{dt}=v(t)=\frac{\Delta x(t+h)+\Delta x(t)}{2h}, \tag{8}$$

which is derived from (4) and (5). In this paper we compare the accuracy of integration from the original formulas (3) and (4) with that from the revised formulas (5) to (8).

3. Evaluation of accuracy

In order to examine accuracy of the Verlet algorithm, a motion of harmonic oscillator has been simulated as a simple case. The oscillator has the following equation of motion:

$$\frac{d^2x(t)}{dt^2}=-x(t). \tag{9}$$

where $x(t)$, dimension of which is one, is the displacement of the oscillator from equilibrium position of it. In integrating the equation, the following initial conditions have been used:

$$x(0)=1,$$
$$v(0)=0. \tag{10}$$

These conditions give the exact solutions

$$x_e(t)=\cos(t)$$

$$v_e(t) = -\sin(t), \tag{11}$$

representing an oscillation period is 2π. The motion of the oscillator has been simulated with the original and the revised formulas up to 1×10^6 steps respectively. The time mesh h has been taken to be $2\pi/200$ which corresponds to 1/200 of the period for both of the formulas. The simulation period, i. e. 1×10^6 steps, corresponds to the period for 5000 sycles in this system.

First let us see the variation of the total energy of the oscillator. The energy is the conserved quantity in the system. The energy $E(t)$ at time t is obtained from

$$E(t) = x^2(t) + v^2(t), \tag{12}$$

In the case of the exact solutions (11), the energy $E_e(t)$ is conserved at the constant value 1 :

$$E_e(t) = x_e^2(t) + v_e^2(t) = 1. \tag{13}$$

Figure 1 shows the variations of the energy differences $\Delta E(t)$ between $E(t)$ and $E_e(t)$:

$$\Delta E(t) = E(t) - E_e(t) = E(t) - 1. \tag{14}$$

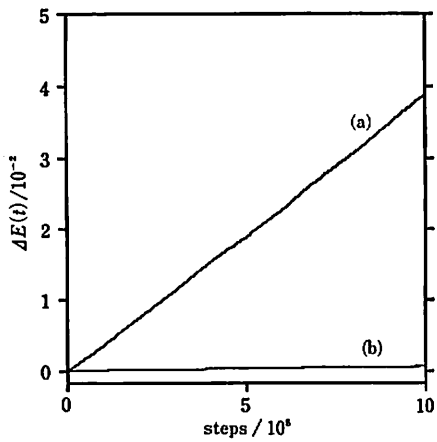

Fig. 1. Variations of the differences $\Delta E(t)$ between the simulated and the exact total energies as a function of time steps. Line (a) is for the original formulas and (b) for the revised formulas.

The difference (a) is for the original formulas and (b) for the revised formulas. The difference (a) is 0 at 0 step. The difference begins to increase linearly with time at the step. The difference at 1×10^5 steps has been 0.0389 which is almost 3.9% of the energy $E_e(t)$. On the other hand, the difference (b) is almost 0 through whole time range: the difference at 1×10^6 steps has been 0.0006 which is only 0.06% of $E_e(t)$. This shows the revised formulas give accurate total energy rather than the original formulas. The drift behavior, which is the deviation from the initial energy with time, is attributed to the cancelling error during iteration.

Here we examine the accuracy of the integration directly by appreciating the differences between simulated and exact solutions on the time deveropments of position $x(t)$ and the velocity $v(t)$ of the oscillator. First the maximum error $|\Delta x(t)|_{max}$ of position has been examined as

$$|\Delta x(t)|_{max}=\max(|x(0)-x_e(0)|,\ |x(h)-x_e(h)|,\ |x(2h)-x_e(2h)|,\cdots,\ |x(t-h)-x_e(t-h)|,\ |x(t)-x_e(t)|). \tag{15}$$

This is the maximum absolute value of the difference between the simulated and the exact positions up to time t. The result is shown in Fig. 2. The difference (a) is for the original formulas and (b) for the revised formulas. Both of the two lines (a) and (b) increase linearly with time. For the original formulas, the difference at 1×10^6 steps has been 1.1892 which is 119% of the amplitude of the oscillator. The difference has been 1.2042 for the revised formulas at the steps, which is 120% of the amplitude. This is almost the same percentage as the difference for the original formulas. The same relation has appeared in the maximum absolute value of the differences $|\Delta v(t)|_{max}$ of velocities. The difference at 1×10^6 steps for the original formulas has been 1.1883 which is almost 119 % of the maximum velocity $v_{max}=1$. The difference for the revised formulas at the steps has been 1.2041 which is 120% of the velocity.

Although the revised formulas have given the conserved total energy (within 0.06%) in this simulation, the position and velocity have included a large error (about 120%) accumlated with iteration. This suggests that the total energy, which has been used as a measure of accuracy, is not detectable for the integration error during long-time simulation with

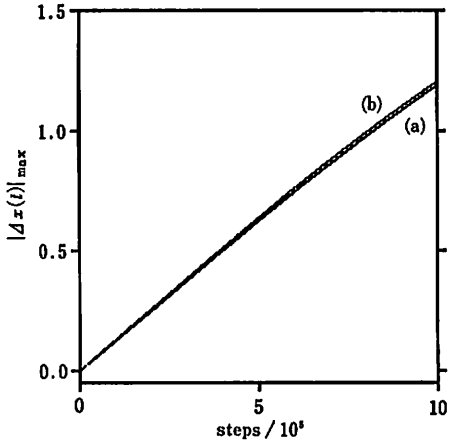

Fig. 2. Variations of the maximum absolute value $|\Delta x(t)|_{max}$ of the differences between the simulated and the exact positions as a function of time steps. Line (a) is for the original formulas and (b) for the revised formulas.

the Verlet algorithm. This may be attributed to the global (or accumlated) truncation error on the algorithm. Further analysis will be reported elsewhere[6].

4. Concluding remarks

Integration error has been evaluated for the original and the revised formulas of the Verlet algorithm by simulating the movement of harmonic oscillator up to 1×10^6 steps. The revised formulas, which has been proposed in order to avoid the cancelling error in iteration, have given accurate total energy in the simulation: the deviation of the energy was only 0.06% at the steps indicating conservation of the energy. The drift behavior, which is the deviation of the energy with time, has been found to be attributed to the cancelling error during iteration. The positions have included a large error for both of the revised and the original formulas each other: the deviations of the position have been almost 120% of the amplitude of the oscillator at the steps for both of the formulas. This

relation has been valid for the deviations of the velocity. These suggest that the total energy, which has been used as a measure of accuracy, is inefficient in detecting the integration error with the Verlet algorithm.

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