差分スキームに対する誤差解析〔英文〕

渡辺, 誠 / Watanabe, Makoto

(出版者 / Publisher)
法政大学教養部
(雑誌名 / Journal or Publication Title)
法政大学教養部紀要 / 法政大学教養部紀要
(巻 / Volume)
88
(開始ページ / Start Page)
13
(終了ページ / End Page)
19
(発行年 / Year)
1994-02
(URL)
https://doi.org/10.15002/00003619

Bull. Fac. Lib. Arts
Hosei Univ., No. 88, 1994

Error analysis for Verlet's difference scheme

Makoto S. Watanabe
Faculty of Liberal Arts, Hosei University,
Fujimi, Chiyoda-ku, Tokyo 102, Japan

Abstract

Integration error is analyzed for Verlet's difference scheme by simulating the movement of harmonic oscillator as a conservative system. This scheme gives accurate total energy through the long-time simulation of the oscillation, although large error appears in the time development of position and velocity of it. This is attributed to the angle error of simulated oscillator in phase space.

1. Introduction

Verlet's difference scheme[1] (the Verlet algorithm) is one of the useful methods in integrating the equation of motion for dynamical systems. The scheme has been used to simulate movement of atoms in the molecular dynamics simulations not only for classical systems[2] but also for first-principle systems.[3] The feature of it is to have the simple form and to require only one calculation of force in each time step. This indicates the reduction of computing time.

No method has been proposed in evaluating integration error for the equation of motion for dynamical systems. The total energy has been used as a tool for accuracy evaluation in the systems. For instance the time mesh has been chosen by monitoring the energy.[4][5] In a previous

paper, some results of error analysis has been reported for the scheme by integrating the equation of motion for a harmonic oscillator.[6] Total energy for the conservative system has been clarified to be inefficient for detection of the integration error with this scheme: althogh the energy conseved well during long-time simulation, large error appeared in the time development of position and velocity of the oscillator.[6] No origin, however, has been clarified for the scheme.

In this paper, the origin of the behavior will be clarified. In Sec. 2 computational methods will be given. The origin of the behavior will be clarified in Sec. 3. Concluding remarks will be presented in Sec. 4.

2. Computational methods

A motion of harmonic oscillator, as a simple case with exact solutions, has been simulated with Verlet's scheme[1] in order to examine the accuracy of it. The equations of motion for the oscillator with dimensionless form are

$$\frac{dx(t)}{dt}=v(t) \tag{1}$$

and

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

where $x(t)$ is displacement of the oscillator from the equilibrium position and $v(t)$ is velocity of it at time t.

For the Verlet scheme, the time developments of positions $x(t)$ and velocities $v(t)$ are obtained from

$$x(t+h)=2x(t)-x(t-h)+h^2\frac{d^2x(t)}{d^2t} \tag{3}$$

and

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

where h is time mesh for integration. In order to avoid the cancelling error during iteration, the following modified formulas[6] have been used

in the simulations:

$$x(t_m)=x(0)+\sum_{i=1}^{m}\delta x(t_i) \tag{5}$$

and

$$v(t_m)=\frac{\delta x(t_{m+1})+\delta x(t_m)}{2h}, \tag{6}$$

where t_m is time at m steps ($t_m=m\times h$) and $\delta x(t_m)=x(t_m)-x(t_{m-1})$. The $\delta x(t_m)$ is obtained from

$$\delta x(t_m)=\delta x(t_{m-1})+h^2\frac{d^2x(t_{m-1})}{dt^2}. \tag{7}$$

Initial conditions have been chosen to be $x(0)=1$ and $v(0)=0$. These give exact solutions $x_e(t)=\cos(t)$ and $v_e(t)=-\sin(t)$ representing the oscillation period is 2π for the system. The amplitude of the oscillation is $r=1$ for the exact solutions with the conditions. The time mesh h has been chosen to be $2\pi/100$ which corresponds to 1/100 of the period of the oscillation. The time developments of position $x(t)$ and velocity $v(t)$ have been simulated by means of the formulas (5) to (7) up to 1×10^6 steps. This duration corresponds to the period for 10000 cycles of it.

3. Maximum error and total energy

We examine accumulation behavior of integration error with the scheme. Figure 1 (a) shows the variation of the energy difference $\Delta E(t)$ between the simulated and the exact total energies as a function of time steps: $\Delta E(t)=\{x^2(t)+v^2(t)\}-\{x_e^2(t)+v_e^2(t)\}=x^2(t)+v^2(t)-1$. The difference is shown in the figure up to 5×10^5 steps. The difference is 0 through the whole time range in the figure. The same relation has been valid between 5×10^5 and 1×10^6 steps. This indicates no drift appears for the energy in the system with this scheme.

Here let us examine the error on the position $x(t)$ and velocity $v(t)$ directly in the same time range as Fig. 1 (a). Fig. 1 (b) shows the variation of the maximum error $|\Delta x(t)|_{max}$ of position as a function of time steps: $|\Delta x(t)|_{max}=\max(|x(h)-x_e(h)|,\ |x(2h)-x_e(2h)|,\ldots,\ |x(t-h)-x_e(t$

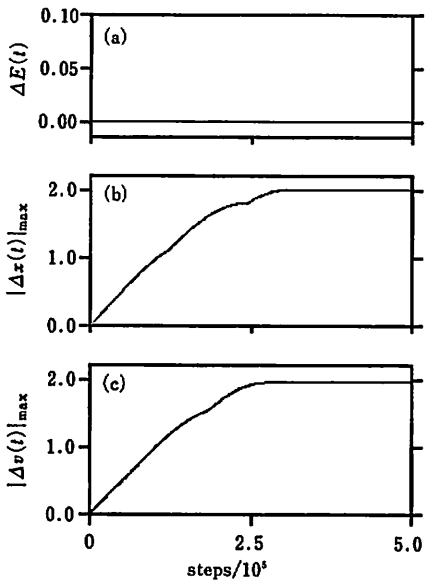

Fig. 1 (a): Variation of the energy difference $\Delta E(t)$ between the simulated and exact total energies as a function of time steps. (b): Variation of the maximum error $|\Delta x(t)|_{max}$ of position up to time t. (c): Variation of the maximum error $|\Delta v(t)|_{max}$ of velocity up to time t.

$-h)|$, $|x(t)-x_e(t)|$). This is the maximum absolute value of the differences between the simulated and the exact positions up to time t. The error increases linearly with time in initial time region. It begins to saturate at around 2.5×10^5 steps and it is constant between 3×10^5 and 5×10^5 steps. The maximum error for the later time region is 2 which is 2 times as large as the amplitudes $r=1$ of the osillation.

Figure 1 (c) shows the variation of the maximum error $|\Delta v(t)|_{max}$ of velocities as a function of time steps: $|\Delta v(t)|_{max}=\max(|v(h)-v_e(h)|, |v(2h)-v_e(2h)|, \ldots, |v(t-h)-v_e(t-h)|, |v(t)-v_e(t)|)$. This is the maximum absolute value of the differences between the simulated and the exact velocities up to time t. The error shows almost the same variation as Fig. 1 (b). The error $|\Delta v(t)|_{max}$ increases linearly with time in initial region. It begins to saturate at around 2.5×10^5 steps and it is constant between 3×10^5 and 5×10^5 steps. The maximum error for the later time region is 2 which is 2 times as large as the maximum velocity $v_{max}=1$ of the oscillator.

We examine why the total energy is conserved at constant value even when the large error (200%) appeares on both of the position and velosity of the oscillator. We clarify the origin in analyzing movement of the oscillator in phase space. The space, dimension of which is 2D,

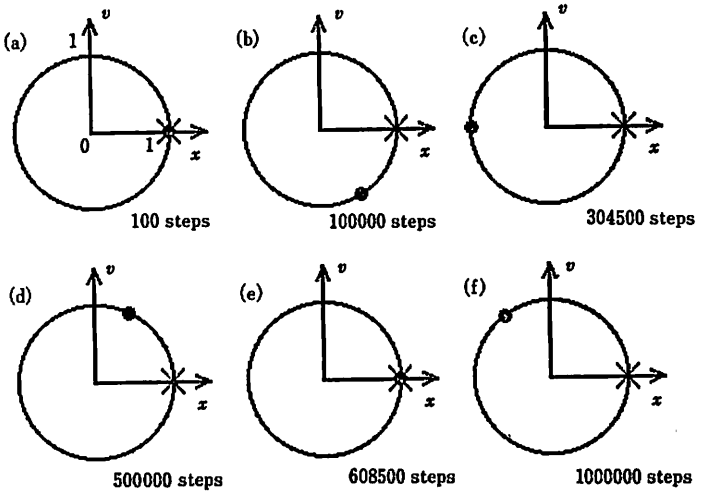

Fig. 2 Positions of phase points for the simulated and exact solutions in phase space at each time step. Filled circle is for the simulated point and cross mark for the exact one. Open circle with radius 1 is the trajectory of them.

has abscissa for the position x and ordinate for the velocity v. In the case of the exact solutions, the phase point rotates on the perfect circle with radius $r=1$ around the origin. Since the total energy is given by square r^2 of the radius, the energy is conserved at $r^2=1$ in this case.

Figure 2 shows the positions for the simulated and exact phase points in the space at each time. Filled circle is for the simulated point and cross mark for the exact one. Open circle shows the trajectory of the phase point with radius $r=1$. For the time 100 steps as shown in Fig. 2 (a), both of the two points locate at the same position $(x, y)=(1, 0)$ each other. This indicates no error appears in the simulated $x(t)$ and $v(t)$ at this time. Figure 2 (b) shows the positions of the points at time 100000 steps. Although the simulated point (filled circle) is on the trajectory, the position of it deviates from the exact point (cross mark). This is attributed to the fact that angular velocity is faster for the filled circle than for the cross mark. This indicates the error appears in the simulated position and velocity, although the total energy is conseved at the constant value.

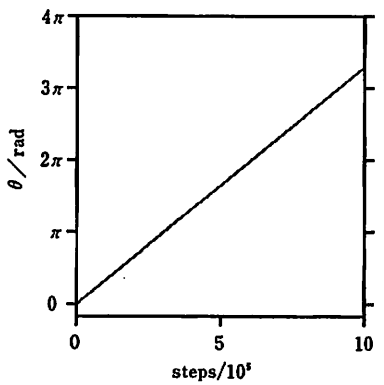

Fig. 3 Variation of angle θ between the simulated and exact phase points around the origin as a function of time steps.

The deviation becomes to be large with simulation time. Figure 2 (c) shows the positions at $t=304500$ steps which corresponds to saturation time of maximum error in Fig. 1 (b) and 1 (c). Filled circle in Fig. 2 (c) is located on the trajectory, showing consevation of the energy. It is at opposite site from the cross mark on the abscissa. This indicates the difference $\Delta x(t)=|x(t)-x_e(t)|$ between the positions is 2 at this time steps, which is 200% of the amplitude of the oscillator. The same relation has been varid for the difference $\Delta v(t)=|v(t)-v_e(t)|$ between velocities at the 304525 steps: filled circle has been located at opposite site from the cross mark on the ordinate. This is the reason why the energy is conseved even when the maximum error becomes 200% for simulated position and velocity: angular velocity is faster for the simulated point than for the exact one.

Here let us examine difference of angular velocity between the simulated and the exact phase points of this oscillator. Figure 3 shows the variation of angle θ between the simulated and the exact points around the origin as a function of time steps. The angle increases linearly with time through the whole time range, indicating difference of anglular velocities is constant between the two points. From the figure, the angle θ is found to be 2π at about 600000 steps. This is the time when the two phase points are located at the same point on the trajectory, as shown in Fig. 2 (e).

4. Concluding remarks

Integration error has been analyzed for Verlet's difference scheme by

simulating the movement of harmonic oscillator up to 1×10^6 steps (10000 cycles). The maximum error on position has been found to be 200% for the amplitude of position of the oscillator. The maximum error on velocity has been the same percentage for the maximum velocity of it. Total energy, however, has been conserved through the whole time range of the simulation. The origin of the behavior has been examined in analyzing movement of the oscillator in phase space. This is attributed to the angle error of simulated phase point, i. e., the angular velocity has been faster for the simulated point than for the exact point in the space.

References

(1) L. Verlet, Phys. Rev. **159**, 98 (1967).
(2) For instance, M. Kimura and F. Yonezawa, Topological Disorder in Condensed Matter, edited by F. Yonezawa and T. Ninomiya (Springer, Berlin, 1983), p. 80.
(3) T. Oguchi and T. Sasaki, Prog. Theor. Phys. Suppl. No. 103, 93 (1991).
(4) A. Ueda, Computer Simulation —atomic motion in macroscopic systems—, (Asakura, Tokyo, 1990), p. 10. (in Japanese).
(5) B. Bernu, J. P. Hansen, Y. Hiwatari, and G. Pastore, Phys. Rev. **A 36**, 4891 (1987).
(6) M. S. Watanaba, Bull. Fac. Lib. Arts, Hosei Univ., No. 84, 29 (1993).