Comparison between Symplectic Integrators and Clean Numerical Simulation for Chaotic Hamiltonian Systems

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Abstract

In this paper we compare the reliability of numerical simulations given by the classical symplectic integrator (SI) and the clean numerical simulation (CNS) for chaotic Hamiltonian systems. The chaotic Hénon-Heiles system and the famous three-body problem are used as examples for comparison. It is found that the numerical simulations given by the symplectic integrator indeed preserves the conservation of the total energy of system quite well. However, their orbits quickly depart away from each other. Thus, the SI can not give a reliable long-term evolution of orbits for these chaotic Hamiltonian systems. Fortunately, the CNS can give the convergent, reliable long-term evolution of solution trajectory with rather small deviations from the total energy. All of these suggest that the CNS could provide us a better and more reliable way than the SI to investigate chaotic Hamiltonian systems, from the microscopic quantum chaos to the macroscopic solar system.

Keywords:
chaos, Hamiltonian system, symplectic integrator, clean numerical simulation (CNS), reliability of computation

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1. Introduction

There are many chaotic Hamiltonian systems in physics, from the microscopic quantum chaos [1] to the macroscopic solar system [2]. However, it is well-known that chaotic dynamic systems have the sensitivity dependence on initial condition (SDIC) [3], say, a tiny difference in initial condition might lead to a significant variation of solution after a long enough time. This is the famous "butterfly-effect", discovered by Lorenz [3]. To make matters even worse, Lorenz [4, 5] further found that chaotic solutions are sensitive not only to initial conditions but also to numerical algorithms: different numerical schemes with different time steps may lead to completely different numerical results of chaos. Lorenz's conclusions were confirmed by other researchers [6]. For example, chaotic numerical simulations of the Lorenz equation given by different schemes were convergent only in a interval less than 30 Lorenz time unit (LTU). This is easy to understand, because the numerical noises, i.e. the truncation error and round-off error, inherently exist at each time-step for all numerical schemes, which are enlarged exponentially due to the SDIC of chaos [3]. So, "computed" dynamic behaviors observed in some nonlinear discrete-time difference equations sometimes might have nothing to do with the "exact" solution of the original continuous-time differential equations at all, as mentioned by some researchers [7]. These numerical phenomena lead to the intense arguments [8, 9] about the reliability of numerical simulations of chaotic systems. A few researchers even believed that "all chaotic responses are simply numerical noise and have nothing to do with the solutions of differential equations" [8]. Thus, due to the SDIC or the butterfly-effect, it is indeed a challenge to accurately simulate chaotic solution of Hamiltonian systems in a long interval of time [10, 11].

Nowadays, the symplectic integrators (SI) are widely applied to numerically solve Hamiltonian systems [12–14], such as solar system [15], spin systems [12] and so on. Especially, the symplectic integrators possess a Hamiltonian as a conserved quantity that often corresponds to the total energy of the system. So, the symplectic integrator schemes have been widely applied to calculate long-term evolution of chaotic Hamiltonian systems in nonlinear dynamics, molecular dynamics, accelerator physics, plasma physics, quantum physics, celestial mechanics and so on. This is mainly because conservation of Hamiltonian quantities is regarded as a criterion of accurate simulations of Hamiltonian systems. For example, the primitive Euler scheme and the classical Runge-Kutta scheme are not symplectic integrators, and thus they

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can not guarantee the conservation of kinetic energy of celestial systems in a long-term evolution. But, the relative energy error, i.e. the deviation from the total energy, becomes much smaller by means of the SI, and therefore the symplectic integrators are widely applied in chaotic Hamiltonian systems.

Are long-term numerical simulations given by the symplectic integrators for chaotic Hamiltonian systems indeed reliable? To check this, one should be able to gain convergent chaotic solution in a long enough interval. This was indeed impossible for the classical schemes, but however currently becomes possible by means of the so-called Clean Numerical Simulation (CNS) [16]. The CNS is based on the arbitrary Taylor series method (TSM) [17, 18] and all data in the arbitrary multiple precision [19], together with a check of solution verification by means of different numerical simulations given by different non-physical parameters such as order of Taylor expansion, time step and so on. Unlike other numerical schemes, the CNS can greatly reduce the truncation and round-off errors by means of high enough order of Taylor expansion and data in multiple-precision with many enough digits, respectively, so that the numerical noises are negligible in a long enough interval of time. As mentioned above, using the Runge-Kutta method, one often gains convergent chaotic solution of Lorenz equation in a rather small interval [0,30] (LTU). However, Liao [16] gained, for the first time, a convergent chaotic solution of the Lorenz equation in a interval [0,1000] (LTU) by means of the CNS using the 400th-order Taylor expansion and data in 800-digit multiple precision. Furthermore, Wang et al. [20] obtained a convergent chaotic solution in the interval [0,2500] (LTU) by means of the CNS using the 1000th-order Taylor expansion and data in the 2100-digit multiple precision. Currently, Liao and Wang [21] successfully obtained a convergent chaotic solution of the Lorenz equation in a rather large interval [0,10000] (LTU) by means of the CNS with the 3500th-order Taylor expansion and data in the 4180-digit multiple precision. This successful application of the CNS has an important meaning in theory: it indicates that, for exactly given initial conditions, the accurate prediction of chaos is *possible* in a rather long interval of time. This is also helpful to quiet down the debate about the reliability of numerical simulations for chaotic systems [7–9]. Thus, from viewpoint of mathematics, the CNS provides us a reliable tool to investigate chaotic dynamic systems, such as three-body problem, Lorenz equation and so on [22, 23].

Considering the wide applications of the symplectic integrators in chaotic Hamiltonian systems from the microscopic quantum chaos [1] to the macro-

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scopic solar system [2], we investigate in this paper the reliability of numerical simulations given by the SI by comparing them with the convergent chaotic solutions given by the CNS. Without loss of generality, the Hénon-Heiles system and the famous three-body problem are used as examples for comparison. It is found that all of the numerical simulations given by the SI indeed preserve the conservation of the total energy quite well in a long interval, but unfortunately their orbits depart from each other quickly due to the inherent numerical noises and the butterfly-effect of chaos. So, in general, even the symplectic integrators can *not* give reliable long-term evolution of orbits of the chaotic Hamiltonian systems. Fortunately, the CNS can give the convergent, reliable long-term evolution of chaotic trajectory with rather small deviation from the total energy. Thus, the CNS is better and more reliable than the symplectic integrators in general.

The basic ideas of the symplectic integrator (SI) for the Homiltonian systems and the clean numerical simulations (CNS) for general nonlinear dynamic systems are briefly described in § 2. Comparisons of the SI and CNS for the Hamiltonian Hénon-Heiles system and the three-body problem are given in § 3. The concluding remarks is provided in § 4.

2. Numerical schemes

2.1. Symplectic integrator (SI)

Consider a generic Hamiltonian system

$$\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}, \quad \dot{\mathbf{q}} = +\frac{\partial H}{\partial \mathbf{p}}, \tag{1}$$

where $\mathbf{q}$ denotes the vector of position coordinates, $\mathbf{p}$ is the vector of momentum coordinates, $H(\mathbf{p}, \mathbf{q})$ is the Hamiltonian that often corresponds to the total energy of the system. Assume that the Hamiltonian is separable, say,

$$H(\mathbf{p}, \mathbf{q}) = T(\mathbf{p}) + V(\mathbf{q}),$$

where $T(\mathbf{p})$ is the kinetic energy and $V(\mathbf{q})$ denotes the potential energy, respectively. We use here the classical 4th-order explicit symplectic integrator:

$$\mathbf{q}_i = \mathbf{q}_{i-1} + h\, c_i\, \frac{\partial T(\mathbf{p}_{i-1})}{\partial \mathbf{p}}, \tag{2}$$

$$\mathbf{p}_i = \mathbf{p}_{i-1} - h\, d_i\, \frac{\partial V(\mathbf{q}_i)}{\partial \mathbf{q}}, \tag{3}$$

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for $i = 1, 2, 3, 4$, where h denotes the time step and

$$c_1 = c_4 = \frac{1}{2(2 - 2^{1/3})}, \quad c_2 = c_3 = \frac{1 - 2^{1/3}}{2(2 - 2^{1/3})},$$

$$d_1 = d_3 = \frac{1}{2 - 2^{1/3}}, \quad d_2 = -\frac{2^{1/3}}{2 - 2^{1/3}}, \quad d_4 = 0 \quad (4)$$

are constant coefficients. For details, please refer to Forest & Ruth [24] and Yoshida [25].

2.2. Clean Numerical Simulation

In order to gain reliable simulations of chaotic dynamic systems in a long but finite interval of time, Liao [16] developed the so-called "Clean numerical simulation" (CNS). The CNS is based on the arbitrary Taylor series method (TSM) [17, 18] and data in the arbitrary multiple precision [19], together with a solution verification check by comparing different numerical simulations. Its basic ideas are simple and straightforward, as mentioned below.

Consider a nonlinear dynamic system

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(t, \mathbf{y}), \quad \mathbf{y}(0) = \mathbf{y}_0, \quad (5)$$

where t is the time, $\mathbf{y}(t)$ is the vector of unknown functions with $\mathbf{y}_0$ being its initial value, $\mathbf{F}$ denotes the vector of nonlinear functions, respectively. Write $t_{n+1} = t_n + h = (n + 1)h$, where h is the time step. Then, we have the Mth-order Taylor expansion

$$\mathbf{y}(t_{n+1}) \simeq \mathbf{y}(t_n) + \frac{d\mathbf{y}(t_n)}{dt}h + \frac{1}{2!}\frac{d^2\mathbf{y}(t_n)}{dt^2}h^2 + ... + \frac{1}{M!}\frac{d^M\mathbf{y}(t_n)}{dt^M}h^M, \quad (6)$$

where the Taylor coefficients can be calculated in a recursive way using (5). Obviously, the higher the order M of the Taylor expansion (6), the smaller the truncation error. Especially, *all* data in the CNS are in the multiple precision with N-digits, so that the round-off error can be reduced to a required level as long as a large enough number N is used. In addition, a verification check is alway necessary: a simulation is acceptable only when it does *not* depart, in the *whole* given interval, from another even better simulation given by the CNS using either higher order (i.e. larger M) of Taylor expansion and/or data in higher precision (i.e. larger N) and/or a smaller time-step h. For the

detailed CNS schemes of the chaotic Hénon-Heiles system and the chaotic three-body problem, please refer to Liao [22, 23].

Note that (5) is *unnecessary* to be a Hamiltonian system. So, the CNS is more general than the SI.

3. Comparison of the SI and CNS

3.1. The Hénon-Heiles system

The motion of stars orbiting in a plane about the galactic centre is governed by the so-called Hénon-Heiles Hamiltonian system of equations [26]:

$$\begin{cases} \ddot{x}(t) = -x(t) - 2x(t)y(t), \\ \ddot{y}(t) = -y(t) - x^2(t) + y^2(t). \end{cases} \tag{7}$$

Here, the Hamiltonian is the total energy, i.e.

$$H = T(\dot{x}, \dot{y}) + V(x, y),$$

where

$$T(\dot{x}, \dot{y}) = \frac{1}{2} \left(\dot{x}^2 + \dot{y}^2 \right)$$

is the kinetic energy,

$$V(x, y) = \frac{1}{2} \left(x^2 + y^2 + 2x^2 y - \frac{2}{3} y^3 \right)$$

is the potential energy, respectively. As pointed out by Sprott [27], its solution is chaotic for some initial conditions, such as

$$x(0) = \frac{14}{25}, \ \ y(0) = 0, \ \ \dot{x}(0) = 0, \ \ \dot{y}(0) = 0, \tag{8}$$

which is considered in this paper.

First of all, we simulated the chaotic orbits of the Hénon-Heiles system (7) with the initial condition (8) in the interval $[0, 1000]$ by means of the 4th-order symplectic integrator using the double precision and the several different time steps $h = 0.001, 0.0001$ and 0.00001, respectively. As mentioned by many researchers [12–14], the relative energy error, i.e. the deviation from the total energy, has been widely used to evaluate the accuracy and reliability of
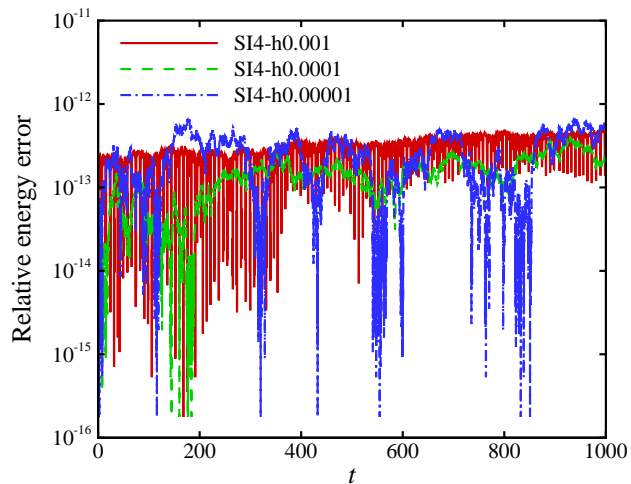
Figure 1: The evolution of relative energy error for the Hénon-Heiles system (7) and (8) given by the 4th-order symplectic integrator using the double precision and the different time steps h. Solid line: $h = 0.001$; Dashed line: $h = 0.0001$; Dash-dotted line: $h = 0.00001$.
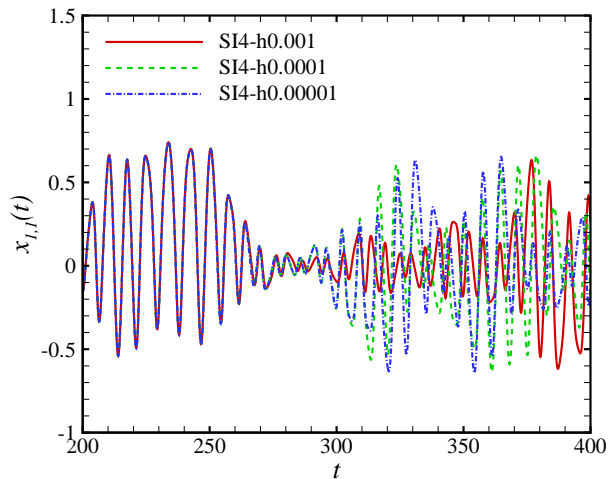

Figure 2: The simulations of the $x(t)$ of the Hénon-Heiles system (7) and (8) given by the 4th-order symplectic integrator using the double precision and the different time steps h. Solid line: $h = 0.001$; Dashed line: $h = 0.0001$; Dash-dotted line: $h = 0.00001$.

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Table 1: The x and the deviation from the total energy at $t = 1000$ by means of the CNS using the different orders of Taylor's expansion, the data in the 100-digit multiple precision and the time step $h = 1/100$.

Order	$x(1000)$	Deviation from the total energy H
20	-0.049	9.1×10^{-48}
25	-0.04915038397848	2.0×10^{-60}
30	-0.0491540383978484	1.8×10^{-73}
40	-0.0491540383978484	2.6×10^{-96}

numerical solutions of Hamiltonian systems. As shown in Fig. 1, the relative energy errors of all these simulations given by the 4th-order SI are rather small in the whole interval $[0, 1000]$, say, less than 10^{-12}. However, as shown in Fig. 2, their orbits depart from each other quickly: the orbits given by the SI using $h = 0.001$ and $h = 0.0001$ separate at about $t = 280$, and the orbits using $h = 0.0001$ and $h = 0.00001$ separate at about $t = 310$, respectively. Therefore, *neither* of these trajectories given by the symplectic integrator are reliable in the interval of $[0, 1000]$, even if the Hamiltonian, i.e. the total energy of the system, is conserved quite well.

However, Liao [22] successfully applied the CNS to gain convergent trajectories of the chaotic Hénon-Heiles system (7) with the initial condition (8) in the interval $[0, 2000]$ by means of the CNS with the 70th-order Taylor expansion and every data in the 140-digit multiple precision using the time step $h = 1/10$. So, following Liao [22], we gain a reliable, convergent orbits of (7) and (8) in the interval $[0, 1000]$ by means of the CNS with the 50th-order Taylor expansion and data in the 100-digit multiple precision using the time step $h = 1/100$, as listed in Table 1. Note that the orbits given by the CNS are convergent in the accuracy of 17 significance digits at the 30th-order ($M = 30$) of Taylor expansion, and the corresponding deviation from the total energy is very small, say, 1.8×10^{-73}, which is 50 orders of magnitude less than that given by the SI (see Fig.1). Therefore, unlike the symplectic integrator, the CNS can give convergent, reliable orbits of the chaotic Hénon-Heiles system with very small deviation from the total energy (i.e. energy preserving) in a long interval $[0, 1000]$. This illustrates that the CNS is better and more reliable for chaotic Hamiltonian systems than the

SI.

Why? This is mainly due to the butterfly-effect of chaos, i.e. the tiny difference at the initial condition enlarges exponentially [3]. Here, we should mention that Liao [22] applied the CNS to gain a convergent solution of the chaotic Hénon-Heiles system (7) with an initial condition

$$x(0) = \frac{14}{25}, \quad y(0) = 10^{-60}, \quad \dot{x}(0) = 0, \quad \dot{y}(0) = 0, \tag{9}$$

which has a tiny difference from (8), but found that this tiny difference at the initial condition indeed leads to the completely different orbits. Unfortunately, the numerical noises (such as the truncation error and round-off error) always exist for the numerical schemes including the symplectic integrators that use the double precision in general with the round-off error at the level 10^{-16} that is much less than 10^{-60}. So, it is reasonable that the symplectic integrators can not give convergent, reliable long-term evolution of chaotic Hénon-Heiles system (7) in some cases.

3.2. three-body problem

Now, let us consider another Hamiltonian system, the famous three-body problem, governed by the Newtonian gravitational law and the motion equations

$$\ddot{x}_{k,i} = \sum_{j=1, j \neq i}^{3} m_j \frac{(x_{k,j} - x_{k,i})}{R_{i,j}^3}, k = 1, 2, 3, \tag{10}$$

where $\mathbf{r}_i = (x_{1,i}, x_{2,i}, x_{3,i})$ denotes the position of the ith body, m_i $(i = 1, 2, 3)$ is the mass of body, and

$$R_{i,j} = \left[\sum_{k=1}^{3} (x_{k,j} - x_{k,i})^2 \right]^{1/2}.$$

Without loss of generality, let us consider here the case $m_1 = m_2 = m_3 = 1$ and the initial condition

$$\begin{cases} \mathbf{r}_1 = (1/10, 0, -1), \mathbf{r}_2 = (0, 0, 0), \mathbf{r}_3 = (0, 0, 1), \\ \\ \dot{\mathbf{r}}_1 = (0, -1, 0), \dot{\mathbf{r}}_2 = (1, 1, 0), \dot{\mathbf{r}}_3 = (-1, 0, 0). \end{cases} \tag{11}$$

Without loss of generality, the 4th-order symplectic integrator with the double precision is used to gain the chaotic orbits of the three-body system
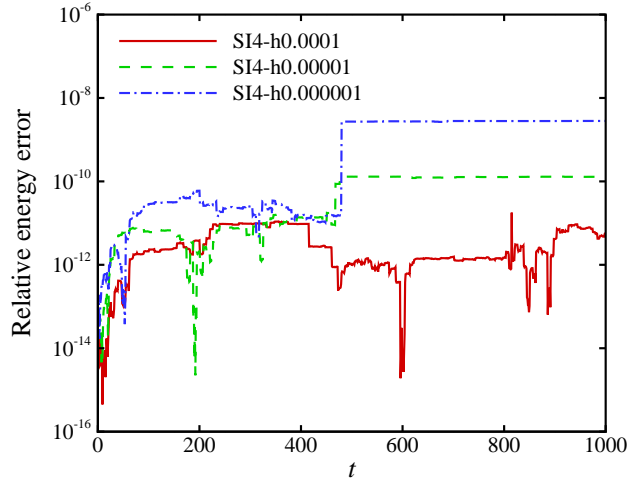
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Figure 3: The evolution of the deviation from the total energy of the three-body problem given by the 4th-order symplectic integrator with the double precision using the different time steps h. Solid line: $h = 10^{-4}$; Dashed line: $h = 10^{-5}$; Dash-dotted line: $h = 10^{-6}$.

Figure 4: The x position of Body-1 given by the 4th-order symplectic integrator with the double precision using the different time steps h. Solid line: $h = 10^{-4}$; Dashed line: $h = 10^{-5}$; Dash-dotted line: $h = 10^{-6}$.
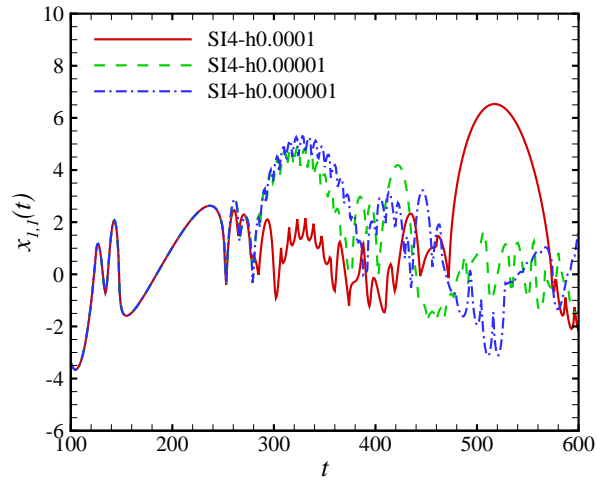
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Table 2: The x position of the Body-1 of the 3-body system (10) and (11) at $t = 1000$ given by the CNS with the different orders (M) of Taylor expansion, the data in 300-digit multiple precision and the time step $h = 10^{-3}$.

Order M	$x_1(1000)$	Deviation from the total energy
40	-16.8	1.63×10^{-17}
50	-16.82869	7.88×10^{-22}
60	-16.8286925389	2.05×10^{-26}
70	-16.82869253894194	1.12×10^{-31}
80	-16.82869253894194	1.90×10^{-35}

(10) and (11) in the interval [0,1000] by means of the four different time steps $h = 10^{-4}, 10^{-5}$ and 10^{-6}, respectively. Since the 3-body problem is a Hamiltonian system, its total energy must be conserved for a reliable simulation. As shown in Fig. 3, the deviation from the total energy of the three-body problem given by the symplectic integrator is indeed rather small in the whole interval [0,1000], at a level less than 10^{-8}. Unfortunately, this can *not* guarantee the reliability of the chaotic trajectory of the 3-body system given by the symplectic integrator! A shown in Fig. 4, the x position of the Body-1 given by the time step $h = 10^{-4}$ departs at $t \approx 270$ from that given by $h = 10^{-5}$, and the x positions given by $h = 10^{-5}$ and $h = 10^{-6}$ depart from each other at $t \approx 310$, respectively. Therefore, the long-term evolutions of the chaotic orbits of the three-body problem (10) and (11) given by the 4th-order symplectic integrator are *not* reliable in the interval [0,1000].

By means of the CNS with the 80th-order Taylor expansion, data in 300-digit multiple precision and the time step $h = 10^{-2}$, Liao [23] successfully gained the reliable orbits of a similar chaotic three-body problem in the interval [0,1000]. Similarly, following Liao [23], we obtained a convergent long-term evolution of the three-body system (10) and (11) in the interval [0,1000] by means of the CNS. Indeed, by means of the CNS using the up-to 80th-order Taylor expansion and data in the 300-digit multiple precision with the time step $h = 10^{-3}$, we gain convergent orbits of the three-body system in the time interval [0, 1000], as shown in Table 2. Note that the orbits at $t = 1000$ given by the CNS at the 40th to 60th-order of Taylor expansion are convergent in the accuracy of 3, 7 and 12 significance digits, respectively.

Especially, the orbits given by the CNS at the 70th and 80th-order Taylor expansion are convergent in the accuracy of 16 significance digits, with very small deviations from the total energy at the level 10^{-31} and 10^{-35}, respectively. Thus, unlike the symplectic integrator, the CNS can give a reliable long-term evolution of the chaotic orbits of the three-body system (10) and (11), together with a rather small deviation from the total energy. It should be emphasized that, for the three-body problem, it is very important to give an accurate prediction of orbits.

This example further illustrates that the CNS is better than the symplectic integrators for some chaotic Hamiltonian systems.

4. Concluding remarks

In this paper we compare the reliability of numerical results given by the classical symplectic integrator (SI) with the double precision and the clean numerical simulation (CNS) for chaotic Hamiltonian systems. The chaotic Hénon-Heiles system and three-body problem are used as examples for comparison. It is found that the numerical simulations given by the symplectic integrator indeed preserves the conservation of the total energy of system quite well. However, their orbits quickly depart away from each other. So, the symplectic integrator can *not* give a reliable long-term evolution of solution trajectory for these chaotic Hamiltonian systems! Fortunately, the CNS can give the convergent, reliable long-term evolution of solution trajectory with a rather small deviation from the total energy. It should be emphasized that, for the Hénon-Heiles system and the three-body problem, it is very important to give an accurate prediction of orbits. All of these suggest that the CNS could provide us a better and more reliable way than the SI to investigate some chaotic Hamiltonian systems.

Note that the symplectic integrator scheme has been widely applied to calculate long-term evolution of chaotic Hamiltonian systems in nonlinear dynamics, molecular dynamics, accelerator physics, plasma physics, quantum physics, celestial mechanics and so on. So, the CNS should find its wide applications in these important fields with reliability, although it needs more CPU times.

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