

Several fourth-order force gradient symplectic algorithms *

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Abstract By adding force gradient operators to symmetric compositions, we build a set of explicit fourth-order force gradient symplectic algorithms, including those of Chin and coworkers, for a separable Hamiltonian system with quadratic kinetic energy T and potential energy V . They are extended to solve a gravitational n -body Hamiltonian system that can be split into a Keplerian part H_0 and a perturbation part H_1 in Jacobi coordinates. It is found that the accuracy of each gradient scheme is greatly superior to that of the standard fourth-order Forest-Ruth symplectic integrator in $T + V$ -type Hamiltonian decomposition, but they are both almost equivalent in the mean longitude and the relative position for $H_0 + H_1$ -type decomposition. At the same time, there are no typical differences between the numerical performances of these gradient algorithms, either in the splitting of $T + V$ or in the splitting of $H_0 + H_1$. In particular, compared with the former decomposition, the latter can dramatically improve the numerical accuracy. Because this extension provides a fast and high-precision method to simulate various orbital motions of n -body problems, it is worth recommending for practical computation.

Key words: celestial mechanics — methods: numerical

1 INTRODUCTION

Recently, there have been a large number of papers written on the subject of numerically solving a gravitational n -body Hamiltonian problem in planetary dynamics. They are mainly divided into two fields. One deals with manifold correction schemes (Nacozy 1971; Fukushima 2003; Wu et al. 2006, 2007; Ma et al. 2008a,b, 2009; Zhong & Wu 2009), and the other relates to symplectic integrators (Wisdom 1982, 1983; Wisdom & Holman 1991; Wu et al. 2003a,b; Zhu et al. 2007; McNeil & Nelson 2009). In order to effectively suppress the fast expansion of various numerical errors, the mechanism of the former is to force the numerical path to go back to the original hypersurfaces by adding the control terms associated with integrals or quasi-integrals to the numerical solution at the end of each time step. The latter can also conserve the integral of energy. Above all, unlike the former, the latter does preserve the symplectic structure of phase-space, that is, the so-called structure-preserving geometrical integration algorithms. Due to these advantages, symplectic algorithms are especially adapted to qualitative research on the longtime evolution of Hamiltonian systems in dynamical astronomy.

Pioneering work on symplectic integration algorithms can be found in existing references (Ruth 1983; Wisdom 1982, 1983; Feng 1986) from the early eighties. As typical examples, explicit symplectic methods for separable Hamiltonian systems mainly involve the mapping method based on

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the averaging principle by which Wisdom (1982, 1983) studied the motion of asteroids near the 3:1 mean-motion resonance with Jupiter, and the second- and third-order symplectic algorithms of Ruth (1983) where a Hamiltonian is divided into two integrable parts, kinetic energy T and potential energy V . Then there are the fourth-order symplectic integrators of Candy & Rozmus (1991) and of Forest & Ruth (1990), and the higher-order symplectic schemes of Yoshida (1990). It should be emphasized that the celebrated Wisdom-Holman (1991) leapfrog symplectic integrator copes with the significant limitations of the mapping method through a gravitational n -body Hamiltonian separated into an unperturbed Keplerian Hamiltonian H_0 and a perturbation H_1 in Jacobi coordinates. In addition, these algorithms constructed in the splitting of $T + V$ can be directly applied to the separable form of $H_0 + H_1$. As is well known, the same symplectic integrator has a different numerical performance with the two decompositions, in which the latter is greatly superior to the former in terms of accuracy. Along this direction, the symplectic correctors of Wisdom et al. (1996), the pseudo-high-order symplectic integrators of Chambers & Murison (2000), and so on, were developed and have been popular in the solar system. A common character of these methods is that they are attributed to standard symplectic integration algorithms that use some negative time steps except for first- and second-order algorithms.

On the other hand, an unusual symplectic integrator, a third-order force gradient explicit symplectic algorithm, was born at the same time when the standard third-order explicit symplectic algorithm was first given by Ruth (1983). The gradient algorithm has only positive time steps, but requires computation of the force gradient with the force. Its implementation is in the splitting of $T + V$. However, few researchers have recognized it and considered its application and development. This is because it is not necessary to use purely positive time steps in classical dynamics that are time reversible, and it may not be convenient to use the force gradient. In contrast, the demand for positive time steps is vital when one solves time-irreversible equations such as imaginary time Schrödinger equations. Because of this, Chin and coworkers (Chin 1997, 2004, 2006, 2007; Chin & Kidwell 2000; Chin & Chen 2001, 2005) developed this kind of gradient algorithm and extended it to the fourth order. Each of the algorithms has been confirmed to have 10 to 80 times better accuracy than a standard Forest-Ruth method of the same order (Chin 1997), and also to be very efficient in solving the circular restricted three-body problem as a gravitational few-body problem with an explicit time-dependent force field (Chin & Chen 2005), as well as both classical and quantum dynamical problems (Chin & Chen 2001).

In this paper, we shall give some fourth-order force gradient symplectic algorithms in the splitting of $T + V$ and extend them to solve a gravitational many-body Hamiltonian problem with the splitting of $H_0 + H_1$ in Jacobi coordinates. Our main aim is to understand the efficiency of these gradient algorithms in this case, and identify whether the accuracy of each gradient integrator is still far superior to that of the standard fourth-order Forest-Ruth method. The rest of this paper is organized as follows. In Section 2, we establish two types of fourth-order gradient symplectic algorithms in terms of different compositions of the force gradient operators. Then they are extended to work out both a perturbed Kepler problem and an n -body problem in the two types of Hamiltonian decompositions. Details of implementing the algorithms are also given. In Section 3, we use two physical models to evaluate the performance of these gradient algorithms. Finally, Section 4 gives our conclusions and discussions.

2 FOURTH-ORDER FORCE GRADIENT SYMPLECTIC ALGORITHMS FOR SOLVING N -BODY PROBLEMS

Let X , Y and Z be non-commutative operators. The Baker-Campbell-Hausdorff (BCH) formula (Blanes et al. 2008; Casas & Murua 2009) relates to the expansion of Z with the product of two exponential functions, $e^X e^Y = e^Z$, expressed as

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}([X, X, Y] + [Y, Y, X]) + \frac{1}{24}[X, Y, Y, X]$$

$$\begin{aligned}
 & - \frac{1}{720}([Y, Y, Y, Y, X] + [X, X, X, X, Y]) + \frac{1}{360}([Y, X, X, X, Y] + [X, Y, Y, Y, X]) \\
 & + \frac{1}{120}([X, X, Y, Y, X] + [Y, Y, X, X, Y]) + \dots, \quad (1)
 \end{aligned}$$

where the commutators $[X, Y] = XY - YX$, and $[X, X, Y] = [X, [X, Y]]$, etc. It is possible to compute the product of more operators like these. In particular, for the symmetric composite operators $e^X e^Y e^X = e^W$, W reads easily as

$$\begin{aligned}
 W &= 2X + Y + \frac{1}{6}([Y, Y, X] - [X, X, Y]) + \frac{1}{360}(7[X, X, X, X, Y] - [Y, Y, Y, Y, X]) \\
 &+ \frac{1}{90}[X, Y, Y, Y, X] + \frac{1}{45}[Y, X, X, X, Y] - \frac{1}{60}[X, X, Y, Y, X] + \frac{1}{30}[Y, Y, X, X, Y] + \dots. \quad (2)
 \end{aligned}$$

Next, in this way, let us build fourth-order force gradient explicit symplectic algorithms, and be engaged in studying their effectiveness in solving gravitational n -body problems in Jacobi coordinates.

2.1 Construction of Fourth-Order Gradient Integrators in the Splitting of $T + V$

Usually, a Hamiltonian H is a summation of kinetic energy $T(\mathbf{p})$ and potential energy $V(\mathbf{q})$, namely,

$$H = T(\mathbf{p}) + V(\mathbf{q}). \quad (3)$$

Assume that T is only a positive definite quadratic function with respect to momentum \mathbf{p} , i.e. $T(\mathbf{p}) = \mathbf{p}^2/2$, and V stands for a function of position \mathbf{q} . We also define the Lie derivatives \hat{T} and \hat{V} associated with T and V as $\hat{T} = \mathcal{D}_T = \{ \cdot, T \}$ and $\hat{V} = \mathcal{D}_V = \{ \cdot, V \}$ (symbol $\{ \cdot, \cdot \}$ being the Poisson bracket), equivalently,

$$\hat{T} = \sum_{i=1}^3 p_i \frac{\partial}{\partial q_i}, \quad \hat{V} = \sum_{i=1}^3 f_i \frac{\partial}{\partial p_i} \quad (4)$$

with $f_i = -\partial V/\partial q_i$, where q_i and p_i represent, respectively, the i th generalized coordinate and momentum, and f_i is the i th component of the force. It can be easily inferred that

$$[\hat{V}, \hat{T}, \hat{V}] = \{ \cdot, \{ \{ V, T \}, V \} \} = 2 \sum_{i,j,k=1}^3 V_{ij} V_k T_{jk} \frac{\partial}{\partial p_i} = 2 \sum_{i,j=1}^3 f_j \frac{\partial f_i}{\partial q_j} \frac{\partial}{\partial p_i} = \sum_{i=1}^3 \nabla_i |\mathbf{f}|^2 \frac{\partial}{\partial p_i}, \quad (5)$$

where $V_k = \frac{\partial V}{\partial q_k}$, $V_{ij} = \frac{\partial^2 V}{\partial q_i \partial q_j}$ and $T_{jk} = \frac{\partial^2 T}{\partial p_j \partial p_k}$. Obviously, operator $[\hat{V}, \hat{T}, \hat{V}]$ refers to the gradient of force \mathbf{f} . See also the article of Chin (1997).

Now, we add the gradient operator to one operator \hat{V} or two, and then consider two different symmetric compositions of operators \hat{V} , \hat{T} and $[\hat{V}, \hat{T}, \hat{V}]$, like the construction of the standard higher-order symplectic algorithms of Yoshida (1990).

2.1.1 A-type algorithms: the gradient operator is arranged at the midpoint of compositions

Let us consider symmetric combinatorial operators in the form

$$e^{a_1 \tau \hat{T}} e^{b_1 \tau \hat{V}} e^{a_2 \tau \hat{T}} e^{\tilde{V}} e^{a_2 \tau \hat{T}} e^{b_1 \tau \hat{V}} e^{a_1 \tau \hat{T}} = e^{\tau W}, \quad (6)$$

where $\tilde{V} = b_2 \tau \hat{V} + b_3 \tau^3 [\hat{V}, \hat{T}, \hat{V}]$, τ is the timestep, and a_i and b_i are a set of positive time coefficients that we shall determine. Carrying out the recurrent derivation from the middle of composition (6) in terms of Equation (2), we have

$$\begin{aligned}
 W &= 2(a_1 + a_2)\hat{T} + (2b_1 + b_2)\hat{V} + \left[b_3 + \frac{a_2}{3}(b_1^2 + b_1 b_2 - \frac{1}{2}b_2^2) - \frac{a_1}{6}(2b_1 + b_2)^2 \right] \tau^2 [\hat{V}, \hat{T}, \hat{V}] \\
 &+ \left[\frac{1}{6}a_2^2(b_2 - 4b_1) + \frac{1}{3}a_1 a_2(2b_1 + b_2) + \frac{1}{6}a_1^2(2b_1 + b_2) \right] \tau^2 [\hat{T}, \hat{V}, \hat{T}] + \mathcal{O}(\tau^4), \quad (7)
 \end{aligned}$$

where terms smaller than $\mathcal{O}(\tau^3)$ are neglected. The fourth-order conditions should satisfy the following relations

$$2(a_1 + a_2) = 1, \tag{8}$$

$$2b_1 + b_2 = 1, \tag{9}$$

$$b_3 + \frac{a_2}{3}(b_1^2 + b_1b_2 - \frac{1}{2}b_2^2) - \frac{a_1}{6}(2b_1 + b_2)^2 = 0, \tag{10}$$

$$\frac{1}{6}a_2^2(b_2 - 4b_1) + \frac{1}{3}a_1a_2(2b_1 + b_2) + \frac{1}{6}a_1^2(2b_1 + b_2) = 0. \tag{11}$$

Clearly, the above four constraints turn out to indicate that the five coefficients must have a wide freedom of choice in terms of possible values, so that an infinite number of fourth-order integrators can be obtained. For example, given a group of time coefficients, $a_1 = 1/6$, $a_2 = 1/3$, $b_1 = 3/8$, $b_2 = 1/4$ and $b_3 = 1/192$, composition method (6) just corresponds to the fourth-order algorithm C of Chin (1997) of the form

$$(A1) \quad e^{\frac{\tau}{6}\hat{T}} e^{\frac{3\tau}{8}\hat{V}} e^{\frac{\tau}{3}\hat{T}} e^{\frac{\tau}{4}\hat{V}} + \frac{\tau^3}{192}[\hat{V}, \hat{T}, \hat{V}] e^{\frac{\tau}{3}\hat{T}} e^{\frac{3\tau}{8}\hat{V}} e^{\frac{\tau}{6}\hat{T}}. \tag{12}$$

Without loss of generality, a_2 is assumed to be an autonomous coefficient. Given an additional constraint that the sum of squares of some of these time coefficients as functions of a_2 is required to be minimized, we can get several new fourth-order algorithms with known positive time coefficients listed in Table 1.

Table 1 Several Groups of Positive Time Coefficients for A-Type Fourth Order Algorithms

Algorithm constraint $\Gamma'(a_2) = 0$	a_1 b_1	a_2 b_2	b_3
A2 $\Gamma(a_2) = b_1^2 + b_2^2$	$\frac{1}{2} - \frac{\sqrt{15}}{12}$ $\frac{2}{5}$	$\frac{\sqrt{15}}{12}$ $\frac{1}{5}$	$\frac{1}{12} - \frac{\sqrt{15}}{50}$
A3 $\Gamma(a_2) = a_1^2 + a_2^2$ $+b_1^2 + b_2^2 + b_3^2$	0.181441601770871 0.410592148470405	0.318558398229129 0.178815703059189	0.0062402144046793
A4 $\Gamma(a_2) = b_3$	$\frac{1}{2} - \frac{\sqrt{2}}{4}$ $\frac{1}{3}$	$\frac{\sqrt{2}}{4}$ $\frac{1}{3}$	$\frac{1}{12} - \frac{\sqrt{2}}{18}$

2.1.2 B-type algorithms: the gradient operators are arranged at the ends of compositions

For the following combinatorial operators

$$e^{\tilde{V}} e^{a_1\tau\hat{T}} e^{b_3\tau\hat{V}} e^{a_2\tau\hat{T}} e^{b_3\tau\hat{V}} e^{a_1\tau\hat{T}} e^{\tilde{V}} = e^{\tau W} \tag{13}$$

with $\tilde{V} = b_1\tau\hat{V} + b_2\tau^3[\hat{V}, \hat{T}, \hat{V}]$, W , like that of the A-type algorithms, is easily written as

$$W = (2a_1 + a_2)\hat{T} + 2(b_1 + b_3)\hat{V} + \left[\frac{b_3}{3}(a_1^2 + a_1a_2 - \frac{1}{2}a_2^2) - \frac{b_1}{6}(2a_1 + a_2)^2 \right] \tau^2[\hat{T}, \hat{V}, \hat{T}] + \left[\frac{1}{6}b_3^2(a_2 - 4a_1) + 2b_2 + \frac{1}{3}b_1b_3(2a_1 + a_2) + \frac{1}{6}b_1^2(2a_1 + a_2) \right] \tau^2[\hat{V}, \hat{T}, \hat{V}] + \mathcal{O}(\tau^4). \tag{14}$$

Still, the fourth-order conditions should be as follows:

$$2a_1 + a_2 = 1, \tag{15}$$

$$2(b_1 + b_3) = 1, \tag{16}$$

$$\frac{b_3}{3}(a_1^2 + a_1a_2 - \frac{1}{2}a_2^2) - \frac{b_1}{6}(2a_1 + a_2)^2 = 0, \tag{17}$$

$$\frac{1}{6}b_3^2(a_2 - 4a_1) + 2b_2 + \frac{1}{3}b_1b_3(2a_1 + a_2) + \frac{1}{6}b_1^2(2a_1 + a_2) = 0. \tag{18}$$

At once, we achieve some coefficients of B-type algorithms in Table 2. Note that algorithm B1 with the form

$$(B1) \quad e^{\frac{\tau}{8}\hat{V} + \frac{\tau^3}{384}[\hat{V}, \hat{T}, \hat{V}]} e^{\frac{\tau}{3}\hat{T}} e^{\frac{3\tau}{8}\hat{V}} e^{\frac{\tau}{3}\hat{T}} e^{\frac{3\tau}{8}\hat{V}} e^{\frac{\tau}{3}\hat{T}} e^{\frac{\tau}{8}\hat{V} + \frac{\tau^3}{384}[\hat{V}, \hat{T}, \hat{V}]} \tag{19}$$

is just scheme D of Chin & Chen (2001).

Table 2 Several Groups of Positive Time Coefficients on B-Type Fourth-Order Algorithms

Algorithm constraint $\Gamma'(a_2) = 0$	a_1 b_1	a_2 b_2	b_3
B1 $\Gamma(a_2) = b_2$	$\frac{1}{3}$ $\frac{1}{8}$	$\frac{1}{3}$ $\frac{1}{384}$	$\frac{3}{8}$
B2 $\Gamma(a_2) = a_1^2 + a_2^2$	$\frac{2}{5}$ $\frac{71}{72}$	$\frac{1}{5}$ $\frac{17}{5184}$	$\frac{25}{72}$
B3 $\Gamma(a_2) = a_1^2 + a_2^2 + b_2^2$	0.399986824812539 0.152773965219889	0.200026350374923 0.0032790562731969	0.347226034780111
B4 $\Gamma(a_2) = a_1^2 + a_2^2 + b_1^2 + b_2^2 + b_3^2$	0.409715409973947 0.155431946448732	0.180569180052107 0.0034888368094941	0.344568053551268

Properly speaking, the above-mentioned symplectic integrators, besides the methods proposed by Chin (1997), are all constructed in the decomposition of $T + V$. They need calculation of the gradient of force, and coefficients in the combinatorial operators are all positive. In contrast, some negative coefficients have to appear in the combinatorial operators of the standard higher-order symplectic methods given by Yoshida (1990) and Forest & Ruth (1990). In other words, a positive step length of each substep for the former is admissible to adopt, but a negative step length of at least one substep for the latter cannot be avoided. It should be pointed out that the splitting method of a Hamiltonian function plays an important role in the accuracy of a symplectic integrator. As Wisdom & Holman (1991) confirmed, a standard symplectic algorithm in the splitting of an unperturbed Keplerian Hamiltonian and a perturbative one brings a more notable improvement in the computational efficiency and the numerical accuracy than it does in the decomposition similar to Equation (3). Therefore, it is very significant to apply these algorithms to the perturbative decomposition.

2.2 Extending the Algorithms to Integrate a Perturbed Kepler Problem

Consider a perturbed Kepler problem

$$H = H_0(\mathbf{q}, \mathbf{p}) + \varepsilon H_1(\mathbf{q}), \tag{20}$$

where H_0 , as a primary, integrable Keplerian part, is of the expression $H_0 = T(\mathbf{p}) + V_0(\mathbf{q})$ with $T(\mathbf{p}) = \mathbf{p}^2/2$ and $V_0(\mathbf{q}) = -\mu/r$ ($r = |\mathbf{q}|$, and μ is a constant connected with mass and gravity), and H_1 is regarded as a secondary, perturbation part. In addition, ε is a small perturbation parameter used as a mark of H_1 being much smaller than H_0 . If the system still adopts the decomposition of Equation (3), we employ the above force gradient symplectic integrators to work it out without any difficulty as Chin (1997) did. Still, there is an open problem of whether the integrators are useful for the decomposition of Equation (20). In order to answer this, an in-depth exploration will be necessary.

2.2.1 Implementation Details

We specify the Lie derivatives \hat{H}_0 and \hat{H}_1 as follows:

$$\hat{H}_0 = \{ \cdot, H_0 \} = \sum_{i=1}^3 (p_i \frac{\partial}{\partial q_i} + g_i \frac{\partial}{\partial p_i}), \quad \hat{H}_1 = \{ \cdot, H_1 \} = \sum_{i=1}^3 f_i \frac{\partial}{\partial p_i}, \quad (21)$$

where $g_i = -\partial V_0 / \partial q_i$ and $f_i = -\partial H_1 / \partial q_i$. If \hat{T} and \hat{V} mentioned above give place to \hat{H}_0 and \hat{H}_1 , respectively, the force gradient symplectic algorithms are easily rewritten in the expressional forms. As an example, here we provide the modified versions of Algorithms A1 and B1 in the following

$$(\varepsilon\text{-A1}) \quad e^{\frac{\tau}{6}\hat{H}_0} e^{\frac{3}{8}\tau\varepsilon\hat{H}_1} e^{\frac{\tau}{3}\hat{H}_0} e^{\frac{\tau}{4}\varepsilon\hat{H}_1 + \frac{\tau^3}{192}\varepsilon^2[\hat{H}_1, \hat{H}_0, \hat{H}_1]} e^{\frac{\tau}{3}\hat{H}_0} e^{\frac{3}{8}\tau\varepsilon\hat{H}_1} e^{\frac{\tau}{6}\hat{H}_0}, \quad (22)$$

and

$$(\varepsilon\text{-B1}) \quad e^{\frac{\tau}{8}\varepsilon\hat{H}_1 + \frac{\tau^3}{384}\varepsilon^2[\hat{H}_1, \hat{H}_0, \hat{H}_1]} e^{\frac{\tau}{3}\hat{H}_0} e^{\frac{3}{8}\tau\varepsilon\hat{H}_1} e^{\frac{\tau}{3}\hat{H}_0} e^{\frac{3}{8}\tau\varepsilon\hat{H}_1} e^{\frac{\tau}{3}\hat{H}_0} e^{\frac{\tau}{8}\varepsilon\hat{H}_1 + \frac{\tau^3}{384}\varepsilon^2[\hat{H}_1, \hat{H}_0, \hat{H}_1]}. \quad (23)$$

For emphasis, the key point for the use of the ε -type algorithms is how to treat the operator $[\hat{H}_1, \hat{H}_0, \hat{H}_1]$. In fact, the computation of the operator is completely the same as that of $[\hat{V}, \hat{T}, \hat{V}]$, that is,

$$\begin{aligned} [\hat{H}_1, \hat{H}_0, \hat{H}_1] &= \{ \cdot, \{ \{ H_1, H_0 \}, H_1 \} \} = \{ \cdot, \{ \{ H_1, T + V_0 \}, H_1 \} \} = \{ \cdot, \{ \{ H_1, T \}, H_1 \} \} \\ &= 2 \sum_{i,j=1}^3 f_j \frac{\partial f_i}{\partial q_j} \frac{\partial}{\partial p_i} = \sum_{i=1}^3 \nabla_i |\mathbf{f}|^2 \frac{\partial}{\partial p_i}. \end{aligned} \quad (24)$$

2.2.2 Discrete difference formulae

According to the different decompositions of the Hamiltonian function, we design difference schemes of the symplectic algorithms from a twofold point of view.

Case 1: Decomposition of $T + V$. — For the perturbed Kepler problem with splitting of kinetic energy T and potential energy $V = V_0(\mathbf{q}) + \varepsilon H_1(\mathbf{q})$, we have $f_i = -\partial V / \partial q_i$. Then, we still use Algorithms A1 and B1 as examples to illustrate the mechanism of the difference schemes. The difference scheme of Equation (12) is of the version

$$\begin{aligned} (\text{A1}) \quad \mathbf{q}^* &= \mathbf{q}_{s-1} + \frac{\tau}{6} \mathbf{p}_{s-1}, \\ \mathbf{p}^* &= \mathbf{p}_{s-1} + \frac{3}{8} \tau \mathbf{f}(\mathbf{q}^*), \\ \mathbf{q}^{**} &= \mathbf{q}^* + \frac{\tau}{3} \mathbf{p}^*, \\ \mathbf{p}^{**} &= \mathbf{p}^* + \frac{\tau}{4} \left[\mathbf{f}(\mathbf{q}^{**}) + \frac{\tau^2}{48} \nabla |\mathbf{f}(\mathbf{q}^{**})|^2 \right], \\ \mathbf{q}^{***} &= \mathbf{q}^{**} + \frac{\tau}{3} \mathbf{p}^{**}, \\ \mathbf{p}_s &= \mathbf{p}^{**} + \frac{3}{8} \tau \mathbf{f}(\mathbf{q}^{***}), \\ \mathbf{q}_s &= \mathbf{q}^{***} + \frac{\tau}{6} \mathbf{p}_s, \end{aligned} \quad (25)$$

where $s (=1, 2, \dots)$ is the number of integration step points. Meanwhile, that of Equation (19) reads

$$\begin{aligned}
 & \text{(B1)} \\
 \mathbf{p}^* &= \mathbf{p}_{s-1} + \frac{\tau}{8} \left[\mathbf{f}(\mathbf{q}_{s-1}) + \frac{\tau^2}{48} \nabla |\mathbf{f}(\mathbf{q}_{s-1})|^2 \right], \\
 \mathbf{q}^* &= \mathbf{q}_{s-1} + \frac{\tau}{3} \mathbf{p}^*, \\
 \mathbf{p}^{**} &= \mathbf{p}^* + \frac{3}{8} \tau \mathbf{f}(\mathbf{q}^*), \\
 \mathbf{q}^{**} &= \mathbf{q}^* + \frac{\tau}{3} \mathbf{p}^{**}, \\
 \mathbf{p}^{***} &= \mathbf{p}^{**} + \frac{3}{8} \tau \mathbf{f}(\mathbf{q}^{**}), \\
 \mathbf{q}_s &= \mathbf{q}^{**} + \frac{\tau}{3} \mathbf{p}^{***}, \\
 \mathbf{p}_s &= \mathbf{p}^{***} + \frac{\tau}{8} \left[\mathbf{f}(\mathbf{q}_s) + \frac{\tau^2}{48} \nabla |\mathbf{f}(\mathbf{q}_s)|^2 \right].
 \end{aligned} \tag{26}$$

Case 2: Decomposition of $H_0 + H_1$. — When the Hamiltonian has a separable form like Equation (20), the Keplerian part, H_0 , as a main piece, from the initial state $(\mathbf{q}_0, \mathbf{p}_0)$ to time τ has the analytic solution, $\mathbf{q} = \text{Kepler1}(\mathbf{q}_0, \mathbf{p}_0, \tau)$ and $\mathbf{p} = \text{Kepler2}(\mathbf{q}_0, \mathbf{p}_0, \tau)$, expressed by Gaussian functions. See the book by Murray & Dermott (1999) for more details. Given $\mathbf{f} = -\partial H_1 / \partial \mathbf{q}$, Equations (22) and (23) correspond to the following difference schemes:

$$\begin{aligned}
 & \text{(\varepsilon-A1)} \\
 \mathbf{q}^* &= \text{Kepler1}(\mathbf{q}_{s-1}, \mathbf{p}_{s-1}, \frac{\tau}{6}), \\
 \mathbf{p}^* &= \text{Kepler2}(\mathbf{q}_{s-1}, \mathbf{p}_{s-1}, \frac{\tau}{6}), \\
 \mathbf{p}^\dagger &= \mathbf{p}^* + \frac{3}{8} \tau \varepsilon \mathbf{f}(\mathbf{q}^*), \\
 \mathbf{q}^{**} &= \text{Kepler1}(\mathbf{q}^*, \mathbf{p}^\dagger, \frac{\tau}{3}), \\
 \mathbf{p}^{**} &= \text{Kepler2}(\mathbf{q}^*, \mathbf{p}^\dagger, \frac{\tau}{3}), \\
 \mathbf{p}^\ddagger &= \mathbf{p}^{**} + \frac{\tau \varepsilon}{4} \left[\mathbf{f}(\mathbf{q}^{**}) + \frac{\tau^2 \varepsilon}{48} \nabla |\mathbf{f}(\mathbf{q}^{**})|^2 \right], \\
 \mathbf{q}^{***} &= \text{Kepler1}(\mathbf{q}^{**}, \mathbf{p}^\ddagger, \frac{\tau}{3}), \\
 \mathbf{p}^{***} &= \text{Kepler2}(\mathbf{q}^{**}, \mathbf{p}^\ddagger, \frac{\tau}{3}), \\
 \mathbf{p}^\# &= \mathbf{p}^{***} + \frac{3}{8} \tau \varepsilon \mathbf{f}(\mathbf{q}^{***}), \\
 \mathbf{q}_s &= \text{Kepler1}(\mathbf{q}^{***}, \mathbf{p}^\#, \frac{\tau}{6}), \\
 \mathbf{p}_s &= \text{Kepler2}(\mathbf{q}^{***}, \mathbf{p}^\#, \frac{\tau}{6}),
 \end{aligned} \tag{27}$$

and

$$\begin{aligned}
 & \text{(\varepsilon-B1)} \\
 \mathbf{p}^\clubsuit &= \mathbf{p}_{s-1} + \frac{\tau \varepsilon}{8} \left[\mathbf{f}(\mathbf{q}_{s-1}) + \frac{\tau^2 \varepsilon}{48} \nabla |\mathbf{f}(\mathbf{q}_{s-1})|^2 \right],
 \end{aligned}$$

$$\begin{aligned}
\mathbf{q}^* &= \text{Kepler1}(\mathbf{q}_{s-1}, \mathbf{p}^\clubsuit, \frac{\tau}{3}), \\
\mathbf{p}^* &= \text{Kepler2}(\mathbf{q}_{s-1}, \mathbf{p}^\clubsuit, \frac{\tau}{3}), \\
\mathbf{p}^\diamond &= \mathbf{p}^* + \frac{3}{8}\tau\varepsilon\mathbf{f}(\mathbf{q}^*), \\
\mathbf{q}^{**} &= \text{Kepler1}(\mathbf{q}^*, \mathbf{p}^\diamond, \frac{\tau}{3}), \\
\mathbf{p}^{**} &= \text{Kepler2}(\mathbf{q}^*, \mathbf{p}^\diamond, \frac{\tau}{3}), \\
\mathbf{p}^\spadesuit &= \mathbf{p}^{**} + \frac{3}{8}\tau\varepsilon\mathbf{f}(\mathbf{q}^{**}), \\
\mathbf{q}_s &= \text{Kepler1}(\mathbf{q}^{**}, \mathbf{p}^\spadesuit, \frac{\tau}{3}), \\
\mathbf{p}^{***} &= \text{Kepler2}(\mathbf{q}^{**}, \mathbf{p}^\spadesuit, \frac{\tau}{3}), \\
\mathbf{p}_s &= \mathbf{p}^{***} + \frac{\tau\varepsilon}{8} \left[\mathbf{f}(\mathbf{q}_s) + \frac{\tau^2\varepsilon}{48} \nabla|\mathbf{f}(\mathbf{q}_s)|^2 \right].
\end{aligned} \tag{28}$$

Besides the perturbed two-body problem, these algorithms can further be extended to treat the case of multiple bodies in planetary dynamics. In the following, we list the details of this extension.

2.3 Extending the Algorithms to Solve an n -body Problem in Jacobi Coordinates

In the barycentric coordinate frame, an n -body problem in the solar system has the Hamiltonian function

$$H = \sum_{i=0}^{n-1} \frac{|\mathbf{p}_i|^2}{2m_i} - \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \frac{Gm_i m_j}{q_{ij}} \tag{29}$$

with $q_{ij} = |\mathbf{q}_i - \mathbf{q}_j|$ as the distance between body i and body j . Note that $i = 0$ denotes the Sun, m_i is the mass of body i , and G is the gravitational constant. Equation (29) itself looks to be the separation of $T + V$ ¹, but one had better consider the algorithms in the separation like Equation (20), as discussed above. In view of this, Wisdom & Holman (1991) gave a method to successfully implement the desired separation. By taking advantage of the Jacobi coordinates

$$\mathbf{q}'_i = \begin{cases} \mathbf{q}_i - \frac{1}{M_{i-1}} \sum_{j=0}^{i-1} m_j \mathbf{q}_j & (0 < i < n), \\ \frac{1}{M_{n-1}} \sum_{j=0}^{n-1} m_j \mathbf{q}_j & (i = 0), \end{cases} \tag{30}$$

where

$$M_i = \sum_{j=0}^i m_j, \tag{31}$$

and

$$m'_i = \begin{cases} M_{i-1} m_i / M_i & (0 < i < n) \\ M_{n-1} & (i = 0), \end{cases} \tag{32}$$

¹ Generally speaking, direct integration of Equation (29) in the barycentric coordinate system is not ideal for this Hamiltonian separation because the Sun is too close to the center of mass. Instead, numerical integrations are usually implemented in the heliocentric system, where the evolution of the Sun is not considered. After each integration step it must be considered by means of the constant laws of both the center of mass and the total momentum.

they rewrote the Hamiltonian as

$$H = H_0 + H_1, \quad (33)$$

$$H_0 = \sum_{i=1}^{n-1} \left(\frac{|\mathbf{p}'_i|^2}{2m'_i} - \frac{Gm_0m_i}{q'_i} \right), \quad (34)$$

$$H_1 = \sum_{i=1}^{n-1} \left(\frac{Gm_0m_i}{q'_i} - \frac{Gm_0m_i}{q_{i0}} \right) - \sum_{i=0}^{n-2} \sum_{j=i+1}^{n-1} \frac{Gm_im_j}{q_{ij}}. \quad (35)$$

For an illustration, $q'_i = |\mathbf{q}'_i|$, and barycentric coordinate \mathbf{q}_i does not appear in Equation (35) at all when it is expressed by Jacobi coordinate \mathbf{q}'_i in Equation (30). H_0 is the Keplerian part, and H_1 represents the interplanetary interactive part. In particular, the former is much larger than the latter.

By comparison of Equations (33) and (20), it is easy to understand that the force gradient symplectic integrators are also suitable for the n -body system in Jacobi coordinates. Here is a brief introduction to this problem.

For the decomposition of $T + V$ in Jacobi coordinates, kinetic energy T and potential energy V are described as

$$T = \sum_{i=1}^{n-1} \frac{|\mathbf{p}'_i|^2}{2m'_i}, \quad (36)$$

$$V = - \sum_{i=1}^{n-1} \frac{Gm_0m_i}{q_{i0}} - \sum_{i=0}^{n-2} \sum_{j=i+1}^{n-1} \frac{Gm_im_j}{q_{ij}}. \quad (37)$$

Then, we have

$$\hat{T} = \sum_{i=1}^{n-1} \sum_{j=1}^3 \frac{p'_{ij}}{m'_i} \frac{\partial}{\partial q'_{ij}}, \quad \hat{V} = \sum_{i=1}^{n-1} \sum_{j=1}^3 f_{ij} \frac{\partial}{\partial p'_{ij}}, \quad (38)$$

$$[\hat{V}, \hat{T}, \hat{V}] = 2 \sum_{i,\ell=1}^{n-1} \sum_{j,k=1}^3 \frac{f_{ik}}{m'_i} \frac{\partial f_{\ell j}}{\partial q'_{ik}} \frac{\partial}{\partial p'_{\ell j}} = \sum_{\ell=1}^{n-1} \sum_{j=1}^3 \nabla_{\ell j} \left(\sum_{i=1}^{n-1} \frac{|\mathbf{f}_i|^2}{m'_i} \right) \frac{\partial}{\partial p'_{\ell j}}. \quad (39)$$

In the above equations, $f_{ij} = -\partial V / \partial q'_{ij}$, index i (or ℓ) stands for planet i , index j (or k) denotes the j th component, and symbol $\nabla_{\ell j}$ is the gradient vs. the j th coordinate component of planet ℓ . In this case, either A-type algorithms or B-type algorithms like Equations (12) and (19) are easy to implement, as in the case of the perturbed two-body problem.

On the other hand, for the Hamiltonian decomposition of Equation (33), the implementation of the ε -type algorithms like Equations (22) and (23) is typically similar to that in the case of the perturbed two-body problem. Here, it is worth stressing that $f_{ij} = -\partial H_1 / \partial q'_{ij}$, and the computation of H_0 should still use the analytic solution of the pure Kepler problem. In addition, ε does not appear in Equations (22) and (23) or Equations (27) and (28) as a factor, but it plays a book-keeping role only for the perturbation and in fact refers to mass factors of planets.

From a theoretical point of view, the extension of both A-type algorithms and B-type algorithms to the perturbed Kepler problem and the n -body gravitational system in the splitting of $H_0 + H_1$ sounds very reasonable. What about its effectiveness in real computations? This awaits checking of our numerical experiments.

3 NUMERICAL SIMULATIONS

In this section, let us numerically evaluate the performance of these algorithms, such as A1, A4, B1 and B2, in comparison with the Forest-Ruth (1990) standard fourth-order symplectic method

$$(\text{FR}) \quad e^{\frac{\tau}{2c}X} e^{\frac{\tau}{c}Y} e^{\frac{1-k}{2c}\tau X} e^{\frac{-k}{c}\tau Y} e^{\frac{1-k}{2c}\tau X} e^{\frac{\tau}{c}Y} e^{\frac{\tau}{2c}X} \quad (40)$$

with $k = 2^{\frac{1}{3}}$, $c = 2 - k$, $X = \hat{T}$ and $Y = \hat{V}$ (or $X = \hat{H}_0$ and $Y = \hat{H}_1$). The physical models we choose are a perturbed two-body problem and a three-body problem made of the Sun, Jupiter and Saturn, in each of which there are two Hamiltonian splitting types, $T + V$ like in Equation (3) and $H_0 + H_1$ in Equation (20).

3.1 Perturbed Two-body Problem

The dynamics of a satellite moving around a slightly oblate spherical planet is viewed as a simple perturbed two-body problem. The physical model can be described by the following Hamiltonian (Blanes et al. 2008)

$$H = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{r} - \frac{\varepsilon}{2r^3} \left(1 - \frac{3q_1^2}{r^2}\right), \quad (41)$$

where $r = \sqrt{q_1^2 + q_2^2}$, and ε is a small parameter. In the case of $\varepsilon = 0$, Equation (41) is just a pure integrable Kepler problem. When ε is small, system (41) is near-integrable. As mentioned in Section 2, the Hamiltonian has two splitting methods: one is separable into two solvable parts, kinetic energy $T = (p_1^2 + p_2^2)/2$ and potential energy $V = -1/r - \varepsilon(1 - 3q_1^2/r^2)/(2r^3)$, and the other deals with the perturbative decomposition, including the Kepler problem $H_0 = (p_1^2 + p_2^2)/2 - 1/r$ and the small perturbation $\varepsilon H_1 = -\varepsilon(1 - 3q_1^2/r^2)/(2r^3)$.

Now, we take $\varepsilon = 0.001$ and initial conditions $q_1 = 1 - e$, $q_2 = 0$, $p_1 = 0$ and $p_2 = \sqrt{(1+e)/(1-e)}$, with $e = 0.2$ as the eccentricity of the unperturbed Kepler part H_0 . The fixed time step is 6.98×10^{-2} , 1/90 of the orbital period for the Kepler problem. Each of the algorithms, FR, A1, A4, B1 and B2, is applied to solve system (41) in the two Hamiltonian decompositions. Its relative energy error $\Delta E/E$ is plotted in Figure 1, where the left-hand side relates to that of the $T + V$ decomposition, and the right-hand side deals with that of the ε -type algorithms, i.e. that of the $H_0 + H_1$ decomposition. It can be clearly observed that each integrator retains an important character of a symplectic algorithm: that the energy error varies not secularly but rather periodically with time. In addition, Figure 1(a), (c), (e), (g) and (i) display that in the $T + V$ decomposition, the energy error for each gradient integrator is approximately 10 to 1000 times smaller than the standard fourth-order Forest-Ruth method. This is basically in agreement with the result of Chin (1997). However, not all of the algorithms have significant differences in the energy error in the case of the $H_0 + H_1$ decomposition, as shown in Figure 1(b), (d), (f), (h) and (j). It should be particularly emphasized that the accuracy of energy for any algorithm in the $H_0 + H_1$ -type decomposition is explicitly superior to one in the $T + V$ -type decomposition.

What would happen if these algorithms were applied to real many-body problems in the solar system? See the further numerical experiment for more information.

3.2 Three-body Problem

As a representative example of n -body problems, a three-body problem consisting of the Sun, Jupiter and Saturn is considered. In the Jacobi coordinate system, the Hamiltonian has two classes of separable forms, $T + V$ and $H_0 + H_1$ types, as introduced in Section 2. All the initial conditions and physical parameters are taken from JPL's planetary ephemeris DE405 at J2000.0. Note that the initial epoch in the heliocentric coordinate system should be changed into one in the barycentric coordinate system, and then it is re-given in the Jacobi coordinate system, where the various above-mentioned symplectic algorithms are used.

Figure 2 describes the evolution of the relative error of the total energy with time for each integrator. Here, the fixed time step is 36.525 d which is about 1/120 of Jupiter's orbital period, and the error must be computed in the barycentric coordinate frame because the total energy is constant only in this frame. Like the left-hand side of Figure 1, that of Figure 2 still gives the same fact that any gradient integrator is always greatly superior to the FR method in the accuracy of energy in

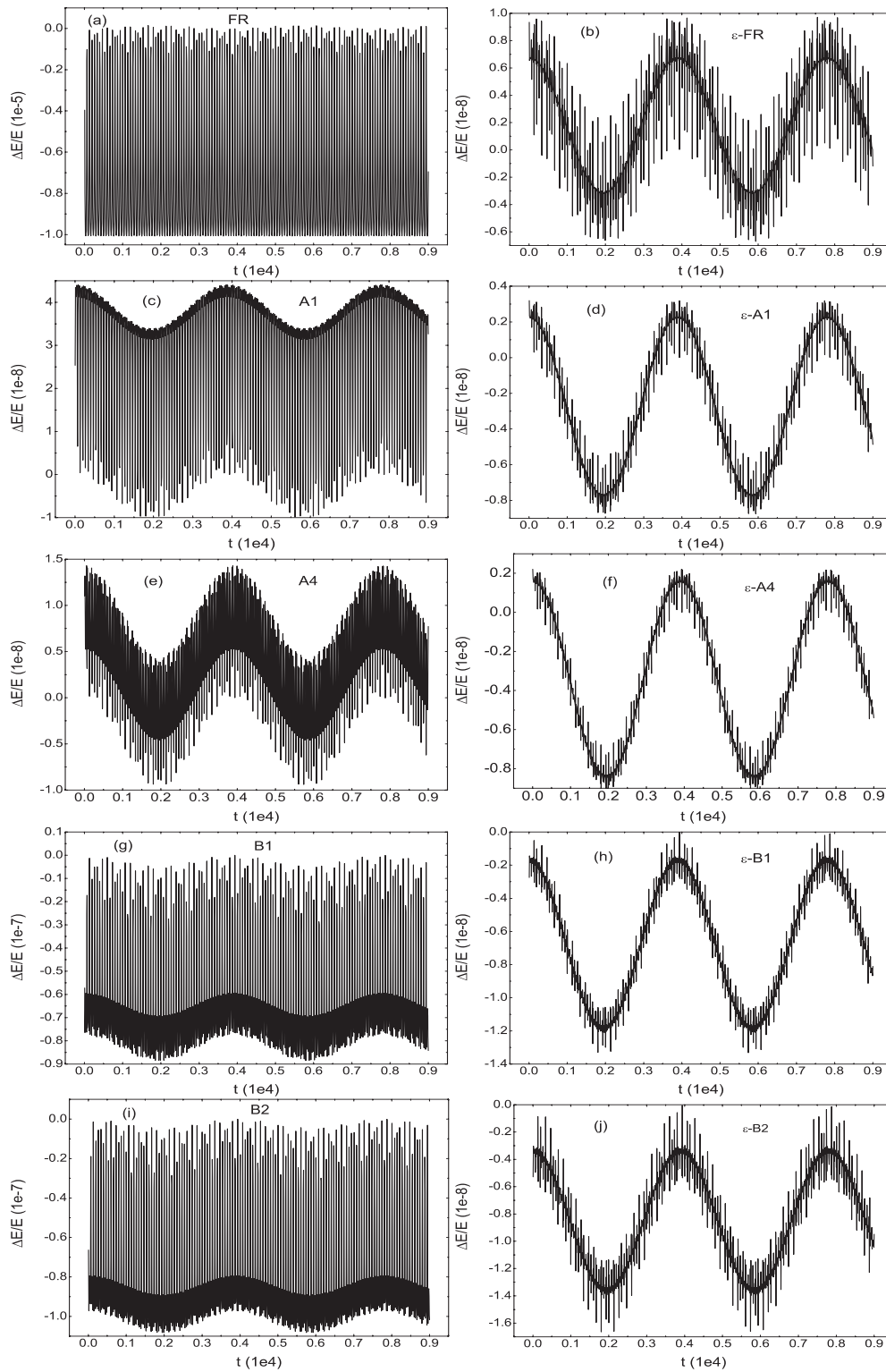


Fig.1 Relative energy errors $\Delta E/E$ of several symplectic integrators for solving the perturbed two-body problem in the two Hamiltonian decompositions. The left panels refer to those in the $T + V$ -type decomposition, and the right ones are those in the $H_0 + H_1$ -type decomposition, i.e. the ε -type algorithms.

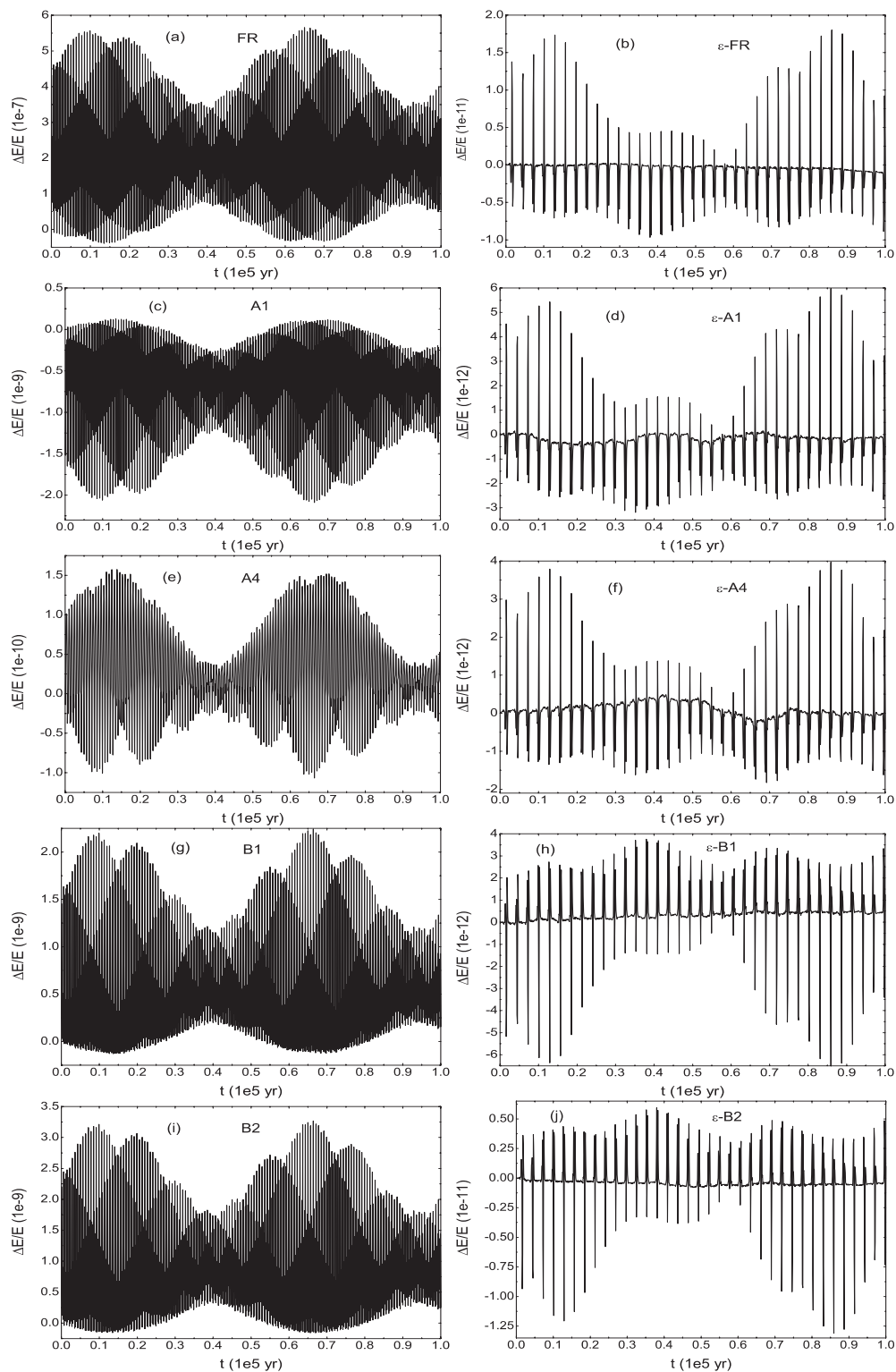


Fig. 2 Same as Fig. 1 but solving the three-body problem of the Sun, Jupiter and Saturn.

$T + V$ -type decomposition. However, the performance of the former is slightly better than that of the latter in $H_0 + H_1$ -type decomposition. See the right-hand side of Figure 2 for more information. In particular, compared with the $T + V$ -type decomposition, $H_0 + H_1$ -type decomposition gives each integrator a drastic improvement in energy accuracy of several orders of magnitude. In practice, an explicit answer to this can be given from the truncation errors of the Hamiltonian function in the two kinds of decompositions. The error of each fourth-order integrator is $\mathcal{O}(\tau^4)$ in the $T + V$ -type decomposition, but it is $\mathcal{O}(\varepsilon\tau^4)$ ($\varepsilon = |H_1/H_0| \approx 10^{-4}$ for the Sun-Jupiter-Saturn system) in the $H_0 + H_1$ -type decomposition.

Certainly, the mean longitude error, $\Delta\lambda = \Delta(M + \Omega + \omega)$ (where M , Ω and ω denote the mean anomaly, the longitude of ascending node and the argument of perihelion, respectively), as the along-track error (Huang & Innanen 1983), grows faster than the energy error. This implies that it is more important to use $\Delta\lambda$ as the evaluation of these symplectic integrators. To get this error, one needs a higher precision reference orbit that can be achieved by applying a 12th-order Cowell method to solve the three-body problem in the heliocentric coordinate system. The step size is 36.525 d for the Cowell method, while it is 365.25 d for each symplectic scheme. Hereafter, the related errors are all given in the heliocentric coordinate system. As in Figure 2, the same results in Figure 3 are that the mean longitude error of Jupiter for each force gradient method is smaller by two to three orders of magnitude than that for the FR scheme in $T + V$ -type decomposition, but they are both basically equivalent in $H_0 + H_1$ -type decomposition. It is clear that the latter decomposition decreases the mean longitude error of the former decomposition by about three orders of magnitude for the same gradient integrator. These facts can also be seen from Figure 4, which shows the relative position error of Jupiter for each symplectic integrator in the two types of Hamiltonian decompositions.

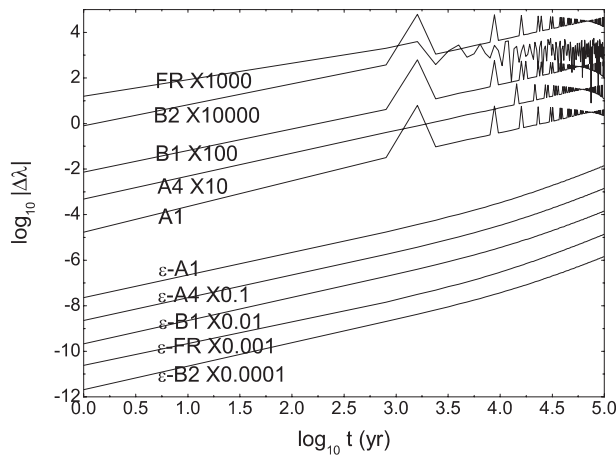


Fig. 3 Mean longitude errors of Jupiter. The details of the related symbols are as follows. For example, $A4 \times 10$ means that the errors compared with the real ones are enlarged by 10 times for A4, and $\varepsilon-A4 \times 0.1$ denotes that the errors are decreased by 10 times for $\varepsilon-A4$.

Perhaps someone believes that each gradient algorithm needs a great deal of additional computational time in the decomposition of $H_0 + H_1$. An answer can be found from Table 3, which compares the computational cost of the algorithms mentioned in Figure 2. Without a doubt, the computation of the force gradient operator $[\hat{H}_1, \hat{H}_0, \hat{H}_1]$ needs a little additional computational cost but is not very expensive. As to the same scheme, of course much more CPU time is needed for the decomposition of $H_0 + H_1$ than in the splitting of $T + V$ because the computation of the H_0 part deals

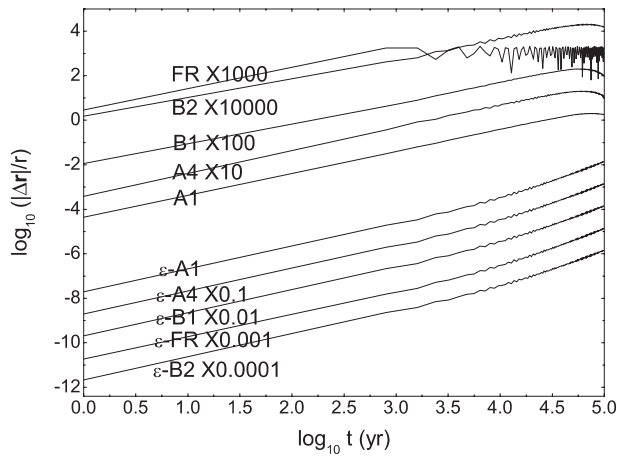


Fig. 4 Errors of the relative position of Jupiter.

Table 3 Comparison between computational cost, say, CPU times (units: min and s), for each algorithm with a fixed time step of $\tau = 36.525$ d between the two Hamiltonian decompositions of the three-body problem. As an illustration, the integration time of each scheme is 10^6 yr.

Algorithm	$T + V$	$H_0 + H_1$
FR	0'41''	2'20''
A1	1'12''	2'52''
A4	1'13''	2'52''
B1	1'44''	3'04''
B2	1'42''	3'00''

Table 4 CPU times of the related symplectic algorithms in the splitting of $T + V$. Here, each of these methods must use a suitably smaller time step so that it has the same accuracy as in the decomposition of $H_0 + H_1$ in Table 3.

Algorithm	Time step	$T + V$
FR	36.525/9 d	6'07''
A1	36.525/4 d	4'48''
A4	36.525/4 d	4'53''
B1	36.525/4 d	6'56''
B2	36.525/4 d	6'52''

with the use of the analytic method, where a certain iteration method is frequently used to solve the nonlinear Kepler equation. In spite of this, the cost is not expensive at all compared to the case of the $T + V$ -type decomposition in which each algorithm is required to have the same accuracy as in the decomposition of $H_0 + H_1$ in Table 3. See the detailed CPU times in Table 4.

4 CONCLUSIONS AND DISCUSSION

In this work, by different arrangements of the force gradient operators in combinatorial operators, two types of explicit fourth-order force gradient symplectic integrators, including those of Chin and coworkers, are specifically designed for a Hamiltonian system with a separation of kinetic energy T (as a quadratic function of momentum \mathbf{p}) and potential energy V (as a function of position \mathbf{q}). One relates to A-type algorithms in which the gradient operator is added to the midpoint of compositions, and the other relates to B-type algorithms where the gradient operators are arranged at the ends of compositions. Unlike the standard symplectic integrators, the two types of algorithms use fully positive time coefficients as the construction of composite operator factorizations. These algorithms are then extended to solve the perturbed Kepler problem, and the gravitational n -body problem with the splitting of the primary Keplerian part H_0 and the secondary perturbation part H_1 in the Jacobi coordinate system. The difficulty in treating the force gradient operator $[\hat{H}_1, \hat{H}_0, \hat{H}_1]$ for the Hamiltonian decomposition is dealt with from a theoretical point of view, and practical, efficient schemes for the implementation of these gradient algorithms are set up. As shown in numerical simulations, the standard fourth-order Forest-Ruth symplectic method is always greatly inferior to each gradient integrator in terms of the numerical accuracy when $T+V$ -type Hamiltonian decomposition is used, but it is almost equivalent when the case of $H_0 + H_1$ -type decomposition is adopted. In addition, there are not typical differences between the numerical performances of these gradient algorithms, either in $T+V$ -type decomposition or in $H_0 + H_1$ -type decomposition. Above all, the latter decomposition compared with the former decomposition can dramatically improve the accuracy of symplectic integrators.

The force gradient operator $[\hat{H}_1, \hat{H}_0, \hat{H}_1]$ seems to be more complicated in the formal expression than the operator \hat{H}_0 , so that doubt could be cast on the force gradient symplectic algorithms in terms of convenience of application. This is indeed a misunderstanding. In fact, the computation of commutator $[\hat{H}_1, \hat{H}_0, \hat{H}_1]$ by Equation (24) or Equation (39) with $f_{ij} = -\partial H_1 / \partial q'_{ij}$ becomes much simpler than that of the H_0 part, and it needs a little additional (but not very expensive) computational cost and labor for its implementation compared to that of perturbation H_1 . In view of this point and the above-mentioned facts, we recommend this kind of force gradient symplectic algorithm as a numerical integration tool for studying the long-term qualitative evolution of gravitational n -body Hamiltonian problems in Jacobi coordinates. These fourth-order gradient algorithms can easily be used to build higher-order gradient algorithms like the methods of Yoshida (1990), to introduce the symplectic correctors of Wisdom et al. (1996) and Wisdom (2006), and to develop the pseudo-high-order symplectic integrators of Chambers & Murison (2000), etc. It is worth pointing out that they cannot work in the Hamiltonian splitting method of Duncan et al. (1998), where by means of the heliocentric coordinates and the barycentric momenta, the n -body Hamiltonian is decomposed into three integrable parts, the Keplerian motion H_0 , motion H_1 of the Sun versus the barycenter and interactive potential H_2 between the planets, because of the difficulty in solving commutator $[\hat{H}_1, \hat{H}_0, \hat{H}_2]$.

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