RECENT PROGRESS IN THE THEORY AND APPLICATION OF SYMPLECTIC INTEGRATORS

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Abstract. In this paper various aspect of symplectic integrators are reviewed. Symplectic integrators are numerical integration methods for Hamiltonian systems which are designed to conserve the symplectic structure exactly as the original flow. There are explicit symplectic schemes for systems of the form $H = T(p) + V(q)$, and implicit schemes for general Hamiltonian systems. As a general property, symplectic integrators conserve the energy quite well and therefore an artificial damping (excitation) caused by the accumulation of the local truncation error cannot occur. Symplectic integrators have been applied to the Kepler problem, the motion of minor bodies in the solar system and the long-term evolution of outer planets.

Key words: Numerical integration methods – long time evolution – symplectic mapping

1. Introduction

1.1. MOTIVATION

For a given system of differential equations,

$$\frac{dz}{dt} = f(z), \tag{1}$$

we try to get an approximate solution from z at $t = 0$ to z' at $t = \tau$ in the form $z' = \psi(z, \tau)$, where τ is called the step size and assumed to be small. The most primitive one is called the Euler method which makes use of the mapping

$$z' = \psi(z, \tau) = z + \tau f(z). \tag{2}$$

This Euler method has the 1st order accuracy, since (2) agrees with the Taylor expansion of the true solution,

$$z' = z + \tau f(z) + \frac{\tau^2}{2} f'(z) f(z) + \frac{\tau^3}{6} \left(f''(z) f(z) + f'(z)^2 \right) f(z) + \dots \tag{3}$$

up to the 1st order of τ. We call a mapping $z' = \psi(z, \tau)$ an n-th order integration scheme (integration method, integrator), if it agrees with the Taylor expansion (3) up to the order of τ^n. The well-known classical Runge-Kutta method, which avoids the evaluation of higher derivatives of $f(z)$, is the 4th order in this sense.

When we apply these conventional integration methods to Hamiltonian systems, there occur an artificial excitation or damping which comes from the integration method itself. For example, for the one-dimensional harmonic oscillator with the Hamiltonian

$$H = (1/2)(p^2 + q^2), \tag{4}$$

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we know the exact solution

$$\begin{pmatrix} q(\tau) \\ p(\tau) \end{pmatrix} = \begin{pmatrix} \cos\tau & \sin\tau \\ -\sin\tau & \cos\tau \end{pmatrix} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix}. \tag{5}$$

On the other hands, the Euler method (2) approximates (5) as

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} 1 & \tau \\ -\tau & 1 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}. \tag{6}$$

One finds easily that at each step, the value of the energy is multiplied by $(1+\tau^2)$ with the Euler method (6), i.e.,

$$(p'^2 + q'^2) = (1+\tau^2)(p^2+q^2), \tag{7}$$

which leads to an indefinite increase of the energy. When we use the 4th order Runge-Kutta method we find, on the contrary, an artificial damping,

$$(p'^2 + q'^2) = (1 - \frac{1}{72}\tau^6 + ...)(p^2+q^2). \tag{8}$$

This artificial excitation or damping makes the result of long-time integration quite unreliable. Therefore it is desirable to use some special integration scheme for Hamiltonian systems.

For autonomous Hamiltonian systems

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}, \tag{9}$$

in general, we know that (i) the value of energy (Hamiltonian) is conserved, and that (ii) the mapping from (q,p) at $t=0$ to (q',p') at $t=\tau$ along the solution is symplectic (canonical),

$$dp \wedge dq = dp' \wedge dq', \tag{10}$$

i.e., the symplectic structure is conserved. The Euler method and Runge-Kutta method violate not only the conservation of energy but also the conservation of symplectic structure.

Then it is quite natural to search a numerical integration scheme which keeps the above two properties, (i) $H = const.$ and (ii) $dp \wedge dq = const.$. Unfortunately, according to Ge and Marsden (1988), there cannot exist such an integration scheme for non-integrable Hamiltonian systems in general. They claims that if such a scheme $z' = \psi(z,\tau)$ exists then it should coincides with the exact solution up to a reparametrization of the independent variable τ.

Now as a compromise, one may search schemes which keep one of the conservation properties. As for the Hamiltonian-conserving methods, there have been a lot of works by now and they will not be discussed in this paper. See Itoh and Abe (1988, 1989) and references therein. A scheme which conserves the symplectic structure (10) exactly is called a symplectic integration method (symplectic integrator) which will be reviewed from now on in detail.

1.2. History of Symplectic Integrators

The research on symplectic integrators originates from three independent groups. The first one is by Feng and his collaborators in Beijing who developed implicit symplectic schemes based on the generating function. See Feng and Qin (1987) for a review. This implicit method was later applied by Channell and Scovel (1990) extensively.

The second group of research starts with Sanz-Serna (1988) and Lasagni (1988). They found a condition for implicit Runge-Kutta methods to be symplectic. As a result, the family of Gauss-Legendre Runge-Kutta methods (Dekker and Verwer, 1984) are shown to be symplectic. The simplest one is known as the implicit midpoint rule.

As for the third group, Ruth(1983) developed an idea of explicit symplectic schemes for Hamiltonian of the form $H = T(p) + V(q)$. Along the line of Ruth(1983), higher order integrators were presented by Forest(1987), Neri(1988) and Yoshida(1990) later on.

In the next two sections, these implicit and explicit schemes will be explained in more detail. For a general review of symplectic integrators, see MacKay (1991), Sanz-Serna (1991) and Scovel (1991).

One important topic which will not be described in this paper is related to multistep methods. In fact, Eirola and Sanz-Serna (1990) proposed a multistep method which conserves the symplectic structure. On the other hand, Quinlan and Tremaine (1990) worked out with the symmetric multistep method which shows a good behavior on the conservation of energy, and might be understood as a kind of symplectic method. For this method, see also Kinoshita and Nakai (1991), and Quinlan and Toomre (1991).

2. Implicit Schemes

2.1. Generating Function Methods

For an arbitrary function of mixed variables $W = W(q, p')$, the mapping $(q, p) \to (q', p')$ defined implicitly by the relations

$$p = \frac{\partial W}{\partial q}, \quad q' = \frac{\partial W}{\partial p'}, \tag{11}$$

is symplectic (canonical transformation). The function W is called the generating function (of Von-Zeipel type). If we take

$$W = qp' + \tau H(q, p'), \tag{12}$$

then (11) implies

$$q' = q + \tau \frac{\partial H}{\partial p'}, \quad p' = p - \tau \frac{\partial H}{\partial q}, \tag{13}$$

which gives a 1st order implicit symplectic integrator. For the 2nd order integrator, take

$$W(q,p') = qp' + \tau H(q,p') + (\tau^2/2)H_{p'}H_q. \tag{14}$$

and the implicit scheme

$$\begin{aligned} q' &= q + \tau H_{p'} + (\tau^2/2)(H_{p'p'}H_q + H_{p'}H_{p'q}), \\ p' &= p - \tau H_q - (\tau^2/2)(H_{p'q}H_q + H_{p'}H_{qq}). \end{aligned} \tag{15}$$

follows. Higher order integrators ($n > 2$) are similarly obtained by choosing the generating function $W(q,p')$ properly so that the mapping $(q,p) \to (q',p')$ agrees with the Taylor expansion of the solution up to the order of τ^n.

Feng and Qin (1987) derived the generating functions $W(q,p')$ and the corresponding symplectic schemes up to the 4th order, and Channell and Scovel (1990), up to the 6th order. Since it becomes very difficult to write down the computer program by hand for these higher order integrators, Channell and Scovel (1990) developed a preprocessor to generate the FORTRAN source code.

2.2. Implicit Runge-Kutta Methods

For the system of differential equations (1) in general, an s-stage Runge-Kutta method (generally implicit), which is a natural generalization of the classical 4-th order one, is defined as follows. First, vectors k_i are determined by solving the simultaneous algebraic equations

$$k_i = f(z + \tau \sum_{j=1}^{s} a_{ij}k_j), \tag{16}$$

$(i = 1, ..., s)$, then the mapping $z \to z'$ is

$$z' = z + \tau \sum_{j=1}^{s} b_j k_j. \tag{17}$$

Here a_{ij} and b_j are scalar constants which characterize the scheme. The so-called Butcher table which lists a_{ij} and b_j as an $s+1$ by s matrix is often used to specify a given Runge-Kutta method. Note that if $a_{ij} = 0$ for $i \leq j$, then the scheme is explicit. These constants a_{ij} and b_j are determined by the order conditions which are derived by the postulate that the mapping $z \to z'$ should agree with the Taylor expansion of the solution up to the desired order of τ.

Suppose now that (1) is Hamiltonian. For general Runge-Kutta methods, the mapping (17) is not symplectic. Sanz-Serna(1988) and Lasagni(1988) found that if the constants satisfies the conditions

$$M_{ij} := b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad (1 \leq i,j \leq s) \tag{18}$$

identically, then the mapping is symplectic. Notice that for (18) to be satisfied, the scheme must be implicit.

The simplest solution (1-stage, $s = 1$) which satisfies the conditions (18) is given by

$$a_{11} = \frac{1}{2}, \quad b_1 = 1, \tag{19}$$

and we have the scheme,

$$k_1 = f(z + \frac{\tau}{2}k_1), \quad z' = z + \tau k_1 \tag{20}$$

or, more concisely,

$$z' = z + \tau f(\frac{z + z'}{2}), \tag{21}$$

which is known as the implicit midpoint rule, and has order 2. For the 2-stage method we have, for example,

$$(a_{ij}) = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \end{pmatrix}, \quad (b_j) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} \tag{22}$$

and the order is 4. Pullin and Saffman (1991) applied this 4th order implicit Runge-Kutta method to the motion of four vortex motion successfully. These schemes are simplest examples of the family of Gauss-Legendre method and the s-stage Gauss-Legendre method has order 2s (Dekker and Verwer, 1984). This family has a good stability property. For further references in this direction of research, see Sanz-Serna(1991), Sanz-Serna and Abia (1991), and Saito et al. (1992).

3. Explicit Schemes

3.1. RUTH(1983)

For Hamiltonian systems of the form

$$H = T(p) + V(q), \tag{23}$$

there exist explicit symplectic algorithms. As for the 1st order one, a small change of the Euler method (2) makes it exactly symplectic. In fact, take

$$q' = q + \tau \left(\frac{\partial T}{\partial p}\right)_{p=p}, \quad p' = p - \tau \left(\frac{\partial V}{\partial q}\right)_{q=q'}. \tag{24}$$

This mapping is symplectic because it is composed of two symplectic mappings $(q, p) \to (q', p)$ and $(q', p) \to (q', p')$.

The idea to construct higher order schemes is simply to approximate the original Hamiltonian flow by a composition of trivial symplectic mappings,

$$S_T(c_i\tau): \quad q' = q + c_i\tau \left(\frac{\partial T}{\partial p}\right), \quad p' = p, \tag{25}$$

and

$$S_V(d_i\tau): \quad q' = q, \quad p' = p - d_i\tau\left(\frac{\partial V}{\partial q}\right), \tag{26}$$

repeatedly. Here numerical coefficients $(c_i, d_i), (i = 1, ...k)$ are determined so that the composed mapping $(q,p) \to (q',p')$ coincides with the Taylor expansion of the solution up to the order of τ^n. Thus an n-th order explicit symplectic integrator is obtained. For example, a second order scheme $(q,p) \to (q',p')$ is attained by

$$q* = q + \frac{\tau}{2}\left(\frac{\partial T}{\partial p}\right)_{p=p}, \quad p' = p - \tau\left(\frac{\partial V}{\partial q}\right)_{q=q*}, \quad q' = q + \frac{\tau}{2}\left(\frac{\partial T}{\partial p}\right)_{p=p'} \tag{27}$$

which corresponds to the choice $c_1 = c_2 = 1/2, d_1 = 1, d_2 = 0$, and this scheme has been known as the leap-frog method. Ruth(1983) first derived the algebraic equations of (c_i, d_i) for the 3rd order integrator and obtained a solution,

$$c_1 = \frac{7}{24}, c_2 = \frac{3}{4}, c_3 = -\frac{1}{24}, d_1 = \frac{2}{3}, d_2 = -\frac{2}{3}, d_3 = 1. \tag{28}$$

Candy and Rozmus (1991) directly extended the idea of Ruth to obtain the coefficients of the 4th order integrator, and demonstrated the advantage of symplectic schemes in various examples.

3.2. NERI(1987)

The above problem to derive explicit symplectic integrator was reformulated by Neri(1987) in terms of Lie algebraic language. First rewrite the Hamilton equation in the form

$$\frac{dz}{dt} = \{z, H(z)\}, \tag{29}$$

where braces stand for the Poisson bracket, $\{F,G\} = F_qG_p - F_pG_q$. If we introduce a differential operator D_G by $D_GF := \{F,G\}$, then (29) is written as $\dot{z} = D_Hz$, so the formal solution, or the exact time evolution of $z(t)$ from $t = 0$ to $t = \tau$ is given by

$$z(\tau) = [\exp(\tau D_H)]z(0). \tag{30}$$

For a Hamiltonian of the form (23), $D_H = D_T + D_V$ and we have the formal solution

$$z(\tau) = \exp[\tau(A + B)]z(0). \tag{31}$$

where $A := D_T$ and $B := D_V$, and these operators A and B do not commute in general.

Suppose (c_i, d_i), $(i = 1,2,...,k)$ is a set of real numbers which satisfies the equality

$$\exp[\tau(A + B)] = \prod_{i=1}^{k} \exp(c_i\tau A)\exp(d_i\tau B) + o(\tau^{n+1}), \tag{32}$$

for a given integer n, which corresponds to the order of integrator. Now consider a mapping from $z = z(0)$ to $z' = z(\tau)$ given by

$$z' = \left[\prod_{i=1}^{k} \exp(c_i \tau A) \exp(d_i \tau B)\right] z. \tag{33}$$

This mapping is symplectic because it is just a product of elementary symplectic mappings, and approximates the exact solution (31) up to the order of τ^n. Furthermore (33) is explicitly computable. In fact (33) gives the succession of the mappings

$$q_i = q_{i-1} + \tau c_i \left(\frac{\partial T}{\partial p}\right)_{p=p_{i-1}}, \quad p_i = p_{i-1} - \tau d_i \left(\frac{\partial V}{\partial q}\right)_{q=q_i}, \tag{34}$$

for $i = 1$ to $i = k$, with $(q_0, p_0) = z$ and $(q_k, p_k) = z'$. An n-th order symplectic integrator (integration scheme) is thus realized. For example when $n = 1$, a trivial solution is $c_1 = d_1 = 1$, $(k = 1)$, which corresponds to the identity

$$\exp[\tau(A + B)] = \exp(\tau A) \exp(\tau B) + o(\tau^2). \tag{35}$$

and gives the 1st order symplectic integrator (24). When $n = 2$, we find easily a solution $c_1 = c_2 = 1/2, d_1 = 1, d_2 = 0$, $(k = 2)$, which comes from

$$\exp[\tau(A + B)] = \exp(\frac{\tau}{2} A) \exp(\tau B) \exp(\frac{\tau}{2} A) + o(\tau^3). \tag{36}$$

and implies the 2nd order integrator (27). Forest(1987), Forest and Ruth(1990), Candy and Rozmus(1991) obtained a 4th order integrator in a rather straightforward way with the result,

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

$$d_1 = d_3 = \frac{1}{2 - 2^{1/3}}, \quad d_2 = \frac{-2^{1/3}}{2 - 2^{1/3}}, \quad d_4 = 0. \tag{37}$$

Notice that this 4th order integrator requires the evaluation of force function only 3-times in a step, although the classical 4th order Runge-Kutta method needs 4-times.

3.3. YOSHIDA(1990)

Yoshida(1990) first noticed that the 4th order integrator found by Forest (1987) is composed of the 2nd order ones. With use of the notation

$$S_2(\tau) := \exp(\frac{\tau}{2} A) \exp(\tau B) \exp(\frac{\tau}{2} A), \tag{38}$$

the 4th order integrator $S_4(\tau)$ can be written as

$$S_4(\tau) = S_2(x_1\tau)S_2(x_0\tau)S_2(x_1\tau) \tag{39}$$

where

$$x_0 = \frac{-2^{1/3}}{2-2^{1/3}}, \quad x_1 = \frac{1}{2-2^{1/3}}. \tag{40}$$

In fact, x_0 and x_1 are determined as the solution of algebraic equations,

$$x_0 + 2x_1 = 1, \quad x_0^3 + 2x_1^3 = 0, \tag{41}$$

and this interpretation gives the simplest derivation of the 4th order integrator (37). Forest et al.(1991) noticed that this idea of composition can be used also to obtain higher order implicit integrators in the previous section.

The above fact was found independently, and *even earlier*, by Suzuki (1990) from a completely different motivation which shares the same mathematical problem (32). Suzuki (1991) further proved the very strong statement that there cannot exist any solution of (32) with all positive (c_i, d_i) when $n \geq 3$. Therefore, the presence of some negative numbers in (28) and (37) is unavoidable. For the 6th order integrator, Yoshida (1990) put

$$S_6(\tau) = S_2(w_3\tau)S_2(w_2\tau)S_2(w_1\tau)S_2(w_0\tau)S_2(w_1\tau)S_2(w_2\tau)S_2(w_3\tau) \tag{42}$$

and three sets of (w_0, w_1, w_2, w_3) were obtained numerically. Five sets for the 8th order integrator were also found. This construction of higher order integrators with minimum number of force evaluation was recently generalized to arbitrary orders by Suzuki (1992).

For other researches on finding explicit symplectic integrators, see Abia and Sanz-Serna (1990), McLachlan and Atela (1991) and Okunbor and Skeel (1991, 1992, 1992a).

4. General Property

4.1. Conservation of Energy

The original Hamiltonian flow conserves the Hamiltonian (Energy) exactly and it is desirable that numerical integration methods respect this fact.

For the family of symplectic Runge-Kutta methods with condition (18), all the quadratic integrals are conserved exactly (Sanz-Serna, 1988). Thus for linear systems with a quadratic Hamiltonian, the symplectic Runge-Kutta scheme conserves the Hamiltonian and the symplectic structure at the same time. This is possible because linear Hamiltonian systems are integrable. For general non-integrable systems one cannot expect the conservation of energy exactly at each step (Ge and Marsden, 1988). Nevertheless there is an advantage for symplectic schemes.

Let us apply the 1st order explicit symplectic scheme (24) to the one-dimensional harmonic oscillator (4). Then we have the symplectic mapping

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} 1 & \tau \\ -\tau & 1-\tau^2 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}. \tag{43}$$

One finds easily that although the value of energy is not conserved exactly by the iteration of symplectic mapping (43), the error has no secular increase and it is bounded of the order of τ for moderate small values of τ.

For the one-dimensional harmonic oscillator case, this phenomenon is explained by the existence of a conserved quantity (integral of motion) of the mapping (43), which has the expression

$$\frac{1}{2}(p^2+q^2)+\frac{\tau}{2}pq = const. \tag{44}$$

If one starts with the initial condition $(q,p) = (1,0)$ with a fixed small value of τ, the points obtained by iterating the mapping (43) must lie on an ellipse in the (q,p) plane, $q^2+p^2+\tau pq = 1$, which differs from the trajectory of the exact solution, $q^2+p^2 = 1$, only of the order of τ permanently. Thus the error of the energy caused by the local truncation error cannot grow. Indeed, we have a more general statement;

THEOREM 1. *The symplectic mapping (24) exactly describes the time-τ evolution of an associated Hamiltonian system $\tilde{H}$, which is close to the original Hamiltonian (23) and has the expression of a formal power series in τ,*

$$\tilde{H} = H + \tau H_1 + \tau^2 H_2 + \tau^3 H_3 + ... \tag{45}$$

where H is the original Hamiltonian (23), and

$$H_1 = \frac{1}{2}H_p H_q,\ H_2 = \frac{1}{12}(H_{pp}H_q^2 + H_{qq}H_p^2),\ H_3 = \frac{1}{12}H_{pp}H_{qq}H_pH_q,\ \ldots \tag{46}$$

In particular, (24) conserves $\tilde{H}$ in (45) exactly.

As far as the author knows, this fact was first mentioned by Dragt and Finn (1976) without any motivation on numerical integration methods. See also Dragt et al.(1988). The series (45) reflects on the Baker-Campbell-Hausdorff (BCH) formula (Varadarajan, 1974) for the product of two exponential functions of non-commuting operators X and Y;

$$\exp X \exp Y = \exp Z \tag{47}$$

with

$$Z = X+Y+\frac{1}{2}[X,Y]+\frac{1}{12}([X,[X,Y]]+[Y,[Y,X]])+\frac{1}{24}[X,[Y,[Y,X]]]+\ldots \tag{48}$$

and $[X,Y] := XY - YX$, etc. For the 1st order symplectic integrator (24), one can apply BCH formula (47) to obtain

$$(\exp \tau D_T)(\exp \tau D_V) = \exp \tau D_{\tilde{H}} \,. \tag{49}$$

where

$$\tilde{H} = T+V+\frac{\tau}{2}\{V,T\}+\frac{\tau^2}{12}(\{\{T,V\},V\}+\{\{V,T\},T\})+\frac{\tau^3}{24}\{\{\{T,V\},V\},T\}+\ldots$$

$$= H + \frac{\tau}{2}H_pH_q + \frac{\tau^2}{12}(H_{pp}H_q^2 + H_{qq}H_p^2) + \frac{\tau^3}{12}H_{pp}H_{qq}H_pH_q + \ldots \tag{50}$$

which proves the theorem. For the 2nd order integrator (27), one obtains

$$(\exp \frac{\tau}{2}D_T)(\exp \tau D_V)(\exp \frac{\tau}{2}D_T) = \exp \tau D_{\tilde{H}_{2nd}}, \tag{51}$$

where

$$\tilde{H}_{2nd} = T + V + \tau^2\left(\frac{1}{12}\{\{T,V\},V\} - \frac{1}{24}\{\{V,T\},T\}\right) + o(\tau^4)$$

$$= H + \tau^2\left(\frac{1}{12}H_q^2H_{pp} - \frac{1}{24}H_p^2H_{qq}\right) + o(\tau^4). \tag{52}$$

In general, for an n-th order integrator, one has the associated Hamiltonian

$$\tilde{H}_{nth} = H + \tau^n H_n + o(\tau^{n+1}), \tag{53}$$

so that the error of the energy remains of the order of τ^n. Notice, however, that the rigorous convergence of the series (45), (52), (53) are not guaranteed for nonlinear systems in general. Some related works are found in Auerbach and Friedman (1991), and Friedman and Auerbach (1991).

As for the implicit schemes by the generating function method, i.e., for (13) and (15), a similar argument is possible. A near-identity symplectic mapping defined by the generating function, (12) or (14), can be written into the explicit form

$$z' = (\exp \tau D_{\tilde{H}})z, \tag{54}$$

by the equivalence of von-Zeipel and Hori perturbation methods (Mersman 1971, Giacaglia 1972). Thus $\tilde{H}$, which is again a formal power series in τ, is conserved.

For the symplectic Runge-Kutta method with condition (18), the present author does not know any similar statement how to write down the associated Hamiltonian $\tilde{H}$ from the original Hamiltonian H.

5. Application to Specific Problems

5.1. KEPLER PROBLEM

Kinoshita et al.(1991) applied the 4th order explicit symplectic integrator (SI4) to the Kepler problem

$$H = \frac{1}{2}p^2 - \frac{1}{r}, \tag{55}$$

with the eccentricity, $e = 0.1$, and compared with the results obtained by the classical 4th order Runge-Kutta method (RK4).

For a short time (10 orbital periods), the errors in the semi-major axis $\triangle a$ and in the eccentricity $\triangle e$ by SI4 are much bigger than those by RK4. The superiority of SI4 over RK4 can be seen after a long time (2000 periods), since $\triangle a$ and $\triangle e$ by RK4 grow secularly in time. The errors in the inclination $\triangle i$ and the longitude of node $\triangle\Omega$ come from the round-off error only, since these elements are conserved exactly. As for the error in the mean anomaly $\triangle l$, RK4 allows the quadratic increase in time although SI4 allows only the linear growth. This difference becomes significant for a long time integration. There is one problem with the error in the argument of pericenter $\triangle\omega$. Both integrators give linear growth of $\triangle\omega$, and the error by SI4 is much larger than that by RK4. RK4 is too good by some unknown reason for $\triangle\omega$, since the 6th order symplectic integrator (SI6) and the 6th order explicit Runge-Kutta method (RK6) give almost the same error in $\triangle\omega$ (Kinoshita and Nakai, 1991).

Gladman et al.(1991) also applied SI4 to the Kepler problem and obtained similar results.

5.2. SOLAR SYSTEM

The idea of explicit symplectic integrator can be applied also to the system of the form

$$H = H_0(q,p) + H_1(q,p) \tag{56}$$

where H_0 and H_1 are integrable in the absence of other parts. A Hamiltonian of the form, $H = T(p) + V(q)$, is the simplest case of this situation. Since H_0 and H_1 are integrable, $\exp \tau D_{H_0}$ and $\exp \tau D_{H_1}$ can be computed without error by introducing the action-angle variables, (I_0, θ_0) and (I_1, θ_1) for each part. Sometimes, however, the change of variables between these two sets of action-angle variables is really time-consuming (Kinoshita et al. 1991) and may decrease the advantage of this treatment.

Wisdom and Holman (1991) write the Hamiltonian of the n-body problem (outer planets)

$$H = \sum_{i=0}^{n-1} \frac{p_i^2}{2m_i} - \sum_{i<j} \frac{Gm_i m_j}{r_{ij}}, \tag{57}$$

into the form

$$H = H_0 + H_1 = H_{Kepler} + H_{Interaction} \tag{58}$$

using the Jacobi coordinates and applied the 2nd order symplectic integrator (27) in the sense above with the step size, $\tau = 1$ year to integrate for 10^9 years. For the computation of $\exp \tau D_{H_0}$, the f and g functions of Gauss were used. The authors claimed that they reproduced all the principal results of Sussman and Wisdom (1988) and confirmed that the motion of Pluto is chaotic with much fewer CPU time.

Gladman and Duncan (1990) simulated the evolution of test particles in the outer solar system using the 4th order explicit symplectic integrator (37) to explain the apparent absence of a large number of minor bodies between the giant planets.

6. Miscellaneous Problems

6.1. Variable Time Step

When integrating, for example, a very eccentric orbit in the Kepler problem, one often uses a variable time step to obtain better accuracy. What happens if symplectic integrators are used with a variable step ? The result is, unfortunately, a decrease in efficiency, and the error of energy starts to increase without any bound like the result by a traditional integration method.

Let us define the new independent variable s, for example, by

$$adt = rds \tag{59}$$

where a is the semi-major axis of elliptic orbit. This introduction of new variable s implies that when $r < a$ (i.e., near the pericenter where the motion is fast), ds is bigger that dt and more steps are used than the average. On the other hand when $r > a$ (i.e., near the apocenter where the motion is slow), fewer steps are used to integrating the orbit.

If one compares the constant step and the variable step using RK4, there is an obvious advantage in the variable step method (Figure 1). The error of energy (although it grows linearly) decreases one order using the variable step while total number of steps are kept constant. On th other hand, with use of symplectic integrator (SI4), one finds the secular grows in the error of energy which did not exist with the constant step integration. The argument in the previous section to ensure the lack of secular increase in the error of energy has assumed a constant step size τ, or just an iteration of mapping, and is not valid when the step size is changed. Thus one must say that there is no advantage to use a variable step when integrating by known symplectic methods.

More detailed analysis on this subject can be found in Calvo and Sanz-Serna (1991, 1991a). See also Gladman et al.(1991).

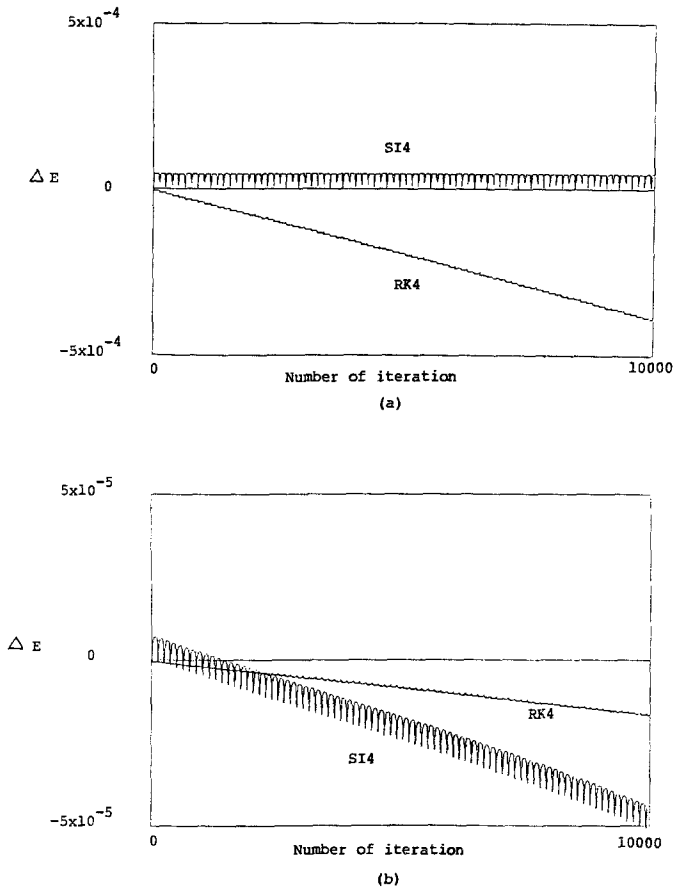

Fig. 1. (a) : The error of energy in the Kepler problem (55) by RK4 and by SI4 ($a = 1, e = 0.5$). The constant step size is $\tau = 0.05$ and the number of iteration is 10000 (80 orbital periods). The error growth by RK4 is almost linear and periodic by SI4. (b) : The same couple as in (a) using the variable step size (59). The scale of ordinate is 1/10 of that of (a). The energy growth by SI4 is no more periodic.

6.2. Large Time Step and Chaos

With a constant time step, symplectic integrators do not produce any secular growth in the error of energy. This fact allows one to use a relatively large step size. Of course, if the step size is too large so that the series (45), (52), (52) really diverge (or, far from convergent) the associated Hamiltonian $\tilde{H}$ never represents the numerical solution and the good conservation of energy is no more guaranteed.

Take an example of the simple pendulum

$$H = \frac{1}{2}p^2 + \cos q. \tag{60}$$

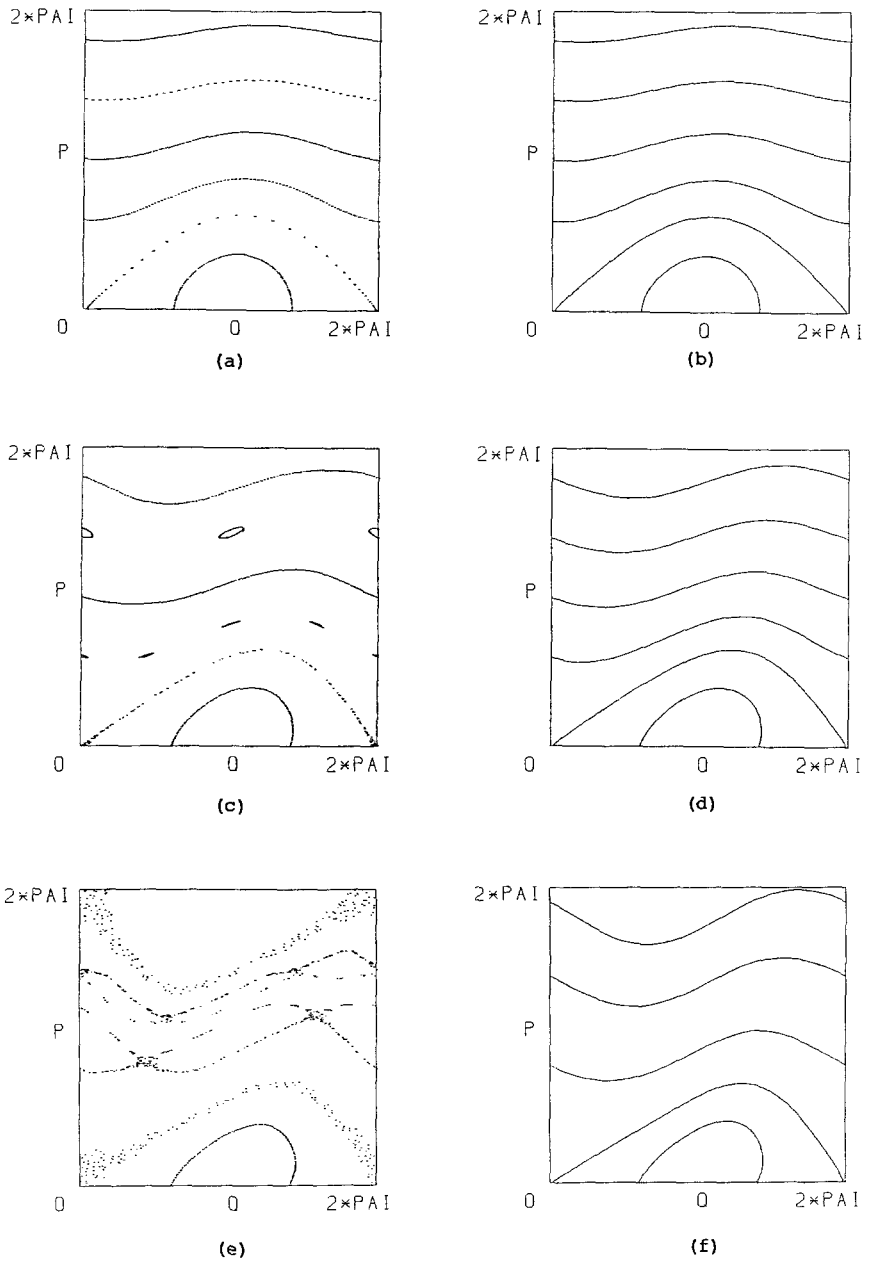

Fig. 2. (a) : Points generated by the iteration of symplectic mapping (61) when $\tau = 0.2$. (b) : Contour lines of $\tilde{H} = const.$ given by (63) when $\tau = 0.2$. (c) : Same as (a) when $\tau = 0.7$. (d) : Same as (b) when $\tau = 0.7$. (e) : Same as (a) when $\tau = 1.0$. (f) : Same as (b) when $\tau = 1.0$.

The 1st order explicit symplectic integrator, the dual of (24), gives the mapping

$$p' = p + \tau \sin q, \quad q' = q + \tau p', \tag{61}$$

which is equivalent (unless $\tau = 0$) to the so-called standard mapping (Greene 1979)

$$P' = P + k \sin Q, \quad Q' = Q + P'. \tag{62}$$

In fact, (60) and (61) are related by the change of scale $\tau p = P$, $q = Q$ and $\tau^2 = k$. The associated Hamiltonian (45) has the expression

$$\tilde{H} = \frac{1}{2}p^2 + \cos q + \frac{\tau}{2} p \sin q + \frac{\tau^2}{12}(\sin^2 q - p^2 \cos q) - \frac{\tau^3}{12} p \sin q \cos q + o(\tau^4). \tag{63}$$

Figure 2 shows the comparison between the points generated by the iteration of the mapping (61) and the contour lines of $\tilde{H}(q,p) = const.$ given by (63) for the values $\tau = 0.2$, $\tau = 0.7$, and $\tau = 1.0$. To draw contour lines, only the terms of up to the order τ^3 are used in (63) and higher terms are neglected. The good agreement of two pictures when $\tau = 0.2$ indicates (but not proves) that the series (63) *practically* converges for this value of τ and in the range of (q,p) shown. When $\tau = 0.7$ there are already some discrepancy between the iterated points and the contour lines $\tilde{H} = const.$ This discrepancy becomes larger when $\tau = 1.0$. For this value of τ, the series (63) never represents the conserved quantity of the mapping (61) except for the small region around the elliptic fixed point $(q,p) = (\pi, 0)$. For most initial conditions, the iterated points show chaotic behaviors, which cannot be approximated by the perturbation series (63) at all.

These phenomena reminds us of a famous result of Gustavson on the Hénon-Heiles Hamiltonian (Gustavson 1966). He showed that the set of points (obtained by the Poincaré map) on the surface of section has a good agreement with the truncated formal integral obtained by the perturbation series for small energy (small perturbation) but not for large energy, where the Poincaré map becomes chaotic.

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