Symplectic Integrators for Hamiltonian Systems : Basic Theory

HARUO YOSHIDA

National Astronomical Observatory, Mitaka, Tokyo 181, Japan

Abstract. Symplectic integrators are numerical integration methods for Hamiltonian systems, which conserves the symplectic 2-form exactly. With use of symplectic integrators there is no secular increase in the error of the energy because of the existence of a conserved quantity closed to the original Hamiltonian. Higher order symplectic integrators are obtained by a composition of 2nd order ones.

Key words: Numerical integration method - Symplectic mapping - Conserved quantity

1. Introduction

The exact solution of Hamiltonian equations of motion

$$\dot{q} = H_p, \quad \dot{p} = -H_q \tag{1}$$

has the following properties. The mapping from (q, p) at $t = 0$ to (q', p') at $t = \tau$ along the solution is

(i) exactly symplectic, i.e., $\Sigma dp \wedge dq = \Sigma dp' \wedge dq'$

and

(ii) conserves the energy, i.e., $H(q, p) = H(q', p')$.

If we use a traditional integration method (such as the Euler method or the Runge-Kutta method) which does not respect the Hamiltonian nature, the above two properties are easily violated. For example, the one-dimensional harmonic oscillator with the Hamiltonian

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

has the exact solution

$$\begin{pmatrix} q(\tau) \\ p(\tau) \end{pmatrix} = \begin{pmatrix} \cos\tau & \sin\tau \\ -\sin\tau & \cos\tau \end{pmatrix} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix}, \tag{3}$$

which, of course, enjoy the above two properties.

The most primitive integration method (i.e., Euler method) approximates (3) as

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} 1 & \tau \\ -\tau & 1 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}. \tag{4}$$

This mapping $(q, p) \to (q', p')$ is not exactly symplectic, and at each step, the value of the energy is multiplied by $(1 + \tau^2)$, i.e.,

$$(p'^2 + q'^2) = (1 + \tau^2)(p^2 + q^2), \tag{5}$$

which leads to the indefinite increase of the energy. The situation is, more or less, the same when one uses a higher order integrator, such as the 4th order Runge-Kutta method.

S. Ferraz-Mello (ed.), Chaos, Resonance and Collective Dynamical Phenomena in the Solar System, 407–411.

2. First Order Symplectic Integrator

A small change in (4) makes the mapping exactly symplectic. Indeed, take

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} 1 & \tau \\ -\tau & 1-\tau^2 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}. \tag{6}$$

This mapping is obviously symplectic (det = 1), and has the same local accuracy (1st order) as the Euler method. In general, for a Hamiltonian of the form

$$H = T(\mathbf{p}) + V(\mathbf{q}), \tag{7}$$

a first order symplectic integrator (a symplectic mapping which approximates the exact solution up to the order of τ) is given by

$$\mathbf{q}' = \mathbf{q} + \tau \left(\frac{\partial T}{\partial \mathbf{p}}\right)_{p=p}, \quad \mathbf{p}' = \mathbf{p} - \tau \left(\frac{\partial V}{\partial \mathbf{q}}\right)_{q=q'} \tag{8}$$

This mapping $(q,p) \to (q',p')$ is symplectic because it is composed of two symplectic mappings, $(q,p) \to (q',p)$ and $(q',p) \to (q',p')$. One finds easily that although the value of the energy is not conserved exactly with use of the symplectic integrator, the error has no secular increase and it is bounded of the order 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 (6), which has the expression

$$\frac{1}{2}(p^2+q^2) + \frac{\tau}{2}pq = const. \tag{9}$$

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 (6) must lie on an ellipse in the (q,p) plane, $q^2 + p^2 + \tau pq = 1$, which differ 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

The symplectic mapping (8) describes the exact time-τ evolution of a Hamiltonian system $\tilde{H}$, which is close to the original Hamiltonian (7) and has the expression of a formal power series in τ,

$$\tilde{H} = H + \tau H_1 + \tau^2 H_2 + \tau^3 H_3 + ... \tag{10}$$

where,

$$H_1 = \frac{1}{2}H_p H_q, \; H_2 = \frac{1}{12}(H_{pp}H_q^2 + H_{qq}H_p^2), \; H_3 = \frac{1}{12}H_{pp}H_{qq}H_p H_q, \; \ldots \tag{11}$$

In particular, (8) conserves $\tilde{H}$ exactly.

Therefore with use of the symplectic integrator, there is no secular accumulation in the error of the energy.

https://doi.org/10.1017/S0074180900091440 Published online by Cambridge University Press

3. Higher Order Symplectic Integrators

From a practical point of view, higher order symplectic schemes are important. Introducing the notation, $z = (\mathbf{q}, \mathbf{p})$, the Hamilton equation is written in the form

$$\dot{z} = \{z, H(z)\}, \tag{12}$$

where braces stand for the Poisson bracket, $\{F, G\} = F_q G_p - F_p G_q$. If we introduce a differential operator D_G by $D_G F := \{F, G\}$, (12) is written as $\dot{z} = D_H z$, so the formal solution, or the exact time evolution of $z(t)$ from $t = 0$ to $t = \tau$ is given by

$$z(\tau) = [\exp(\tau D_H)] z(0). \tag{13}$$

For a Hamiltonian of the form (7), $D_H = D_T + D_V$ and we have the formal solution

$$z(\tau) = \exp[\tau(A + B)] z(0). \tag{14}$$

where $A := D_T$, and $B := D_V$.

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

$$\exp[\tau(A + B)] = \prod_{i=1}^{k} \exp(c_i \tau A) \exp(d_i \tau B) + o(\tau^{n+1}). \tag{15}$$

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

$$z' = \left[\prod_{i=1}^{k} \exp(c_i \tau A) \exp(d_i \tau B) \right] z. \tag{16}$$

This mapping is symplectic because it is just a product of elementary symplectic mappings, and approximates the exact solution (14) up to the order $o(\tau^n)$. Furthermore, (16) is explicitly computable although (14) is only formal. In fact (16) gives the succession of the mappings

$$\mathbf{q}_i = \mathbf{q}_{i-1} + \tau c_i \left(\frac{\partial T}{\partial \mathbf{p}} \right)_{p=p_{i-1}}, \quad \mathbf{p}_i = \mathbf{p}_{i-1} - \tau d_i \left(\frac{\partial V}{\partial \mathbf{q}} \right)_{q=q_i} \tag{17}$$

for $i = 1$ to $i = k$, with $(\mathbf{q}_0, \mathbf{p}_0) = z$ and $(\mathbf{q}_k, \mathbf{p}_k) = z'$. An n-th order symplectic integrator (integration scheme) is thus obtained. For example when $n = 1$, a trivial solution is $c_1 = d_1 = 1$, $(k = 1)$, and we have

$$\exp[\tau(A + B)] = \exp(\tau A) \exp(\tau B) + o(\tau^2). \tag{18}$$

which gives the first order integrator (8). When $n = 2$, we find that $c_1 = c_2 = 1/2, d_1 = 1, d_2 = 0$, $(k = 2)$, thus

$$\exp[\tau(A + B)] = \exp(\frac{\tau}{2} A) \exp(\tau B) \exp(\frac{\tau}{2} A) + o(\tau^3). \tag{19}$$

https://doi.org/10.1017/S0074180900091440 Published online by Cambridge University Press

Forest and Ruth(1990) obtained a 4th order integrator in a rather straightforward way with the result,

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

$$d_1 = d_3 = \frac{1}{2-2^{1/3}},\ d_2 = \frac{-2^{1/3}}{2-2^{1/3}},\ d_4 = 0. \tag{20}$$

Yoshida(1990) found that this 4th order integrator is composed of the 2nd order ones. With use of the notation

$$S_2(\tau) := \exp(\frac{\tau}{2}A)\exp(\tau B)\exp(\frac{\tau}{2}A), \tag{21}$$

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

$$S_4(\tau) = S_2(x_1\tau)S_2(x_0\tau)S_2(x_1\tau) \tag{22}$$

where

$$x_0 = \frac{-2^{1/3}}{2-2^{1/3}},\ \ x_1 = \frac{1}{2-2^{1/3}}. \tag{23}$$

Furthermore, if a 2n-th order integrator $S_{2n}(\tau)$ is known which enjoyes the property,

$$S_{2n}(\tau)S_{2n}(-\tau) = 1, \tag{24}$$

a (2n+2)-th order integrator is obtained by a composition

$$S_{2n+2}(\tau) := S_{2n}(z_1\tau)S_{2n}(z_0\tau)S_{2n}(z_1\tau), \tag{25}$$

where

$$z_0 = \frac{-2^{1/(2n+1)}}{2-2^{1/(2n+1)}},\ \ z_1 = \frac{1}{2-2^{1/(2n+1)}}. \tag{26}$$

Thus there exists an explicit symplectic integrator of any even order. For more details, see Yoshida(1990). Recently, Forest et al.(1991) remarked that this idea can be used also to desine an implicit integrator for arbitrary Hamiltonian systems.

For the application of symplectic integrators, see Kinoshita et al.(1991), Channel and Scovel(1990), Candy and Rozmus(1991), and Pullin and Saffman(1991).

References

Candy, J. and Rozmus, W.: 1991, 'A symplectic integration algorithm for separable Hamiltonian functions', *J. Comp. Phys.* **92**, 230

Channel, P.J. and Scovel, J.C.: 1990, 'Symplectic integration of Hamiltonian systems', *Nonlinearity* **3**, 231

Forest, E. and Ruth, R.D.: 1990, 'Fourth-order symplectic integration', *Physica D* **43**, 105

Forest, E., Brengtsson, J. and Reusch M.F.: 1991, 'Application of the Yoshida-Ruth techniques to implicit integration and multi-map explicit integration', *Phys. Lett. A* **158**, 99

Kinoshita, H., Yoshida, H. and Nakai, H: 1991, 'Symplectic integrators and their application to dynamical astronomy', *Celest. Mech.* **50**, 59

Pullin, D.I. and Saffman, P.G.: 1991, 'Long time symplectic integration, the example of four-vortex motion', *Proc. R. Soc. London A* **432**, 481

Yoshida, H: 1990, 'Construction of higher order symplectic integrators', *Phys. Lett. A* **150**, 262

Discussion

J. Wisdom – Both your presentation and that of Kinoshita mention only Hamiltonians of the form $H = T(p) + V(q)$. I would like to emphasize that the same coefficient achieve high order for Hamiltonians of the more general form $H = H_0(\mathbf{p}, \mathbf{q}) + H_1(\mathbf{p}, \mathbf{q})$ provided that H_0 and H_1 are individually integrable, as I presented in my talk.

H. Yoshida – Yes, of course. Indeed one section of our recent publication (Kinoshita, Yoshida and Nakai, *Celest. Mech. Dyn. Astron.* **50**,59-71, 1991) is devoted to such case.

J. Wisdom – The doubling method of solving the coefficient equations to high order is very impressive, but it may be that there are other solutions with fewer function evaluations that can achieve the same order.

H. Yoshida – I Agree with you completely. What I have shown is just the existence of at least one integrator of any even order, by forgetting economy completely. But I have no idea how to search such solution systematically.

J. Wisdom – It has not been mentioned, but of course the conservation of energy is purely formal. In reality there is accumulation of numerical error that must lead to, at least, square root of time error growth in energy and 3/2 power of time in the mean longitudes.

https://doi.org/10.1017/S0074180900091440 Published online by Cambridge University Press