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Energy Conserving, Liouville, and Symplectic Integrators

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In this paper, we construct an integrator that converves volume in phase space. We compare the results obtained using this method and a symplectic integrator. The results of our experiments do not reveal any superiority of the symplectic over strictly volume-preserving integrators. We also investigate the effect of numerically conserving energy in a numerical process by rescaling velocities to keep energy constant at every step. Our results for Henon–Heiles problem show that keeping energy constant in this way destroys ergodicity and forces the solution onto a periodic orbit. © 1995 Academic Press, Inc.

1. INTRODUCTION

The problem of interest is that of a computer solution of a Hamiltonian dynamical system of the form

$$\frac{dz}{dt} = J\nabla H(z, t), \quad z(t_0) = z_0, \tag{1}$$

where $z \in \mathcal{R}^{2\nu}$, t is time, H (called the Hamiltonian) is a scalar function, J is the skew-symmetric matrix $\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ and the two identity matrices I are of equal dimension. We assume that the function $H(z, t)$ is sufficiently smooth to ensure the existence of a unique solution. The value ν is the number of the degrees of freedom of the system. This value may sometimes be large, especially in systems obtained from N-body motion and spatial discretization of partial differential questions.

Hamiltonian systems have qualitative features that are very important when they are being integrated. Most of the conventional numerical integrators such as the classical 4-stage, fourth-order Runge–Kutta method do not capture these qualitative features of the systems. Seemingly, all the features exhibited by the flow of the Hamiltonian system are consequences of just one property, namely, the property that the flow of the system is *symplectic*. The flow is the mapping from a set of initial values to a set of solution values at some time later. In differential geometry, the solution of the system would be said to have *symplectic* structure.

The construction of symplectic integrators for Hamiltonian has been the interest of several researchers. Ruth [14] and Feng [3] were the first, independently, to give published reports on the possibility of symplectic numerical integration of Hamiltonian systems. Ruth [14] discovered 1-, 2-, and 3-stage methods of orders ≤ 3. Ruth's work was followed by a considerable research in the area of constructing higher order symplectic integrators [2–4, 12, 15, 17, 18]. Forest and Ruth [4] derived a symmetric explicit 3-stage symplectic integrator of order 4. Yoshida [18] proved the possibility of constructing symplectic 3^k-stage partitioned Runge–Kutta method having order $2k + 2$ using a composition of symplectic 1-stage method of order 2. He derived numerically 7- and 15-stage symplectic integrators, respectively, of orders 6 and 8 using a Lie group approach. Using the discrete variable approach, several Runge–Kutta–Nyström methods of orders at most 8, some of which are equivalent to the Yoshida's methods have been constructed by Okunbor and Skeel [13].

This paper is not about the derivation of symplectic integrators, detailed treatment of this are found in [12] and the references therein. We focus on the analysis of existing symplectic integrators. The analyses presented in this paper are different from those available in the literature [1]. So far, the emphasis has been on the comparison between symplectic integrators and nonsymplectic integrators [12, 15] and the effect of variable stepsize implementation of symplectic integrators [1]. There are basically two issues that will be presented in this paper. The first is that of energy conservation. Can the qualitative behavior of symplectic integrators be explained by linearized stability or simply by energy conservation? As reported by Ge and Marsden [5], symplectic integrators do not conserve energy. However, the property of being symplectic surpasses energy conservation. In Section 2, we investigate the effect of numerically conserving energy. To do this, we rescale velocities to keep energy constant at every step. Our results for Hénon–Heiles problem show that keeping energy constant in this way destroys ergodicity and forces the solution onto a periodic orbit.

The second issue is that of volume preservation. It is well known that methods that are symplectic preserve volume in phase space. The construction of integrators that merely preserve volume in phase space was considered by Suris [16]. This poses the question as to whether or not volume preservation is all that a numerical integrator requires to represent the qualitative behavior of the flow of the system. We examine this ques-

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tion in somewhat incomplete manner in Section 3. We apply a merely volume-preserving and a symplectic integrator to a two degrees-of-freedom Kepler problem and 16 degrees-of-freedom pseudospectral discretization of a sine–Gordon equation. The results of these experiments do not reveal any superiority of the symplectic over the volume-preserving integrator.

2. CONSERVATION OF ENERGY

The value of the Hamiltonian $H(q, p)$ of a Hamiltonian system is a conserved quantity for given initial conditions $\begin{pmatrix} q(0) \\ p(0) \end{pmatrix}$, that is, $H(q(t), p(t)) = H(q(0), p(0))$ for all time t, where $\begin{pmatrix} q(t) \\ p(t) \end{pmatrix}$ is the solution of the system. Usually H corresponds to the energy of the system. Several numerical integrators for dynamical systems, not necessarily symplectic, that conserve energy have been proposed (see [6–8, 11]). Sanz-Serna [15] claims that the conservation of energy forces the solution orbits of the Hamiltonian system to be in the $(2\nu - 1)$-dimensional surface, thereby allowing them to be free within the surface and, therefore, it may not be as important as the property of being symplectic.

In fact, it has been proved by Ge and Marsden [5] for Hamiltonian systems having no integrals other than the energy that if a symplectic integrator always conserves energy, then it must agree with the map of the exact Hamiltonian system up to a reparametrization of the time.

A simple-minded way to conserve energy is to rescale velocities at every step using the formula

$$p_n = sp_n, \quad s = \sqrt{(H_0 - V(q_n))/T(p_n)},$$

where $T(p_n)$ and $V(q_n)$ are, respectively, the kinetic energy and potential energy at time t_n and H_0 is the initial energy. To find the effect that rescaling velocities might have on a numerical integrator, we consider the Hénon–Heiles problem with the initial condition $(q_1, q_2, p_1, p_2) = (0, 0.2, 0.4483395, 0)$ giving energy 0.117835. We compute the solutions using the symplectic 3-stage third-order RKN method derived above, a G-symmetric 5-stage fourth-order method (acronym, RO) with the following coefficient was constructed by Okunbor and Skeel [12]

$$\begin{array}{lcccccc} c: & \frac{7}{48} & \frac{25}{48} & \frac{24}{48} & \frac{23}{48} & \frac{41}{48} & 1 \\ B: & \frac{1}{3} & -\frac{1}{3} & 1 & -\frac{1}{3} & \frac{1}{3} & 0 \end{array}$$

and the nonsymplectic 3-stage, fourth-order RKN method taken from [9]

$$Q_2 = q_n + \tfrac{1}{2}h\dot{q}_n + \tfrac{1}{8}h^2 f(q_n),$$
$$Q_3 = q_n + h\dot{q}_n + \tfrac{1}{2}h^2 f(Q_2),$$

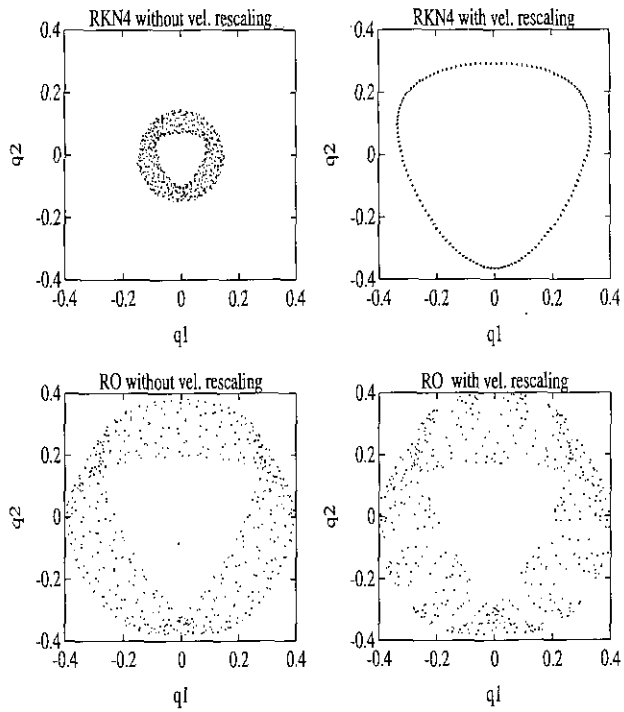

FIG. 1. *The effect of numerically conserving energy.*

$$q_{n+1} = q_n + h\dot{q}_n + \tfrac{1}{6}h^2 f(q_n) + \tfrac{1}{3}h^2 f(Q_2),$$
$$\dot{q}_{n+1} = \dot{q}_n + \tfrac{1}{6}h(f(q_n) + f(Q_2) + f(Q_3))$$

(acronym, RKN 4). It can be shown that velocity rescaling destroys the symplectic property of RO. Different scaled time steps (actual time step is equal to the scaled time step times the number of stages) but we depict in Fig. 1 the results for RKN 4 and RO with and without rescaling velocities using scaled time step of $\frac{1}{18}$. From Fig. 1 we see that keeping the energy constant for the case of RKN 4 destroys the ergodicity and forces the solution onto a periodic orbit. Therefore, to conserve energy numerically does not make the results obtained by nonsymplectic to be comparable to that obtained using a symplectic integrator. The RO method with velocity rescaling is not better than the RO method without rescaling.

3. LIOUVILLE VERSUS SYMPLECTIC INTEGRATORS

The property of being symplectic can give rise to many qualitative characteristics of Hamiltonian systems. One of these characteristics is the preservation of volume in phase space. The volume element $\Pi_z = dz_1 dz_2 \cdots dz_{2\nu}$ of z is related to the volume element $\Pi_{\bar{z}} = d\bar{z}_1 d\bar{z}_2 \cdots d\bar{z}_{2\nu}$ of $\bar{z}$ by

$$\Pi_{\bar{z}} = |\det S| \Pi_z,$$

where S is the Jacobian matrix of the tansformation. Since $S^T J S = J$, then $\det S = \pm 1$, implying that the volume is invariant under a symplectic transformation. This result is important when sampling phase space.

A transformation which conserves volume in phase space is called a Liouville transformation. We say that a consistent integrator is *Liouville* if it gives rise to a Liouville transformation. Clearly, all symplectic integrators are Liouville, but the converse is not in general true. In this section we examine in more detail the usefulness, if any, of the symplectic property over the property of being Liouville. In other words, what additional gain does one achieve from the symplectic property. Is the Liouville property all that a numerical integrator needs to represent qualitatively the behavior of the flow of the system? The motivation for such a consideration arises from the fact that the conditions for a method to be Liouville are less restrictive. It is clear that symplectic RKN methods form a subset of Liouville RKN methods. For example, consider a general explicit 2-stage RKN method. The Jacobian matrix S of this method is

$$S = \begin{pmatrix} I + h^2 b_1 D_1 + h^2 b_2 D_2 + h^4 b_2 a_{21} D_1 D_2 & hI + h^3 b_1 c_1 D_1 + h^3 b_2 c_2 D_2 + h^5 b_2 a_{21} c_1 D_1 D_2 \\ hB_1 D_1 + hB_2 D_2 + h^3 B_2 a_{21} D_1 D_2 & I + h^2 B_1 c_1 D_1 + h^2 B_2 c_2 D_2 + h^4 B_2 a_{21} c_1 D_1 D_2 \end{pmatrix},$$

where D_1 and D_2 are the derivatives of $f(y)$ with respect to y evaluated at $q + c_1 hp$ and $q + c_2 hp + h^2 a_{21} f(q + c_1 hp)$, respectively. To obtain the necessary conditions to be Liouville, we consider the scalar case, and we get three equations, namely,

$$b_1 - B_1 + B_1 c_1 = 0, \quad (2)$$

$$b_2 - B_2 + B_2 c_2 = 0, \quad (3)$$

$$(b_2 - B_2 + B_2 c_1) a_{21} + (B_2 b_1 - B_1 b_2)(c_2 - c_1) = 0. \quad (4)$$

With Eqs. (2) and (3) satistifed, Eq. (4) becomes

$$(-B_2 a_{21} + B_2 b_1 - B_1 b_2)(c_2 - c_1) = 0.$$

To be symplectic, the method must satisfy $B_2 a_{21} + B_2 b_1 - B_1 b_2 = 0$. However, to be Liouville, this is not necessary if $c_2 = c_1$. What this means is that if we choose c_1 so that it is equal to c_2, then the method is Liouville but it may or may not be symplectic. The method

$$\begin{array}{c|cc} \frac{1}{2} & 0 & \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & \frac{1}{4} & \frac{1}{4} \\ & \frac{1}{2} & \frac{1}{2} \end{array}$$

is Liouville but not symplectic. One can show that this method is Liouville for systems. This method is of order 2. It has an accuracy comparable to the Störmer–Verlet method but it requires twice as much work. In what follows, we perform numerical experiments in an attempt to compare symplectic and Liouville integrators. From the numerical results, there is no noticeable difference between a symplectic integrator and the above Liouville method. However, there is a difficulty in constructing methods that are Liouville without assuming the symplectic property. The conditions for the Liouville property are not explicitly expressible in terms of the method parameters.

In our experiments we compare the above Liouville method and the Störmer–Verlet method. Both methods have the same P-stability threshold. Therefore, using the same timestep for both methods does not pose any serious consequences. We consider two Hamiltonian systems. The first is the 2-body problem with

$$H(q, p) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}} \quad (5)$$

and the initial condition $(0.5, 0, 0, \sqrt{3})$. The timestep in this case is 0.0001 and total time of the experiment in terms of periods is 3000. The global errors in the trajectory against time for both methods are indicated in Fig. 2. We see from the figure that both the Liouville and symplectic integrators have linear

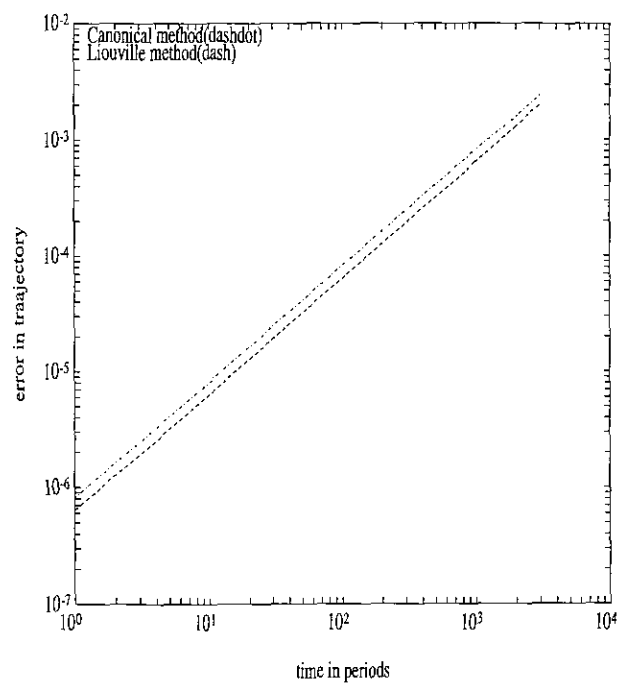

FIG. 2. Two-Body problem: Liouville versus symplectic.

growth in error. We did not see any noticeable difference between both methods for all the time steps that were tried for this problem.

The second problem is the sine–Gordon equation,

$$u_{tt} + u_{xx} + \sin u = 0,$$
$$u(x, 0) = \pi + 0.1 \cos(\mu x), \quad u_t(x, 0) = 0, \tag{6}$$

where $\mu = 2\pi/L$ and $L = 2\sqrt{2}\pi$. The solution is periodic in x with period L. This is considered to be a more difficult problem. The paper by Herbst and Ablowitz [10] describes the application of a pseudospectral method to (6). The Hamiltonian of the pseudospectral spatial discretization in Fourier space is

$$H = \frac{1}{2} \sum_{k=-(1/2)N}^{(1/2)N-1} [p_k p_{-k} + \mu_k^2 q_k q_{-k}] - \frac{1}{N} \sum_{j=-(1/2)N}^{(1/2)N-1} \cos U_j, \tag{7}$$

where

$$U_j = (F^{-1})_j\{q_k\} := \sum_{k=-(1/2)N}^{(1/2)N-1} q_k \exp(i\mu_k x_j),$$

$q_{N/2} := q_{-N/2}$, $p_{N/2} := p_{-N/2}$, $\mu_k = 2\pi k/L$, $x_j = L_j/N$, and N is even. The Hamiltonian system is

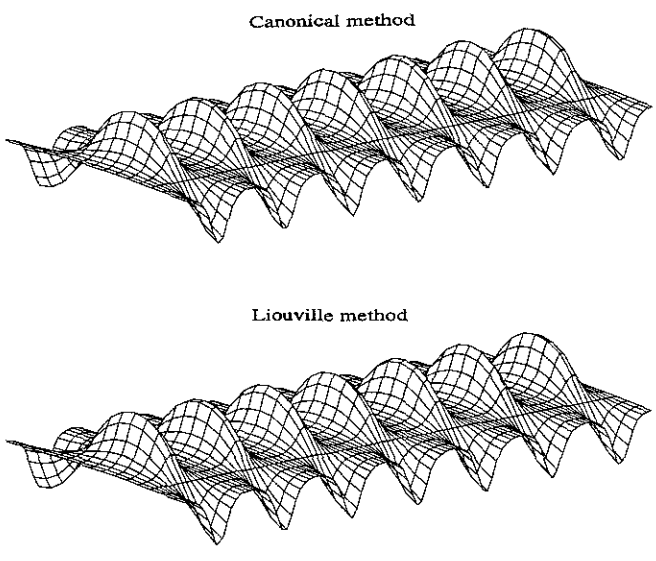

FIG. 3. Sine–Gordon equation: Liouville versus symplectic.

$$\dot{q}_k = p_k, \quad \dot{p}_k = -(\mu_k^2 q_k + F_k\{\sin U_j\}), \quad k = -\tfrac{1}{2}\mathrm{N}, \ldots, \tfrac{1}{2}N - 1,$$

where

$$F_k\{v_j\} := \frac{1}{N} \sum_{j=-(1/2)N}^{(1/2)N-1} v_j \exp(-i\mu_k x_j).$$

We choose $N = 16$. Although, several time steps were tried for this problem, we only present in Fig. 3 the solution obtained using a time spacing of 0.02 for a total of 5000 steps for the two methods. Again, there is no remarkable difference between the two methods. On the basis of these two sets of experiments, it may be tempting to say that the reason why symplectic methods perform the way they did might be due to the preservation of volume in phase space. In any case, more needs to be done in this regard.

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