Symplectic-Energy-Momentum Preserving Variational Integrators

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August, 1998; this version: May 13, 1999
Journal of Mathematical Physics **40**, 1999, 3353–3371

Abstract

The purpose of this paper is to develop variational integrators for conservative mechanical systems that are symplectic, energy and momentum conserving. To do this, a spacetime view of variational integrators is employed and time step adaptation is used to impose the constraint of conservation of energy. Criteria for the solvability of the time steps and some numerical examples are given.

Contents

1 Introduction

The purpose of this paper is to develop variational integrators for conservative mechanical systems with adaptive time steps. The resulting algorithms are symplectic, energy preserving and they also preserve the momentum maps (Noether quantities) associated with symmetry groups.

An important idea for how to develop such integrators comes from the paper of Marsden, Patrick, and Shkoller [1] in which the spacetime view is stressed. This viewpoint is very important for two main reasons:

1. One must avoids conflicts with well know theorems (Ge and Marsden [2]), which limit the possiblitity that *constant time stepping* algorithms be symplectic, energy and momentum preserving.

2. To give meaning to the term *symplectic* in the context of adaptive time stepping algorithms since the algorithm is not given by a single mapping associated with a constant time step.

The basic algorithm itself consists of two parts. First, to update positions, the variational approach of Veselov [3], [4], and Moser and Veselov [5] is adopted; these ideas were implemented numerically in Wendlandt and Marsden [6]. Second, to compute the time steps themselves, energy preservation is imposed. Roughly speaking, we make use of the fact that time and energy are conjugate variables.

In this paper, our main purpose is the following:

1. To set up the basic algorithm that implements these symplectic-energy-momentum (SEM) integrators

2. To make precise the sense in which the algorithms are symplectic

3. To investigate the solvability conditions for the time step.

4. To give some simple numerical examples.

With regard to solving for the time step, we shall indicate how the solvability conditions are closely related to the positivity of the numerically computed kinetic energy. In particular, when one is close to a location with zero velocity (roughly speaking, "turning points"), our solvability criterion and examples indicate that one should move through such points using a criterion other than energy preservation. Numerically, this causes a slight adjustment to the energy. How one should best

treat these points requires further investigation. *It is not the purpose of this paper to give any extensive numerical tests or implementations of these methods.* This is a nontrivial task, but clearly needs to be done, and is planned for other publications.

In future papers we will also investigate the use of these ideas in our collision algorithms[7] and how one can incorporate dissipative effects.

2 Brief Review of Variational Integrators

In this section, we recall some of the essential features of variational integrators that are needed in this paper. For additional details, see Wendlandt and Marsden [6] and Marsden, Patrick, and Shkoller [1].

Limitations on Mechanical Integrators. There has been a large literature developing on the use of energy-momentum and symplectic-momentum integrators. We shall not attempt to survey this all here, but rather refer the reader to some of the recent literature, such as the collection of papers in Marsden, Patrick, and Shadwick [8] and Sanz-Serna and Calvo [9]. We do mention that for time stepping algorithms with fixed time steps, the theorem of Ge and Marsden [2] has led to a general division of algorithms into those that are energy-momentum preserving and those that are symplectic-momentum preserving. One of our main points is that if one takes a spacetime view of variational integrators, as is advocated in Marsden, Patrick and Shkoller [1], then one can have all three of these properties. Papers typified by Simo and Tarnow [10], Simo, Tarnow, and Wong [11] and Gonzalez [12] have focussed on energy preserving algorithms, but they presumably fail (except, perhaps, in special cases, such as integrable systems) to be symplectic. Other approaches based on Hamilton's principle are those of Shibberu[13] and Lewis[14]. See also Lee [15].

Accuracy of Solutions. We should, at the outset make another point clear. We are not claiming anything about accuracy of individual trajectories. Indeed, it is well known that structure preservation alone does not guarantee this. (See, e.g., Ortiz [16] and Simo and Gonzalez [17]. For systems with complicated, unstable, or chaotic trajectories, it is not clear that accuracy of individual trajectories is the correct question to ask. Rather one should probably concentrate on statistical properties of solutions. These are deep questions that we do not attempt to address here, but one hopes that by preserving as much of the structure as possible, one is closer to addressing such issues. In some cases the advantage of symplectic is clear; for instance, the condition of being symplectic guarantees that the phase space volume is preserved and this can be an obvious limitation on many integrators; even after relatively short times, one can see phase space volume not preserved in many integrators.

Some Common Integrators. In structural mechanics, the $\beta = 0$, $\gamma = 1/2$ member of the widely used Newmark family is a variational integrator (see, for example, Simo, Tarnow, and Wong [11]) and therefore is symplectic and momentum preserving. One can, in fact, the whole Newmark family of algorithms is variational [18] Our methods can be used to make these integrators also preserve energy by

using time adaptive stepping. We also mention that the popular Verlet methods and shake algorithms are variational integrators (see [6] and [18] for further discussion and references).

Dissipation and Constraints. While dissipation and forcing are of course very important, as we have mentioned, we leave their discussion for future publications. One possibility is that dissipative effects can be dealt with by means of product formulas, as in Armero and Simo [19], [20], [21] for example. Another is to incorporate the dissipative effects into the variational principle, as in [22] and [18].

Constraints are also very important for integrators. We also do not discuss these in any detail in this paper. However, we do mention that variational integrators handle constraints in a simple and efficient way.

Variational methods also generalize to pde's using multisymplectic geometry with the result being a class of multisymplectic momentum integrators. See Marsden, Patrick, and Shkoller [1] for details and numerical examples. This type of approach should untimately be of use in elastodynamics as well as ocean dynamics, for example.

Symmetry and Reduction. We should also mention that for mechanical systems with symmetry, the investigation of discrete versions of reduction theory, such as Euler–Poincaré reduction[23] are of current interest.[24], [25] We will not be making use of this reduction theory in this paper, but it is related since our integrators are intended to preserve symmetry. It would be of interest to develop time adapted integrators in the sense of the present paper in the general context of discrete reduction.

The Discrete Variational Principle. Given a *configuration space* Q, a ***discrete Lagrangian*** is a map

$$L_d : Q \times Q \to \mathbb{R}.$$

In practice, L_d is obtained by approximating a given Lagrangian as we shall discuss later, but regard L_d as given for the moment. The time step information will be contained in L_d and we regard L_d as a function of two nearby points (q_k, q_{k+1}).

For a positive integer N, the ***action sum*** is the map $S_d : Q^{N+1} \to \mathbb{R}$ defined by

$$S_d = \sum_{k=0}^{N-1} L_d\left(q_k, q_{k+1}\right),$$

where $q_k \in Q$ and k is a nonnegative integer. The action sum is the discrete analog of the action integral in mechanics.

The ***discrete variational principle*** states that the evolution equations extremize the action sum given fixed end points, q_0 and q_N. Extremizing S_d over $q_1, \cdots, q_{N-1}$ leads to the ***discrete Euler-Lagrange (DEL) equations***:

$$D_1 L_d\left(q_k, q_{k+1}\right) + D_2 L_d\left(q_{k-1}, q_k\right) = 0$$

for all $k = 1, \cdots, N-1$. We can write this equation in terms of a discrete ***algorithm***

$$\Phi : Q \times Q \to Q \times Q$$

defined implicitly by

$$D_1 L_d \circ \Phi + D_2 L_d = 0,$$

i.e.,

$$\Phi\left(q_{k-1}, q_k\right) = \left(q_k, q_{k+1}\right).$$

If, for each $q \in Q$, $D_1 L_d(q,q) : T_q Q \to T_q^* Q$ is invertible, then $D_1 L_d : Q \times Q \to T^*Q$ is locally invertible and so the algorithm Φ, which flows the system forward in discrete time, is well defined for small time steps.

Variational Algorithms are Symplectic. To explain the sense in which the algorithm is symplectic, first define the ***fiber derivative*** (or the discrete Legendre transform) by

$$\mathbb{F}L_d : Q \times Q \to T^*Q; \quad (q_0, q_1) \mapsto \left(q_0, D_1 L_d\left(q_0, q_1\right)\right)$$

and define the 2-form ω on $Q \times Q$ by pulling back the canonical 2-form $\Omega_{\mathrm{CAN}} = dq^i \wedge dp_i$ from T^*Q to $Q \times Q$:

$$\omega = \mathbb{F}L_d^*\left(\Omega_{\mathrm{CAN}}\right).$$

The fiber derivative is analogous to the standard Legendre transform.

The coordinate expression for ω is:

$$\omega = \frac{\partial^2 L_d}{\partial q_k^i \partial q_{k+1}^j}\left(q_k, q_{k+1}\right) dq_k^i \wedge dq_{k+1}^j.$$

A fundamental fact is that

The algorithm Φ exactly preserves the symplectic form ω.

One proof of this is to simply verify it with a straightforward calculation—see Wendlandt and Marsden [6] for the details. Another is to derive the same conclusion directly from the variational structure, as is done in Marsden, Patrick, and Shkoller [1].

The Algorithm Preserves Momentum. Recall that *Noether's theorem* states that a continuous symmetry of the Lagrangian leads to conserved quantities, as with linear and angular momentum. A nice way to derive these conservation laws (the way Noether did it) is to use the *invariance of the variational principle*.

Assume that the discrete Lagrangian is invariant under the action of a Lie group G on Q, and let $\xi \in \mathfrak{g}$, the Lie algebra of G. By analogy with the continuous case, define the ***discrete momentum map***, $\mathbf{J}_d : Q \times Q \to \mathfrak{g}^*$ by

$$\left\langle \mathbf{J}_d(q_k, q_{k+1}), \xi \right\rangle := \left\langle D_1 L_d(q_k, q_{k+1}), \xi_Q(q_k) \right\rangle,$$

A second fundamental fact is that

The algorithm Φ exactly preserves the momentum map.

Construction of Mechanical Integrators. Assume we have a mechanical system with a constraint manifold, $Q \subset V$, where V is a real finite dimensional vector space, and that we have an unconstrained Lagrangian, $L : TV \to \mathbb{R}$ which, by restriction of L to TQ, defines a ***constrained Lagrangian***, $L^c : TQ \to \mathbb{R}$. Roughly speaking, V is a containing vector space in which the computer arithmetic will take place. In particular, coordinate charts on Q are *not* chosen for this purpose. In fact, apart from the use of the containing vector space V, the algorithms developed here are independent of the use of coordinates on Q.

We also assume that we have a vector valued ***constraint function***, $g : V \to \mathbb{R}^k$, such that our constraint manifold is given by $g^{-1}(0) = Q \subset V$, with 0 a regular value of g. The dimension of V is denoted n, and therefore, the dimension of Q is $m = n - k$.

Define a ***discrete, unconstrained Lagrangian***, $L_d : V \times V \to \mathbb{R}$ in some consistent manner, such as

$$L_d(x, y) = L\left(\gamma x + (1-\gamma)y, \frac{y-x}{h}\right), \tag{2.1}$$

where $h \in \mathbb{R}_+$ is the time step and $0 \leq \gamma \leq 1$ is an interpolation parameter.

The corresponding discrete Euler-Lagrange equations give an algorithm closely related to (in a sense made precise in [18]) the ***Newmark algorithm*** for the standard choice of Lagrangian given by kinetic minus potential energy. We get the *central difference method* for $\gamma = 1/2$ and we get the *shake* algorithm with $\gamma = 1$ (the *Verlet* algorithm is the unconstrained version of the shake algorithm). We also note that the *Moser-Veselov discrete Lagrangian* for the rigid body is constructed using either $\gamma = 1$ or $\gamma = 0$ (see Marsden, Pekarsky, and Shkoller [24] for details).

We remark in passing that other choices for discrete Lagrangian are also possible, such as

$$L_d(x, y) = \sigma L\left(\gamma_1 x + (1-\gamma_1)y, \frac{y-x}{h}\right) + (1-\sigma)L\left(\gamma_2 x + (1-\gamma_2)y, \frac{y-x}{h}\right),$$

where σ, λ_1 and λ_2 are between 0 and 1. These other choices, which give algorithms such as the midpoint rule, are not investigated here (see [18]). Alternative choices, of which this is an example, as well as issues of local truncation error and accuracy are investigated in West [26].

The ***unconstrained action sum*** is defined by

$$S_d = \sum_{k=0}^{N-1} L_d\left(x_k, x_{k+1}\right).$$

Extremize $S_d : V^{N+1} \to \mathbb{R}$ *subject to the constraint* that $x_k \in Q \subset V$ for $k = 1, \cdots, N-1$, *i.e.,* solve

$$D_1 L_d\left(x_k, x_{k+1}\right) + D_2 L_d\left(x_{k-1}, x_k\right) + \lambda_k^T Dg\left(x_k\right) = 0$$

(no sum on k) with $g\left(x_k\right) = 0$ for $k = 1, \cdots, N-1$. Here, the λ_k are *Lagrange multipliers*, chosen to enforce the constraints.

Thus, the algorithm is defined by starting with x_k and x_{k-1} in $Q \subset V$, *i.e.,* $g(x_k) = 0$ and $g(x_{k-1}) = 0$, and solving

$$D_1 L_d(x_k, x_{k+1}) + D_2 L_d(x_{k-1}, x_k) + \lambda_k^T Dg(x_k) = 0$$

subject to $g(x_{k+1}) = 0$, for x_{k+1} and λ_k. In terms of the *unconstrained Lagrangian*, the algorithm reads as follows:

$$\begin{aligned}
&\frac{1}{h}\left[\frac{\partial L}{\partial \dot{x}}\left(\gamma x_{k-1} + (1-\gamma)x_k, \frac{x_k - x_{k-1}}{h}\right)\right. \\
&\left. - \frac{\partial L}{\partial \dot{x}}\left(\gamma x_k + (1-\gamma)x_{k+1}, \frac{x_{k+1} - x_k}{h}\right)\right] \\
&+ (1-\gamma)\frac{\partial L}{\partial x}\left(\gamma x_{k-1} + (1-\gamma)x_k, \frac{x_k - x_{k-1}}{h}\right) \\
&+ \gamma\frac{\partial L}{\partial x}\left(\gamma x_k + (1-\gamma)x_{k+1}, \frac{x_{k+1} - x_k}{h}\right) + D^T g(x_k)\,\lambda_k = 0
\end{aligned}$$

together with $g(x_{k+1}) = 0$.

Example. If the continuous Lagrangian is

$$L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q)$$

with constraint $g(q) = 0$, where M is a constant mass matrix, and V is the potential energy, then the DEL equations are

$$\begin{aligned}
M\left(\frac{x_{k+1} - 2x_k + x_{k-1}}{h^2}\right) &+ (1-\gamma)\frac{\partial V}{\partial q}\left(\gamma x_{k-1} + (1-\gamma)x_k\right) \\
&+ \gamma\frac{\partial V}{\partial q}\left(\gamma x_k + (1-\gamma)x_{k+1}\right) \\
&- D^T g(x_k)\,\lambda_k = 0
\end{aligned}$$

with $g(x_{k+1}) = 0$.

Wendlandt and Marsden [6] show that *the algorithm defined using Lagrange multipliers coincides with that defined intrinsically using the constrained discrete Lagrangian on $Q \times Q$, so it is symplectic and momentum preserving.*

An Intrinsic Variational Viewpoint. Recall that given a Lagrangian function $L : TQ \to \mathbb{R}$, we construct the corresponding ***action functional*** $\mathfrak{S}$ on C^2 curves $q(t)$ by (using coordinate notation)

$$\mathfrak{S}\big(q(\cdot)\big) \equiv \int_a^b L\left(q^i(t), \frac{dq^i}{dt}(t)\right) dt. \tag{2.2}$$

The action functional depends on a and b, but this is not explicit in the notation. Hamilton's principle seeks the curves $q(t)$ for which the functional $\mathfrak{S}$ is stationary under variations of $q^i(t)$ with fixed endpoints. It will be useful to recall this calculation; namely, we seek curves $q(t)$ which satisfy

$$\mathbf{d}\mathfrak{S}\big(q(t)\big) \cdot \delta q(t) \equiv \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \mathfrak{S}\big(q(t) + \epsilon\delta q(t)\big) = 0 \tag{2.3}$$

for all $\delta q(t)$ with $\delta q(a) = \delta q(b) = 0$. Abbreviating $q_\epsilon \equiv q + \epsilon \delta q$, and using integration by parts, the calculation is

$$\begin{aligned} \mathbf{d}\mathfrak{S}\big(q(t)\big) \cdot \delta q(t) &= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \int_a^b L\left(q_\epsilon^i(t), \frac{dq_\epsilon^i}{dt}(t)\right) dt \\ &= \int_a^b \delta q^i \left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} \right) dt + \left. \frac{\partial L}{\partial \dot{q}^i} \delta q^i \right|_a^b . \end{aligned} \tag{2.4}$$

The last term in (2.4) vanishes since $\delta q(a) = \delta q(b) = 0$, so that the requirement (2.3) for $\mathfrak{S}$ to be stationary yields the ***Euler-Lagrange equations***

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} = 0. \tag{2.5}$$

Notice that the boundary term in the first variation of the action is the canonical one form $p_i \dot{q}^i$. This is the starting point for the variational proof that the algorithm is symplectic. The idea is to restrict $\mathfrak{S}$ to the space of solutions and to use the general identity $d^2\mathfrak{S} = 0$ to derive the symplectic nature of flow of the Euler-Lagrange equations. The point is that *this type of derivation also is valid for the discrete case*, as is shown in Marsden, Patrick, and Shkoller [1].

We also mention that one can similarly give a derivation of the conservation of momentum maps entirely based on the variational principle as well.

We end this section with one further important remark. Namely, one may think that the discrete symplectic form and momentum map that are conserved by the variational algorithm are somehow "concocted" to be conserved. This is not the case. Indeed, one can, via the discrete Legendre transform, transfer the algorithm to position-momentum space. Transferred to these variables, the algorithm will preserve the *standard* symplectic form $dq^i \wedge dp_i$ and the *standard* momentum map. As M. West pointed out to us, to get a corresponding algorithm that is consistent with the corresponding continuous Hamiltonian system on T^*Q, and one that is also in line with our discrete energy developed below, one should really use the map

$$(q_0, q_1) \mapsto (q_0, -hD_1 L_d\,(q_0, q_1))\,.$$

where h is the time step, but this does not affect the results here.

3 Review of Energy and Symplecticity Conservation in the Continuous Case

The main issue addressed in the following section is how we can achieve conservation of energy using adaptive time steps. We shall see that apart from some exceptional circumstances, which we can algorithmically identify, one can achieve this.

To address these issues, we first consider the continuous time case.

Conservation of Energy. We will first recall how conservation of energy is derived directly from Hamilton's principle in the case where $L(q, \dot{q})$ is time independent. This provides a clue about how one should proceed with the time adaptive steps.

Assume that $q(t)$ is a solution of the Euler-Lagrange equations. Let $s_\varepsilon(t)$ be a family of functions of t depending on the parameter ε and with $s_0(t) = t$ and with $s_\varepsilon(a) = a, s_\varepsilon(b) = b$. Let

$$\delta s(t) = \frac{d}{d\varepsilon} s_\varepsilon \Big|_{\varepsilon=0}.$$

We consider the associated family of curves $q(s_\varepsilon(t))$ which has the variation

$$\delta q(t) = \delta s(t) \dot{q}(t).$$

Hamilton's principle $\left(\delta \int L dt = 0\right)$ in this case gives us:

$$\int \frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} (\dot{\delta q}) = \int \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \delta q \tag{3.1}$$

Using the special form of the variation, this becomes

$$\int \frac{\partial L}{\partial q} \dot{q} \delta s - \left(\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \dot{q} \delta s \, dt = 0 \tag{3.2}$$

Equation (3.2) gives:

$$\frac{\partial L}{\partial q} \dot{q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \dot{q} = 0 = \frac{dE}{dt} \tag{3.3}$$

where, as usual,

$$E = \frac{\partial L}{\partial \dot{q}} \dot{q} - L(q, \dot{q}) \tag{3.4}$$

The point here is that we see a sense in which the Hamiltonian H arises naturally when one considers variations of the curve $q(t)$ that are given by time reparametrizations.

Symplecticity in the Spacetime Sense. In Marsden, Patrick, and Shkoller [1] it is shown how the variational principle naturally leads to boundary terms in both the continuous and the discrete case that leads to a deeper understanding of why the Euler-Lagrange and Hamilton equations themselves preserve the symplectic structure, as well as their discrete counterparts. We shall make use of this type of argument below in the discrete case. To help motivate the result, we make some relevant remarks here.

Consider a (possibly time dependent) Hamiltonian $H(q, p, t)$ in the canonically conjugate variables q^i, p_i and introduce an extended Hamiltonian $\bar{H}$, a function of q, p and two new real variables q_0 and p_0 by

$$\bar{H}(q, p, q_0, p_0) = H(q, p, q_0) + p_0.$$

Hamilton's equations for this new autonomous Hamiltonian agree with the time dependent equations for the original H if we identify q_0 with the time and p_0 with

$-H$. In addition, this leads one to the conservation of the canonical symplectic structure in the spacetime sense, namely

$$\Omega_H = \omega + dH \wedge dt,$$

where $\omega = \sum_i dq^i \wedge dp_i$ is the canonical symplectic form. What is interesting for us later is the following remark in case H is time independent (so H is conserved). Consider the flow $\bar{F}_s$ of the extended Hamiltonian $\bar{H}$, which is given by advancing the time by an amount s:

$$(q(t), p(t), t, H) \mapsto (q(t+s), p(t+s), t+s, H),$$

where q and p advance by the flow F_s of the original Hamiltonian system. Imagine, for later purposes that s is a function of the initial point and t, so that ds is a nontrivial differential. Then the statement that the flow $\bar{F}_s$ preserves the symplectic form above reads: $\bar{F}_s^* \Omega_H = \Omega_H$ or, equivalently,

$$F_s^* \omega + dH \wedge d(t+s) = \omega + dH \wedge dt$$

Cancelling $dH \wedge dt$, this reads

$$F_s^* \omega + dH \wedge ds = \Omega_0. \tag{3.5}$$

If we think of s as the time advancement, or the time step, then below we will prove a discrete analogue of this identity, which is how we will interpret symplectic in the time dependent sense.

Following the arguments in the discrete case later, or the methods of Marsden, Patrick, and Shkoller [1], one can also derive a Lagrangian version of this identity from the variational principle.

4 The Variational-Energy Algorithm

We consider a discrete Lagrangian that is (possibly) time dependent and has an associated time step h_1 that may be coupled to the current choice of points (q_1, q_2); we denote this discrete Lagrangian by $L_{h_1}(q_1, q_2) := L_d(q_1, q_2, h_1)$.

Given (q_0, q_1, h_0), we seek to find (q_1, q_2, h_1). In general, this will give us a way to pass from data (q_{k-1}, q_k, h_{k-1}) to (q_k, q_{k+1}, h_k).

This set up differs from the usual discrete Lagrangian procedures in the inclusion of time step information h_k that is coupled to the current configuration data (q_k, q_{k+1}).

We will find q_2 and h_1 together, by solving an equation similar to the discrete Euler-Lagrange equation for q_2, while we solve for h_1 using the equation $E_d(q_0, q_1, h_0) = E_d(q_1, q_2, h_1)$ where E_d is the discrete energy function, defined below.

The Discrete Action. One choice of discrete action is obtained by just using the following approximation to the action integral for the first two sets of points, (q_0, q_1, h_0) and (q_1, q_2, h_1):

$$[h_0 L_d(q_0, q_1, h_0) + h_1 L_d(q_1, q_2, h_1)] \tag{4.1}$$

One could also use other, more accurate methods to approximate the action integral. This might lead to some interesting new, more accurate algorithms, but we shall not explore them in this paper.

The Discrete Algorithm. To derive the algorithm, we consider the same discrete variational principle as before, but now parametrized by the time step information:

$$\frac{\partial}{\partial q_1} [h_0 L_d(q_0, q_1, h_0) + h_1 L_d(q_1, q_2, h_1)] = 0 \tag{4.2}$$

We also write this as

$$h_0 D_2 L_d(q_0, q_1, h_0) + h_1 D_1 L_d(q_1, q_2, h_1) = 0.$$

In this relation, the time steps h_0, h_1 are held fixed. We will later derive the symplectic relation by considering variations of solutions, just as in the continuous case.

The Discrete Energy. The above variational equation (4.2) will be coupled with an energy equation that will enable us to solve for both q_2 and h_2.

We define the ***discrete energy*** as follows:

$$\begin{aligned} E_d(q_0, q_1, h_0) &= -h_0 D_3 L_d(q_0, q_1, h_0) - L_d(q_0, q_1, h_0) \\ &= -\frac{\partial}{\partial h_0} [h_0 L_d(q_0, q_1, h_0)] \end{aligned} \tag{4.3}$$

This intrinsic definition is motivated in part by the fact that for Lagrangians of the form of kinetic minus potential energy, and with the choice of discrete Lagrangian given by (2.1), the discrete energy is given by the expression one would naturally think of, namely it is easily verified that in this case, we have

$$E_d(q_0, q_1, h_0) = \frac{1}{2} \left(\frac{q_1 - q_0}{h_0} \right)^T M \left(\frac{q_1 - q_0}{h_0} \right) + V\left(\gamma q_0 + (1-\gamma) q_1\right) \tag{4.4}$$

In this case, this can also be written as

$$E_d(q_0, q_1, h_0) = E\left(\gamma q_0 + (1-\gamma) q_1, \left(\frac{q_1 - q_0}{h_0} \right) \right) \tag{4.5}$$

where $E(q, \dot{q})$ is the energy associated with the original Lagrangian $L(q, \dot{q})$. As pointed out to us by Matt West, one can also motivate this definition of the energy using the variational principle or a discrete form of the Hamilton-Jacobi equation.

The main second equation defining the algorithm is

$$E_d(q_0, q_1, h_0) = E_d(q_1, q_2, h_1). \tag{4.6}$$

or, with algorithmic notation,

$$E_{k-1} := E_d(q_{k-1}, q_k, h_{k-1}) = E_d(q_k, q_{k+1}, h_k) := E_k. \tag{4.7}$$

For example, in the case the Lagrangian equals kinetic plus potential energy, and using the midpoint, the condition $E_0 = E_1$ is equivalent to:

$$h_1^2 = \frac{(q_2 - q_1)^T M (q_2 - q_1)}{2\left[E_0 - V\left(\gamma q_1 + (1-\gamma) q_2\right)\right]} \tag{4.8}$$

For this to remain meaningful as we compute, we need to make sure that the *computed kinetic energy*

$$E_0 - V\left(\gamma q_1 + (1-\gamma) q_2\right) \tag{4.9}$$

remains positive.

To realize this condition, one can consider verifying it a posteriori; that is,

1. First compute the square of the new time step h_1
2. Substitute h_1^2 in the relation

$$h_0 D_2 L_{h_0}(q_0, q_1) + h_1 D_1 L_{h_1}(q_1, q_2) = 0 \tag{4.10}$$

   which gives an implicit equation for q_2.
3. Compute q_2 implicitly
4. Verify from the formula for h_1^2 that one gets a positive answer.
5. If so, we proceed. If not, we keep the time step from the last iterate and proceed.

This approach will of course induces an energy variation in such cases. As we shall see below in greater detail, *this will only happen near "turning points"; that is, near points where the velocity is nearly zero.*

In the specific example, the equation for q_2 reads

$$\begin{aligned} m\left[\frac{(q_1 - q_0)}{h_0^2} - (1-\gamma) V'\left(\gamma q_0 + (1-\gamma) q_1\right)\right] h_0 \\ + \left[-\frac{m}{h_1^2}(q_2 - q_1) - \gamma V'\left(\gamma q_1 + (1-\gamma) q_2\right)\right] h_1 = 0 \end{aligned}$$

We define $B(q_0, q_1, h_0)$ to be:

$$B(q_0, q_1, h_0) := \left[m\frac{(q_1 - q_0)}{h_0^2} - (1-\gamma) V'\left(\gamma q_0 + (1-\gamma) q_1\right)\right] h_0$$

and we let, for notational convenience $u = \gamma q_1 + (1-\gamma)q_2$, we have

$$B = \left[2(1-\gamma)\frac{M(E_0 - V(u))}{(u-q_1)^T M(u-q_1)}(u-q_1) + \gamma V'(u)\right]\sqrt{2\frac{(u-q_1)^T M(u-q_1)}{E_0 - V(u)}} \tag{4.11}$$

In the particular case where $\gamma = \frac{1}{2}$ and q_1, q_2 are scalars, this expression simplifies to:

$$B = \left[\frac{E_0 - V(u)}{u-q_1} + \frac{1}{2}V'(u)\right]\sqrt{\frac{2(u-q_1)^2 M}{E_0 - V(u)}} \tag{4.12}$$

In other words:

$$E_0 - V(u) + \frac{1}{2}V'(u)(u-q_1) - \frac{\sqrt{E_0 - V(u)}}{\sqrt{2M}}B = 0 \tag{4.13}$$

We solve the previous equation for u then q_2 follows in a straightforward way.

5 Time Step Solvability and an Optimization Method

We have seen previously that the condition $E_0 - V(u) > 0$ should be verified in order to compute the next time step h_1, given h_0. To clarify the exposition, we write $E_0 = K_0 + V_0$ and we take : $V_1 = V(u)$. It follows that

$$E_0 - V(u) = K_0 + V_0 - V_1$$

Our condition for solvability is therefore

$$K_0 + V_0 - V_1 > 0 \tag{5.1}$$

If K_0 is large and the time step small, then in this case (5.1) is automatically verified. Indeed, K_0 large and $V_0 \simeq V_1$ implies that the computed kinetic energy is positive. If $q_1 \simeq q_2$ and h_0 is not so small, this is a rather delicate situation but can be explored by writing

$$\frac{1}{2}\frac{(q_1-q_0)^T m(q_1-q_0)}{h_0^2} + V\left(\gamma q_0 + (1-\gamma)q_1\right) - V\left(\gamma q_1 + (1-\gamma)q_2\right). \tag{5.2}$$

Taylor expanding the potential terms when $\gamma = \frac{1}{2}$ gives:

$$V\left(\frac{q_0+q_1}{2}\right) - V\left(\frac{q_1+q_2}{2}\right) = -\frac{1}{2}V'\left(\frac{q_0+q_1}{2}\right)\frac{q_2-q_0}{2}. \tag{5.3}$$

When the kinetic term is small, the condition should reduces to the condition that $q_2 - q_0$ has the same sign as $-V'((q_0+q_1)/2)$. This tells one in which direction q_2 should move.

An Optimization Method. An alternative strategy to deal with this issue of how to compute the time steps near turning points, which is the one we adapt in this paper, is to adopt the following optimization technique. Given h_0, q_0, q_1 we have to find h_1, q_2 such that q_2 is determined by the DEL equations

$$g(q_0, q_1, q_2, h_0, h_1) := h_0 D_2 L(q_0, q_1, h_0) + h_1 D_1 L(q_1, q_2, h_1) = 0 \tag{5.4}$$

and the energy condition

$$f(q_0, q_1, q_2, h_0, h_1) := E(q_1, q_2, h_1) - E(q_0, q_1, h_0) = 0 \tag{5.5}$$

The basic equations we want to solve are thus

$$f(q_0, q_1, q_2, h_0, h_1) = 0 \tag{5.6}$$
$$g(q_0, q_1, q_2, h_0, h_1) = 0, \tag{5.7}$$

to be solved for the variables q_2 and h_1 as a function of q_0, q_1, and h_0. The technique we use is to minimize the quantity

$$\mathcal{B} = [f(q_0, q_1, q_2, h_0, h_1)]^2 + [g(q_0, q_1, q_2, h_0, h_1)]^2 \tag{5.8}$$

over the variables h_1, q_2, with the other variables given, and *subject to the constraint* $h_1 > 0$. As above, this constraint means, in practice, that the computed kinetic energy is positive. Of course this is then iterated and defines our algorithm as a map

$$(q_{k-1}, q_k, h_{k-1}) \mapsto (q_k, q_{k+1}, h_k).$$

This method may be implemented in a standard way using a quasi-Newton algorithm, as in Byrd, Lu, Nocedal, and Zhu [27] (see also Zhu, Byrd, Lu, and Nocedal [28]). Of course other methods for efficiently solving the system of equations (8.9) can be considered as well, but as we have mentioned, we do not carry out any extensive comparitive or implementation tests in this paper. In the simple examples we do give in the section below, we use this optimization method.

6 Symplectic Nature of the Algorithm

We now show the sense in which the algorithm above is symplectic. This will be in the form of an identity that the mapping

$$\bar{\Phi} : Q \times Q \times \mathbb{R} \to Q \times Q \times \mathbb{R}$$

defined by

$$(q_0, q_1, h_0) \mapsto (q_1, q_2, h_1)$$

where, as we have seen, q_2 and h_1 are defined by

$$h_0 D_2 L_d(q_0, q_1, h_0) + h_1 D_1 L_d(q_1, q_2, h_1) = 0$$

and

$$E_d(q_0, q_1, h_0) = E_d(q_1, q_2, h_1),$$

where we recall that the discrete energy is defined by

$$E_d(q_0, q_1, h_0) = -D_{h_0}[h_0 L_d(q_0, q_1, h_0)].$$

To determine the symplectic nature of the mapping $\bar{\Phi}$, we follow the general line of reasoning in Marsden, Patrick, and Shkoller [1]. Namely, we consider the action sum

$$S = [h_0 L_d(q_0, q_1, h_0) + h_1 L_d(q_1, q_2, h_1)]$$

and take its full differential as a function of all the variables, keeping in mind that h_1 and q_2 are functions of (q_0, q_1, h_0). Using the definition of the discrete energy, we get

$$\begin{aligned} dS = {} & h_0 D_1 L_d(q_0, q_1, h_0) dq_0 + h_0 D_2 L_d(q_0, q_1, h_0) dq_1 \\ & + h_1 D_1 L_d(q_1, q_2, h_1) dq_1 + h_1 D_2 L_d(q_1, q_2, h_1) dq_2 \\ & - E_d(q_0, q_1, h_0) dh_0 - E_d(q_1, q_2, h_1) dh_1 \end{aligned}$$

Because of the discrete Euler-Lagrange equations, this simplifies to

$$\begin{aligned} dS = {} & h_0 D_1 L_d(q_0, q_1, h_0) dq_0 + h_1 D_2 L_d(q_1, q_2, h_1) dq_2 \\ & - E_d(q_0, q_1, h_0) dh_0 - E_d(q_1, q_2, h_1) dh_1. \end{aligned}$$

In view of the equations defining the algorithm, we can write this as

$$dS = \Theta_L^- + \bar{\Phi}^* \Theta_L^+ \tag{6.1}$$

where the one forms Θ_L^- and Θ_L^+ are defined by

$$\Theta_L^-(q_0, q_1, h_0) = h_0 D_1 L_d(q_0, q_1, h_0) dq_0 - E_d dh_0$$

and

$$\Theta_L^+(q_0, q_1, h_0) = h_0 D_2 L_d(q_0, q_1, h_0) dq_1 - E_d dh_0$$

Now notice that because of the definition of E_d, we have

$$\Theta_L^-(q_0, q_1, h_0) + \Theta_L^+(q_0, q_1, h_0) = d[h_0 L_d] - E_d dh_0 \tag{6.2}$$

Substituting (6.2) into (6.1) gives

$$dS = d[h_0 L_d] - \theta_d^+ + \bar{\Phi}^* \Theta_L^+ \tag{6.3}$$

where θ_d^+ is the discrete analogue of the canonical one form, $p_i dq^i$, namely

$$\begin{aligned} \theta_d^+ &= \Theta_d^+ + E_d dh_0 \\ &= h_0 D_2 L_d(q_0, q_1, h_0) dq_1 \end{aligned}$$

Taking the differential of (6.3), using $d^2 = 0$ and the fact that pull back commutes with the differential gives our final identity, namely

$$\bar{\Phi}^* \Omega_d = \omega_d, \tag{6.4}$$

where

$$\Omega_d = -d\Theta_d^+$$

is the discrete analogue of the spacetime symplectic form and where

$$\omega_d = -d\theta_d^+$$

is the discrete analogue of the phase space symplectic form. Notice that the identity (6.4) is the discrete analogue of the identity (3.5) in the continuous case. Thus, we may interpret the identity (6.4) as the symplectic nature of the algorithm.

Momentum Conservation. We note that one proves conservation of momentum for algorithms invariant under a symmetry group in the same way as usual, following, Marsden, Patrick, and Shkoller [1]; we need not repeat the argument.

7 Summary of the features of the Algorithm

In this section we summarize the three main features of the algorithm.

1. The algorithm conserves energy
2. The algorithm is symplectic in the sense spelled out in the previous section
3. The algorithm conserves momentum.

We have designed it to preserve energy. The discrete version of the arguments given in the continuous case shows the "spacetime" sense in which the algorithm is symplectic, as we have explained.

8 Numerical Examples

The first example is one dimensional and integrable and the second example consists of the first one coupled to an oscillator.

In each case, we will compare the constant time step method, which will show the orbits in phase space and variations in the energy as a function of time, with the corresponding results for the adaptive time step algorithm.

8.1 One Degree of Freedom Example

We will use a Lagrangian that is of the standard form kinetic minus potential, namely

$$L(q, \dot{q}) = \frac{m}{2}\dot{q}^2 - V(q)$$

where q and $\dot{q}$ are real numbers, with the corresponding discrete Lagrangian (with $\gamma = 1/2$) given by

$$L_d(q_0, q_1, h) = \frac{1}{2}m\left(\frac{q_1 - q_0}{h}\right)^2 - V\left(\frac{q_0 + q_1}{2}\right),$$

where q_0, q_1 and $h > 0$ are also real numbers. The corresponding energy, according to formula (4.4) is given by

$$E_h(q_0, q_1) = \frac{1}{2}m\left(\frac{q_1 - q_0}{h}\right)^2 + V\left(\frac{q_0 + q_1}{2}\right)$$

Constant time step algorithm. We find q_2 using the DEL equations:

$$h\left[D_2L(q_0, q_1) + D_1L(q_1, q_2)\right] = 0 \tag{8.1}$$

As $h \neq 0$, equation (8.1) leads to:

$$\frac{m}{h^2}(q_1 - q_0) - \frac{1}{2}V'\left(\frac{q_0 + q_1}{2}\right) - \frac{m}{h^2}(q_2 - q_1) - V'\left(\frac{q_1 + q_2}{2}\right) = 0 \tag{8.2}$$

to be solved for q_2. Keeping h fixed, this is the variational integrator that we use for the constant time step algorithm.

Adaptive time step algorithm. Given h_0, q_0, q_1 we have to find h_1, q_2 such that q_2 is determined by the DEL equations

$$h_0D_2L(q_0, q_1, h_0) + h_1D_1L(q_1, q_2, h_1) = 0 \tag{8.3}$$

and the energy condition:

$$E(q_0, q_1, h_0) = E(q_1, q_2, h_1) \tag{8.4}$$

We write the energy condition as follows. Define

$$\begin{aligned} f(q_0, q_1, q_2, h_0, h_1) &= E(q_1, q_2, h_1) - E(q_0, q_1, h_0) \\ &= \frac{1}{2}m\frac{(q_2 - q_1)^2}{h_1^2} + V\left(\frac{q_1 + q_2}{2}\right) - E(q_0, q_1, h_0). \end{aligned} \tag{8.5}$$

The energy equation is written this way because $E_0 := E(q_0, q_1, h_0)$ will have been computed and stored at the previous step.

The DEL equation (8.3) is written as follows:

$$g(q_0, q_1, q_2, h_0, h_1) = h_0B_0 + h_1\left[-m\frac{q_2 - q_1}{h_1^2} - \frac{1}{2}V'\left(\frac{q_1 + q_2}{2}\right)\right], \tag{8.6}$$

where

$$B_0 = \left[m\frac{q_1 - q_0}{h_0^2} - \frac{1}{2}V'\left(\frac{q_0 + q_1}{2}\right)\right], \tag{8.7}$$

again, a quantity that will have been computed at the previous step.

The numerical technique. The basic equations we want to solve are the following:

$$f(q_0, q_1, q_2, h_0, h_1) = 0 \tag{8.8}$$

$$g(q_0, q_1, q_2, h_0, h_1) = 0, \tag{8.9}$$

to be solved for the variables q_2 and h_1 as a function of q_0, q_1, and h_0. The technique we use is to minimize the quantity

$$\mathcal{B} = [f(q_0, q_1, q_2, h_0, h_1)]^2 + [g(q_0, q_1, q_2, h_0, h_1)]^2 \tag{8.10}$$

over the variables h_1, q_2, with the other variables given, and subject to the constraint $h_1 > 0$. As mentioned in the general theory, this method is implemented using descent methods, following Byrd, Lu, Nocedal, and Zhu [27] and Zhu, Byrd, Lu, and Nocedal [28].

The Double Well Potential. To illustrate the procedures, we choose $m = 1$ and take

$$V(q) = \frac{1}{2}(q^4 - q^2). \tag{8.11}$$

We study three regions of phase space as shown in Figure 8.1. The axes show the computed position $q = (q_k + q_{k+1})/2$ and the computed velocity $\dot{q} = (q_{k+1} - q_k)/h_k$ as functions of time. The orbit in figure (a) is a periodic orbit that oscillates around the stable equilibrium position $q = 1/\sqrt{2}, \dot{q} = 0$. That in (b) is a periodic orbit with high period just inside the homoclinic orbit in the positive q half space, while that in (c) is a periodic orbit just outside the homoclinic orbit.

The energy errors for both the constant time step and the adaptive time step algorithms are shown in Figure 8.2. The amplitude in the variation of the energy depends on the time step. The smaller the time step, the smaller the amplitude, but we note that there is not a big difference in the periods. The same sort of behavior can also be seen in the corresponding plots in Wendlandt and Marsden [6].

The small changes in the energy are, we believe, due to the effect of the turning points as we explained earlier. Of course one can contemplate methods whereby these can be compensated or reduced further, but it we do not explore these issues in this paper.

8.2 A Two Degree of Freedom Example

Now we consider an oscillator coupled with our previous double well potential example. The system now has chaotic orbits, so is somewhat more interesting.

The continuous Lagrangian we choose is given by:

$$L(x, y, \dot{x}, \dot{y}) = \frac{1}{2}\dot{x}^2 - V(x) + \frac{1}{2}\dot{y}^2 - \frac{1}{2}y^2 + \varepsilon xy \tag{8.12}$$

Where ε introduces a small perturbation. This is a very simple example of a chaotic system arising as a perturbation of an integrable one. Shortly we will choose V to be the potential used in the preceding subsection.

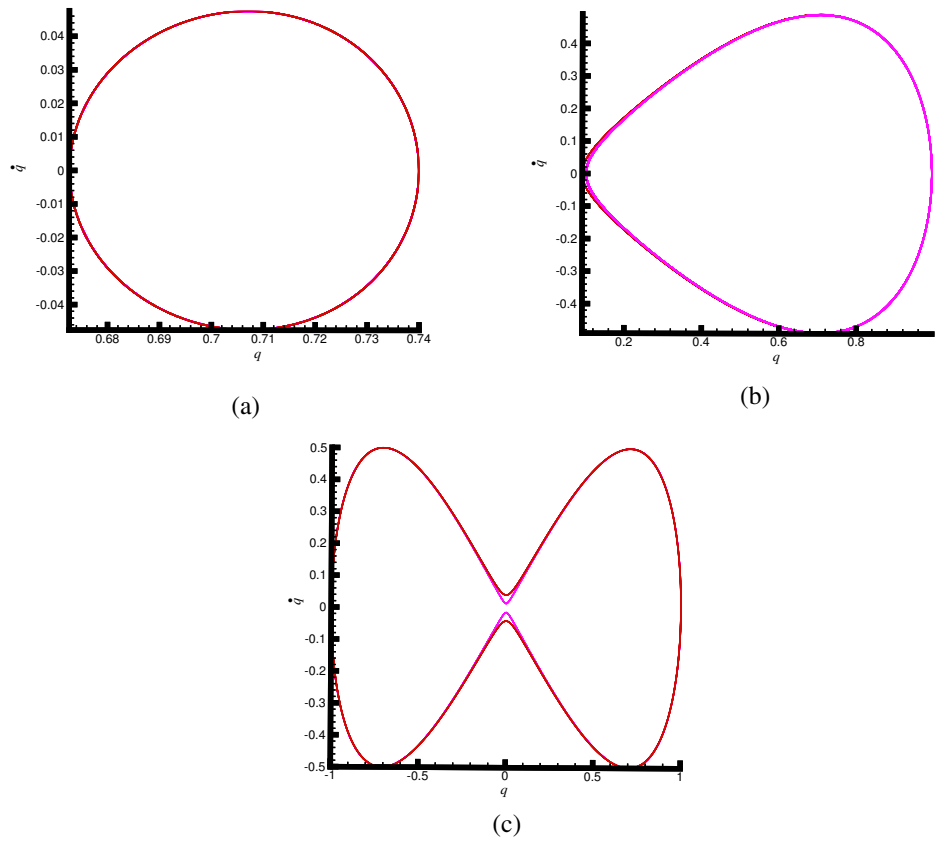

Figure 8.1: Three initial conditions are studied for the particle in the double well potential. The orbits for both the fixed time step and the adaptive time step algorithms are plotted. The initial time step used in all cases is $h_0 = 0.1$. The initial data is (a) $q_0 = q_1 = 0.74$. (b) $q_0 = q_1 = 0.995$. (c) $q_0 = 1.0, q_1 = 1.0$. The two orbits in each figure are nearly indistinguishable to the eye, but the adaptive time step computation is somewhat more accurate.

Using the notation

$$q_0 = (x_0, y_0), q_1 = (x_1, y_1),$$

the corresponding discrete Lagrangian is

$$\begin{aligned} L_d(x_0, y_0, x_1, y_1, h_0) = & \frac{1}{2}\frac{(x_1 - x_0)^2}{h_0^2} - V\left(\frac{x_0 + x_1}{2}\right) \\ & + \frac{1}{2}\frac{(y_1 - y_0)^2}{h_0^2} - \frac{1}{2}\left(\frac{y_0 + y_1}{2}\right) \\ & + \epsilon\left(\frac{x_0 + x_1}{2}\right)\left(\frac{y_0 + y_1}{2}\right). \end{aligned} \tag{8.13}$$

Given h_0, x_0, y_0, x_1, y_1 we have to find h_1, x_2, y_2 such that the DEL equations

$$h_0 D_2 L(x_0, y_0, x_1, y_1, h_0) + h_1 D_1 L(x_1, y_1, x_2, y_2, h_1) = 0 \tag{8.14}$$

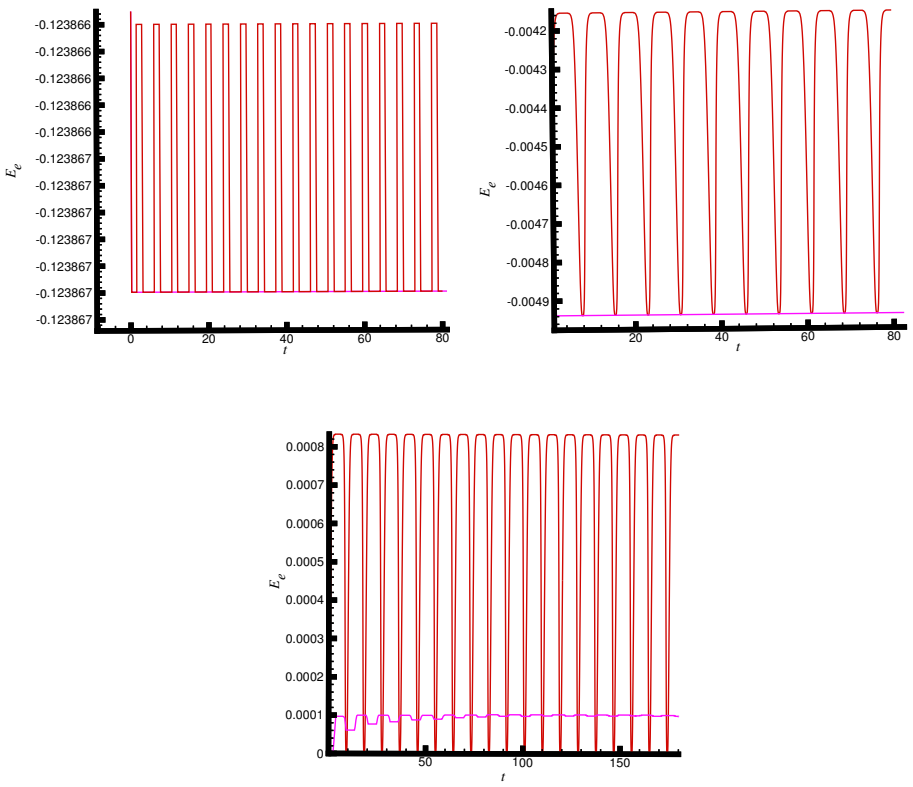

Figure 8.2: The relatively large amplitude curve shows the (small) energy error for the constant time step algorithm as a function of time, while the lower curve shows the energy error for the adaptive time step algorithm. The initial data correspond to the three regions shown in the preceding figure.

and the energy condition:

$$E(x_0, y_0, x_1, y_1, h_0) = E(x_1, y_1, x_2, y_2, h_1) \tag{8.15}$$

We write the energy condition in the form $f = 0$ as follows. Define

$$\begin{aligned} f(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1) \\ &= E(x_1, y_1, x_2, y_2, h_1) - E(x_0, y_0, x_1, y_1, h_0) \\ &= \frac{1}{2}\frac{(x_2 - x_1)^2}{h_1^2} + V\left(\frac{x_1 + x_2}{2}\right) \\ &\quad + \frac{1}{2}\frac{(y_2 - y_1)^2}{h_1^2} + \frac{1}{2}\left(\frac{y_1 + y_2}{2}\right)^2 \\ &\quad - \epsilon\left(\frac{x_1 + x_2}{2}\right)\left(\frac{y_1 + y_2}{2}\right) - E(x_0, y_0, x_1, y_1, h_0). \end{aligned} \tag{8.16}$$

The DEL equation (8.14) is written in the form of a system $g = 0, k = 0$ as

follows. Define g by

$$g(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1)$$
$$= h_0 B_0 + h_1 \left[-\frac{x_2 - x_1}{h_1^2} - \frac{1}{2} V' \left(\frac{x_1 + x_2}{2} \right) + \frac{\epsilon}{2} \left(\frac{y_1 + y_2}{2} \right) \right], \tag{8.17}$$

where

$$B_0 = \left[\frac{x_1 - x_0}{h_0^2} - \frac{1}{2} V' \left(\frac{x_0 + x_1}{2} \right) + \frac{\epsilon}{2} \left(\frac{y_0 + y_1}{2} \right) \right]. \tag{8.18}$$

Define k by

$$k(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1)$$
$$= h_0 C_0 + h_1 \left[-\frac{y_2 - y_1}{h_1^2} - \frac{1}{2} \left(\frac{y_1 + y_2}{2} \right) + \frac{\epsilon}{2} \left(\frac{x_1 + x_2}{2} \right) \right], \tag{8.19}$$

where

$$C_0 = \left[\frac{y_1 - y_0}{h_0^2} - \frac{1}{2} \left(\frac{y_0 + y_1}{2} \right) + \frac{\epsilon}{2} \left(\frac{x_0 + x_1}{2} \right) \right]. \tag{8.20}$$

The numerical technique. The basic equations we want to solve are the following:

$$f(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1) = 0 \tag{8.21}$$
$$g(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1) = 0,$$
$$k(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1) = 0 \tag{8.22}$$

to be solved for the variables x_2, y_2 and h_1 as a function of x_0, y_0, x_1, y_1 and h_0.

The technique used is to minimize the quantity

$$\mathcal{B} = [f(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1)]^2 + [g(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1)]^2 \tag{8.23}$$

over the variables h_1, x_2, y_2, with the other variables given, and subject to the constraint $h_1 > 0$. This method is then implemented by the same method as in the preceding example.

The Double Well Potential Coupled with an Oscillator. To illustrate the procedures, we choose, as before,

$$V(x) = \frac{1}{2}(x^4 - x^2). \tag{8.24}$$

We study a single chaotic orbit shown in Figure 8.3. The different projections of the orbit, to the $x, \dot{x}$, the $y, \dot{y}$ spaces and to the configuration space, x, y are shown.

In this plot, the initial conditions used were $x_0 = y_0 = x_1 = y_1 = 1.00$, $h_0 = 0.1$ and $\epsilon = 0.01$.

Figure 8.4 shows the energy behavior, as before, for the standard variational integrator verses our symplectic-energy algorithm.

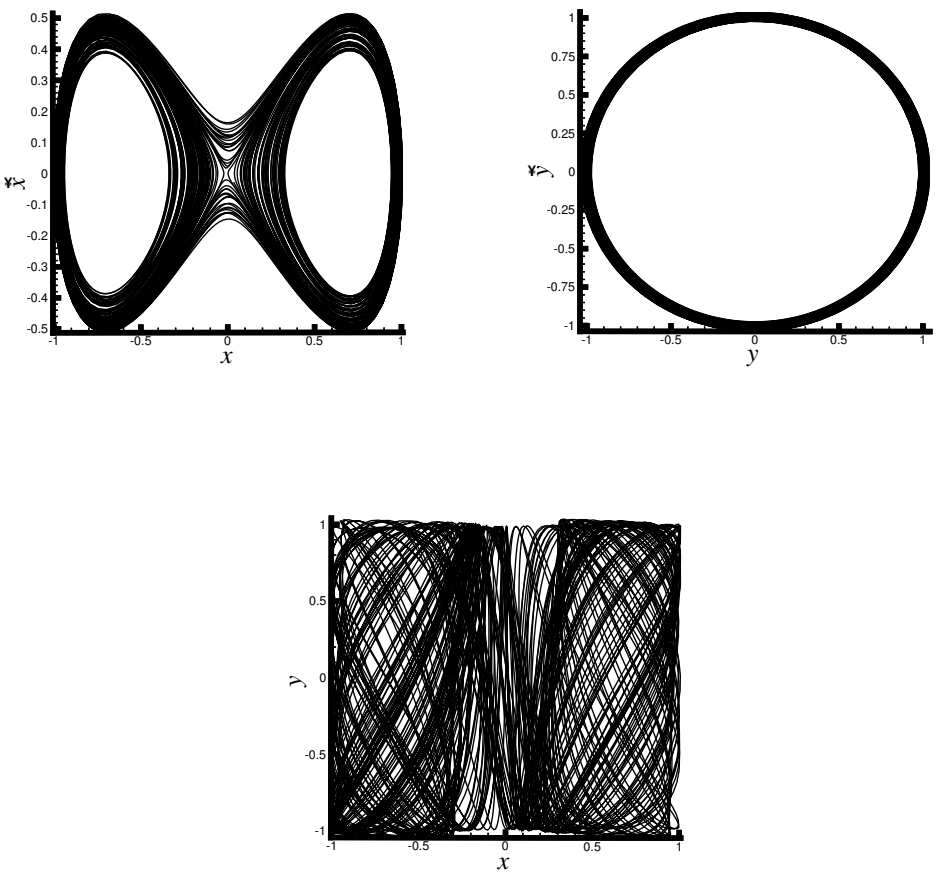

Figure 8.3: An orbit in the coupled double well – oscillator system.

Finally, figure 8.5 shows how the time step varies with the iteration.

Acknowledgments. We thank Debra Lewis, Robert McLachlan, George Patrick, Steve Shkoller, and Matt West for useful remarks.

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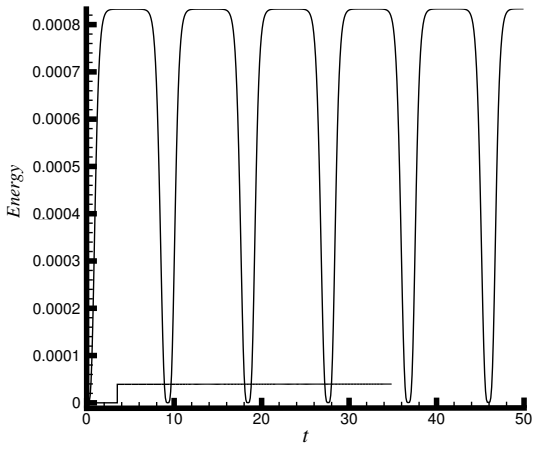

Figure 8.4: The energy behavior for the variational verses the symplectic-energy method in the coupled double well – oscillator system.

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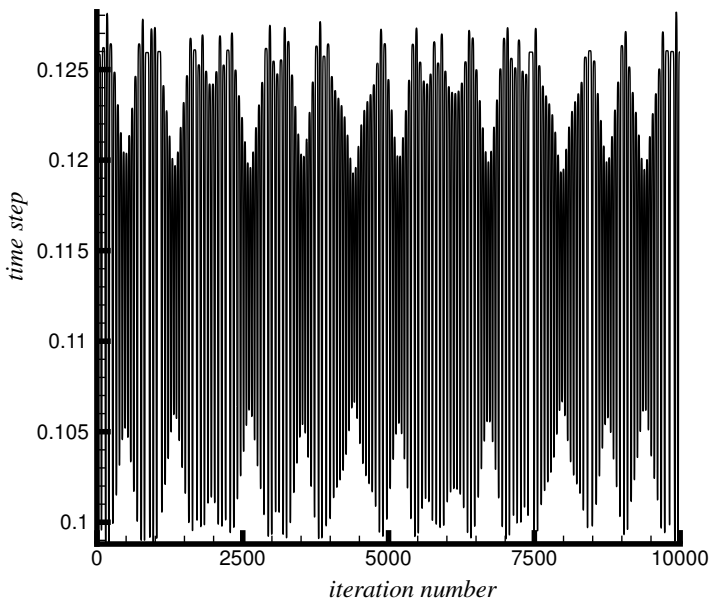

Figure 8.5: The time step verses the iteration number for the symplectic-energy method.

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