Symplectic-energy-momentum preserving variational integrators

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(Received 20 January 1999; accepted for publication 3 February 1999)

The purpose of this paper is to develop variational integrators for conservative mechanical systems that are symplectic and energy and momentum conserving. To do this, a space–time 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. © 1999 American Institute of Physics.

I. 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 in which the space–time view is stressed. This viewpoint is very important for two main reasons:

1. to avoid conflicts with well-known theorems (Ge and Marsden), which limit the possibility that constant time stepping algorithms be symplectic and 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, and Moser and Veselov is adopted; these ideas were implemented numerically by Wendlandt and Marsden. 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; and
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 and
how one can incorporate dissipative effects.

II. 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 Refs. 6 and 1.

A. 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 Ref. 8 and Ref. 9. We do mention
that for time stepping algorithms with fixed time steps, the theorem of Ge and Marsden 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 space–time
view of variational integrators, as is advocated in Ref. 1, then one can have all three of these
properties. Papers typified by Simo and Tarnow, Simo, Tarnow, and Wong, and Gonzalez have focused 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 and Lewis. See also the work by Lee.

B. Accuracy of solutions

We should, at the outset, make another point clear. We are not claiming anything about the
accuracy of individual trajectories. Indeed, it is well known that structure preservation alone does
not guarantee this. (See, e.g., Refs. 16, 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 being
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.

C. Some common integrators

In structural mechanics, the $\beta = 0, \gamma = \frac{1}{2}$ member of the widely used Newmark family is a
variational integrator (see, for example, Ref. 11) and therefore is symplectic and momentum
preserving. In fact, the whole Newmark family of algorithms is variational. 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
Refs. 6 and 18 for further discussion and references).

D. 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 Refs. 19–21, for example. Another is to incorporate the
dissipative effects into the variational principle, as in Refs. 18 and 22.

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 partial differential equations (PDE's) using multisymplectic geometry with the result being a class of multisymplectic momentum integrators. See Ref. 1 for details and numerical examples. This type of approach should ultimately be of use in elastodynamics as well as ocean dynamics, for example.

E. 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, are of current interest. 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.

F. 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 2 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

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

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 $q_1, \ldots, q_{N−1}$ leads to the discrete Euler–Lagrange (DEL) equations:

$$D_1L_d(q_k, q_{k+1}) + D_2L_d(q_{k−1}, q_k) = 0$$

for all $k = 1, \ldots, N−1$. We can write this equation in terms of a discrete algorithm $\Phi : Q \times Q \to Q \times Q$ defined implicitly by

$$D_1L_d \circ \Phi + D_2L_d = 0,$$

i.e.,

$$\Phi(q_{k−1}, q_k) = (q_k, q_{k+1}).$$

If, for each $q \in Q$, $D_1L_d(q, q) : T_qQ \to T_q^*Q$ is invertible, then $D_1L_d : Q \times Q \to T^*Q$ is locally invertible and so the algorithm $\Phi$, which flows the system forward in discrete time, is well defined for small time steps.

G. 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

$$Fl_d : Q \times Q \to T^*Q ; \ (q_0, q_1) \mapsto (q_0, D_1L_d(q_0, q_1)).$$
and define the two-form $\omega$ on $Q \times Q$ by pulling back the canonical two-form $\Omega_{\text{CAN}} = dq^i \wedge dp_i$ from $T^*Q$ to $Q \times Q$:

$$\omega = \mathcal{F}L^*_d(\Omega_{\text{CAN}}).$$

The fiber derivative is analogous to the standard Legendre transform.

The coordinate expression for $v$ is

$$v = F_L dq^i \wedge dp_i.$$

A fundamental fact is that the algorithm $\Phi$ exactly preserves the symplectic form $\omega$.

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

H. 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, $J_d: Q \times Q \to \mathfrak{g}^*$ by

$$\langle J_d(q_k, q_{k+1}), \xi \rangle = \langle D_1 L_d(q_k, q_{k+1}), \xi(q_k) \rangle.$$

A second fundamental fact is that the algorithm $\Phi$ exactly preserves the momentum map.

I. 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, $L^*: TQ \to \mathbb{R}$. 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

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

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 Ref. 18) the Newmark algorithm for the standard choice of Lagrangian given by kinetic minus potential energy. We get the central difference method for $\gamma = \frac{1}{2}$ and we get the shake algorithm with $\gamma = 1$ (the Verlet algorithm is the unconstrained version of the shake algorithm).
algorithm). We also note that the \textit{Moser–Veselov discrete Lagrangian} for the rigid body is constructed using either \( \gamma = 1 \) or \( \gamma = 0 \) (see Ref. 24 for details).

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

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

where \( \alpha, \lambda_1, \) and \( \lambda_2 \) are between 0 and 1. These other choices, which give algorithms such as the midpoint rule, are not investigated here (see Ref. 18). Alternative choices, of which this is an example, as well as issues of local truncation error and accuracy are investigated in Ref. 26.

The \textbf{unconstrained action sum} is defined by

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

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

\[
D_1 L_d(x_k, x_{k+1}) + D_2 L_d(x_{k-1}, x_k) + \lambda_k^T D g(x_k) = 0
\]

(no sum on \( k \)) with \( g(x_k) = 0 \) for \( k = 1,...,N-1 \). Here, the \( \lambda_k \) are \textit{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

\[
D_1 L_d(x_k, x_{k+1}) + D_2 L_d(x_{k-1}, x_k) + \lambda_k^T D g(x_k) = 0
\]

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

\[
\frac{1}{h} \left[ \frac{\partial L}{\partial x} \left[ \gamma x_{k-1} + (1 - \gamma) x_k, \frac{x_k - x_{k-1}}{h} \right] - \frac{\partial L}{\partial x} \left[ \gamma x_k + (1 - \gamma) x_{k+1}, \frac{x_{k+1} - x_k}{h} \right] \right]
\]

\[
\times (1 - \gamma) \frac{\partial L}{\partial x} \left[ \gamma x_{k-1} + (1 - \gamma) x_k, \frac{x_k - x_{k-1}}{h} \right] + \gamma \frac{\partial L}{\partial x} \left[ \gamma x_k + (1 - \gamma) x_{k+1}, \frac{x_{k+1} - x_k}{h} \right] + D^T g(x_k) \lambda_k = 0
\]

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

\[
M \left( \frac{x_{k+1} - 2x_k + x_{k-1}}{h^2} \right) + (1 - \gamma) \frac{\partial V}{\partial q} (\gamma x_{k-1} + (1 - \gamma) x_k)
\]

\[
+ \gamma \frac{\partial V}{\partial q} (\gamma x_k + (1 - \gamma) x_{k+1}) - D^T g(x_k) \lambda_k = 0
\]

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

Wendlandt and Marsden\(^6\) show that the \textit{algorithm defined using Lagrange multipliers coincides with that defined intrinsically using the constrained discrete Lagrangian on} \( Q \times Q \), \textit{so it is symplectic and momentum preserving}.
J. An intrinsic variational viewpoint

Recall that given a Lagrangian function $L: TQ \rightarrow \mathbb{R}$, we construct the corresponding action functional $\mathcal{S}$ on $C^2$ curves $q(t)$ by (using coordinate notation)

$$\mathcal{S}(q(\cdot)) = \int_{a}^{b} L(q^i(t), \frac{dq^i}{dt}(t)) dt.$$  \hfill (II.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 $\mathcal{S}$ 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

$$d\mathcal{S}(q(t)) \cdot \delta q(t) = \frac{d}{d\epsilon} \left. \mathcal{S}(q(t) + \epsilon \delta q(t)) \right|_{\epsilon = 0} = 0$$  \hfill (II.3)

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

$$d\mathcal{S}(q(t)) \cdot \delta q(t) = \frac{d}{d\epsilon} \int_{a}^{b} L(q^i_\epsilon(t), \frac{dq^i_\epsilon}{dt}(t)) dt = \int_{a}^{b} \delta q^i \left( \frac{\partial L}{\partial q^i} \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} + \frac{\partial L}{\partial \dot{q}^i} \frac{\partial L}{\partial q^i} \right) dt + \frac{\partial L}{\partial \dot{q}^i} \delta q^i \bigg|_{a}^{b}.$$  \hfill (II.4)

The last term in (II.4) vanishes since $\delta q(a) = \delta q(b) = 0$, so that the requirement (II.3) for $\mathcal{S}$ to be stationary yields the Euler–Lagrange equations

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} = 0.$$  \hfill (II.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 $\mathcal{S}$ to the space of solutions and to use the general identity $d^2 \mathcal{S} = 0$ 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 Ref. 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

$$\begin{pmatrix} q_0 \cdot q_1 \end{pmatrix} \rightarrow \begin{pmatrix} q_0 \cdot -hD_1L_d(q_0, q_1) \end{pmatrix},$$

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

III. 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.
A. 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 \( s(\varepsilon) \) be a family of functions of \( t \) depending on the parameter \( \varepsilon \) and with \( s_0(t) = t \) and with \( s_\varepsilon(a) = a, \ s_\varepsilon(b) = b \). Let

\[
\delta \dot{s}(t) = \frac{d}{d\varepsilon} s_\varepsilon \bigg|_{\varepsilon = 0}.
\]

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

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

Hamilton’s principle (\( \delta \int L \, dt = 0 \)) in this case gives us

\[
\int \frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} (\delta \dot{q}) = \int \left( \frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \delta q.
\]

(III.1)

Using the special form of the variation, this becomes

\[
\int \frac{\partial L}{\partial q} \delta q - \left( \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \dot{q} \delta s \, dt = 0.
\]

(III.2)

Equation (III.2) gives

\[
\frac{\partial L}{\partial q} \dot{q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = 0 \quad \Rightarrow \quad \frac{dE}{dt} = 0,
\]

(III.3)

where, as usual,

\[
E = \frac{\partial L}{\partial \dot{q}} \dot{q} - L(q, \dot{q}).
\]

(III.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.

B. Symplecticity in the space–time sense

In Ref. 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 \( \hat{H} \), a function of \( q, \ p \) and two new real variables \( q_0 \) and \( p_0 \) by

\[
\hat{H}(q, p, q_0, p_0) = H(q, p, q_0) + p_0.
\]

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 space–time sense, namely,

\[
\Omega_H = \omega + dH \wedge dt,
\]
where $\omega = \sum dq_i \wedge dp_i$ 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 $F_s$ 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 $F_s$ preserves the symplectic form above reads: $F_s^* \Omega_H = \Omega_H$ or, equivalently,

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

Cancelling $dH \wedge dt$, this reads

$$F_s^* \omega + dH \wedge ds = \Omega_0.$$  \hspace{1cm} (III.5)

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

Following the arguments in the discrete case later, or the methods of Marsden et al., one can also derive a Lagrangian version of this identity from the variational principle.

### IV. 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 $L_{d_1}(q_1,q_2) = L_d(q_1,q_2,h_1)$.

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 setup differs from the usual discrete Lagrangian procedures in the inclusion of time step information $h_1$ 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.

(a) 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 $(q_1,q_2,h_1)$:

$$[h_0 L_d(q_0,q_1,h_0) + h_1 L_d(q_1,q_2,h_1)].$$  \hspace{1cm} (IV.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.

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

$$\frac{\partial}{\partial q_1} [h_0 L_d(q_0,q_1,h_0) + h_1 L_d(q_1,q_2,h_1)] = 0.$$  \hspace{1cm} (IV.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.
A. The discrete energy

The above variational equation (IV.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:

\[
E_d(q_0, q_1, h_0) = -h_0 D_2 L_d(q_0, q_1, h_0) - L_d(q_0, q_1, h_0) = -\frac{\partial}{\partial h_0} [h_0 L_d(q_0, q_1, h_0)]. \tag{IV.3}
\]

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 (II.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

\[
E_d(q_0, q_1, h_0) = \frac{1}{2} \left( \frac{q_1 - q_0}{h_0} \right)^T M \left( \frac{q_1 - q_0}{h_0} \right) + V(\gamma q_0 + (1 - \gamma) q_1). \tag{IV.4}
\]

In this case, this can also be written as

\[
E_d(q_0, q_1, h_0) = E(\gamma q_0 + (1 - \gamma) q_1). \tag{IV.5}
\]

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 and a discrete version of the Hamilton-Jacobi equation.

The main second equation defining the algorithm is

\[
E_d(q_0, q_1, h_0) = E_d(q_1, q_2, h_1), \tag{IV.6}
\]

or, with algorithmic notation,

\[
E_{k-1} = E_d(q_{k-1}, q_k, h_{k-1}) = E_d(q_k, q_{k+1}, h_k) = E_k. \tag{IV.7}
\]

For example, in the case the Lagrangian equals kinetic plus potential energy, the condition \( E_0 = E_1 \) is equivalent to

\[
h_1^2 = \frac{(q_2 - q_1)^T M (q_2 - q_1)}{2[ E_0 - V(\gamma q_1 + (1 - \gamma) q_2) ]}. \tag{IV.8}
\]

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

\[
E_0 - V(\gamma q_1 + (1 - \gamma) q_2) \tag{IV.9}
\]

remains positive.

To realize this condition, one can consider verifying it *a posteriori* as follows.

(1) First compute the square of the new time step \( h_1 \).

(2) Substitute \( h_1^2 \) in the relation

\[
h_0 D_2 L_{h_0}(q_0, q_1) + h_1 D_1 L_{h_1}(q_1, q_2) = 0, \tag{IV.10}
\]

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 induce 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 particular case where \( g \) is large and \( K \) is small, this will only happen near ‘‘turning points;’’ that is, near points where the velocity is nearly zero. This approach will of course induce 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

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

We define \( B(q_0, q_1, h_0) \) to be

\[
B(q_0, q_1, h_0) = \left[ m \left( \frac{(q_1 - q_0)}{h_0^2} - (1 - \gamma)V'(\gamma q_0 + (1 - \gamma)q_1) \right) h_0 + \left[ -\frac{m}{h_0^2} (q_2 - q_1) - \gamma V'(\gamma q_1 + (1 - \gamma)q_2) \right] h_1 \right] h_0,
\]

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

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

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

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

In other words,

\[
E_0 - V(u) + \frac{1}{2} V'(u)(u - q_1) - \frac{\sqrt{E_0 - V(u)}}{\sqrt{2} M} B = 0.
\]

We solve the previous equation for \( u \). Then \( q_2 \) follows in a straightforward way.

\[V. \text{ TIME STEP SOLVABILITY AND AN OPTIMIZATION METHOD}\]

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

\[
K_0 + V_0 - V_1 > 0. \quad (V.1)
\]

If \( K_0 \) is large and the time step small, then in this case (V.1) is automatically verified. Indeed, \( K_0 \) large and \( V_0 = V_1 \) implies that the computed kinetic energy is positive. If \( q_1 = q_2 \) and \( h_0 \) is not so small, this is a rather delicate situation but can be explored by writing

\[
\frac{1}{2} \frac{(q_1 - q_0)^2 M(q_1 - q_0)}{h_0^2} + V(\gamma q_0 + (1 - \gamma)q_1) - V(\gamma q_1 + (1 - \gamma)q_2).
\]

Taylor expanding the potential terms when \( \gamma = \frac{1}{2} \) gives

\[
V \left( \frac{q_0 + q_1}{2} \right) - V \left( \frac{q_1 + q_2}{2} \right) = -\frac{1}{2} V' \left( \frac{q_0 + q_1}{2} \right) \left( \frac{q_2 - q_0}{2} \right). \quad (V.3)
\]
When the kinetic term is small, the condition should reduce 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.

(a) 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

\[
g(q_0, q_1, q_2, h_0, h_1) := h_0 D_2 L(q_0, q_1, h_0) + h_1 D_1 L(q_1, q_2, h_1) = 0
\]

and the energy condition

\[
f(q_0, q_1, q_2, h_0, h_1) := E(q_1, q_2, h_1) - E(q_0, q_1, h_0) = 0.
\]

The basic equations we want to solve are thus

\[
f(q_0, q_1, q_2, h_0, h_1) = 0,
\]

\[
g(q_0, q_1, q_2, h_0, h_1) = 0,
\]

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

\[
B = [f(q_0, q_1, q_2, h_0, h_1)]^2 + [g(q_0, q_1, q_2, h_0, h_1)]^2
\]

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

\[
(q_{k-1}, q_k, h_k) \rightarrow (q_k, q_{k+1}, h_{k+1}).
\]

This method may be implemented in a standard way using a quasi-Newton algorithm, as in Ref. 27 (see also Ref. 28). Of course, other methods for efficiently solving the system of equations (VIII.9) can be considered as well, but as we have mentioned, we do not carry out any extensive competitive or implementation tests in this paper. In the simple examples we do give in the section below, we use this optimization method.

VI. 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

\[
\Phi: Q \times Q \times R \rightarrow Q \times Q \times R
\]

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
\[ E_d(q_0, q_1, h_0) = -D_h[h_0L_d(q_0, q_1, h_0)]. \]

To determine the symplectic nature of the mapping \( \Phi \), we follow the general line of reasoning in Ref. 1. Namely, we consider the action sum

\[ S = h_0L_d(q_0, q_1, h_0) + h_1L_d(q_1, q_2, h_1) \]

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

\[
dS = h_0D_1L_d(q_0, q_1, h_0)dq_0 + h_1D_2L_d(q_1, q_2, h_1)dq_2 - E_d(q_0, q_1, h_0)dh_0 - E_d(q_1, q_2, h_1)dh_1.
\]

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

\[
dS = h_0D_1L_d(q_0, q_1, h_0)dq_0 + h_1D_2L_d(q_1, q_2, h_1)dq_2 - E_d(q_0, q_1, h_0)dh_0 - E_d(q_1, q_2, h_1)dh_1.
\]

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

\[
dS = \Omega_L^- + \Phi^* \Omega_L^+,
\]

where the one-forms \( \Omega_L^- \) and \( \Omega_L^+ \) are defined by

\[
\Omega_L^-(q_0, q_1, h_0) = h_0D_1L_d(q_0, q_1, h_0)dq_0 - E_ddh_0
\]

and

\[
\Omega_L^+(q_0, q_1, h_0) = h_1D_2L_d(q_0, q_1, h_0)dq_1 - E_ddh_0.
\]

Now notice that because of the definition of \( E_d \), we have

\[
\Omega_L^-(q_0, q_1, h_0) + \Omega_L^+(q_0, q_1, h_0) = d[h_0L_d] - E_ddh_0. \tag{VI.2}
\]

Substituting (VI.2) into (VI.1) gives

\[
dS = d[h_0L_d] - \theta_d^+ + \Phi^* \Omega_L^+ \tag{VI.3},
\]

where \( \theta_d^+ \) is the discrete analog of the canonical one form, \( p_idq^i \), namely

\[
\theta_d^+ = \Omega_d^+ + E_ddh_0 = h_0D_2L_d(q_0, q_1, h_0)dq_1.
\]

Taking the differential of (VI.3), using \( d^2 = 0 \) and the fact that pull back commutes with the differential gives our final identity, namely

\[
\Phi^* \Omega_d = \omega_d \tag{VI.4},
\]

where

\[
\Omega_d = -d\theta_d^+.
\]

is the discrete analog of the space–time symplectic form and where

\[
\omega_d = -d\theta_d^+.
\]
is the discrete analog of the phase space symplectic form. Notice that the identity (VI.4) is the discrete analog of the identity (III.5) in the continuous case. Thus, we may interpret the identity (VI.4) as the symplectic nature of the algorithm.

(a) **Momentum conservation.** We note that one proves conservation of momentum for algorithms invariant under a symmetry group in the same way as usual, following, Ref. 1; we need not repeat the argument.

**VII. 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 "space–time" sense in which the algorithm is symplectic, as we have explained.

**VIII. 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.

**A. One degree of freedom example**

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

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

where \( q \) and \( \dot{q} \) are real numbers, with the corresponding discrete Lagrangian (with \( \gamma = \frac{1}{2} \)) 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 (IV.4) is given by

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

(a) **Constant time step algorithm.** We find \( q_2 \) using the DEL equations:

\[ h [D_2 L(q_0, q_1) + D_1 L(q_1, q_2)] = 0. \] (VIII.1)

As \( h \neq 0 \), Eq. (VIII.1) leads to

\[ \frac{m}{h^2} (q_1 - q_0) - \frac{1}{2} V\left( \frac{q_0 + q_1}{2} \right) - \frac{m}{h^2} (q_2 - q_1) - V\left( \frac{q_1 + q_2}{2} \right) = 0 \] (VIII.2)

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

\[
h_0 D_2 L(q_0, q_1, h_0) + h_1 D_1 L(q_1, q_2, h_1) = 0 \tag{VIII.3}
\]

and the energy condition

\[
E(q_0, q_1, h_0) = E(q_1, q_2, h_1). \tag{VIII.4}
\]

We write the energy condition as follows. Define

\[
f(q_0, q_1, q_2, h_0, h_1) = E(q_1, q_2, h_1) - E(q_0, q_1, h_0)
\]

\[
= \frac{1}{2} m \frac{(q_2 - q_1)^2}{h_1^2} + V\left(\frac{q_1 + q_2}{2}\right) - E(q_0, q_1, h_0). \tag{VIII.5}
\]

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 (VIII.3) is written as follows:

\[
g(q_0, q_1, q_2, h_0, h_1) = h_0 B_0 + h_1 \left[ -m \frac{q_2 - q_1}{h_1^2} - \frac{1}{2} V\left(\frac{q_1 + q_2}{2}\right) \right]. \tag{VIII.6}
\]
where

\[ B_0 = \left[ m \frac{q_1 - q_0}{h_0} - \frac{1}{2} V(\frac{q_0 + q_1}{2}) \right]. \]  

(VIII.7)

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

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

\[ f(q_0, q_1, q_2, h_0, h_1) = 0, \]  

(VIII.8)

\[ g(q_0, q_1, q_2, h_0, h_1) = 0, \]  

(VIII.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

\[ E = [f(q_0, q_1, q_2, h_0, h_1)]^2 + [g(q_0, q_1, q_2, h_0, h_1)]^2 \]  

(VIII.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 et al.\textsuperscript{27} and Zhu et al.\textsuperscript{28}

(d) The double well potential. To illustrate the procedures, we choose \( m = 1 \) and take

\[ V(q) = \frac{1}{2} q^4 - q^2. \]  

(VIII.11)
We study three regions of phase space as shown in Fig. 1. The axes show the computed position $q_5 = (q_k + q_{k+1})/2$ and the computed velocity $q_5 = (q_{k+1} - q_k)/h_k$ as functions of time. The orbit in Fig. 1(a) is a periodic orbit that oscillates around the stable equilibrium position $q = 1/\sqrt{2}$, $q = 0$. That in Fig. 1(b) is a periodic orbit with high period just inside the homoclinic orbit in the positive $q$ half-space, while that in Fig. 1(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 Fig. 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 Ref. 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 we do not explore these issues in this paper.

B. 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 it is somewhat more interesting.

The continuous Lagrangian we choose is given by

$$L(x,y,\dot{x},\dot{y}) = \frac{1}{2}\dot{x}^2 - V(x) + \frac{1}{2}\dot{y}^2 - \frac{1}{2}y^2 + \epsilon xy,$$  \hspace{1cm} (VIII.12)

where $\epsilon$ 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.

Using the notation...
the corresponding discrete Lagrangian is

\[ L_d(x_0, y_0, x_1, y_1, h_0) = \frac{1}{2} \left( \frac{x_1 - x_0}{h_0^2} \right)^2 + \frac{1}{2} \left( \frac{y_1 - y_0}{h_0^2} \right)^2 + \frac{1}{2} \left( \frac{y_0 + y_1}{h_0^2} \right)^2 \]

\[ + \epsilon \left( \frac{x_0 + x_1}{2} \right) \left( \frac{y_0 + y_1}{2} \right). \]  \hspace{1cm} \text{(VIII.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

\[ h_0 D_2 L(x_0, y_0, x_1, y_1, h_0) + h_1 D_1 L(x_1, y_1, x_2, y_2, h_1) = 0 \]  \hspace{1cm} \text{(VIII.14)}

and the energy condition

\[ E(x_0, y_0, x_1, y_1, h_0) = E(x_1, y_1, x_2, y_2, h_1). \]  \hspace{1cm} \text{(VIII.15)}

We write the energy condition in the form \( f = 0 \) as follows. Define

\[ f(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1) = E(x_1, y_1, x_2, y_2, h_1) - E(x_0, y_0, x_1, y_1, h_0) \]

\[ = \frac{1}{2} \left( \frac{x_2 - x_1}{h_1^2} \right)^2 + V\left( \frac{x_1 + x_2}{2} \right) + \frac{1}{2} \left( \frac{y_2 - y_1}{h_1^2} \right)^2 + \frac{1}{2} \left( \frac{y_1 + y_2}{h_1^2} \right)^2 \]

\[ - \epsilon \left( \frac{x_1 + x_2}{2} \right) \left( \frac{y_1 + y_2}{2} \right) - E(x_0, y_0, x_1, y_1, h_0). \]  \hspace{1cm} \text{(VIII.16)}

The DEL equation (VIII.14) is written in the form of a system \( g = 0, k = 0 \) as follows. Define \( g \) by

\[ g(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1) = h_0 B_0 + h_1 \left[ - \frac{x_2 - x_1}{h_1^2} - \frac{1}{2} V'\left( \frac{x_1 + x_2}{2} \right) + \epsilon \left( \frac{y_1 + y_2}{2} \right) \right], \]  \hspace{1cm} \text{(VIII.17)}

where
Define $k$ by

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

(VIII.19)

where

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

(VIII.20)

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

$$ f(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1) = 0, $$

(VIII.21)

$$ g(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1) = 0, $$

(VIII.22)

$$ k(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1) = 0, $$

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

$$ B = [f(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1)]^2 + [g(x_0, y_0, x_1, y_1, x_2, y_2, h_0, h_1)]^2 $$

(VIII.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.

(f) The double well potential coupled with an oscillator. To illustrate the procedures, we choose, as before,

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

(VIII.24)
We study a single chaotic orbit shown in Fig. 3. The different projections of the orbit, to the $x$, $\dot{x}$ and the $y$, $\dot{y}$ spaces and to the configuration space $x$, $y$, are shown.

Figure 4 shows the energy behavior, as before, for the standard variational integrator versus our symplectic-energy algorithm.

Finally, Fig. 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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