A Non-Existence Result for Hamiltonian Integrators

P. F. Tupper

Department of Mathematics and Statistics, McGill University,
Montréal QC, H3A 2K6 Canada.

Abstract

We consider the numerical simulation of Hamiltonian systems of ordinary differential equations. Two features of Hamiltonian systems are that energy is conserved along trajectories and phase space volume is preserved by the flow. We want to determine if there are one-step integration schemes that preserve these two properties for all Hamiltonian systems, or at least for all systems in a wide class. This paper provides a negative result in the case of two dimensional (one degree of freedom) Hamiltonian systems, for which phase space volume is identical to area. Our main theorem shows that there are no computationally reasonable one-step integrators for which all Hamiltonian systems of one degree of freedom can be integrated while conserving both area and energy. Before proving this result we define what we mean by a computationally reasonable one-step integrator. We then consider what obstructions this result places on the existence of volume- and energy-conserving integrators for Hamiltonian systems with an arbitrary number of degrees of freedom.

Key words: ordinary differential equations, numerical integration, Hamiltonian systems, geometric integration, no-go theorems, volume-conservation, energy-conservation
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1 Introduction

We consider a system of Hamiltonian differential equations on $\mathbb{R}^{2n}$

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q}, \tag{1}$$

Email address: tupper@math.mcgill.ca (P. F. Tupper).
URL: www.math.mcgill.ca/~tupper (P. F. Tupper).

defined by the Hamiltonian function $H : \mathbb{R}^{2n} \to \mathbb{R}$. We denote the time t flow map of these equations by S^t. The flow of these differential equations has two important features. The first is that H is conserved along trajectories. That is, $H(S^t(q, p)) = H(q, p)$, for all $t \in \mathbb{R}$ and all $(q, p) \in \mathbb{R}^{2n}$. The second is that phase space volume is conserved by the flow: if $A \subset \mathbb{R}^{2n}$ is a bounded open set, then $\text{vol}(S^t(A)) = \text{vol}(A)$ for all t. The latter property is a consequence of the symplecticity of the flow. (See, for example, [4]).

For certain molecular dynamics applications, the ideal numerical integrator would be a one-step integrator that retained these two properties of the flow [8]. That is, if the integrator with time step Δt defines a map $\Phi^{\Delta t}$ on $\mathbb{R}^{2n}$, we would like both $H(\Phi^{\Delta t}(q, p)) = H(q, p)$ for all (q, p) (energy conservation) and $\text{vol}(\Phi^{\Delta t}(A)) = \text{vol}(A)$ for all bounded open subsets A of $\mathbb{R}^{2n}$ (volume conservation).

Symplectic integrators such as the implicit midpoint rule conserve volume exactly for all Hamiltonian systems, with any number of degrees of freedom, but do not conserve energy [4]. It has already been shown that in certain circumstances it is unreasonable to expect that symplectic integrators which also conserve energy exist [9]. However, volume-conservation is a weaker property than symplecticity for Hamiltonian systems of more than one degree of freedom ($n > 1$). Thus it seems plausible that there is a consistent one-step integration scheme which for any Hamiltonian function H and time step Δt yields a map $\Phi^{\Delta t}$ which conserves both volume and energy.

In this article we will argue that there is no such integration scheme. We do this by showing that no one-step numerical integrator is able to integrate *all* Hamiltonian systems in $\mathbb{R}^2$ while simultaneously conserving energy and phase space volume. For special Hamiltonian systems in $\mathbb{R}^2$ such an integrator is possible. (See [6] for examples of such systems of any number of degrees of freedom.) However, our theorem states that for any energy-conserving one-step numerical integrator from a very broad class, and applied with any positive steplength, there will be at least one Hamiltonian system on $\mathbb{R}^2$ (and in fact very many) for which it does not conserve phase space volume.

Before stating and proving our main theorem, in Section 2 we will define what we mean by a one-step integrator for Hamiltonian systems. From the class of one-step integrators we then define the *computationally reasonable* one-step integrators. This will include any explicit or implicit formula for defining a new state (q^{k+1}, p^{k+1}) as a function of a state (q^k, p^k) and a timestep Δt such that the only information used about H is its value and the value of its derivatives at a finite number of points $(r^j, s^j) \in \mathbb{R}^{2n}$, $j = 1, \ldots, m$. (The points (r^j, s^j) could be the internal stages of a Runge-Kutta method, for example.) In Section 3 we will state and prove our main result in terms of this definition. We imagine that a numerical analyst has devised a computationally reasonable one-step

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integrator that is energy-conserving for all Hamiltonian systems in $\mathbb{R}^2$. We apply this integrator to the system with Hamiltonian function $H(q,p) = p^2/2$ in $\mathbb{R}^2$. For two different inputs we observe at which points $(r^j, s^j), j = 1, \ldots, m$ the integrator depends on the function H and its derivatives. Using this information, we construct another Hamiltonian function $\widetilde{H}(q,p) = p^2/2 + V(q)$ which is arbitrarily close to H and has the following property: the numerical integrator cannot be volume-conserving for both H and $\widetilde{H}$.

The main result demonstrates that there is no one-step integration scheme that conserves volume and energy for arbitrary Hamiltonian systems of any number of degrees of freedom. However, we cannot conclude that there is no scheme that is energy- and volume-conserving for Hamiltonian systems in a particular number of dimensions $2n$, $n > 1$. This question remains open. To partially address this issue, in Section 4 we will show that under some reasonable — but not essential — conditions on an integrator, the problem reduces to that of the $n = 1$ case. Thus, there is no energy- and volume-conserving one-step integrator for fixed n that satisfies these additional assumptions.

We now explain the relation between the results here and those of the well-known paper of Zhong and Marsden [9]. In that paper the authors consider a Hamiltonian system for which there are no invariants except energy. They show that any one-step integrator that is both symplectic and energy-conserving actually computes exact trajectories of the system up to a time reparametrization. From this result they conclude that energy-conserving symplectic integration is not possible in general, since presumably the set of Hamiltonians for which one could compute trajectories exactly up to a time reparametrization are very small. Though this argument is very plausible, it leaves open two questions:

(1) How do we make mathematically precise the idea of something not being possible for any numerical integrator?
(2) Is it possible to perform energy-conserving and symplectic/volume-conserving integration for general Hamiltonians when we restrict ourselves to the $\mathbb{R}^2$ case?

The importance of the latter question is that if it were possible, then volume- and energy-conserving integration would be possible for general Hamiltonian systems via J-splitting [6,3].

We provide an answer to the first question in Section 2 with the definition of a computationally reasonable one-step integrator. As for the second question, since volume-conservation and symplecticity are identical in $\mathbb{R}^2$, Zhong and Marsden's result shows that in $\mathbb{R}^2$ volume- and energy-conserving integration is equivalent to solving the original system exactly up to a time-reparametrization. (This result is stated and proved for this case as Lemma 3

in Section 3.) The main result of our paper answers the second question in the negative by showing that it is not possible for general Hamiltonian systems in $\mathbb{R}^2$ using computationally reasonable one-step integrators.

Before we begin we discuss some interesting related work. Even though energy and volume conserving integrators may not exist, the paper [3] does the next best thing. There the authors show how to approximate any Hamiltonian function arbitrarily well by a special piece-wise smooth function of a form described by [6] whose trajectories can be integrated while conserving volume and energy. The original Hamiltonian function is not conserved. However, unlike for standard symplectic methods, a modified Hamiltonian function close to the original is conserved exactly for all time [3].

Results similar to those presented here have been derived for B-series methods [1,2,5]. In particular, [2] and [5] show that B-series methods cannot be volume-preserving for general source-free flows. Though the class of B-series integrators and the class of computationally reasonable one-step integrators have an intersection that includes most integrators used in practice, neither class is a subset of the other. The class of B-series methods does not include projection methods, for example. On the other hand, the higher coefficients of a B-series method could be chosen more or less arbitrarily in order to prevent the resulting one-step method from being computationally reasonable. Thus neither result follows from the other.

2   What is a one-step integrator for Hamiltonian systems?

A one-step integrator for a Hamiltonian system of ordinary differential equations takes a Hamiltonian H, a step length Δt, and an initial value $(q^k, p^k) \in \mathbb{R}^{2n}$, and produces a value $(q^{k+1}, p^{k+1}) \in \mathbb{R}^{2n}$. Typically, (q^{k+1}, p^{k+1}) depends on H through components of ∇H and perhaps H itself. If (q^k, p^k) is an approximation to $(q(k\Delta t), p(k\Delta t))$, we take (q^{k+1}, p^{k+1}) to be an approximation to $(q((k+1)\Delta t), p((k+1)\Delta t))$.

Definition 1 *A one-step integrator Φ for Hamiltonian systems is a function that takes arguments $H : \mathbb{R}^{2n} \to \mathbb{R}$, $\Delta t \in [0, \infty)$, $(q^k, p^k) \in \mathbb{R}^{2n}$ and either returns $(q^{k+1}, p^{k+1}) \in \mathbb{R}^{2n}$ or is not defined. We write*

$$(q^{k+1}, p^{k+1}) = \Phi(H, (q^k, p^k), \Delta t).$$

We have allowed the integrator to not be defined for certain input values. This is often the case for implicit integrators when the vector field is insufficiently smooth or the time step is too large.

In order to get meaningful constraints on what is computationally reasonable, we cannot let arbitrary maps be included in the class of algorithms we study. After all, the exact flow map has all the qualitative features one could want, but it is not feasible to compute it (even to machine precision) for most applications. We would like our definition to be broad enough to include most existing numerical integrators.

Informally, we say a one-step integrator for Hamiltonian systems Φ is *computationally reasonable* if for each (q^k, p^k) and Δt, $(q^{k+1}, p^{k+1}) = \Phi(H, (q^k, p^k), \Delta t)$ depends on H only through its value and the value of its derivatives at a finite number of points $(r^j, s^j) \in \mathbb{R}^{2n}$, $j = 1, \ldots, n$. In the following formal definition we use multi-index notation to define higher-order derivatives: for $H : \mathbb{R}^{2n} \to \mathbb{R}$ and $\alpha \in \mathbb{N}_0^{2n}$ we let

$$\partial_\alpha H := \frac{\partial^{\alpha_1}}{\partial q_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_n}}{\partial q_n^{\alpha_n}} \frac{\partial^{\alpha_{n+1}}}{\partial p_1^{\alpha_{n+1}}} \cdots \frac{\partial^{\alpha_{2n}}}{\partial p_n^{\alpha_{2n}}} H$$

Definition 2 *An integrator Φ is* computationally reasonable *if for each $H : \mathbb{R}^{2n} \to \mathbb{R}$, $(q^k, p^k) \in \mathbb{R}^{2n}$ and $\Delta t \geq 0$ there exists*

(1) $m \in \mathbb{N}_0$,
(2) $(r^j, s^j) \in \mathbb{R}^{2n}, j = 1, \ldots, m$,
(3) $\alpha^j \in \mathbb{N}_0^{2n}, j = 1, \ldots, m$,

such that for any function $\widetilde{H} : \mathbb{R}^{2n} \to \mathbb{R}$ that satisfies

$$\partial_{\alpha^j} \widetilde{H}(r^j, s^j) = \partial_{\alpha^j} H(r^j, s^j), \quad j = 1, \ldots, m$$

either $\Phi(H, (q^k, p^k), \Delta t) = \Phi(\widetilde{H}, (q^k, p^k), \Delta t)$ or both are not defined.

In the remainder of this section we discuss examples of the class of computationally reasonable integrators for Hamiltonian systems.

First note that all explicit methods fit into this class. We informally define an integrator to be explicit if it can be implemented by an algorithm that terminates in a finite number of steps using function evaluations of H or its derivatives, arithmetic operations, and logical operations. This includes all of the explicit Runge-Kutta and partitioned Runge-Kutta methods, for example. It also includes integrators that collect information adaptively to perform a step, such as the Bulirsch-Stoer method [7]. Taylor series methods are also included.

The class of computationally reasonable integrators also includes implicit methods, such as the implicit Runge-Kutta methods. Here we define an implicit method to be one where (q^{k+1}, p^{k+1}) is specified by requiring it to be the solution to a nonlinear system of equations in H and its derivatives. Im-

plicit algorithms cannot in general be implemented exactly in a finite number of steps, but they still fit into the framework of Definition 2. To see this, note that even though solving a system of nonlinear equations exactly typically requires looking at H and its derivatives at an infinite number of points (while performing the Newton Iteration, for example), determining if we have a solution to a nonlinear system of equations only requires examining a finite number of points. So if (q^{k+1}, p^{k+1}) solves the equations for H, it will still solve the equation for any $\widetilde{H}$ which is identical to H at the points. Similarly, step-and-project methods are included in this class. These are methods that consist of one step of a simpler method followed by a projection onto a manifold [4, IV.4]. This is probably the most important class of methods that are not an example of B-series methods.

What integrators do not satisfy Definition 2? Integrators that require the exact computation of integrals of H or its derivatives do not. Computing the integral of a general function requires knowing its value at an infinite set of points on the domain of integration. Unlike in the case of solving nonlinear equations, if we are given a value for the integral, there is no finite set of points at which we can examine the function to verify that the value is correct. Of course, it is possible to define a numerical integrator that uses integrals of functions, but the actual computation of these integrals for general Hamiltonian systems would require numerical quadrature. This in turn would require sampling the function at a finite number of points, and introducing truncation error. The new method with this additional truncation error does form a computationally reasonable integrator, while the original method with the exact integral does not.

3   Main Theorem

To prove our main result Theorem 5 we use the following lemma. It shows that for a Hamiltonian system in $\mathbb{R}^2$, the map defined by an energy and area preserving integrator is just a time-reparametrization of the flow map. As discussed in the introduction, this is essentially Zhong and Marsden's result [9] in the two dimensional case. The only addition is that we show that the time-reparametrization is just a constant rescaling of time where locally the constant does not depend on energy.

Lemma 3 *Let $H : \mathbb{R}^2 \to \mathbb{R}$ be a smooth function and S^t its induced Hamiltonian flow map. Let $E \in \mathbb{R}$ be a particular energy. Let U be an open set whose intersection with $\{(q, p)|H(q, p) = E\}$ is a simple curve Γ. Suppose that $\nabla H \neq 0$ on Γ. Let $\Phi^{\Delta t}$, $\Delta t > 0$ be a differentiable area-conserving map defined on U that conserves H. Then there is a constant c such that $\Phi^{\Delta t}(q, p) = S^{c\Delta t}(q, p)$ for all $(q, p) \in \Gamma$.*

Remark: Note that the constant c does *not* depend on the $(q, p) \in \Gamma$, though it may depend on E through Γ.

Proof: On U we can define canonical action-angle coordinates (θ, ϕ) in which the Hamiltonian function is $H(\theta, \phi) = H(\theta)$. The flow map is then $S^t(\theta, \phi) = (\theta, \phi + tH'(\theta))$, where $H'(\theta) \neq 0$, since we still have $[H'(\theta), 0]^T = \nabla H \neq 0$ in the new coordinates. To study the Jacobian of $\Phi^{\Delta t}$ in the coordinates (θ, ϕ) we let $(\theta_1, \phi_1) = \Phi^{\Delta t}(\theta_0, \phi_0)$ for $(\theta_0, \phi_0) \in U$. Then the Jacobian of $\Phi^{\Delta t}$ is

$$\begin{bmatrix} 1 & 0 \\ \frac{\partial \phi_1}{\partial \theta_0} & \frac{\partial \phi_1}{\partial \phi_0} \end{bmatrix}.$$

Area conservation implies that the determinant is 1 and so $\partial \phi_1 / \partial \phi_0 = 1$ for all θ_0, ϕ_0. This yields $\phi_1 = \phi_0 + \tau$ for all ϕ_0 for some τ which may depend on θ_0. Hence, if we choose c so that $c\Delta t / H'(\theta_0) = \tau$ we have

$$\Phi^{\Delta t}(\theta_0, \phi_0) = (\theta_0, \phi_0 + \tau) = S^{c\Delta t}(\theta_0, \phi_0),$$

for all $(\theta_0, \phi_0) \in \Gamma$, as required. $\diamond$

For the main result we will use the following very weak definition of consistency.

Definition 4 *Let S^t be the flow map for the Hamiltonian $H : \mathbb{R}^{2n} \to \mathbb{R}$. A one-step integrator Φ is consistent at $(q, p) \in \mathbb{R}^{2n}$ if*

$$\lim_{\Delta t \to 0} \frac{\|S^{\Delta t}(q, p) - \Phi(H, (q, p), \Delta t)\|}{\Delta t} = 0.$$

Theorem 5 *Let Φ be a one-step integrator for a Hamiltonian system in $\mathbb{R}^2$. Let $H(q, p) = p^2/2$. Let U be an open neighbourhood of $\{(q, 1)|q \in \mathbb{R}\}$. Suppose:*

(1) Φ is consistent at $(0, 1)$ (Definition 4).
(2) Φ is computationally reasonable (Definition 2).
(3) Φ conserves energy for any H, (q, p), and Δt for which it is defined.
(4) For $\Delta t \leq \Delta t_0$, $\Phi(H, (q, p), \Delta t)$ is defined, is differentiable with respect to (q, p), and conserves volume on U.

Then for all sufficiently small Δt there is a C_0^∞ function $V : \mathbb{R} \to \mathbb{R}$ such that if $\widetilde{H}(q, p) = p^2/2 + V(q)$ then $\Phi(\widetilde{H}, \cdot, \Delta t)$ is not simultaneously defined, differentiable, and volume-conserving on U.

Remark: Note that for each such Δt, the V constructed can be replaced by λV for $\lambda \in (0, 1)$ and the same result holds. This means that any derivatives of V can be chosen as small as desired, independently of Δt.

Proof: For any $\Delta t \in (0, \Delta t_0]$, since $\Phi(H, \cdot, \Delta t)$ conserves energy and is differentiable on U, the set $\{(q,1)|q \in \mathbb{R}\}$ is mapped onto itself. As $\Phi(H, \cdot, \Delta t)$ conserves volume, Lemma 3 shows that it is identical to the flow of the original Hamiltonian system on $\{(q,1)|q \in \mathbb{R}\}$ with a rescaling of time:

$$\Phi(H, (q,1), \Delta t) = (q + c\Delta t, 1),$$

for all $q \in \mathbb{R}$, where c does not depend q. The consistency condition at $(0,1)$ implies that for small enough Δt we have that $c > 0$. From now on, we assume Δt is small enough so that $c > 0$.

Consider the integrator applied to H at the point $(q, p) = (0, 1)$. Since Φ is computationally reasonable (Definition 2), there are a finite number of points $(r^j, s^j) \in \mathbb{R}^2$, $j = 1, \ldots, m$, such that Φ only depends on H at these points. Choose a $q_0 \in \mathbb{R}$ big enough so that the interval $[q_0, q_0 + c\Delta t]$ contains none of the points $r^j, j = 1, \ldots, m$ and is disjoint from the interval $[0, c\Delta t]$.

Consider the integrator applied to H at the point $(q_0, 1)$. There are points $(\bar{r}^j, \bar{s}^j), j = 1, \ldots, \bar{m}$ such that $\Phi(H, (q_0, 1), \Delta t)$ only depends on H at these points. Let V be a C_0^∞ function such that

(1) $V(q) = 0$ for q not in $[q_0, q_0 + c\Delta t]$, and $V(\bar{r}^j) = 0, j = 1, \ldots, \bar{m}$,
(2) $0 \leq V(q) < 1/2$ for all q,
(3) for some $\epsilon > 0$, $V(q) > 0$ for $q \in (q_0, q_0 + \epsilon)$.

Note that multiplying V by any factor in $(0,1)$ gives a function satisfying the same conditions.

Let $\widetilde{H}(q, p) = p^2/2 + V(q)$ and let $\widetilde{S}^t$ denote the flow map of the system with this Hamiltonian. Now if $\Phi(\widetilde{H}, \cdot, \Delta t)$ were defined, differentiable and volume-conserving on U, then by Lemma 3

$$\Phi(\widetilde{H}, (q,1), \Delta t) = \widetilde{S}^{d\Delta t}(q, 1)$$

for all $q \in \mathbb{R}$ for some constant d not depending on q. We will show that this is impossible.

First note that the integrator gives the same result for both Hamiltonians at $(0,1)$. This is because here the result of the integrator only depends on H only at the points (r^j, s^j), at which H and $\widetilde{H}$ agree. Since

$$(d\Delta t, 1) = \Phi(\widetilde{H}, (0,1), \Delta t) = \Phi(H, (0,1), \Delta t) = (c\Delta t, 1)$$

we must have $c = d$.

On the other hand, the integrators also give the same results for both Hamiltonians at $(q_0, 1)$. This implies $c \neq d$ in the following way. We have that

$$
\begin{aligned}
(q_0 + c\Delta t, 1) &= \Phi(H, (q_0, 1), \Delta t) \\
&= \Phi(\widetilde{H}, (q_0, 1), \Delta t) \\
&= \widetilde{S}^{d\Delta t}(q_0, 1) \\
&\neq S^{d\Delta t}(q_0, 1) \\
&= (q_0 + d\Delta t, 1).
\end{aligned}
$$

The inequality follows from Lemma 6, since the Hamiltonians differ on the interval $[q_0, q_0 + \epsilon]$. So $c \neq d$. This is a contradiction. Therefore, $\Phi(\widetilde{H}, \cdot, \Delta t)$ cannot be simultaneously defined, differentiable, and volume-conserving on U. $\diamond$

The following lemma asserts the intuitively clear fact that if $V(q)$ is positive for $q \in [q_0, q_0 + \epsilon]$ then the flows starting from $(q_0, 1)$ corresponding to H and $\widetilde{H}$ are different for positive times.

Lemma 6 *Let $V : \mathbb{R}^{2n} \to \mathbb{R}$ be C_0^∞ with $V(q_0) = 0$, $1/2 > V(q) \geq 0$ for all $q \in \mathbb{R}$ and $V(q) > 0$ for all $q \in [q_0, q_0 + \epsilon]$. Let $H(q, p) = p^2/2$ and $\widetilde{H}(q, p) = p^2/2 + V(q)$. Let S^t and $\widetilde{S}^t$ be the respective Hamiltonian flow maps of H and $\widetilde{H}$. Then $S^t(q_0, 1) \neq \widetilde{S}^t(q_0, 1)$ for $t > 0$.*

Proof. The trajectory for the Hamiltonian H as a function of time is $(q(t), p(t)) = (t, 1)$ for all t. Letting $\tilde{q}(t)$ describe the position for the Hamiltonian $\widetilde{H}$, the usual solution technique gives

$$
t = \int_{q_0}^{\tilde{q}} \frac{1}{\sqrt{1 - 2V(x)}} dx =: \widetilde{F}(\tilde{q})
$$

The function $\widetilde{F}$ is strictly increasing and so has a well defined inverse. We can write $\tilde{q}(t) = \widetilde{F}^{-1}(t)$. Now $\widetilde{F}'(\tilde{q}) > 1$ for $\tilde{q} > 0$, so $\tilde{q}'(t) < 1$ for $t > 0$. Hence $\tilde{q}(t) < t$ for $t > 0$ and the two flow maps cannot be equal for $t > 0$. $\diamond$

4   Multiple Degrees of Freedom

In the previous section we showed that there can be no general energy- and volume-conserving one-step integration schemes because there are no one-step integrators that conserve energy and volume for all Hamiltonians in $\mathbb{R}^2$. However, suppose we ask if such integrators exists for Hamiltonian systems of dimension $2n$, $n > 1$. We conjecture that a result like Theorem 5 still holds in

this case. However, the method of proof for the $n = 1$ case does not extend to this case.

Instead we will state two conditions on a one-step integrator, either one of which prevents it from being volume- and energy-conserving for general Hamiltonian systems in $\mathbb{R}^{2n}$. Both of these conditions are desirable for an integrator to have, but unlike computational reasonability, it is not difficult to imagine a practical integrator that did not satisfy them. The proof of the theorems in this section will work by showing that, if a computational reasonable energy-conserving one-step integrator with either condition exists, a special Hamiltonian in $\mathbb{R}^{2n}$ can be constructed for which it does not conserve volume.

In the following, fix $n \geq 2$. Let $q, p \in \mathbb{R}^n$ have components $q_i, p_i \in \mathbb{R}$. Define the projections π_i, $i = 1, \ldots, n$ by $\pi_i(q, p) = (q_i, p_i)$.

The first condition asserts that if variables (q_i, p_i) do not occur in the Hamiltonian function then the integrator does not change their value.

Condition 7 *If $H(q, p)$ is independent of the variables (q_i, p_i) then*

$$\pi_i \Phi(H, (q, p), \Delta t) = (q_i, p_i)$$

for all (q, p) and Δt for which Φ is defined.

Theorem 8 *Let Φ be a one-step integrator for Hamiltonian systems in $\mathbb{R}^{2n}$. Let $H(q, p) = p_1^2/2$. Let U be an open neighbourhood of the set*

$$\{((q_1, 0, \ldots, 0), (1, 0, \ldots, 0)) \, | \, q_1 \in \mathbb{R}\} .$$

Suppose

(1) Φ is consistent (Definition 3).
(2) Φ is computationally reasonable (Definition 2).
(3) Φ conserves energy for any H, (q, p) and Δt for which it is defined.
(4) Φ satisfies Condition 7
(5) For sufficiently small Δt, $\Phi(H, (q, p), \Delta t)$ is defined, differentiable, and conserves volume for $(q, p) \in U$.

Then for sufficiently small Δt, there is a C_0^∞ function $V : \mathbb{R} \to \mathbb{R}$ such that if $\widetilde{H}(q, p) = p_1^2 + V(q_1)$, then $\Phi(\widetilde{H}, \cdot, \Delta t)$ is not simultaneously defined, differentiable, and volume-conserving on U. For each such Δt, the V constructed can be replaced by λV for $\lambda \in (0, 1)$ and the same result holds.

Proof: We will use the hypothesized integrator on $\mathbb{R}^{2n}$ to construct an integrator ϕ on $\mathbb{R}^2$ satisfying the conditions of Theorem 5. Let $H : \mathbb{R}^2 \to \mathbb{R}$ be

a given Hamiltonian function. Define $H^* : \mathbb{R}^{2n} \to \mathbb{R}$ by $H^*(q, p) = H(q_1, p_1)$. We define the integrator ϕ by

$$\phi(H, (q_1, p_1), \Delta t) = \pi_1 \Phi(H^*, ((q_1, 0, \ldots, 0), (p_1, 0, \ldots, 0)), \Delta t).$$

Let $\bar{U} \subset \mathbb{R}^2$ be given by

$$\bar{U} := \{(q_1, p_1) | ((q_1, 0, \ldots, 0), (p_1, 0, \ldots, 0)) \in U\}.$$

It is straightforward to check that ϕ satisfies the conditions of Theorem 5 on $\bar{U}$. Thus, by the theorem, we have an arbitrarily small C_0^∞ function V such that ϕ is not simultaneously defined, differentiable, and volume-conserving on $\bar{U}$ for $\widehat{H}(q_1, p_1) = p_1^2 + V(q_1)$.

Let $\widetilde{H}^*(q, p) = p_1^2/2 + V(q_1)$ for $(q, p) \in \mathbb{R}^{2n}$. Now suppose that $\Phi(\widetilde{H}^*, \cdot, \Delta t)$ is defined, differentiable, and volume preserving on U. We will derive a contradiction by showing this implies that $\phi(\widehat{H}, \cdot, \Delta t)$ is, in fact, defined, differentiable, and volume-conserving on $\bar{U}$.

First note that $\Phi(\widetilde{H}^*, \cdot, \Delta t)$ being defined and differentiable on U implies that $\phi(\widehat{H}, \cdot, \Delta t)$ is defined and differentiable on $\bar{U}$. To check volume conservation, note that the Jacobian of the map $\Phi(\widetilde{H}^*, \cdot, \Delta t)$ has structure

$$\begin{bmatrix} J_{11} & J_{12} \\ 0 & I \end{bmatrix}$$

where we have put the variables in order $(q_1, p_1, \ldots, q_n, p_n)$ and J_{11} is a 2-by-2 matrix. Since the determinant of this matrix is 1 by volume-conservation, the determinant of J_{11} must be 1. But J_{11} is the Jacobian of $\phi(\widehat{H}, \cdot, \Delta t)$, so this latter map must be area preserving. This contradicts our earlier assumption. $\diamond$

The second condition states that if the Hamiltonian system consists of n identical uncoupled one-degree-of-freedom systems, then the integrator itself should consist of n identical uncoupled maps on the state-space of each subsystem.

Condition 9 *If $H(q, p) = \sum_{i=1}^n h(q_i, p_i)$ then there is a one-step integrator ϕ on $\mathbb{R}^2$ such that*

$$\pi_i \Phi(H, (q, p), \Delta t) = \phi(h, (q_i, p_i), \Delta t)$$

for $i = 1, \ldots, n$, for any (q, p) and Δt for which the integrator is defined.

Though this is certainly a nice property for the integrator to have (since the flow map has the same property) there are many integrators for which it does not hold. For example, step-and-project methods may not satisfy this condition, even if the underlying one-step method does.

Theorem 10 *Let Φ be a one-step integrator for Hamiltonian systems in $\mathbb{R}^{2n}$. Let $H(q, p) = \sum_i p_i^2/2$. Let $U \subset \mathbb{R}^{2n}$ be an open neighbourhood of the set*

$$\{((q_1, \ldots, q_1), (1, \ldots, 1)) \,|\, q_1 \in \mathbb{R}\}.$$

Suppose

(1) Φ is consistent (Definition 3).
(2) Φ is computationally reasonable (Definition 2).
(3) Φ conserves energy for any H, (q, p) and Δt for which it is defined.
(4) Φ satisfies Condition 9
(5) For sufficiently small Δt, $\Phi(H, (q, p), \Delta t)$ is defined, differentiable, and conserves volume for $(q, p) \in U$.

Then for sufficiently small Δt, there is a C_0^∞ function $V : \mathbb{R} \to \mathbb{R}$ such that if $\widetilde{H}(q, p) = \sum_{i=1}^n (p_i^2 + V(q_i))$ then $\Phi(\widetilde{H}, \cdot, \Delta t)$ is not simultaneously defined, differentiable, and volume-conserving on U. For each such Δt, the V constructed can be replaced by λV for $\lambda \in (0, 1)$ and the same result holds.

Proof: This theorem is proven analogously to the previous theorem. For any $H : \mathbb{R}^2 \to \mathbb{R}$ we define $H^* : \mathbb{R}^{2n} \to \mathbb{R}$ by $H^*(q, p) = \sum_i H(q_i, p_i)$. We define the integrator ϕ by

$$\phi(H, (q_1, p_1), \Delta t) = \pi_1 \Phi(H^*, ((q_1, \ldots, q_1), (p_1, \ldots, p_1)), \Delta t).$$

We define $\bar{U} \in \mathbb{R}^2$ by

$$\bar{U} := \{(q_1, p_1) \,|\, ((q_1, \ldots, q_1), (p_1, \ldots, p_1)) \in U\}.$$

As in the proof of the previous theorem, ϕ and $\bar{U}$ satisfy the conditions of Theorem 5. Thus, by the theorem, we have an arbitrarily small C_0^∞ function V such that ϕ is not defined differentiable and volume-conserving on $\bar{U}$ for $\widetilde{H} = p_1^2 + V(q_1)$.

Let $\widetilde{H}^*(q, p) = \sum_i (p_i^2/2 + V(q_i))$ for $(q, p) \in \mathbb{R}^{2n}$. Now suppose that $\Phi(\widetilde{H}^*, \cdot, \Delta t)$ is defined, differentiable, and volume preserving on U. We will derive a contradiction.

Now $\phi(\widetilde{H}, \cdot, \Delta t)$ is defined and differentiable on $\bar{U}$. To check volume conserva-

tion, note that the Jacobian of the map $\Phi(\widetilde{H}^*, \cdot, \Delta t)$ in this case has structure

$$
\begin{bmatrix}
J_{11} & 0 & \ldots & 0 \\
0 & J_{22} & \ldots & 0 \\
\vdots & \vdots & \ddots & 0 \\
0 & \ldots & 0 & J_{nn}
\end{bmatrix}
$$

where we have put the variables in order $(q_1, p_1, \ldots, q_n, p_n)$ and each J_{ii} is 2-by-2. Since the determinant of this matrix must be 1 by volume-conservation and the determinants of the J_{ii} are identical, the determinant of J_{11} must be ± 1. As in the proof of the previous theorem this implies $\phi(\widetilde{H}, \cdot, \Delta t)$ is area conserving on $\bar{U}$ which is a contradiction. $\diamond$

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