Computing Statistics for Hamiltonian Systems: A Case Study

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Abstract

We present the results of a set of numerical experiments designed to investigate the appropriateness of various integration schemes for molecular dynamics simulations. In particular, we wish to identify which numerical methods, when applied to an ergodic Hamiltonian system, sample the state-space in an unbiased manner. We do this by describing two Hamiltonian system for which we can analytically compute some of the important statistical features of its trajectories, and then applying various numerical integration schemes to them. We can then compare the results from the numerical simulation against the exact results for the system and see how closely they agree. The statistic we study is the empirical distribution of particle velocity over long trajectories of the systems. We apply four methods: one symplectic method (Störmer-Verlet) and three energy-conserving step-and-project methods. The symplectic method performs better on both test problems, accurately computing empirical distributions for all step-lengths consistent with stability. Depending on the test system and the method, the step-and-project methods are either no longer ergodic for any step length (thus giving the wrong empirical distribution) or give the correct distribution only in the limit of step-size going to zero.

Key words: symplectic integrators, Hamiltonian systems, invariant measures, long-time integration, step-and-project methods
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1 Introduction

Researchers in molecular dynamics use numerical simulations to extract information about microscopic systems of particles. A typical model in such studies

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is a Hamiltonian system of ordinary differential equations. The equations are numerically integrated over long time intervals and the trajectories are analysed to obtain information about the system. Given a single long trajectory, a researcher may look at the fraction of time the system occupies different states, the rate of transition between different states, or the correlation between different functions of the state of the system. We refer to these different data as statistical information about the trajectory. The computed trajectories are not accurate given the duration of the simulation and the step lengths used; in general the true solution to the differential equations and the numerical solution will diverge exponentially fast. Nevertheless, statistical information is often believed to be accurately computed when appropriate methods are used [1,5]. One goal of current research in numerical analysis is to understand how— and for which methods— this is possible [12].

Standard numerical methods are inappropriate for long-time simulation of Hamiltonian systems. They tend to either systematically add or systematically remove energy from the system [11,7]. There are two alternatives commonly proposed. One is the use of *symplectic* methods. This class of methods, which includes the popular Störmer-Verlet or leapfrog method, has been shown to have many desirable properties for the simulation of Hamiltonian systems. They exactly conserve phase space volume, and conserve to very high accuracy a modified Hamiltonian energy function [2,10,7]. However, they do not conserve the original Hamiltonian function. This motivates the other alternative for simulation of Hamiltonian systems: the step-and-project methods [7]. The strategy is to use a standard method but to project the solution after each step onto the manifold of states of the correct energy. Thus any method can be turned into an energy-conserving method, while the order of the original method is preserved [14].

The symplectic Störmer-Verlet method is the leading choice for simulations in molecular dynamics. In addition to being used for thousands of simulations with good empirical results [1,5] there is much theoretical evidence that these methods compute statistical properties accurately, despite not conserving energy exactly [10,15]. Thus it is generally believed that it is more important to preserve the symplectic structure of the Hamiltonian flow than it is to exactly preserve the Hamiltonian function— at least when computing statistical information about a system. However, there has been little direct evidence to show that this is so. Our paper has two goals in this regard:

(1) To demonstrate that step-and-project methods can perform significantly worse than the Störmer-Verlet method for the computation of statistical information.
(2) To exhibit some of the pathologies possible when integrating Hamiltonian systems with step-and-project methods.

We will achieve these goals by presenting the results of a set of numerical experiments intended to illuminate these issues. We apply four numerical methods to two simple Hamiltonian systems for which we can analytically determine some of their statistical properties. This allows us to compare statistical features computed with numerical methods with the actual statistics of the system. Thus we are able to directly evaluate various methods' performance as integrators for molecular dynamics, and for other situations where statistical features of Hamiltonian dynamics are important.

We focus on one particular statistical feature of the trajectories of our systems: the *empirical distribution* of a function of the state-space of the system. Given a stable system of ordinary differential equations and an initial condition, we can compute a trajectory of arbitrary length. Given a function of state-space, for each finite trajectory we can look at the distribution of the values the function takes along the trajectory. One way to visualize this information is as a histogram for the value of the function. For fixed initial conditions we can look at the limit of this distribution as the length of the trajectory goes to infinity (if it exists). We define this to be the empirical distribution for the function for this initial condition. We say that the system is ergodic if the empirical distribution does not depend on the initial condition. In this case we refer to this limit as the empirical distribution of the system.

In order to assess various methods' ability to compute empirical measures we have chosen Hamiltonian systems which are nearly ergodic and for which we can analytically determine the empirical measure of a particular function: specifically the velocity of a single particle in the system. In Section 2 we describe the two Hamiltonian systems we consider. The first consists of two particles interacting on a two-dimensional domain with reflecting walls. The second consists of three particles interacting on a two-dimensional domain with periodic boundaries. Whenever two particles are far from each other and any bounding walls, there is no force on the particles. This allows us to analytically determine the empirical measure of velocities in these states. We describe the invariant measure in Section 3.

We have deliberately not chosen for our study realistic Hamiltonian systems from the point of view of molecular dynamics. The main reason is that our comparison of methods consists of studying the difference of the analytically known empirical measure of the original system with that of the numerically computed trajectories. For realistic molecular systems exact invariant measures (on a particular energy level-set) are not available. Moreover, we suspect that these effects will be much less noticeable for systems of many interacting particles. (Though not always; see [16] for a one-dimensional example of a many particle system where projection methods destroy the systems statistics.) Finally, we believe that there is an advantage to presenting as simple an example as possible in order that the fundamental difficulties are easily

understandable.

In Section 4 we describe the numerical methods which we consider and in Section 5 we present the numerical results of their application to the test problems. We consider one symplectic method (Störmer-Verlet) and three step-and-project methods. The Störmer-Verlet method is a second-order method that uses one force evaluation per step. Since we will see that it has nearly perfect properties with respect to our tests, we do not consider any higher order symplectic methods. The three step-and-project methods we consider are the projected versions of forward Euler, backward Euler, and the 4th-order Runge-Kutta method RK4. We have chosen forward Euler since it is explicit, like Störmer-Verlet requires only one force evaluation per step. We include backward Euler to show that the poor behaviour of forward Euler is not due to it somehow being unstable. Finally, we study RK4 to show that some of the problems associated with the Euler methods persist for higher order methods. There are, of course, other numerical methods that preserve the Hamiltonian exactly [7,14], but we have not considered them here.

We conclude in Section 6 with a discussion of how the results of our experiments tie in with the current theoretical knowledge. We also briefly discuss the relevance of our experiments to practical molecular dynamics simulations.

2 Model Systems

We consider two model Hamiltonian systems in our investigation. Both are systems of circular particles interacting on two-dimensional domains. The first system consists of two discs in a two-dimensional box. The dimensions of the box are 1-by-1 units, and the radius of the discs are both $r = 0.1$ units. When the discs do not overlap the walls of the box or each other, no force acts upon them and they move at constant velocity. However, when they overlap each other or the walls, there is a restoring force that pushes them apart. The strength of the force varies linearly with the amount of overlap of the two objects.

To formally specify the first model system we let $q_i \in \mathbb{R}^2$ denote the position of the ith particle, $i = 1, 2$. Likewise, $p_i \in \mathbb{R}^2$ denotes the momentum of the ith particle. We let q, p denote the vectors of length 4 that hold the states of both particles. The Hamiltonian for the first system is

$$H(q, p) = \frac{1}{2}\|p\|^2 + U(q)$$

with equations of motion

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} = p, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q} = -\nabla U(q).$$

The potential U is given by

$$U(q) = U_{\text{inter}}(q_1, q_2) + \sum_{i=1,2} U_{\text{walls}}(q_i).$$

The function U_{inter} gives the potential energy of the interaction between the two balls. If d_{12} is the distance between the centres of the two balls then

$$U_{\text{inter}}(q_1, q_2) = \frac{1}{2}k^2(2r - d_{12})_+^2. \tag{1}$$

Here $(x)_+$ denotes the maximum of 0 and x. The value $U_{\text{walls}}(q_i)$ is the energy of interaction of particle i with the walls. In particular

$$U_{\text{walls}}(q_i) = \frac{1}{2}k^2 \sum_{j=1,2} [(q_{ij} - 1)_+^2 + (-q_{ij})_+^2].$$

We always choose the initial condition to have energy $H(q_0, p_0) = 1/2$.

The second model system is also a two-dimensional system but now consists of three discs interacting on a square periodic domain $\mathbb{T}^2$. By a periodic domain, we mean that if a particle exits the square on one side, it re-enters at the opposite side with the same velocity. The size of the domain and the particles remain the same, and the particles interact through the same potential. The positions q_i, and momenta p_i, $i = 1, 2, 3$ (and q and p) are defined analogously. The Hamiltonian of the system is

$$H(q, p) = \frac{1}{2}\|p\|^2 + \sum_{m<n} U_{\text{inter}}(q_m, q_n),$$

with U_{inter} defined as in (1), with d_{mn} the distance (in the minimal geodesic sense) between the centres discs m and n on the periodic domain.

Besides the total energy, the second model system has two additional conserved quantities, the total momentum in the x direction and the total momentum in the y direction. Moreover, if we start with zero total momentum, the sum of the x-coordinates of the discs is always conserved, as is the sum of the y-coordinates. We always start our system with a total energy of $1/2$, with zero total momentum and with the sums of the x- and y-coordinates set both set to zero. Thus the state-space for our system is the set of all $(q, p) \in \mathbb{T}^{2\times 3} \times \mathbb{T}^6$ such that $H(q, p) = 1$ and

$$q_1 + q_2 + q_3 = 0, \quad p_1 + p_2 + p_3 = 0. \tag{2}$$

For both systems k is a parameter that controls how stiff the interaction between the particles is. In both cases as $k \to \infty$ their flows approach those of a billiard system (that is, a Hamiltonian system with instantaneous collisions.) In each case the limiting billiard system has been shown to be ergodic. (See [13, p.59] for the two disc in a box, and [8] for three discs on a periodic domain.) It is unlikely that either of the model systems is ergodic on any of its energy level surfaces for finite k [9,3]. However, we conjecture that for large k the systems are indistinguishable from being ergodic up to the accuracy of our calculations [15]. This is borne out by numerical simulations. Hence, from now on in this paper we will use the term empirically ergodic to denote this approximate, empirical notion of ergodicity.

3 Empirical Distributions

For both systems we study the empirical distribution of the velocity of one of the particles. Specifically, we shall examine

$$v := \frac{p_{1,1}}{\sqrt{\sum_i \|p_i\|^2}},$$

i.e. the velocity in the x direction of the first particle, normalized by the total kinetic energy of the system. (We perform this normalization in order to minimize the effect of numerical energy drift, which is a separate issue.) When the total energy of the system is conserved, as it is for the original system and with the step-and-project methods, the normalization is irrelevant and $v = p_{1,1}$. In all cases we shall only sample the variable v when no particles or walls are interacting. These choices mean that the empirical distributions of the systems are analytically determinable and that that they independent of k.

For the first system the full state-space is the set of all states with total energy $1/2$. When we restrict to states where no objects are interacting we are left with the product of a configuration space (q variables) and a momentum space which is just the unit sphere in $\mathbb{R}^4$. This allows us to exactly sample v from the true empirical distribution in the following manner.

Let η_i, $i = 1, \ldots, 4$ be independent standard Gaussian random variables.
Let $v = \eta_1 / \sqrt{\sum_{i=1,\ldots,4} \eta_i^2}$.

The empirical distribution of the random variable generated this way is shown by the thick grey line in Figure 1.

For the second system, restricting to states without interaction means that again the state-space factors into configuration and momentum spaces. The

momentum space consists of 6-vectors of unit length such that the momentum constraint $p_1 + p_2 + p_3 = 0$ is satisfied. We can sample directly from this distribution by the following procedure.

Let $\tilde{\eta}_i$, $i = 1, \ldots, 6$ be independent standard Gaussian random variables.
Let $\eta_i = \tilde{\eta}_i - (\tilde{\eta}_1 + \tilde{\eta}_2 + \tilde{\eta}_3)/3$, for $i = 1, 2, 3$.
Let $\eta_i = \tilde{\eta}_i - (\tilde{\eta}_4 + \tilde{\eta}_5 + \tilde{\eta}_6)/3$, for $i = 4, 5, 6$.
Let $v = \eta_1 / \sqrt{\sum_{i=1,\ldots,6} \eta_i^2}$

The empirical distribution of v that is sampled by this procedure is shown by the thick grey line in Figure 3.

4 Numerical Methods

We apply four numerical methods to our two test systems: the Störmer-Verlet method, and each of forward Euler, backward Euler, and RK4 projected to conserve energy.

Applying the Störmer-Verlet method to our systems gives

$$\begin{aligned} q_{n+1/2} &= q_n + \Delta t p_n/2, \\ p_{n+1} &= p_n - \Delta t \nabla U(q_{n+1/2}), \\ q_n &= q_{n+1/2} + \Delta t p_{n+1}/2. \end{aligned}$$

It is a symplectic method [11], and as a consequence it conserves phase space volume.

The three step-and-project methods are derived by projecting onto the correct energy manifold after a step of a standard method. Starting from the state (q_n, p_n) we apply the standard method to get (q_*, p_*). The forward Euler method gives

$$q_* = q_n + \Delta t p_n, \quad p_* = p_n - \Delta t \nabla U(q_n),$$

and the backward Euler method is the solution to

$$q_* = q_n + \Delta t p_*, \quad p_* = p_n - \Delta t \nabla U(q_*).$$

See [6] for the description of RK4. Then, for each, we let

$$[q_{n+1} \;\; p_{n+1}]^{\mathrm{T}} = [q_* \;\; p_*]^{\mathrm{T}} + t\mathbf{s}^{\mathrm{T}} \tag{3}$$

where $\mathbf{s}$ is a vector search direction and t is a scalar chosen so that

$$H(q_{n+1}, p_{n+1}) = H(q_n, p_n). \tag{4}$$

We determine t with a Newton-Raphson iteration.

For each projected method it is necessary to choose a projection direction $\mathbf{s}$. The standard choice: $\mathbf{s} = \nabla H(q_*, p_*) = [\nabla U(q_*) \quad p_*]^{\mathrm{T}}$ is unsuitable because it scales badly in the $k \to \infty$ limit. Instead we choose $s = [\nabla U(q_*)/k^2 \quad p_*]^{\mathrm{T}}$ for all our numerical experiments in order to give the projected methods their best chance of success.

There is one final feature of our experiments we need to describe. For non-smooth Hamiltonian systems, the energy error of symplectic methods can be quite severe over long time intervals [4]. If left unchecked this can eventually lead to explosively unstable trajectories. This occurs in our experiments with Störmer-Verlet with the step-sizes we use. Accordingly, we project the numerically computed solution onto the set of states with the correct energy after every 1000 Störmer-Verlet steps. We use the same projection technique as for the step-and-project methods. For smoother Hamiltonian systems this would not be necessary and we do not recommend the practice in general.

5 Results

For each simulation run we choose a stiffness k, a time-step Δt, and a time interval T. For sufficiently large k, if k was doubled, the same histograms were observed if instead Δt were halved. That is, the important parameter in the simulations was $k\Delta t$. Accordingly, we fixed k to be 100 and varied Δt. For each situation we ran with several different randomly selected initial conditions.

First we will summarize the results, and then in two subsections we will provide more details together with plots of computed empirical distributions. For both systems, the Störmer-Verlet method yields the correct empirical distribution for v with no detectable truncation error. The only restriction is that the step-size be small enough so that the energy drift does not cause too much instability. The other methods perform less well for both systems. For the first model system (two balls in a box) the dynamics of projected forward Euler and projected backward Euler are no longer empirically ergodic. Projected forward Euler yields two different, wrong histograms for v depending on the initial conditions. Projected backward Euler yields only one histogram, but it is completely inaccurate. For both methods, the poor behaviour remains no matter how small Δt is. The projected RK4 method does better. Its trajectories appear to be empirically ergodic. However, for large Δt the empirical

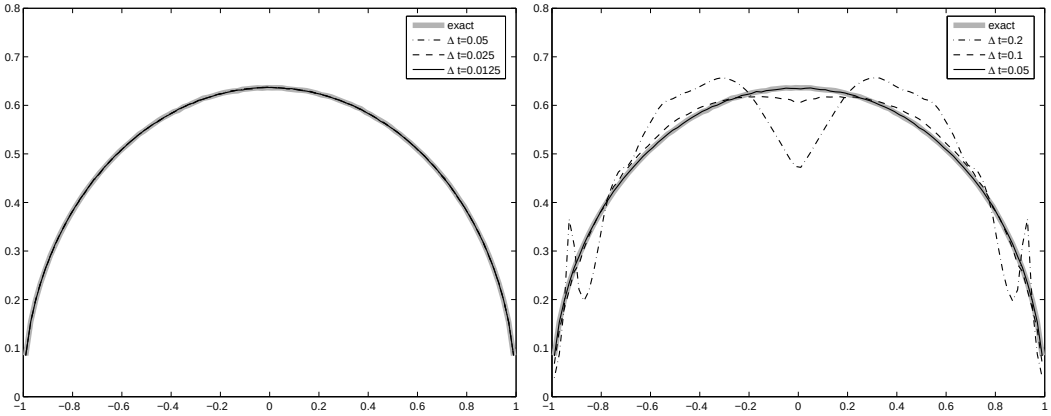

Fig. 1. (Left) Empirical distribution of v for first model system. Shown are the exact solution together with results computed by the Störmer-Verlet algorithm for three different Δt. (Right) Same as left, but with the projected RK4 method.

measure computed is far from the exact answer. As Δt goes to zero, the empirical measure converges to the answer rapidly. For the second model system (three balls on a periodic domain) the projected methods all perform better, but not as well as Störmer-Verlet. They appear to be empirically ergodic, and as Δt goes to zero, the computed empirical distribution converges to the correct empirical distribution. However, they do not exhibit the highly accurate behaviour of Störmer-Verlet.

5.1 First Model System: Two Balls in a Box

Figure 1 (left) shows results of the simulation with the Störmer-Verlet method. The duration of simulations was $T = 0.5 \times 10^9$ time units. We chose Δt to be $0.05, 0.025, 0.0125$. Each histogram generated was insensitive to the initial conditions chosen, so we conclude that the method preserves empirical ergodicity. The histograms are nearly identical to each other, and to the analytically computed histogram.

Figure 1 (right) shows the results of the simulation with the projected RK4 method. The duration of simulations was $T = 0.2 \times 10^7$ time units. We chose Δt to be $0.2, 0.1, 0.05$. This meant that the number of force evaluations per time interval was the same as for the corresponding simulation for the Störmer-Verlet method. In all cases the histogram generated did not depend on the initial condition and so empirical ergodicity appeared to be preserved. For the same number of force evaluations that gave an apparently perfect result for the symplectic method, projected RK4 gives an empirical distribution with spurious peaks and troughs. With approximately 4 times as many force evaluations it gives a reasonable approximation to the empirical measure.

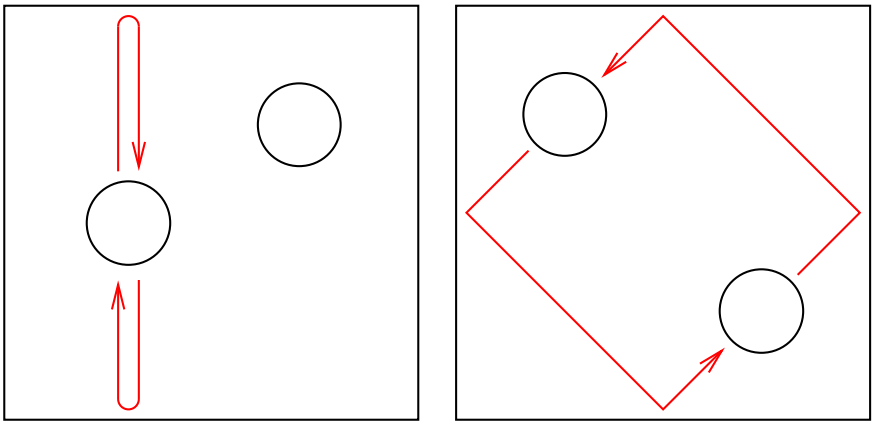

Fig. 2. Schematic diagram showing limit cycles for the first model system numerically integrated with projected forward Euler (left) and projected backward Euler (right).

On the other hand, the results for the two step-and-project methods are disastrous. We first consider the forward Euler with projection. In this case the limiting histogram generated depended on the initial condition of the simulation. There were two possibilities. Either the bin containing $v = 0$ contained all the mass, or else the bins at -1 and 1 each had half the mass. These histograms were observed because in each case the computed trajectory had converged to a stable periodic cycle. One disc was completely motionless, whereas the other was moving back and forth vertically or horizontally between two opposing walls. Figure 2 (left) shows schematically one such limit cycle. We stress that this result did not go away with reduced Δt. However, the smaller Δt was, the longer it took to converge to one of these cycles.

The results for projected backward Euler were similar, though with a different attractive limit cycle. In this case both of the particles eventually moved about the box in a square orbit, not interacting with each other, as shown in Figure 2 (right). This cycle is not unique since the particles may move either clock-wise or counter-clock-wise, depending on the initial condition. The system is therefore not empirically ergodic. However, since we only look at the statistics of v and not other variables, only one limiting histogram is produced: one with two equal delta functions at $\pm 1/2$. The same histogram was generated for all $\Delta t > 0$.

To understand the poor performance of the two first-order step-and-project methods, we must consider how these methods handle collisions. Without the energy projection, each method has a tendency to bias the energy of a colliding particle during a collision. When a collision between a particle and a wall is simulated by the forward Euler method, energy is added unphysically to the colliding particle. When the energy projection is performed the extra energy is removed from the system, but it is now removed from both particles. The net

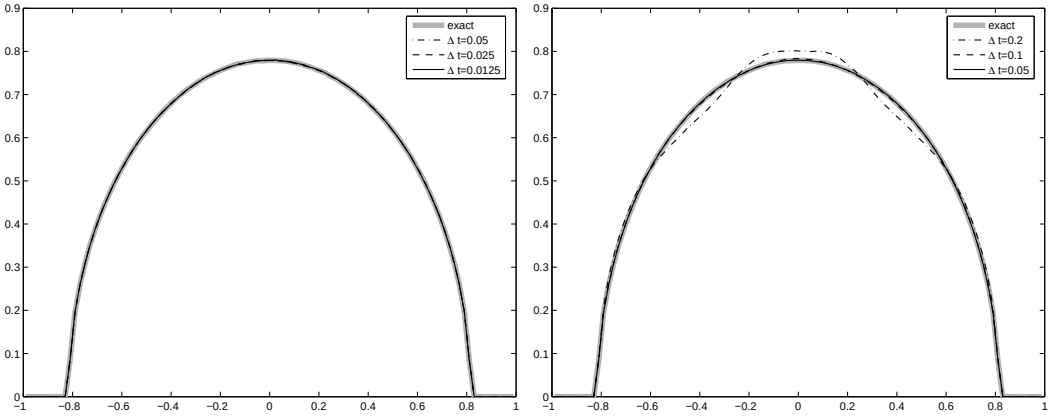

Fig. 3. (Left) Empirical distribution of v for second model system. Shown are the exact solution together with results computed by the Störmer-Verlet algorithm for three different Δt. (Right) Same as left but with projected RK4 method.

result is that the particle that is colliding gains some energy while the other particle loses energy. Since the more energy a particle has, the more often it collides with the wall, and the more energy it gains in turn, eventually all the energy is in one particle and the other is motionless, as in Figure 2(left). A similar phenomenon occurs for the project backward Euler method where in each collision with a wall the colliding particles loses some energy while the other particle gains energy. As a consequence the particles are driven to have the same energy and collide with the walls at the same rate. The net result is that trajectories such as that shown in Figure 2(right) are stable with this method.

5.2 Second Model System: Three Balls on a Periodic Domain

We applied the Störmer-Verlet method to the second model system over a time interval of length $T = 0.5 \times 10^9$ time units, with step-lengths $\Delta t = 0.05, 0.025, 0.0125$. The generated histograms do not depend on the initial condition, so empirical ergodicity is preserved. As Figure 3 (left) shows, the histograms for different step-lengths were indistinguishable from each other and from the exact solution.

The projected RK4 method was applied over a time interval of length $T = 0.2 \times 10^9$ time units, with step-lengths $\Delta t = 0.2, 0.1, 0.05$, again corresponding the the same number of force evaluations per time interval as the simulations with Störmer-Verlet. The generated histograms did not depend on initial condition, so we assume that empirical ergodicity is preserved. The situation as shown in Figure 3 is qualitatively similar to that for the first model system, though the approximation is better for this system.

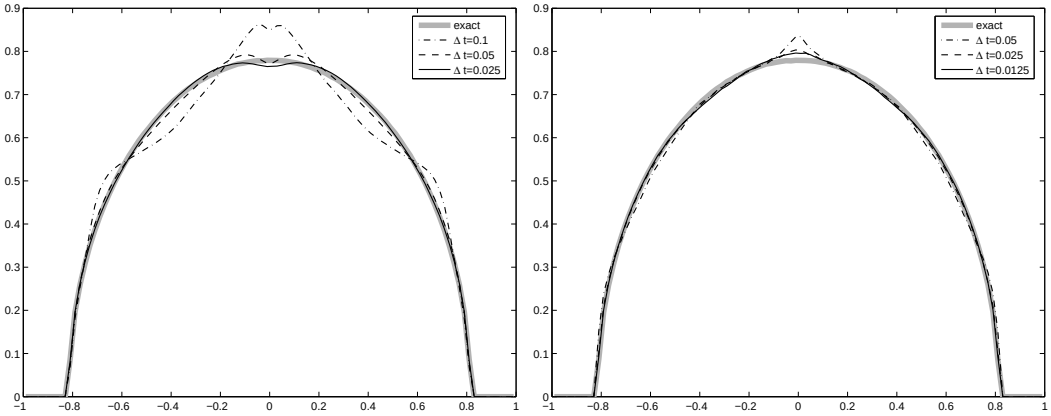

Fig. 4. Empirical distribution of v for second model system. (Left) The exact solution together with results computed by the projected forward Euler method for three different Δt. (Right) Same as left but with the projected backward Euler method.

The projected forward Euler method was applied with step-lengths $\Delta t = 0.1, 0.05, 0.025$ over $T = 10^9$ time units. The projected backward Euler method was applied with step-lengths $\Delta t = 0.05, 0.025, 0.0125$ over $T = 10^9$ time units. (For both methods, the largest step-length we used was determined by how large a step could be taken before the Newton-Raphson iteration failed to converge for some step.) Both methods generated histograms that were independent of the initial data, so empirical ergodicity appeared to be preserved. Figure 4 shows the histograms generated by applying the two first-order step-and-project methods to the system. Like the projected RK4 method, the histograms generated do depend on Δt. As $\Delta t \to 0$ the histograms appear converge to the correct one, but for any finite Δt the histogram is likely incorrect.

6 Discussion

There are three conditions which together are sufficient for a numerical integration method to exactly compute empirical distributions of functions for ergodic Hamiltonian systems [15]:

(1) The numerical method is ergodic when applied to the system.
(2) The numerical method conserves energy.
(3) The numerical method preserves phase space volume.

If any of these conditions fail to hold, we expect some error between the empirical distribution computed with the method and the exact empirical distribution.

Symplectic methods satisfy Condition 3. They do not typically satisfy Condition 2; the Hamiltonian energy H is not conserved. Rather, symplectic meth-

ods very nearly conserves a shadow Hamiltonian $\tilde{H}$ which is $\mathcal{O}(\Delta t^r)$ close to H, where r is the order of the method [2,10,7]. As a consequence, we expect errors in empirical distributions of order Δt^r. In our experiments with Störmer-Verlet, we do not observe any detectable error at all. The reason for this is that we have deliberately chosen our test systems, the statistic v, and our method of sampling so that this error is zero.

Our experiments suggest that the Störmer-Verlet method applied to our systems satisfy Condition 1. In [15] it is shown that a symplectic, approximately energy-conserving method will be empirically ergodic for small enough Δt. What we observe here for Störmer-Verlet shows that this empirical ergodicity can be so good that it is indistinguishable from actual ergodicity. Moreover, extremely small step lengths are not required for this to hold. This phenomenon still requires an explanation.

If we have an exactly energy-conserving method Condition 2 is immediately satisfied, but Condition 3 will very likely not be [17]. At first, one might conjecture that this will be the only problem, and that Condition 1 will not be grossly violated for small step lengths, since the method is convergent. This is what we observe for the second model system with the step-and-project methods. However, the first model system refutes this conjecture. If a method does not preserve phase-space volume, then it is possible for the discretized system to have limit cycles, and thus not be even empirically ergodic in any sense, for any positive Δt.

On a practical note, our experiments add support to the accepted wisdom that symplectic methods are far more appropriate for molecular dynamics than energy-conserving methods. The symplectic Störmer-Verlet method was substantially more accurate than its competitors using the same number of force evaluations per time interval and it was the cheapest of the three by far.

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