

Hamilton-Pontryagin variational integrators

Tomasz M. Tyranowski

Applied & Computational Mathematics
California Institute of Technology

June 5, 2009

1 Introduction

In this paper we discuss the applications of the Hamilton-Pontryagin variational principle for designing time-adaptive variational integrators. First, we review the multisymplectic formalism of field theories. Next, we review the Hamilton-Pontryagin principle and show how it can be used to handle time reparametrizations in a very natural way. Finally, we derive a time-adaptive variational integrator for a mechanical system and present the results of our numerical simulations.

2 Multisymplectic formalism of field theories

2.1 The jet bundle

The tangent bundle is the basic arena for the Lagrangian description of particle mechanics. The analog of the tangent bundle for field theories is the jet bundle. Let us review the basic definitions. For more details see [1]. Let X be an oriented manifold and let $\pi_{XY} : Y \rightarrow X$ be a finite-dimensional fiber bundle called the covariant configuration bundle. In physical applications X represents spacetime. Let Y_x denote the fiber $\pi_{XY}^{-1}(x)$ of Y . The physical fields are sections of this bundle. The role of the tangent bundle is played by J^1Y , the first jet bundle of Y , which we define as follows. Let $\phi_1, \phi_2 \in \Gamma(Y)$ be two sections of Y . We introduce the equivalence relation at $x \in X$

$$\phi_1 \sim_x \phi_2 \quad \Leftrightarrow \quad \phi_1(x) = \phi_2(x) \quad \wedge \quad T_x \phi_1 = T_x \phi_2. \quad (1)$$

We define the first jet bundle as the set of all equivalence classes

$$J^1Y = \left\{ [\phi]_x \mid \phi \in \Gamma(Y), x \in X \right\}. \quad (2)$$

J^1Y can be naturally identified with the affine bundle over Y whose fiber above $y \in Y_x$ consists of those linear mappings $\gamma : T_xX \rightarrow T_yY$ satisfying

$$T\pi_{XY} \circ \gamma = \text{Id}_{T_xX}. \quad (3)$$

The map γ represents the tangent mapping $T_x\phi$ for a section ϕ . The vector bundle underlying this affine bundle is the bundle whose fiber over $y \in Y_x$ is the space of linear mappings $L(T_xX, V_yY)$, where

$$V_yY = \left\{ w \in T_yY \mid T\pi_{XY}(w) = 0 \right\} \quad (4)$$

is the fiber above y of the vertical subbundle $VY \subset TY$. Let $\dim X = n + 1$ and the fiber dimension of Y be N . Let x^μ , $\mu = 0, 1, \dots, n$ be coordinates on X and let y^A , $A = 1, \dots, N$ denote fiber coordinates on Y . These induce coordinates v_μ^A on the fibers of J^1Y . Let $\phi \in \Gamma(Y)$ be a section of Y . We define its first jet prolongation $j^1\phi$ as the section of J^1Y (regarded as a bundle over X) such that

$$j^1\phi : X \ni x \rightarrow T_x\phi \in J_{\phi(x)}^1Y. \quad (5)$$

Such sections are called holonomic. In coordinates $j^1\phi$ is given by

$$x^\mu \rightarrow \left(x^\mu, \phi(x^\mu), \partial_\mu\phi^A(x^\mu) \right). \quad (6)$$

Since later we investigate numerical algorithms for mechanical systems, let us point out what J^1Y is in that case. For a non-relativistic classical particle with configuration space Q , we let $X = \mathbb{R}$ (parameter time) and $Y = \mathbb{R} \times Q$, with $\pi_{XY} : Y \ni (t, q) \rightarrow t \in X$. The first jet bundle J^1Y is the bundle whose holonomic sections are tangents of sections $\phi : X \rightarrow Y$, so we can identify $J^1Y = \mathbb{R} \times TQ$. Coordinates (t, q^A) on $\mathbb{R} \times Q$ induce the coordinates (t, q^A, v^A) on J^1Y .

2.2 The dual jet bundle

Just as the tangent bundle is the arena for Lagrangian dynamics, so is the cotangent bundle for Hamiltonian dynamics. The role of the cotangent bundle for field theories is played by the dual jet bundle J^1Y^* , whose definition we review in what follows. We define J^1Y^* to be the vector bundle over Y whose fiber at $y \in Y_x$ is the set of affine maps from J_y^1Y to $\Lambda_x^{n+1}X$. Since $\Lambda_x^{n+1}X$ is one-dimensional, an affine map can be given in coordinates by

$$v_\mu^A \rightarrow (p + p_A^\mu v_\mu^A) d^{n+1}x, \quad (7)$$

where $d^{n+1}x = dx^0 \wedge \dots \wedge dx^{n+1}$. This induces fiber coordinates (p, p_A^μ) on $J_y^1Y^*$. It turns out that J^1Y^* can be canonically identified with another vector bundle more useful in applications. Namely, let $Z \subset \Lambda^{n+1}Y$ be a subbundle whose fiber over $y \in Y$ is

$$Z_y = \left\{ z \in \Lambda_y^{n+1}Y \mid \mathbf{i}_v \mathbf{i}_w z = 0 \text{ for all } u, v \in V_yY \right\}. \quad (8)$$

Elements of Z can be written uniquely as $z = pd^{n+1}x + p_A^\mu dy^A \wedge d^n x_\mu$, where $d^n x_\mu = \mathbf{i}_{\partial_\mu} d^{n+1}x$. Equating the coordinates (x^μ, y^A, p, p_A^μ) of Z and of J^1Y^* defines a vector bundle isomorphism.

We recall that the cotangent bundle carries a natural symplectic structure. In the same manner a natural ‘multisymplectic’ $(n+2)$ -form can be defined on the dual jet bundle. This canonical $(n+2)$ -form on $J^1Y^* \sim Z$ can be defined in coordinates by

$$\Omega = dy^A \wedge dp_A^\mu \wedge d^n x_\mu - dp \wedge d^{n+1}x. \quad (9)$$

The multisymplectic form can also be defined in a more intrinsic way. For details see [1]. Let us work out what J^1Y^* in the case of particle mechanics is. As mentioned earlier, we have $X = \mathbb{R}$, $Y = \mathbb{R} \times Q$. Then $Z = T^*Y = T^*\mathbb{R} \times T^*Q$ has coordinates $(t, p, q^1, \dots, q^N, p_1, \dots, p_N)$ and the canonical 2-form is

$$\Omega = dq^A \wedge dp_A + dt \wedge dp, \quad (10)$$

that is the multisymplectic approach reduces to the extended state space formulation of classical mechanics.

2.3 Lagrangian dynamics

Let $\mathcal{L} : J^1Y \rightarrow \Lambda^{n+1}X$ be a given smooth bundle map over X , which we are going to call the Lagrangian density. In coordinates

$$\mathcal{L} = L(x^\mu, y^A, v_\mu^A) d^{n+1}x. \quad (11)$$

Our goal is to introduce a multisymplectic structure on the jet bundle J^1Y . We do that by defining the covariant Legendre transform associated with \mathcal{L} . This is a fiber-preserving map

$$\mathbb{F}\mathcal{L} : J^1Y \rightarrow J^1Y^* \sim Z \quad (12)$$

given in coordinates by

$$p_A^\mu = \frac{\partial L}{\partial v_\mu^A}, \quad (13)$$

$$p = L - \frac{\partial L}{\partial v_\mu^A} v_\mu^A. \quad (14)$$

For a more intrinsic definition see [1]. We are now in a position to introduce the canonical $(n+2)$ -form on the jet bundle by pulling back the multisymplectic form on the dual jet bundle

$$\Omega_{\mathcal{L}} = \mathbb{F}\mathcal{L}^*\Omega. \quad (15)$$

In coordinates this gives the expression

$$\Omega_{\mathcal{L}} = dy^A \wedge d\left(\frac{\partial L}{\partial v_\mu^A}\right) \wedge d^n x_\mu - d\left(L - \frac{\partial L}{\partial v_\mu^A} v_\mu^A\right) \wedge d^{n+1}x. \quad (16)$$

Lagrangian dynamics is governed by the least action principle, which states that a field-theoretic system evolves according to a section of the configuration bundle $\phi \in \Gamma(Y)$ iff ϕ is a stationary point of the action functional $S : \Gamma(Y) \rightarrow \mathbb{R}$ given by

$$S[\phi] = \int_X \mathcal{L}(j^1\phi). \quad (17)$$

It can be proved that this holds iff the Euler-Lagrange equations are satisfied in coordinates

$$\frac{\partial L}{\partial y^A}(j^1\phi) - \frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial v_\mu^A}(j^1\phi) \right) = 0. \quad (18)$$

3 Hamilton-Pontryagin principle

Most physical field theories are fully covariant in the sense that no distinction exists between space and time. However, sometimes it is useful to choose one particulate coordinate time, which leads to a slicing of spacetime. A slicing is determined by the lapse function and the shift vector. The lapse function N determines the rate at which the 'proper' time changes from one hypersurface to the next. The shift vector M describes the distortion of the initial hypersurface, if you think of the slicing as a time evolution of the initial hypersurface. This is for instance useful in numerical computations, as one can construct adaptive algorithms for solving field equations. In this section we show how a slicing can be handled in the variational way with the help of the Hamilton-Pontryagin principle on jet bundles. Since in subsequent sections we investigate integrators for mechanical systems, let us restrict ourselves to discussing the Hamilton-Pontryagin approach for particle mechanics only. For a more general discussion see [3].

In addition to the configuration bundle Y and the ject bundle J^1Y (with coordinates (t, q^A, v^B)) described in the previous sections, define the linear dual Π as the bundle over Y whose total space is given by

$$\Pi = T\mathbb{R} \otimes V^*Y = \mathbb{R} \times V^*Y, \quad (19)$$

where V^*Y is the dual of the vertical bundle $VY \subset TY$. The bundle Π has coordinates (t, q^A, p_B) . Given a Lagrangian $L : J^1Y \rightarrow \mathbb{R}$ we introduce a covariant Lagrangian \tilde{L} as follows. We introduce the extended configuration bundle $\tilde{Y} = \mathbb{R} \times Y = \mathbb{R} \times (\mathbb{R} \times Q)$ with coordinates (τ, t, q^A) . This way we put the physical time t on equal footing with the dynamic variables q^A and consider it a function of the new parameter τ . The first jet bundle $J^1\tilde{Y}$ has now coordinates (τ, t, q^A, N, w^B) . We also introduce the bundle $\tilde{\Pi}$ with coordinates (τ, t, q^A, E, p_B) . The Lagrangian L on J^1Y induces a Lagrangian \tilde{L} on $J^1\tilde{Y}$

$$\tilde{L}(\tau, t, q, N, w) = L(t, q, wN^{-1})N. \quad (20)$$

Let us now form the Hamilton-Pontryagin bundle $J^1\tilde{Y} \times_{\tilde{Y}} \tilde{\Pi}$. Consider the action functional S defined on the set of sections of this bundle

$$S = \int_{\tau_1}^{\tau_2} \left[L(t, q, wN^{-1})N - E(\dot{t} - N) + p_A(\dot{q}^A - w^A) \right] d\tau, \quad (21)$$

where the dot denotes derivatives with respect to τ . Note that we have enforced the constraints $\dot{t} = N$ and $\dot{q}^A = w^A$. By the Hamilton-Pontryagin variational principle, we vary this action to obtain the following equations of motion

$$\dot{t} = N \quad (22)$$

$$\dot{q}^A = w^A \quad (23)$$

$$\dot{E} = -\frac{\partial \tilde{L}}{\partial t} = -\frac{\partial L}{\partial t} N \quad (24)$$

$$\dot{p}_A = \frac{\partial \tilde{L}}{\partial q} = \frac{\partial L}{\partial q} N \quad (25)$$

and the constraints

$$p_A = \frac{\partial \tilde{L}}{\partial w^A} = \frac{\partial L}{\partial v^A} \quad (26)$$

$$E = -\frac{\partial \tilde{L}}{\partial N} = \frac{\partial L}{\partial v^B} \frac{w^B}{N} - L. \quad (27)$$

Note that the evolution of N is not specified. In fact N is completely arbitrary, which reflects the reparametrization invariance of particle mechanics. This fact is of great significance for applications in numerical analysis. It gives one the ability to choose N to one's liking, and since the lapse function N determines the rate of change of the physical time with respect to the 'simulation' time, this allows time adaptation of the algorithm used for solving the above equations of motion. Moreover, since the equations of motion have an underlying variational structure, this approach offers a way of constructing time-adaptive variational integrators. We investigate this further in the following section.

4 Time-adaptive variational integrators

In this section we show how the Hamilton-Pontryagin approach can be used to design a time-adaptive variational integrator. We basically reproduce the results obtained by Desbrun et al (see [4]). However, we do that in a different way, starting directly at the continuum level and explicitly showing the variational origin of the algorithm.

Let us consider a 1-dimensional mechanical system described by the Lagrangian of the form

$$L(q, v) = \frac{1}{2}v^2 - V(q), \quad (28)$$

where $V(q)$ is some potential. Let us write the covariant action principle (21)

$$S = \int_{\tau_1}^{\tau_2} \left[\left(\frac{1}{2}v^2 - V(q) \right) N - E(\dot{t} - N) + p(\dot{q} - vN) \right] d\tau, \quad (29)$$

where for computational convenience we stick to the physical velocity v rather than $w = vN$. As pointed out in the previous section, the lapse function N is completely arbitrary at the

continuum level, so we can set $N = N(\tau)$ however we like. Nevertheless, in practice we want the algorithm to adapt the time step according to some criterion depending on the current configuration of the system, that is we want to prescribe some general rule $N = \Gamma(q, v)$. We can enforce this condition by adding an additional Lagrange multiplier in our action functional

$$S = \int_{\tau_1}^{\tau_2} \left[\left(\frac{1}{2} v^2 - V(q) \right) N - E(\dot{t} - N) + p(\dot{q} - vN) + \lambda(N - \Gamma(q, v)) \right] d\tau. \quad (30)$$

We are further going to assume $\Gamma(q, v) = \Gamma(q)$ for simplicity. We discretize (30) on a uniform mesh with the step h in the τ space, i.e. $\tau_{k+1} = \tau_k + h$. Use the following discrete Lagrangian

$$L_d = h \cdot \left[\left(\frac{1}{2} v_k^2 - V(q_k) \right) N_k - E_k \left(\frac{t_{k+1} - t_k}{h} - N_k \right) + p_k \left(\frac{q_{k+1} - q_k}{h} - v_k N_k \right) + \lambda_k \left(N_k - \Gamma(q_k) \right) \right]. \quad (31)$$

The resulting discrete Euler-Lagrange equations are

$$\lambda_m : \quad N_m = \Gamma(q_m) \quad (32)$$

$$E_m : \quad t_{m+1} = t_m + N_m h \quad (33)$$

$$p_m : \quad q_{m+1} = q_m + v_m N_m h \quad (34)$$

$$t_m : \quad E_{m+1} = E_m \quad (35)$$

$$q_m : \quad \frac{p_{m+1} - p_m}{h} = -V'(q_{m+1}) N_{m+1} - \lambda_{m+1} \Gamma'(q_{m+1}) \quad (36)$$

$$N_m : \quad E_m + \lambda_m = p_m v_m - \left(\frac{1}{2} v_m^2 - V(q_m) \right) \quad (37)$$

$$v_m : \quad p_m = v_m. \quad (38)$$

Note that (32) gives us the prescribed time-adaption and (35) states that the quantity E_m is conserved. Looking at (37) we see that E_m is related to the total energy of the system. In fact, as long as λ_m stays small, the numerical energy of the system is approximately conserved. The above numerical algorithm can be put more succinctly

$$t_{m+1} = t_m + N_m h \quad (39)$$

$$q_{m+1} = q_m + v_m N_m h \quad (40)$$

$$\frac{1}{2} v_{m+1}^2 + V(q_{m+1}) - \lambda_{m+1} = \frac{1}{2} v_m^2 + V(q_m) - \lambda_m \quad (41)$$

$$v_{m+1} = v_m - \lambda_{m+1} \Gamma'(q_{m+1}) h - V'(q_{m+1}) \Gamma(q_{m+1}), \quad (42)$$

where the first two equations are explicit update rules and the last two equations have to be simultaneously solved for v_{m+1} and λ_{m+1} . We have implemented this algorithm for the pendulum, that is for the potential

$$V(q) = 1 - \cos q. \quad (43)$$

We have tested two adaption strategies suggested in [4], namely

1. equispaced poses $\Gamma(q_k) = \frac{1}{\sqrt{E_0 - V(q_k) + \epsilon}}$
2. equispaced phase space points $\Gamma(q_k) = \frac{1}{\sqrt{E_0 - V(q_k) + V'(q_k)^2 + \epsilon}}$

where E_0 is the initial energy of the system and ϵ is a regularization parameter preventing the blow-up of $\Gamma(q)$ at the turning points. Since $\epsilon > 0$, the poses/phase space points are only approximately equispaced. The results of the simulations are presented in Fig. 1-12. We used $h = 0.01$ and $\epsilon = 0.01$. Notice the very good behavior of the numerical energy in Fig. 6 and Fig. 12.

5 Final thoughts and future work

Although the algorithm presented in the previous section basically reproduces the results obtained by Desbrun et al, our approach has an important advantage. In Desbrun et al time adaption is introduced *ad hoc* at the discrete level already. In our approach we use the Hamilton-Pontryagin principle to introduce time reparametrization at the continuum level. In this way we exactly know what we are discretizing. Moreover, taking a more sophisticated discretization of our action functional we will end up with an essentially new time-adaptive numerical scheme, otherwise difficult or even impossible to come up with.

The Hamilton-Pontryagin approach also seems to offer a way to design a variational integrator that preserves energy exactly. If we discretize the action functional (29), then one of the discrete Euler-Lagrange equations will be energy conservation. Unfortunately, a one-step method obtained this way has a difficulty near the turning points of the system. While it doesn't technically break down, it ceases to be useful, since the time steps become so small, that the simulation virtually does not progress in time. One way to circumvent this problem could be to design a multistep scheme in which energy preservation is supposed to hold every other step for instance. We have some promising results with an integrator like that, but several other computational issues have to be addressed. This is work in progress.

References

- [1] Gotay M., Isenberg J., Marsden J., Montgomery R., *Momentum maps and classical fields. Part I: Covariant Field Theory*, arXiv:physics/9801019
- [2] Vankerschaver J., Yoshimura H., Marsden J., *A Hamilton-Pontryagin principle for field theories*, in preparation (2009)
- [3] Vankerschaver J., Marsden J., *The Hamilton-Pontryagin principle and the adjoint formalism*, in preparation (2009)
- [4] Kharevych L., Mullen P., Leyendecker S., Tong Y., Marsden J., Desbrun M., *Time adaption strategies for variational integrators*, unpublished (2007)

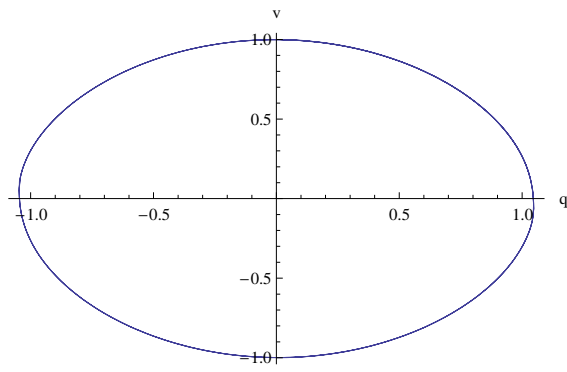


Figure 1: The phase plot of the pendulum (equispaced poses)

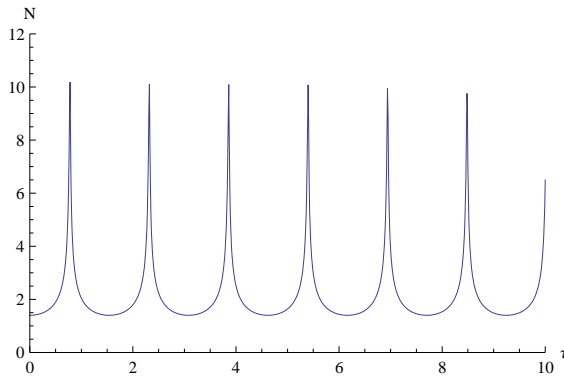


Figure 2: The lapse function versus the parameter time τ (equispaced poses)

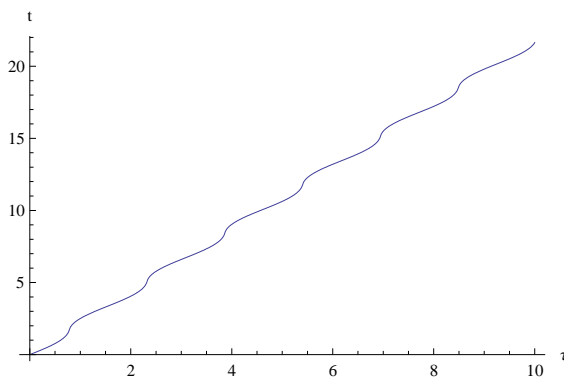


Figure 3: The physical time t versus the parameter time τ (equispaced poses)

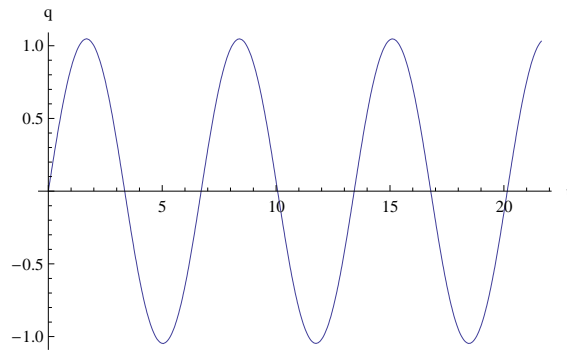


Figure 4: The position of the pendulum versus the physical time t (equispaced poses)

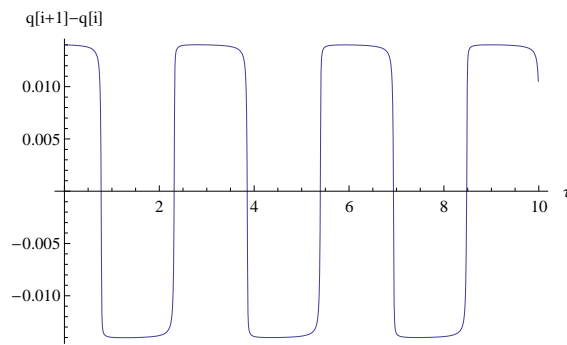


Figure 5: The distance between consecutive positions of the pendulum versus the parameter time τ (equispaced poses)

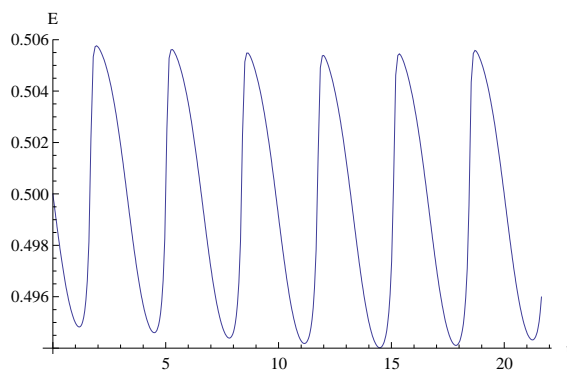


Figure 6: The energy of the pendulum versus the physical time τ (equispaced poses)

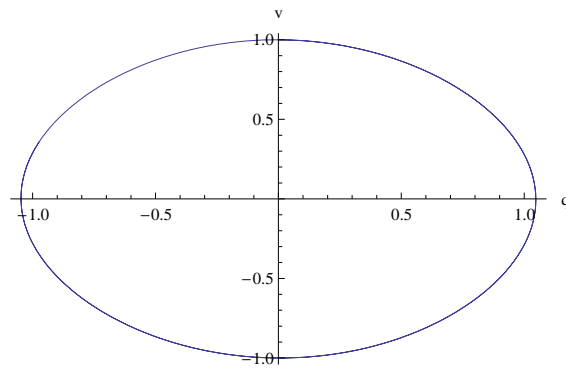


Figure 7: The phase plot of the pendulum (equispaced phase space points)

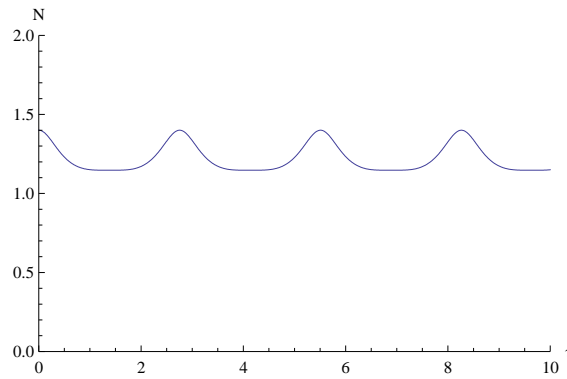


Figure 8: The lapse function versus the parameter time τ (equispaced phase space points)

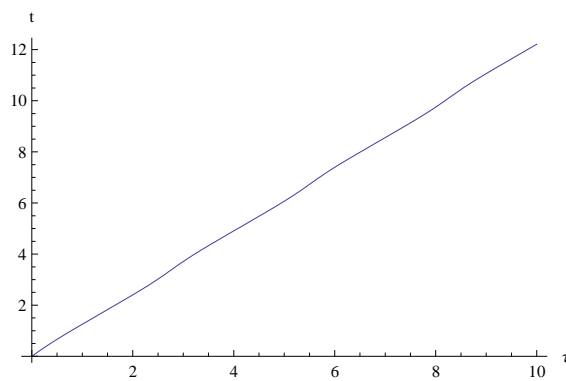


Figure 9: The physical time t versus the parameter time τ (equispaced phase space points)

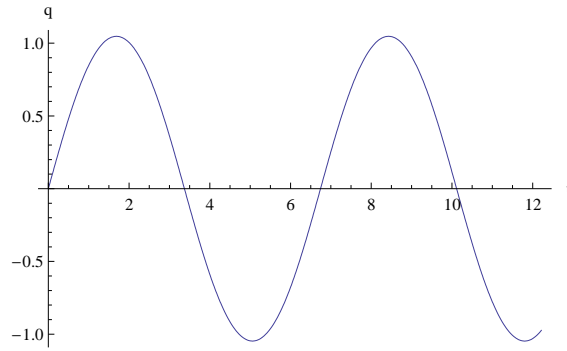


Figure 10: The position of the pendulum versus the physical time t (equispaced phase space points)

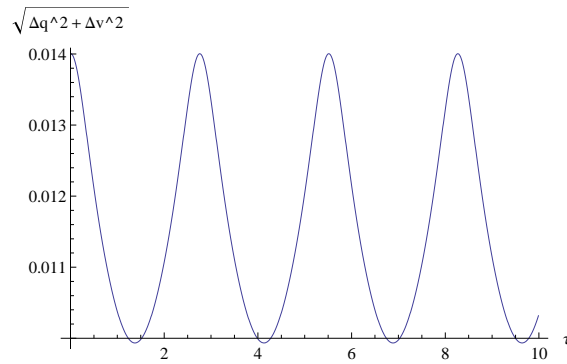


Figure 11: The distance between consecutive points in the phase space versus the parameter time τ (equispaced phase space points)

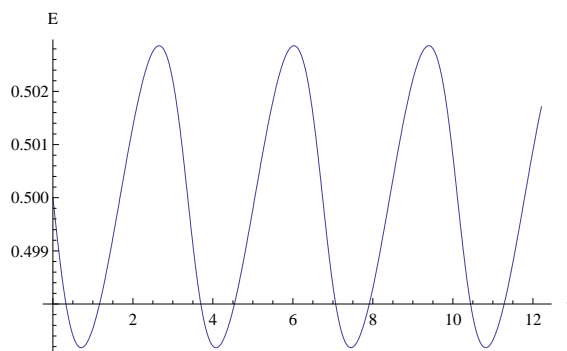


Figure 12: The energy of the pendulum versus the physical time τ (equispaced phase space points)