How to Regularize a Symplectic-Energy-Momentum Integrator

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July 22, 2005

Abstract

We identify ghost trajectories of symplectic-energy-momentum (SEM) integration and show that the ghost trajectories are not time reversible. We explain how SEM integration can be regularized, in a SEM preserving manner, so that it is time reversible. We describe an algorithm for implementing the regularized SEM integrator. Simulation results for the pendulum are given. Coordinate invariance of the regularized SEM integrator is briefly discussed.

Key Words DTH dynamics, symplectic energy momentum integrator, discrete mechanics, discrete time Hamiltonian, discrete variational principles, principle of least action, energy conserving methods, extended phase space, midpoint method.

1 Introduction

Is symplectic-energy-momentum (SEM) integration obstructed by singularities? In 1994, the answer appeared to be yes. SEM integration of the rotations of a pendulum did not appear possible, Shibberu [18]. In this article, we show that SEM integration is actually *not* obstructed by singularities. Difficult to compute, ghost trajectories are identified, but these ghost trajectories are not time reversible. We explain how SEM integration can be regularized, *in a SEM conserving manner,* so that it is time reversible. We begin with a brief review of SEM integration.

A SEM integrator is a symplectic integrator which exactly conserves energy and momentum. Symplecticness implies the integrator can be derived from a discrete variational principle [20]. The discrete variational principle of a symplectic integrator gives it coordinate invariant properties.

SEM integration emerged from two lines of research, symplectic integration and discrete mechanics. Efficient computation is emphasized in symplectic integration. Preservation of the physical laws of nature is the emphasis in discrete mechanics. The term "symplectic-energy-momentum integrator" was coined and popularized by Kane, Marsden and Ortiz [12]. See also Chen, Guo and Wu [3] for related work on higher-order, sympletic-energy integrators. Guibout and Bloch [11] have developed a general framework for deriving many of the published symplectic integrators, including SEM integrators. They also provide an interesting comparison of the various discrete variational principles used.

The author's work on a discrete-time theory for Hamiltonian dynamics (DTH dynamics) [17] predates the work of Kane et. al. [12]. DTH dynamics is a SEM integrator. DTH dynamics originated from an effort to obtain the exact energy and momentum conserving properties of the discrete mechanics of Greenspan [9], [10] from the variational principle used in the discrete mechanics of Lee [14], [15]. DTH dynamics was proved in 1994 (see Shibberu [18], [19]) to be symplectic and hence a SEM integrator. D'Innocenzo, Renna and Rotelli [5] have done work that can also be related to SEM integration.

In the author's work, SEM integration is accomplished by varing the time step of the midpoint scheme to enforce exact energy conservation at the *midpoint* of each step. Symplecticness and momentum conservation occur at the *vertices* of each step. The relationship between the time step and energy conservation originates from the fact that the negative of the energy (Hamiltonian) is the momentum corresponding to time, Shibberu [17], Lee [14].

The requirements of symplectic-energy integration are highly restrictive as illustrated by Ge's Theorem [7], [6]. An early existence and uniqueness result for DTH dynamics was given in Shibberu [17] and an explanation of why Ge's Theorem is not violated was given in Shibberu [19]. The sufficient condition for the existence and uniqueness of DTH trajectories proved in Shibberu [17] does not cover all the points in phase space where the Hamiltonian function is smoothly defined. It first appeared, from simulation results in Shibberu [18], that DTH dynamics was obstructed by points where this sufficient condition does not hold. Kane et. al. [12] later observed similar difficulties near points they refer to as "turning points" and Chen et. al. [3] also mentioned the need to avoid singularities in their algorithm. In this article, we explain how SEM integration can be regularized in a manner which preserves SEM properties and time reversibility at such points.

The outline of this paper is as follows. In section 2, we review the foundations of DTH dynamics. We introduce a discretization of Hamiltonian dynamics which is equivalent to, but simpler than the discretization used in Shibberu [19]. An example of a ghost trajectory of the pendulum is also given. In section 3, we introduce the two complementary variational principles used to regularized DTH dynamics. Regularized DTH equations are derived and shown to preserve SEM properties. Coordinate invariance of the regularized equations is briefly discussed. In section 4, we give a detailed description of an algorithm for solving the regularized DTH equations. Numerical results for the pendulum and Kepler's one-body problem are discussed. Finally, certain peculiarities of regularized DTH dynamics are described.

2 DTH Dynamics

2.1 Foundations of DTH Dynamics

We begin by introducing an extended-phase space version of the principle of least action. Let $H(t, q_1, \ldots, q_n, p_1, \ldots, p_n)$ be the Hamiltonian function of an n-degree of freedom Hamiltonian dynamical system where t is time and q_i and p_i, $i = 1, \ldots, n$, are position and momentum coordinates. Let $q = (q_1, \ldots, q_n, t)^\top$ and $p = (p_1, \ldots, p_n, \wp)^\top$ be extended phase space coordinates where $\wp$ is the momentum conjugate to time. (See [13], [8] or [18] for a description of $\wp$.) Let $z = (q, p)^\top$. Consider the extended-phase space action integral

$$\mathcal{A}(z(\cdot)) = \int_{\tau_0}^{\tau_f} \frac{1}{2} z(\tau)^\top J z'(\tau)^\top \, d\tau, \text{ where } J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

and I is the $n+1$ dimensional identity matrix. The extended-phase space Hamiltonian function is $\mathcal{H}(z) = \wp + H(t, q_1, \ldots, q_n, p_1, \ldots, p_n)$. The principle of least (stationary) action states that the trajectory $z(\tau)$ of a Hamiltonian dynamical system cause the action integral $\mathcal{A}(z(\cdot))$ to be stationary under variations which satisfy the boundary constraints $q(\tau_0) = q_0$, $p(\tau_f) = p_f$ and the Hamiltonian constraint $\mathcal{H}(z) \equiv 0$. (Additional details are given in [19].)

The action integral $\mathcal{A}(z(\cdot))$ is discretized in [19] by evaluating the integral along piecewise-linear, continuous trajectories and then appending boundary terms to account for the boundary conditions. An equivalent discretization

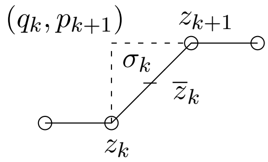


Figure 1: A piecewise-linear, continuous trajectory in extended-phase space.

with no boundary terms is described below. This discretization makes it possible to provide a simpler derivation of the DTH equations.

Lemma 1 *Let $\partial\sigma_k$ represent the boundary of the triangle σ_k in extended-phase space shown in Figure 1. Then, along $\partial\sigma_k$,*

$$\mathcal{A}(z(\cdot)) = \int_{\partial\sigma_k} \frac{1}{2} z(\tau)^\top J z'(\tau)^\top \, d\tau = \frac{1}{2} \Delta q_k{}^\top \Delta p_k.$$

Lemma 1 follows from Stoke's formula [1].

Definition 2 (One Step Action) *The one-step action of a discrete-time Hamiltonian dynamical system is defined to be*

$$\mathcal{A}(z_k, z_{k+1}) = \frac{1}{2} \Delta q_k{}^\top \Delta p_k, \text{ where } z_k = (q_k, p_k)^\top.$$

A discrete-time Hamiltonian (DTH) trajectory is a piecewise-linear, continuous trajectory which satisfies the following discrete variational principle.

Definition 3 (DTH Principle of Stationary Action) *The one-step action $\mathcal{A}(z_k, z_{k+1})$ is stationary along a DTH trajectory for variations which fix q_k and p_{k+1} and satisfy the Hamiltonian constraint $\mathcal{H}(\overline{z}_k) = 0$ where $\overline{z}_k = \frac{1}{2}(z_{k+1} + z_k)$ and $k = 0, \ldots, N-1$.*

Theorem 4 (DTH Equations) *A DTH trajectory is determined by the following equations:*

$$\Delta z_k = \lambda_k J \mathcal{H}_z(\overline{z}_k) \tag{1a}$$
$$\mathcal{H}(\overline{z}_k) = 0. \tag{1b}$$

The proof of Theorem 4 follows from the proof of Theorem 6. The proof that equations (1a)–(1b) is a SEM integrator (i.e. preserve symplecticness and conserve momentum at z_k and conserves energy at $\overline{z}_k$) can be found in [19].

2.2 An Example of SEM Integration

The extended-phase space Hamiltonian function for a pendulum is $\mathcal{H}(q, p, \wp) = \wp + \frac{1}{2}p^2 - \cos(q)$. The corresponding DTH equations are

$$\Delta q_k = \lambda_k \overline{p}_k \tag{2a}$$
$$\Delta t_k = \lambda_k \tag{2b}$$
$$\Delta p_k = -\lambda_k \sin(\overline{q}_k) \tag{2c}$$
$$\Delta \wp_k = 0 \tag{2d}$$
$$0 = \overline{\wp}_k + \frac{1}{2}\overline{p}_k^2 - \cos(\overline{q}_k) \tag{2e}$$

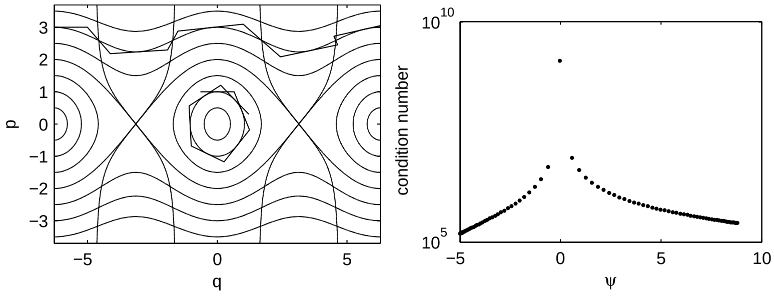
Observe from equation (2b) that λ_k equals the time step Δt_k.

Figure 2(a) shows two DTH trajectories projected onto the phase portrait of the pendulum. Observe that the linear segments of DTH trajectories are tangent to their respective energy-conserving manifolds (except possibly where they cross the v-shaped curves).

A sufficient condition for the existence and (local) uniqueness of solutions to equations (2a)–(2e) is the condition $\psi(z) \neq 0$ where $\psi(z) = (J\mathcal{H}_z)^\top \mathcal{H}_{zz}(J\mathcal{H}_z)$ [17]. The function $\psi(z)$ plays a key role in the regularization of SEM integration. The v-shaped curves in Figure 2(a) are points in phase space where $\psi(z) = 0$ and were first described in [18].

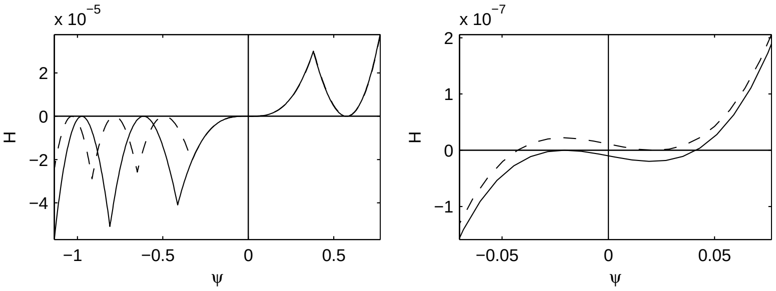
2.3 Ghost Trajectories

Figure 2(b) shows that the DTH equations (2a)–(2e) are poorly conditioned when ψ is near zero. Never the less, these equations determine trajectories which cross the v-shaped curves in Figure 2(a) in a SEM conserving manner. However, these trajectories are not time reversible as is seen in Figure 3. The linear segment crossing $\psi(z) = 0$ forward in time is tangent to the energy-conserving manifold on the left side, but the segment crossing backward in time is tangent on the opposite side. We will call these non-reversible trajectories, ghost trajectories. The trajectory shown crossing the v-shaped curves in Figure 2(a) has been regularized in a SEM conserving manner so that it is time reversible. How this is done is explained in the next section.



(a) Phase portrait (b) Condition number

Figure 2: DTH trajectories for the nonlinear pendulum. The v-shaped curves correspond to points where $\psi = 0$.



(a) View of $\mathcal{H} = 0$, $\psi = 0$ (b) Magnified view of $\mathcal{H} = 0$, $\psi = 0$

Figure 3: A ghost DTH trajectory crossing $\psi = 0$ forward in time (solid curve) and then time-reversed so that it crosses backward in time (dashed curve).

3 Regularized DTH Dynamics

3.1 Regularization

We regularize DTH dynamics by resorting to two complementary variational principles. The first variational principle restricts variations in Definition 3 by the inequality constraint $\psi(\overline{z}_k) \geq \psi_k$ where ψ_k is a constant. The second variational principle restricted variations by the inequality constraint $\psi(\overline{z}_k) \leq \psi_k$. We alternate between the two variational principles to generate trajectories which cross $\psi = 0$ in a time reversible manner.

Definition 5 (Regularized DTH Principle) *The one-step action $\mathcal{A}(z_k, z_{k+1})$ is stationary along a DTH trajectory for variations which fix q_k and p_{k+1} and satisfy the Hamiltonian constraint $\mathcal{H}(\overline{z}_k) = 0$ and the inequality constraint $\psi(\overline{z}_k) \geq \psi_k$ (or $\psi(\overline{z}_k) \leq \psi_k$).*

Theorem 6 (Regularized DTH Equations) *Assume $\mathcal{H}_z(\overline{z}_k)$ and $\psi_z(\overline{z}_k)$ are linearly independent for $k = 0, \ldots, N-1$. A regularized DTH trajectory must satisfy the following equations and inequalities:*

$$\Delta z_k = \lambda_k J \mathcal{H}_z(\overline{z}_k) + \mu_k J \psi_z(\overline{z}_k) \tag{3a}$$

$$\mathcal{H}(\overline{z}_k) = 0 \tag{3b}$$

$$\psi(\overline{z}_k) \geq \psi_k \text{ (or } \psi(\overline{z}_k) \leq \psi_k\text{)} \tag{3c}$$

$$\mu_k \left(\psi(\overline{z}_k) - \psi_k\right) = 0 \tag{3d}$$

$$\mu_k \leq 0 \text{ (or } \mu_k \geq 0\text{)} \tag{3e}$$

Proof. Define the Lagrangian function

$$\mathcal{L}(z_k, z_{k+1}, \lambda_k, \mu_k) = \mathcal{A}(z_k, z_{k+1}) + \lambda_k \mathcal{H}(\overline{z}_k) + \mu_k \psi(\overline{z}_k)$$

where λ_k is a Lagrange multiplier for the equality constraint $\mathcal{H}(\overline{z}_k) = 0$ and μ_k is a Karush-Kuhn-Tucker (KKT) multiplier for the inequality constraint $\psi(\overline{z}_k) \geq \psi_k$ (or $\psi(\overline{z}_k) \leq \psi_k$). Applying the KKT necessary conditions, [2], [4], to the regularized DTH principle results in the following equations:

$$\mathcal{L}_{p_k} = -\frac{1}{2}\Delta q_k + \frac{1}{2}\lambda_k \mathcal{H}_p(\overline{z}_k) + \frac{1}{2}\mu_k \psi_p(\overline{z}_k) = 0 \tag{4a}$$

$$\mathcal{L}_{q_{k+1}} = \frac{1}{2}\Delta p_k + \frac{1}{2}\lambda_k \mathcal{H}_q(\overline{z}_k) + \frac{1}{2}\mu_k \psi_q(\overline{z}_k) = 0 \tag{4b}$$

$$\begin{aligned}
\mathcal{L}_{\lambda_k} &= \mathcal{H}(\overline{z}_k) = 0 \\
\psi(\overline{z}_k) &\geq \psi_k \text{ (or } \psi(\overline{z}_k) \leq \psi_k\text{)} \\
\mu_k \left(\psi(\overline{z}_k) - \psi_k\right) &= 0 \\
\mu_k &\leq 0, \text{ (or } \mu_k \geq 0\text{)}.
\end{aligned}$$

Equations (4a) and (4b) can be rearranged and combined to give equation (3a). ■

Time reversibility of the regularized DTH trajectory follows from the following observation. If the inequality constraint $\psi(\overline{z}_k) \geq \psi_k$ is active forward in time, the inequality constraint $\psi(\overline{z}_k) \leq \psi_k$ is active backward in time. Therefore, the same equation, $\psi(\overline{z}_k) = \psi_k$, applies for both directions in time.

3.2 Symplectic-Energy-Momentum Properties

Next, we show that the regularized DTH equations (3a)–(3e) is a SEM integrator. Conservation of energy (Hamiltonian) follows directly from equation (3b). To prove symplecticness, we identify a generating function which generates symplectic transformations between adjacent vertices of a regularized DTH trajectory.

Theorem 7 (Generating Function) *Assume μ_k and $\psi(\overline{z}_k)$ are not simultaneous equal to zero. Then the function*

$$S(q_k, p_{k+1}) = {q_k}^\top p_{k+1} + \mathcal{L}(z_k, z_{k+1}, \lambda_k, \mu_k)$$

is a generating function which determines a symplectic transformation between the vertices z_k and z_{k+1} of a regularized DTH trajectory for $k = 0, \dots, N-1$. The function $\mathcal{L}(z_k, z_{k+1}, \lambda_k, \mu_k)$ is the Lagrangian function used in the proof of Theorem 6 . The variables q_{k+1}, p_k, λ_k and μ_k are determined by the regularized DTH equations (3a)–(3e).

Proof. We show that $S_{q_k}(q_k, p_{k+1}) = p_k$. The equation $S_{p_{k+1}}(q_k, p_{k+1}) = q_k$ follows in a similar fashion.

$$\begin{aligned} S_{q_k} &= p_{k+1} + \mathcal{L}_{q_k} \\ &= p_{k+1} - \frac{1}{2}\Delta p_k + \frac{1}{2}\lambda_k \mathcal{H}_q(\overline{z}_k) + \frac{1}{2}\mu_k \psi_q(\overline{z}_k) \\ &= p_{k+1} - \frac{1}{2}\Delta p_k - \frac{1}{2}\Delta p_k \\ &= p_k \end{aligned}$$

■

We note that the transformation $z_{k+1}(z_k)$ may not be differentiable when both $\psi(\overline{z}_k)$ and μ_k are equal to zero. Theorem 7 may not be valid for this special case.

The following lemma will be used to prove conservation of momentum. (Conservation of momentum is restricted here to linear and quadratic functions e.g. linear and angular momentum in Cartesian coordinates.)

Lemma 8 *If $L(z)$ is a quadratic function and the Poisson bracket $[L, \mathcal{H}]$ is identically equal to zero, then the Poisson bracket $[L, \psi]$ is identically equal to zero.*

Proof. By assumption, $[L, \mathcal{H}] = L_z^\top J \mathcal{H}_z = J^{i_1 i_2} L_{i_1} \mathcal{H}_{i_2} = 0$. (We use the convention of summing over repeated subscript and superscript indices.) Taking the first and second derivative of $J^{i_1 i_2} L_{i_1} H_{i_2} = 0$ with respect to k th component of z and using the fact that, since $L(z)$ is quadratic, $L_{i_1 k_1 k_2} = 0$, we have

$$J^{i_1 i_2} L_{i_1 k_1} \mathcal{H}_{i_2} + J^{i_1 i_2} L_{i_1} \mathcal{H}_{i_2 k_1} = 0 \tag{5a}$$

$$J^{i_1 i_2} L_{i_1 k_1} \mathcal{H}_{i_2 k_2} + J^{i_1 i_2} L_{i_1 k_2} \mathcal{H}_{i_2 k_1} + J^{i_1 i_2} L_{i_1} \mathcal{H}_{i_2 k_1 k_2} = 0. \tag{5b}$$

Since $\psi = (J\mathcal{H}_z)^\top \mathcal{H}_{zz} (J\mathcal{H}_z) = J^{k_1 j_1} J^{k_2 j_2} \mathcal{H}_{k_1 k_2} \mathcal{H}_{j_1} \mathcal{H}_{j_2}$ we have

$$\begin{aligned} \psi_{i_2} &= J^{k_1 j_1} J^{k_2 j_2} \mathcal{H}_{k_1 k_2 i_2} \mathcal{H}_{j_1} \mathcal{H}_{j_2} + J^{k_1 j_1} J^{k_2 j_2} \mathcal{H}_{k_1 k_2} \mathcal{H}_{j_1 i_2} \mathcal{H}_{j_2} \\ &\quad + J^{k_1 j_1} J^{k_2 j_2} \mathcal{H}_{k_1 k_2} \mathcal{H}_{j_1} \mathcal{H}_{j_2 i_2} \\ &= J^{k_1 j_1} J^{k_2 j_2} \mathcal{H}_{k_1 k_2 i_2} \mathcal{H}_{j_1} \mathcal{H}_{j_2} + 2 J^{k_1 j_1} J^{k_2 j_2} \mathcal{H}_{k_1 k_2} \mathcal{H}_{j_1 i_2} \mathcal{H}_{j_2} \end{aligned} \tag{6}$$

where we combined the last two terms of (6) by renaming indices and using the fact that $\mathcal{H}_{k_2 k_1} = \mathcal{H}_{k_1 k_2}$. Substituting for ψ_{i_2} in the Possion bracket $[L, \psi] = L_z^\top J \psi_z = J^{i_1 i_2} L_{i_1} \psi_{i_2}$ we have

$$\begin{aligned} [L, \psi] = J^{k_1 j_1} J^{k_2 j_2} &\left(J^{i_1 i_2} L_{i_1} \mathcal{H}_{k_1 k_2 i_2} \right) \mathcal{H}_{j_1} \mathcal{H}_{j_2} \\ &+ 2 J^{k_1 j_1} J^{k_2 j_2} \left(J^{i_1 i_2} L_{i_1} \mathcal{H}_{j_1 i_2} \right) \mathcal{H}_{k_1 k_2} \mathcal{H}_{j_2}. \end{aligned}$$

Using equations (5a) and (5b) and $\mathcal{H}_{j_1 i_2} = \mathcal{H}_{i_2 j_1}$, $\mathcal{H}_{k_1 k_2 i_2} = \mathcal{H}_{i_2 k_1 k_2}$, we have

$$\begin{aligned} [L, \psi] &= -J^{k_1 j_1} J^{k_2 j_2} \left(J^{i_1 i_2} L_{i_1 k_1} H_{i_2 k_2} + J^{i_1 i_2} L_{i_1 k_2} H_{i_2 k_1} \right) H_{j_1} H_{j_2} \\ &\quad - 2 J^{k_1 j_1} J^{k_2 j_2} \left(J^{i_1 i_2} L_{i_1 j_1} H_{i_2} \right) H_{k_1 k_2} H_{j_2} \end{aligned} \tag{7}$$

The last term of (7) can be expressed as (8) by rearranging terms, using $J^{k_1 j_1} = -J^{j_1 k_1}$ and renaming indices as shown below.

$$\begin{aligned}
&-2J^{k_1 j_1} J^{k_2 j_2} \left(J^{i_1 i_2} L_{i_1 j_1} H_{i_2}\right) H_{k_1 k_2} H_{j_2} = \\
&-2J^{i_1 i_2} J^{k_2 j_2} \left(J^{k_1 j_1} L_{j_1 i_1} H_{k_1 k_2}\right) H_{i_2} H_{j_2} = \\
&2J^{i_1 i_2} J^{k_2 j_2} \left(J^{j_1 k_1} L_{j_1 i_1} H_{k_1 k_2}\right) H_{i_2} H_{j_2} = \\
&2J^{k_1 j_1} J^{k_2 j_2} \left(J^{i_1 i_2} L_{i_1 k_1} H_{i_2 k_2}\right) H_{j_1} H_{j_2}
\end{aligned} \tag{8}$$

Replacing the last term in (7) with (8) and rearranging we have

$$[L, \psi] = J^{k_1 j_1} J^{k_2 j_2} J^{i_1 i_2} \left(L_{i_1 k_1} H_{i_2 k_2} - L_{i_1 k_2} H_{i_2 k_1}\right) H_{j_1} H_{j_2} \tag{9}$$

Skew-symmetry with respect to the indicies k_1 and k_2 in (9) implies $[L, \psi] = 0$. ■

Theorem 9 (Quadratic Conservation Laws) *Assume $L(z)$ is a quadratic function and $[L, \mathcal{H}]$ is identically equal to zero. Then $L(z)$ is exactly conserved at the vertices of a regularized DTH trajectory.*

Proof. Since $L(z)$ is quadratic, $L(z_{k+1}) - L(z_k) = L_z(\overline{z}_k)^\top \Delta z_k$. From equation (3a) and Lemma 8 we have

$$\begin{aligned}
L(z_{k+1}) - L(z_k) &= L_z(\overline{z}_k)^\top \left[\lambda_k J \mathcal{H}_z(\overline{z}_k) + \mu_k J \psi_z(\overline{z}_k)\right] \\
&= \left(\lambda_k [L, \mathcal{H}] + \mu_k [L, \psi]\right)\big|_{z=\overline{z}_k} \\
&= 0.
\end{aligned}$$

■

Corollary 10 (Quadratic Conservation Laws) *If $L(z)$ is quadratic, L_t and $L_\wp$ are both zero, and the Poisson bracket $[L, H]$ is identically equal to zero, then $L(z)$ is exactly conserved at the vertices of a regularized DTH trajectory.*

Proof. Since $[L, \mathcal{H}] = [L, H] + L_t \mathcal{H}_\wp - L_\wp \mathcal{H}_t$, then $L_t = L_\wp = 0$ implies $[L, \mathcal{H}] = [L, H]$ and the corollary follows from Theorem 9. ■

3.3 Coordinate Invariance

We briefly consider the coordinate invariance of regularized DTH dynamics. In the lemma below, we show that $\psi(z)$ is coordinate invariant with respect to linear, symplectic, coordinate transformations.

Lemma 11 *Let $z = TZ$ be a linear, symplectic, coordinate transformation between old coordinates z and new coordinates Z. Let $\mathcal{H}(z)$ be a Hamiltonian function expressed in the old coordinates and $\mathcal{K}(Z) = \mathcal{H}(TZ)$ be the Hamiltonian function expressed in the new coordinates. Define $\psi^{\mathcal{H}}(z) = (J\mathcal{H}_z)^\top \mathcal{H}_{zz}(J\mathcal{H}_z)$ and $\psi^{\mathcal{K}}(Z) = (J\mathcal{K}_Z)^\top \mathcal{K}_{ZZ}\,(J\mathcal{K}_Z)$. Then $\psi^{\mathcal{K}}(Z) = \psi^{\mathcal{H}}(TZ)$.*

Proof. Since $\mathcal{K}(Z) = \mathcal{H}(TZ)$ we have $\mathcal{K}_Z = T^\top \mathcal{H}_z$ and $K_{ZZ} = T^\top \mathcal{H}_{zz} T$.

$$\begin{aligned}
\psi^K(Z) &= (J\mathcal{K}_Z)^\top \mathcal{K}_{ZZ}\,(J\mathcal{K}_Z) \\
&= \left(JT^\top \mathcal{H}_z\right)^\top \left(T^\top \mathcal{H}_{zz} T\right)\left(JT^\top \mathcal{H}_z\right) \\
&= \mathcal{H}_z^\top \left(TJ^\top T^\top\right)\mathcal{H}_{zz}\left(TJT^\top\right)\mathcal{H}_z
\end{aligned}$$

Since T is symplectic, $TJT^\top = T^\top JT = J$ and we have

$$\begin{aligned}
\psi^K(Z) &= \mathcal{H}_z^\top J^\top \mathcal{H}_{zz} J \mathcal{H}_z \\
&= (J\mathcal{H}_z)^\top \mathcal{H}_{zz}(J\mathcal{H}_z) \\
&= \psi^{\mathcal{H}}(z) \\
&= \psi^{\mathcal{H}}(TZ).
\end{aligned}$$

■

Theorem 12 (Linear Coordinate Invariance) *The regularized DTH equations are coordinate invariant under linear, symplectic, coordinate transformations.*

The proof of Theorem 12 parallels the proof given in [19] for the DTH equations. The only difference is the use of Lemma 11 in the proof of Theorem 12. (We point out that the Lagrange multiplier λ_k and the KKT multiplier μ_k are both coodinate invariant quantities.)

Ge [6] demonstrated the coordinate invariance of a variety of symplectic integrators under linear, symplectic coordinate transformations. Guibout and Bloch [11] demonstrate coordinate invariance using the larger class of linear, symplectic, discrete-time coordinate transformations. In fact, it should be possible to demonstrate coordinate invariance using the even larger class of piecewise-linear, continuous, symplectic coordinate transformations which are consistent with a special triangulation of extended phase space. A procedure for demonstrating the coordinate invariance of DTH dynamics using this larger class of coordinate transformations was described (in a formal sense) in [17]. Theorem 12 implies this procedure is also valid for regularized DTH dynamics. In fact, the regularization described in this article removes the technical difficulty of identifying principle DTH trajectories described in [17].

4 Numerical Results

4.1 An Algorithm for Regularized SEM Integration

An algorithm for solving the regularized DTH equations (3a)–(3e) is outlined in Figure 4. In this section, we will choose $\psi_k = 0$ in equation (3c). Before explaining the algorithm in detail, it would be useful to review the simpler algorithm developed in [17] for solving the DTH equations (1a)–(1b).

Equations (1a)–(1b) are poorly conditioned for small time steps λ_k. A direct application of Newton's method is likely to result in poor convergence. Instead, nested, Newton iterations are used. The function $\overline{z}_k = \overline{z}(\lambda_k, z_k)$ implicity defined by equation (1a), is evaluated using an inner iteration. An outer iteration solves the equation $g(\lambda) = \mathcal{H}(\overline{z}(\lambda, z_k)) = 0$ for λ_k. Quadratic convergence of the iterations is proved in [17] for $\psi(z_k) \neq 0$. The outer Newton iteration exhibits poor convergence near $\psi = 0$.

The algorithm outlined in Figure 4 also uses nested, Newton iterations. Near $\psi = 0$ however, a bracketed, root-finding procedure is used in place of the outer Newton iteration. The algorithm is further complicated by the problem of identifying when $\psi = 0$ has been crossed. The procedural logic needed to compute a DTH trajectory crossing $\psi = 0$ appears to be complex. We now give a more detailed explanation of the algorithm outlined in Figure 4.

The function $\overline{z}(\lambda_k, \mu_k, z_k)$ implicitly defined by equation (3a) is evaluated using Newton's method. When $\psi(\overline{z}_k) \neq 0$, equation (3d) implies $\mu_k = 0$. We use the abbreviation $\overline{z}(\lambda_k, z_k)$ for $\overline{z}(\lambda_k, \mu_k, z_k)$ when $\mu_k = 0$.

The first block in Figure 4 initializes the algorithm. (We assume $\psi(\overline{z}_0) \neq 0$.) The value of $\wp_0$ (the momentum conjugate to time) determines the initial time step λ_0. If $\wp_0$ is chosen so that $\mathcal{H}(z_0) = 0$, then $\lambda_0 = 0$. Therefore, a value for $\wp_0$ should be chosen so that $\mathcal{H}(z_0)$ is sufficiently small but nonzero.

Vertex points z_k, $k = 2, \ldots, N$, are computed within block 2. To avoid ill-conditioning of the equation $\mathcal{H}(\overline{z}(\lambda, z_k)) = 0$ near $\psi = 0$, we solve the equation $\psi(\overline{z}(\lambda, z_k))\mathcal{H}(\overline{z}(\lambda, z_k)) = 0$. Linear segments which do not cross $\psi = 0$ are computed in block 3. If $\psi(\overline{z}(\lambda_k, z_k)) = 0$, the condition $\psi(z_k)\psi(z_{k+1}) \leq 0$ indicates $\psi = 0$ has been crossed and the algorithm enters block 4 where λ_ψ and $\overline{z}_\psi$ are computed and used in block 5. In block 5, a bracketed root-finding procedure is used to solve the now ill-conditioned

1. $\left\{\begin{array}{l} \text{input } z_0, \text{ set } k=0 \\ \text{solve } \psi(\overline{z}(\lambda,z_k))\mathcal{H}(\overline{z}(\lambda,z_k))=0 \text{ for } \lambda\geq 0 \text{ to determine } \lambda_k \\ \overline{z}_k=\overline{z}(\lambda_k,z_k),\ z_{k+1}=2\overline{z}_k-z_k \end{array}\right.$

2. repeat while $k\leq N$

3. $\left\{\begin{array}{l} \text{while } \psi(z_k)\psi(z_{k+1})>0 \text{ and } k\leq N \\ \quad k=k+1 \\ \quad \text{solve } \psi(\overline{z}(\lambda,z_k))\mathcal{H}(\overline{z}(\lambda,z_k))=0 \text{ for } \lambda\geq 0 \text{ to determine } \lambda_k \\ \quad \overline{z}_k=\overline{z}(\lambda_k,z_k),\ z_{k+1}=2\overline{z}_k-z_k \\ \text{end} \end{array}\right.$

4. $\left\{\begin{array}{l} \text{solve } \psi(\overline{z}(\lambda,z_k))=0 \text{ to determine } \lambda_\psi \\ \overline{z}_\psi=\overline{z}(\lambda_\psi,z_k) \end{array}\right.$

5. $\left\{\begin{array}{l} \text{while } \lambda_\psi\geq 0 \text{ and } \mathcal{H}(z_k)\mathcal{H}(\overline{z}_\psi)\leq 0 \text{ and } k\leq N \\ \quad \text{solve } \mathcal{H}(\overline{z}(\lambda,z_k))=0 \text{ for } 0\leq\lambda\leq\lambda_\psi \text{ to determine } \lambda_k \\ \quad \overline{z}_k=\overline{z}(\lambda_k,z_k),\ z_{k+1}=2\overline{z}_k-z_k \\ \quad k=k+1 \\ \quad \text{solve } \psi(\overline{z}(\lambda,z_k))=0 \text{ to determine } \lambda_\psi \\ \quad \overline{z}_\psi=\overline{z}(\lambda_\psi,z_k) \\ \text{end} \end{array}\right.$

6. $\left\{\begin{array}{l} \text{if ghost trajectory and } \mathcal{H}(z_{k-1})\mathcal{H}(z_k)>0 \\ \quad k=k-1 \\ \quad \text{solve } \psi(\overline{z}(\lambda,z_k))=0 \text{ to determine } \lambda_\psi \\ \quad \text{solve } \mathcal{H}(\overline{z}(\lambda,z_k))=0 \text{ for } \lambda\geq\lambda_\psi \text{ to determine } \lambda_k \\ \quad \overline{z}_k=\overline{z}(\lambda_k,z_k),\ z_{k+1}=2\overline{z}_k-z_k \\ \quad k=k+1 \\ \text{end} \end{array}\right.$

7. $\left\{\begin{array}{l} \text{if regularized trajectory} \\ \quad \text{solve } \left\{\begin{array}{l} \mathcal{H}(\overline{z}(\lambda,\mu,z_k))=0 \\ \psi(\overline{z}(\lambda,\mu,z_k))=0 \end{array}\right. \text{ to determine } \lambda_k \text{ and } \mu_k \\ \quad \overline{z}_k=\overline{z}(\lambda_k,\mu_k,z_k),\ z_{k+1}=2\overline{z}_k-z_k \\ \quad k=k+1 \\ \quad \text{solve } \psi(\overline{z}(\lambda,z_k))=0 \text{ to determine } \lambda_\psi \\ \quad \text{solve } \mathcal{H}(\overline{z}(\lambda,z_k))=0 \text{ for } \lambda\geq\max(0,\lambda_\psi) \text{ to determine } \lambda_k \\ \quad \overline{z}_k=\overline{z}(\lambda_k,z_k),\ z_{k+1}=2\overline{z}_k-z_k \\ \quad k=k+1 \\ \text{end} \end{array}\right.$

8. $\left\{\begin{array}{l} \text{solve } \mathcal{H}(\overline{z}(\lambda,z_k))=0 \text{ for } \lambda\geq 0 \text{ to determine } \lambda_k \\ \overline{z}_k=\overline{z}(\lambda_k,z_k),\ z_{k+1}=2\overline{z}_k-z_k \\ k=k+1 \end{array}\right.$

end

Figure 4: Algorithm for computing ghost and regularized DTH trajectories.

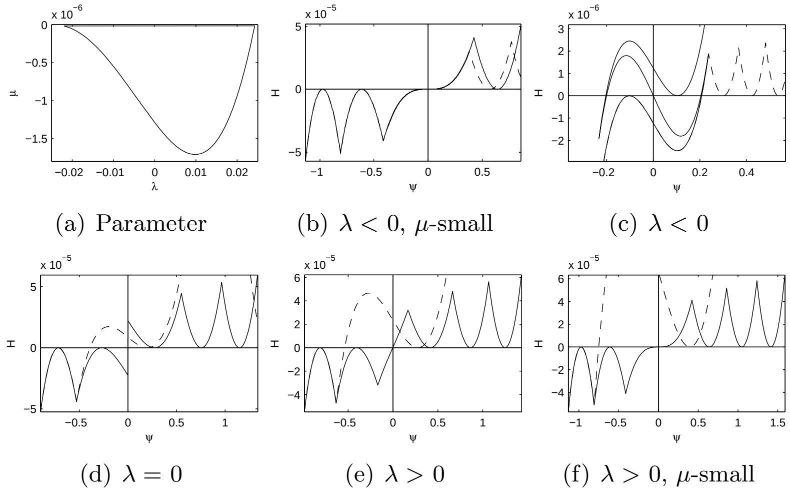


Figure 5: A one parameter family of DTH trajectories crossing $\psi = 0$. Dashed curves are ghost trajectories. Solid curves are regularized trajectories.

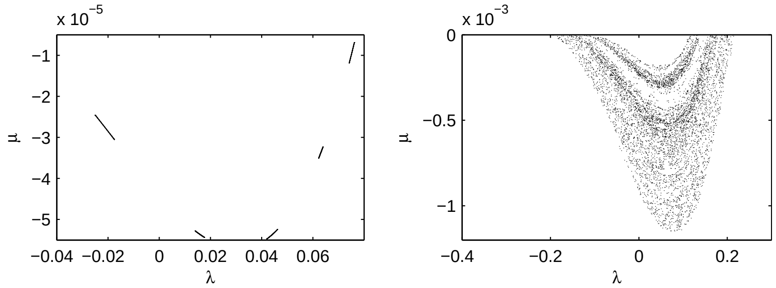
equation $\mathcal{H}(\overline{z}(\lambda, z_k)) = 0$. If a bracket can not be found, the algorithm enters either block 6 and computes a ghost trajectory or block 7 and computes a regularized trajectory. Block 8 is need to prevent the computation of trajectories which immediately recross $\psi = 0$.

Blocks 7 and 8 take into account the different ways DTH trajectories can cross $\psi = 0$. These blocks are best understood after viewing an animation of a one-parameter family of $\psi = 0$ crossings. Snapshots of this animation are given in Figure 5.

Murua [16] has developed an efficient iteration which avoids the nested iterations use to solve $\mathcal{H}(\overline{z}(\lambda, z_k)) = 0$. (Murua has also developed an iteration which does not require evaluation of the Hessian matrix of the Hamiltonian function.) It is likely that the algorithm outlined in Figure 4 could be made significantly more efficient by using Murua's iteration. The author has take a first step in this direction by modifying Murua's iteration so that it can be used to compute regularized segments crossing $\psi = 0$.

4.2 Qualitative Behavior of Regularized SEM Integation

Numerical computations for the pendulum and Kepler's one body problem confirm that the regularization described in this article conserves SEM



(a) $q = 0, p = 3$

(b) $q = 0, p = 2.2$

Figure 6: Behavior of λ vs μ when $\psi = 0$ for a single regularized DTH trjectory of the nonlinear pendulum.

properties. The energy (Hamiltonian) is conserved to roundoff error at midpoints of DTH trajectories. Angular momentum is conserved to roundoff error at vertices for Kepler's problem in Cartesian coordinates. Symplecticness is verified by computing the derivative dz_N/dz_0 of the map $z_N(z_0)$. The matrix $(dz_N/dz_0)^\top J\,(dz_N/dz_0)$ is found to equal J to roundoff error. Time-reversibility is also confirmed to hold to roundoff error. Numerical computations quantifying the accuracy and efficiency of the regularization have not yet been completed.

One of the peculiarities observed in regularized SEM integration is the occurrence of negative time steps. Negative time steps violate the monotonic-increasing property of time. The DTH trajectories become multi-valued functions of time. Lee [15] foresaw this possibility and suggested the remedy of relinking vertices to maintain the monotonicity of time.

Finally, another peculiarity observed for regularized SEM integration, for the case $\psi_k = 0$ in equation (3c), is apparently chaotic behavior near the separatrix of the pendulum. (See Figure 6.) It may be possible to regularize DTH dynamics further by choosing nonzero values for ψ_k.

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