Mechanical Integrators from a Discrete Variational Principle

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Nice report! Getting a 3 body integrator going would be interesting

1 Introduction

In this paper, the intention is to give an introduction to discrete variational mechanics and to mechanical integrators. In particular, we present a systematic construction of mechanical integrators for simulating finite dimensional mechanical systems based on a discretization of Hamilton's principle. Finally, we will apply these principles to the construction of an integrator for the three-body problem.

Variational Integrators for Mechanical Systems. A Veselov-type discretization of Hamilton's principle for mechanics leads naturally to a powerful set of integration algorithms. These algorithms have remarkable respect for the basic invariants of mechanics, preserving in particular the symplectic structure, momentum and energy. These algorithms produce many known and efficient algorithms such as the Newmark algorithm and higher order symplectic partitioned Runge-Kutta schemes. In addition, using a discretization of the Lagrange-d'Alembert principle, one can also produce algorithms for dissipative or forced systems that get the energy decay correct, even over long integration runs. Extensions of these algorithms to the PDE and multisymplectic context are also underway.

2 Variational Principles

We will recall the Lagrangian formulation of mechanics, from which one derives the Euler-Lagrange equations (see [1]). We will then show how to mimic this process on a discrete level.

We work in $\mathbb{R}^n$ or in a configuration space Q and will use vector notation for simplicity, $q = (q^1, q^2, \ldots, q^n)$. One introduces the Lagrangian $L(q, \dot{q}, t)$. We form the action function by integrating L along a curve $q(t)$ and then compute variations of the action while holding the endpoints of the curve $q(t)$ fixed. This gives

$$\delta \int_0^T L(q(t), \dot{q}(t), t)dt = \int_0^T \left[\frac{\partial L}{\partial q} \cdot \delta q + \frac{\partial L}{\partial \dot{q}} \cdot \delta \dot{q} \right] dt \tag{2.1}$$

$$= \int_0^T \left[\frac{\partial L}{\partial q} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) \right] \cdot \delta q \; dt \tag{2.2}$$

where we have used integration by parts and the condition $\delta q(T) = \delta q(0) = 0$. Hamilton's principle states that

$$\delta \int_0^T L(q(t), \dot{q}(t), t)dt = 0. \tag{2.3}$$

Requiring that the variations of the action be zero for all δq implies that the integrand must be zero for each time t, giving the Euler-Lagrange equations

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = 0. \tag{2.4}$$

It is well known that the system described by the Euler-Lagrange equations has many special properties. For instance, the flow on state space TQ is symplectic, i.e. it conserves a particular two-form, and if there are symmetry actions on phase space then there are corresponding conserved quantities of the flow, known as momentum maps.

In what follows, we will see how discrete variational mechanics performs an analogue of the above derivation. Rather than taking a position q and velocity q, consider now two positions q_0 and q_1 and a timestep $h \in \mathbb{R}$. These two positions should be thought of as being two points on a curve at a time h apart, so that $q_0 \approx q(0)$ and $q_1 \approx q(h)$.

2.1 Discrete Variational Principle

A discrete variational principle is presented in this section which leads to evolution equations that are analogous to th Euler-Lagrange equations. We will refer to them as the discrete Euler-Lagrange (DEL) equations. We will follow the results presented in [2] and [3].

Consider a configuration space, Q, but now define a discrete state space to be $Q \times Q$. This contains the same amount of information (i.e. is locally isomorphic to) TQ. A discrete Lagrangian is a function $L_d : Q \times Q \to \mathbb{R}$. It depends on the timestep h, but we will neglect this h dependence except where it is important.

Construct the increasing time series $\{t_k = kh \mid k = 0, \dots, N\} \subset \mathbb{R}$ from the timestep h. We will identify a trajectory with $\{q_k\}_{k=0}^{N} \subset Q$. We now give a procedure that defines the evolution map for the system. The action sum is the map $S_d : Q^{N+1} \to \mathbb{R}$ defined by

$$S_d = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}), \tag{2.5}$$

where $k \in \mathbb{Z}$ is the discrete time. The action sum is a discrete analog of the action integral. The discrete variational principle states that the evolution equations extremize the action sum given fixed end points q_0 and q_N, i.e., $\delta S_d = 0$ with $\delta q_0 = \delta q_N = 0$. Computing δS_d, we get

$$\begin{aligned}
\delta S_d &= \sum_{k=0}^{N-1} \left[D_1 L_d(q_k, q_{k+1}) \cdot \delta q_k + D_2 L_d(q_k, q_{k+1}) \cdot \delta q_{k+1} \right] && (2.6) \\
&= \sum_{k=0}^{N-1} \left[D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) \right] \cdot \delta q_k && (2.7) \\
&\quad + D_1 L_d(q_0, q_1) \cdot \delta q_0 + D_2 L_d(q_{N-1}, q_N) \cdot \delta q_N && (2.8)
\end{aligned}$$

using a discrete integration by parts (rearrangement of the summation). Since $\delta q_0 = \delta q_N = 0$, we have the DEL equations:

$$D_{\mathrm{DEL}} L_d((q_{k-1}, q_k), (q_k, q_{k+1})) = D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0, \tag{2.9}$$

for all $k = 1, \dots, N-1$.

3 Discrete Evolution Operator, Discrete Map, and Symplectic Structure

The discrete object corresponding to $T(TQ)$ is the set $(Q \times Q) \times (Q \times Q)$. We can define the projection operator π and the translator operator σ on $(Q \times Q) \times (Q \times Q)$ to be

$$\pi : ((q_0, q_1), (q_0', q_1')) \mapsto (q_0, q_1) \tag{3.1}$$
$$\sigma : ((q_0, q_1), (q_0', q_1')) \mapsto (q_0', q_1'). \tag{3.2}$$

The discrete second-order submanifold of $(Q \times Q) \times (Q \times Q)$ is defined to be

$$\ddot{Q}_d \equiv \{w_d \in (Q \times Q) \times (Q \times Q) \mid \pi_1 \circ \sigma(w_d) = \pi_2 \circ \pi(w_d)\} \tag{3.3}$$

where π_1 is the first slot of $\pi((q_0, q_1), (q_0', q_1'))$, i.e. q_0 and π_2 is the second slot, i.e. q_1. Note that $\ddot{Q}_d$ has the same information content as (i.e. is locally isomorphic to) $\ddot{Q}$. Concretely, the discrete second-order submanifold is the set of pairs of the form $((q_0, q_1), (q_1, q_2))$.

3.1 Discrete Evolution Operator and Discrete Map

We can introduce a discrete evolution operator X that plays the same role as a continuous vector field and is defined to be any map $X : (Q \times Q) \to (Q \times Q) \times (Q \times Q)$ satisfying $\pi \circ X = id$. The discrete object corresponding to the flow is the discrete map $F : (Q \times Q) \to (Q \times Q)$ defined by $F = \sigma \circ X$. In coordinates, if the discrete evolution operator maps $X : (q_0, q_1) \mapsto (q_0, q_1, q_0', q_1')$ the the discrete map will be $F : (q_0, q_1) \mapsto (q_0', q_1')$.

Lagrangian systems are second-order, so we are interested in discrete evolution operators that are second-order, which is the requirement that $X(Q \times Q) \subset \ddot{Q}_d$. This implies that X has the form $X : (q_0, q_1) \mapsto (q_0, q_1, q_1, q_2)$, and so the corresponding discrete map is $F : (q_0, q_1) \mapsto (q_1, q_2)$. We now restrict to the particular case of a discrete Lagrangian system.

The discrete Lagrangian evolution operator X_{L_d} is a second-order discrete evolution operator satisfying

$$D_{\mathrm{DEL}} L_d \circ X_{L_d} = 0 \tag{3.4}$$

and the discrete Lagrangian map $F_{L_d} : (Q \times Q) \to (Q \times Q)$ is defined by $F_{L_d} = \sigma \circ X_{L_d}$. Thus we rewrite eq. (2.9) as

$$D_2 L_d + D_1 L_d \circ F_{L_d} = 0. \tag{3.5}$$

This defines F_{L_d} implicitly by $F_{L_d}(q_{k-1}, q_k) = (q_k, q_{k+1})$ for points $\{q_k\}_{k=0}^N$ which are a trajectory of eq. (3.5). F_{L_d} is the discrete map that flows the discrete Lagrangian system forward in discrete time.

3.2 Symplectic Structure

We first define a fiber derivative by

$$\mathbb{F}L_d : Q \times Q \to T^*Q \tag{3.6}$$
$$(q_0, q_1) \mapsto (q_1, D_1 L_d(q_0, q_1)) \tag{3.7}$$

and we define the 2-form on $Q \times Q$ by pulling back the canonical 2-form on T^*Q:

$$\Omega_{L_d} = \mathbb{F}L_d^*(\Omega_{\mathrm{CAN}}) \tag{3.8}$$
$$= \mathbb{F}L_d^*(-d\Theta_{\mathrm{CAN}}) \tag{3.9}$$
$$= -d(\mathbb{F}L_d^*(\Theta_{\mathrm{CAN}})). \tag{3.10}$$

The fiber derivative is analogous to the Legendre transform in continuous-time Lagrangian mechanics. In coordinates q^i on Q, and canonical coordinates (q^i, p_i) on T^*Q, the canonical forms are $\Omega_{\mathrm{CAN}} = dq^i \wedge dp_i$ and $\Theta_{\mathrm{CAN}} = p_i dq^i$. Continuing the calculation in eq. (3.10), we have

$$\Omega_{L_d} = -d\left(\frac{\partial L_d}{\partial q_k^i}(q_k, q_{k+1})\right) dq_k^i \tag{3.11}$$

$$= -\frac{\partial^2 L_d}{\partial q_k^i \partial q_{k+1}^j}(q_k, q_{k+1}) dq_{k+1}^j \wedge dq_k^i - \frac{\partial^2 L_d}{\partial q_k^i \partial q_k^j}(q_k, q_{k+1}) dq_k^j \wedge dq_k^i \tag{3.12}$$

$$= \frac{\partial^2 L_d}{\partial q_k^i \partial q_{k+1}^j}(q_k, q_{k+1}) dq_k^i \wedge dq_{k+1}^j \tag{3.13}$$

since the sum $\frac{\partial^2 L_d}{\partial q_k^i \partial q_k^j}(q_k, q_{k+1}) dq_k^j \wedge dq_k^i$ vanishes in eq. (3.12).

To prove that the 2-form Ω_{L_d} is indeed symplectic, we need to show that F_{L_d} preserves Ω_{L_d}, i.e. $F_{L_d}^* \Omega_{L_d} = \Omega_{L_d}$ where $F_{L_d}^*$ is the pullback of F_{L_d}. For clarity, let $F_{L_d}(x, y) = (u, v)$ and write $\Omega_{L_d} = d(p(x, y)dy) = D_{12} L_d(x, y) dx \wedge dy$. In this notation, $y = u = q_k$, $x = q_{k-1}$, and $v = q_{k+1}$. We now show that $F_{L_d}^* \Omega_{L_d} = \Omega_{L_d}$:

$$F_{L_d}^* \Omega_{L_d} = F_{L_d}^*\left(-d\left(\frac{\partial L_d}{\partial u^i}(u, v) du^i\right)\right) \tag{3.14}$$

$$= -d\left(F_{L_d}^*\left(\frac{\partial L_d}{\partial u^i}(u, v) du^i\right)\right) \tag{3.15}$$

$$= -d\left(\frac{\partial L_d}{\partial u^i} \circ F_{L_d}(x, y) d\left(u^i(x, y)\right)\right) \tag{3.16}$$

$$= -d\left(-\frac{\partial L_d}{\partial y^i}(x, y) dy^i\right) \tag{3.17}$$

$$= \frac{\partial^2 L_d}{\partial x^j y^i} dx^j \wedge dy^i \tag{3.18}$$

$$= \Omega_{L_d}. \tag{3.19}$$

We have used eq. (3.5) and $d(u(x, y)) = dy$ in deriving eq. (3.17) from eq. (3.16).

4 Construction of Mechanical Integrators

In this section, we show how to construct mechanical integrators for continuous time Lagrangian systems from the discrete variational principle. We will show how to construct integrators for Lagrangian systems with holonomic constraints by enforcing the constraints through Lagrange multipliers.

We assume that we have a mechanical system with a constraint manifold $Q \subset V$, where V is a real, finite dimensional vector space, and that we have an unconstrained Lagrangian, $L : TV \to \mathbb{R}$ which, by restriction to L of TQ, defines a constrained Lagrangian, $L^c : TQ \to \mathbb{R}$. We also assume that we have a vector valued constraint function, $g : V \to \mathbb{R}^j$, such that $g^{-1}(0) = Q \subset V$ with 0 a regular value of g. Let the dimension of V be n, and therefore, the dimension of Q is $m = n - j$. Also, let Λ be a real, finite dimensional vector space of Lagrange multipliers of dimension j. We first define the discrete, unconstrained Lagrangian to, $L_d : V \times V \to \mathbb{R}$, to be

$$L_d(x, y) = L\left(\frac{x + y}{2}, \frac{y - x}{h}\right), \tag{4.1}$$

where $h \in \mathbb{R}$ is the time step and $h > 0$. The unconstrained action sum is defined by

$$S_d = \sum_{k=0}^{N-1} L_d(v_k, v_{k+1}). \tag{4.2}$$

We then extremeize $S_d : V^{N+1} \to \mathbb{R}$ subject to the constraint that $v_k \in Q \subset V$ for $k \in \{1, \ldots, N-1\}$,

$$\begin{array}{c} \min_{v_k \in V, \lambda_k \in \Lambda} \left(S_d + \sum_{k=1}^{N-1} \lambda_k^T g(v_k) \right) \\ \text{subject to } g(v_k) = 0 \ \text{ forall } k \in \{1, \ldots, N-1\}, \end{array} \tag{4.3}$$

where here T denotes transpose. From this, we derive that

$$\begin{array}{c} D_2 L_d(v_{k-1}, v_k) + D_1 L_d(v_k, v_{k+1}) + \lambda_k^T Dg(v_k) = 0 \text{ (no sum over } k) \\ g(v_k) = 0 \ \text{ for all } k \in \{1, \ldots, N-1\}. \end{array} \tag{4.4}$$

Given v_k and v_{k-1} in $Q \subset V$, i.e. $g(v_k) = g(v_{k-1}) = 0$, we need to solve the following equations

$$\begin{array}{c} D_2 L_d(v_{k-1}, v_k) + D_1 L_d(v_k, v_{k+1}) + \lambda_k^T Dg(v_k) = 0 \\ g(v_{k+1}) = 0 \end{array} \tag{4.5}$$

for v_{k+1} and λ_k.

Suppose $x = v_{k-1}, y = v_k$, and $z = v_{k+1}$. We want to compute z given x and y, thereby iteratively computing the trajectory $\{v_k\}_{k=0}^N \subset Q$. In terms of the original, unconstrained Lagrangian, eq. (4.5) reads as follows:

$$\begin{array}{c} \frac{1}{2}\left[D_1 L\left(\frac{y+x}{2}, \frac{y-x}{h}\right) + D_1 L\left(\frac{z+y}{2}, \frac{z-y}{h}\right)\right] + \\ \frac{1}{h}\left[D_2 L\left(\frac{y+x}{2}, \frac{y-x}{h}\right) - D_2 L\left(\frac{z+y}{2}, \frac{z-y}{h}\right)\right] \\ + \lambda_k^T Dg(y) = 0 \\ g(z) = 0. \end{array} \tag{4.6}$$

Note that when $Q = V$, we have

$$\begin{array}{c} \frac{1}{2}\left[D_1 L\left(\frac{y+x}{2}, \frac{y-x}{h}\right) + D_1 L\left(\frac{z+y}{2}, \frac{z-y}{h}\right)\right] + \\ \frac{1}{h}\left[D_2 L\left(\frac{y+x}{2}, \frac{y-x}{h}\right) - D_2 L\left(\frac{z+y}{2}, \frac{z-y}{h}\right)\right] = 0, \end{array} \tag{4.7}$$

which is an implicit equation for q_{k+1} given q_{k-1} and q_k.

5 Example: Planar Circular Restricted Three-Body Problem

We apply the construction procedure to produce a mechanical integrator for the planar circular restricted three-body problem (PCR3BP). This procedure has been used in [3] to produce mechanical integrators for the rigid body and the double spherical pendulum, with good results. In particular, it has been observed that the energy oscillates around a constant value.

The configuration manifold for the PCR3BP is $Q = V = \mathbb{R}^2 \backslash \{(-\mu, 0) \cup (1-\mu, 0)\}$ where μ is the mass parameter of the system. Thus, we need not deal with a constraint function, and therefore we can use eq. (4.7) to update points. The continuous time Lagrangian $L : TV \to \mathbb{R}$ for the PCR3BP is

$$L(x, y, \dot{x}, \dot{y}) = \frac{1}{2}\left((\dot{x} - y)^2 + (x + \dot{y})^2\right) - U(x, y), \tag{5.1}$$

where

$$U(x, y) = -\frac{1-\mu}{r_1} - \frac{\mu}{r_2} \tag{5.2}$$

$$r_1 = \sqrt{(x+\mu)^2 + y^2} \tag{5.3}$$

$$r_2 = \sqrt{(x+\mu-1)^2 + y^2} \tag{5.4}$$

and $(x, y, \dot{x}, \dot{y}) \in TV \cong V \times \mathbb{R}^2$. From L, one constructs L_d for a given h, via

$$L_d(q_0, q_1) = L\left(\frac{q_1 + q_0}{2}, \frac{q_1 - q_0}{h}\right). \tag{5.5}$$

Could be that there are better choices of L_d!

Taking the derivatives of L, we get

$$\frac{\partial L}{\partial v} = \begin{bmatrix} x + \dot{y} - \frac{\partial U}{\partial x} \\ -\dot{x} + y - \frac{\partial U}{\partial y} \end{bmatrix} \tag{5.6}$$

$$\frac{\partial L}{\partial \dot{v}} = \begin{bmatrix} \dot{x} - y \\ x + \dot{y} \end{bmatrix} \tag{5.7}$$

where

$$\frac{\partial U}{\partial x} = (x + \mu)\frac{1 - \mu}{r_1^3} + (x + \mu - 1)\frac{\mu}{r_2^3} \tag{5.8}$$

$$\frac{\partial U}{\partial y} = y\frac{1 - \mu}{r_1^3} + y\frac{\mu}{r_2^3}. \tag{5.9}$$

To implement the variational integrator scheme for this problem, one would need to solve eq. (4.7) implicitly for $q_{k+1} = (x_{k+1}, y_{k+1})$ given $q_{k-1} = (x_{k-1}, y_{k-1})$ and $q_k = (x_k, y_k)$. One must typically use an iterative technique such as Newton's method. This involves computing a first guess $q_{k+1,0}$ for q_{k+1}, such as $q_{k+1,0} = 2q_k - q_{k-1}$, and then computing the sequence of approximations $q_{k+1,n}, n = 1, 2, \ldots$ until they converge to the solution value q_{k+1}. For Newton's method (see [2]), the iteration rule is given by

$$q^i_{k+1,n+1} = q^i_{k+1,n} - A^{ij}\left[p^j_k + \frac{\partial L_d}{\partial q^j_0}(q_0, q_1)\right] \tag{5.10}$$

where $p_k = -D_1 L_d(q_k, q_{k+1})$ and A^{ij} is the inverse of the matrix

$$A_{ij} = \frac{\partial^2 L_d}{\partial q^i_0 \partial q^j_0}(q_0, q_1). \tag{5.11}$$

While the Newton's method outlined above typically experiences very fast conergence, it is also expensive to have to recompute A^{ij} at each iteration of the method. For this reason, it is typical to use an approximation to this matrix which can be held constant for all iterations of Newton's method.

In the future, we intend to implement this scheme numerically and compare its results to standard Runga-Kutta methods.

References

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