Variational Time Integrators

Symposium on Geometry Processing Course 2015

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Time Integrator

Differential equations in time describe physical paths

Solve for these paths on the computer

Non-damped, Non-Driven Pendulum
Time Integrator

Differential equations in time describe physical paths

Solve for these paths on the computer

Non-damped, Non-Driven Pendulum
Methods of Time Integration

Non-damped, Non-Driven Pendulum

Explicit

Variational

Implicit

“artificial driving”

“reasonable”

“artificial damping”
Methods of Time Integration

Non-damped, Non-Driven Pendulum

- Explicit: “artificial driving”
- Variational: “reasonable”
- Implicit: “artificial damping”
Part One: Reinterpreting Newtonian Mechanics
(what does “variational” mean?)

Part Two: Why Use Variational Integrators?
A Butchering of Feynman’s Lecture

Principle of Least Action
(Feynman Lectures on Physics Volume II.19)

Newtonian Mechanics

Closed mechanical system \( q(t), \dot{q}(t) \)

Kinetic energy \( T(\dot{q}) = \frac{1}{2} m \dot{q}^2 \)

Potential energy \( U(q) \)

Total energy \( T(\dot{q}) + U(q) \)
Newtonian Mechanics

A **physical path** satisfies the vector equation

\[
F = \dot{m} = \ddot{q}
\]

Worked out using force balancing

Difficult to compute with Cartesian coordinates
Lagrangian Reformulation

Goal:
Derive Newton’s equations from a scalar equation

Why?
Works in every choice of coordinates
Highlights variational structure of mechanics
Energy is easy to write down
Particle in a Gravitational Field

“Throw a ball in the air from \((t_1, A)\) catch at \((t_2, B)\)”
What path does the ball take to get from A to B in a given amount of time?
Particle in a Gravitational Field

Physical path is unique and a parabola
Particle in a Gravitational Field

...but there are many possible paths
How are physical paths special among all paths from A to B?
Hamilton’s Principle of Stationary Action

Physical paths are extremal amongst all paths from A to B of a time integral called the action.
Hamilton’s Principle of Stationary Action

Physical paths are extrema of a time integral called the action

$$\int_{t_1}^{t_2} \left[ T(\dot{q}) - U(q) \right] \, dt$$

(Lagrangian is not the total energy $T(\dot{q}) + U(q)$)
Hamilton’s Principle of Stationary Action

Physical paths extremize the action

\[ S = \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}) \, dt \]

...but how we find an extremal path in the space of all paths?

Use Lagrange’s variational calculus
Finding an Extremal Path

1. Action of path
   \[ S(q) \]

2. Differentiate action
   \[ \delta S(q) \]

3. Study when
   \[ \delta S(q) = 0 \]

Analogous to regular calculus
Defining the Variation of an Action

Arbitrary smooth offset $\eta(t)$

Perturbed curve

$$\tilde{q}(t) = q(t) + \varepsilon \eta(t)$$

Curves share endpoints

$$\eta(t_1) = \eta(t_2) = 0$$
Defining the Variation of an Action

**First Variation of the Action (in direction \( \eta \))**

\[
\delta_\eta S(q) := \left. \frac{d}{d\varepsilon} S(q + \varepsilon \eta) \right|_{\varepsilon=0}
\]

Reduce to single variable calculus!
Defining the Variation of an Action

First Variation of the Action (in direction eta)

Differentiating a given path with respect to all smooth variations reduces to single variable calculus.

\[ \delta_{\eta} S(q) \]

Reduce to single variable calculus!
mass = 1

\[ T(\dot{q}) = \frac{\dot{q}^2}{2} \]

\[ \mathcal{L}(q, \dot{q}) = \frac{\dot{q}^2}{2} - U(q) \]

\[ S(q) = \int_{t_1}^{t_2} \frac{\dot{q}(t)^2}{2} - U(q(t)) \, dt \]
Particle Example: Setup

\[ S(q) = \int_{t_1}^{t_2} \frac{\dot{q}(t)^2}{2} - U(q(t)) \, dt \]

\[ \text{mass} = 1 \]

\[ T(\dot{q}) = \frac{\dot{q}^2}{2} \]

\[ \mathcal{L}(q, \dot{q}) = \frac{\dot{q}^2}{2} - U(q) \]
Particle Example: Investigating the Variation

\[ S(q) = \int_{t_1}^{t_2} \frac{\dot{q}(t)^2}{2} - U(q(t)) \, dt \]

\[ \delta_\eta S(q) = \left. \frac{d}{d\varepsilon} S(q + \varepsilon \eta) \right|_{\varepsilon=0} \]

\[ = \int_{t_1}^{t_2} \frac{d}{d\varepsilon} \left( \frac{(\dot{q} + \varepsilon \dot{\eta})^2}{2} - U(q + \varepsilon \eta) \right) \bigg|_{\varepsilon=0} \, dt \]

\[ = \int_{t_1}^{t_2} (\dot{q} + \varepsilon \dot{\eta}) \dot{\eta} - U'(q + \varepsilon \eta) \eta \bigg|_{\varepsilon=0} \, dt \]

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Variational Trick: Essential Integration by Parts

\[
\delta_{\eta} S(q) = \int_{t_1}^{t_2} \dot{q}(t) \dot{\eta}(t) dt - \dot{U}'(q(t)) \eta(t) dt
\]

\[
\int_{t_1}^{t_2} \dot{q}(t) \dot{\eta}(t) dt = \dot{q}(t) \eta(t) \Bigg|_{t_1}^{t_2} - \int_{t_1}^{t_2} \ddot{q}(t) \eta(t) dt
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\[
\delta_{\eta} S(q) = -\int_{t_1}^{t_2} (\ddot{q}(t) + U'(t)) \eta(t) dt
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\delta_\eta S(q) = \int_{t_1}^{t_2} \dot{q}(t)\dot{\eta}(t) - U'(q(t))\eta(t) \, dt
\]

get rid of derivates of the offset

\[
\int_{t_1}^{t_2} \dot{q}(t)\dot{\eta}(t) \, dt = \dot{q}(t)\eta(t) \bigg|_{t_1}^{t_2} - \int_{t_1}^{t_2} \ddot{q}(t)\eta(t) \, dt
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recall offset vanishes at endpoints

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Variational Trick: Essential Integration by Parts

$$\delta_{\eta} S(q) = \int_{t_1}^{t_2} \dot{q}(t) \dot{\eta}(t) - U'(q(t)) \eta(t) \, dt$$

get rid of derivates of the offset

$$\int_{t_1}^{t_2} \dot{q}(t) \dot{\eta}(t) \, dt = \dot{q}(t) \eta(t) \bigg|_{t_1}^{t_2} - \int_{t_1}^{t_2} \ddot{q}(t) \eta(t) \, dt = 0$$

recall offset vanishes at endpoints

$$\delta_{\eta} S(q) = - \int_{t_1}^{t_2} (\ddot{q}(t) + U'(t)) \eta(t) \, dt$$
Variational Trick: Essential Integration by Parts

\[ \delta_{\eta}S(q) = \int_{t_1}^{t_2} \dot{q}(t)\dot{\eta}(t) - U'(q(t))\eta(t) \, dt \]

Integrate by parts to get rid of the derivatives of the smooth offset. This requires the offset to vanish at the boundary.

\[ \delta_{\eta}S(q) = -\int_{t_1}^{t_2} (\ddot{q}(t) + U'(t))\eta(t) \, dt \]
Particle Example: Investigating the Variation

$$\delta_\eta S(q) = - \int_{t_1}^{t_2} (\ddot{q}(t) + U'(q(t))) \eta(t) \, dt$$

When is $\delta_\eta S(q) = 0$ for all offsets $\eta$?
Fundamental Lemma of Variational Calculus

For a continuous function $G$ if

\[ \int_{t_1}^{t_2} G(t) \eta(t) \, dt = 0 \]

for all smooth functions $\eta(t)$ with $\eta(t_1) = \eta(t_2) = 0$,

then $G$ vanishes everywhere in the interval.
Fundamental Lemma of Variational Calculus

For a continuous function $G$ if

$$\int_{t_1}^{t_2} G(t) \eta(t) \, dt = 0$$

for all smooth functions $\eta(t)$ with $\eta(t_1) = \eta(t_2) = 0$, then $G$ vanishes everywhere in the interval.

...believable, but why?
Fundamental Lemma of Variational Calculus

If \( \int_{t_1}^{t_2} G(t) \eta(t) \, dt = 0 \) for all offsets \( \eta(t) \) zero at \( t_1, t_2 \)

then \( G \) vanishes on the interval.

Assume
Fundamental Lemma of Variational Calculus

If \( \int_{t_1}^{t_2} G(t) \eta(t) \, dt = 0 \) for all offsets \( \eta(t) \) zero at \( t_1, t_2 \)

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\[ \int G \eta \, dt \neq 0 \]
Fundamental Lemma of Variational Calculus

If \( \int_{t_1}^{t_2} G(t) \eta(t) \, dt = 0 \) for all offsets \( \eta(t) \) zero at \( t_1, t_2 \)

then \( G \) vanishes on the interval.

\[ G \] must be zero where \( \eta \) is nonzero.
Fundamental Lemma of Variational Calculus

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must hold for every choice of \( \eta \).
Fundamental Lemma of Variational Calculus

If \( \int_{t_1}^{t_2} G(t) \eta(t) \, dt = 0 \) for all offsets \( \eta(t) \) zero at \( t_1, t_2 \)

then \( G \) vanishes on the interval.

So \( G \) vanishes everywhere in the interval.
Particle Example: Deriving Euler-Lagrange Equations

Where were we?

$$\delta_\eta S(q) = - \int_{t_1}^{t_2} (\ddot{q}(t) + U'(q(t))) \eta(t) \, dt$$

When is $$\delta_\eta S(q) = 0$$ for all offsets $$\eta$$?
Particle Example: Deriving Euler-Lagrange Equations

\[ \delta_\eta S(q) = - \int_{t_1}^{t_2} (\ddot{q}(t) + U'(q(t))) \eta(t) \, dt \]

Apply Fundamental Lemma

\[ \delta_\eta S(q) = 0 \iff \ddot{q}(t) + U'(q(t)) = 0 \]

Euler-Lagrange equations
Apply the Fundamental Lemma to see when the derivative vanishes and recover the **Euler-Lagrange equations**.

$$\delta \eta S(q) = \int_{t_1}^{t_2} (\ddot{q}(t) + U'(q(t))) \eta(t) \, dt$$

$$\delta \eta S(q) = \int G(q, \dot{q}, \ddot{q}) \eta \, dt = 0$$
Particle Example: Lagrangian Reformulation

δS(q) = 0 ⇔ \ddot{q}(t) + U'(q(t)) = 0

Euler-Lagrange equations
Particle Example: Lagrangian Reformulation

\[ \delta S(q) = 0 \iff \ddot{q}(t) + U'(q(t)) = 0 \]

Euler-Lagrange equations

Wait... this looks familiar!
Particle Example: Lagrangian Reformulation

\[ \delta S(q) = 0 \iff \ddot{q}(t) + U'(q(t)) = 0 \]

Euler-Lagrange equations

Wait... this looks familiar!

\[ m \ddot{q}(t) + U'(q(t)) = 0 \]

is Newton’s law (reinserting mass)

(force is derivative of potential energy)
Lagrangian Reformulation Summary

**Principle of Stationary Action**
A path connecting two points is a physical path precisely when the first derivative of the action is zero.

\[ \mathcal{L}(q, \dot{q}) = T(\dot{q}) - U(q) \]

**Lagrangian**

\[ S = \int_{t_1}^{t_2} \mathcal{L}(q(t), \dot{q}(t)) \, dt \]

**Action**

\[ \delta S(q) = 0 \iff F = m\ddot{q} \]

**Euler-Lagrange Equations**

**Fundamental Lemma**
(general) Principle of Stationary Action

“Variational principles” apply to many systems, e.g., special relativity, quantum mechanics, geodesics, etc.

Key is to find Lagrangian $\mathcal{L}(t, q(t), \dot{q}(t))$

$$\delta S(q) = 0 \iff \frac{d\mathcal{L}(t, q, \dot{q})}{dq} - \frac{d}{dt} \left( \frac{d\mathcal{L}(t, q, \dot{q})}{d\dot{q}} \right) = 0$$

Fundamental Lemma

so general Euler-Lagrange equations are the equations of interest
(general) Principle of Stationary Action

"Variational principles" apply to many systems, e.g., special relativity, quantum mechanics, geodesics, etc.

The Euler-Lagrange equations for a general Lagrangian $\mathcal{L}(t, q(t), \dot{q}(t))$ are

$$\frac{d}{dq} \frac{d\mathcal{L}(t, q, \dot{q})}{dq} - \frac{d}{dt} \left( \frac{d\mathcal{L}(t, q, \dot{q})}{dq} \right) = 0$$

so general Euler-Lagrange equations are the equations of interest
Noether’s Theorem

Continuous symmetries of the Lagrangian imply **conservation laws** for the physical system.

<table>
<thead>
<tr>
<th>Continuous Symmetry</th>
<th>Conserved Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Translational</td>
<td>Linear momentum</td>
</tr>
<tr>
<td>Rotational (one dimensional)</td>
<td>Angular momentum</td>
</tr>
<tr>
<td>Time</td>
<td>Total energy</td>
</tr>
</tbody>
</table>
Lagrangian Paths are **Symplectic**

![Diagram showing Lagrangian paths and energy levels](image)

- **Position**: \( x \)
- **Momentum**: \( p = \text{mass} \times \text{velocity} \)
- **Energy Levels**
Lagrangian Paths are **Symplectic**

energy
levels

momentum
(mass x velocity)

position
Lagrangian Paths are **Symplectic**

Image from Hairer, Lubich, and Wanner 2006

in 2D equivalent to area conservation in phase space
(in higher dimensions implies volume conservation)
Lagrangian Paths are **Symplectic**

Image from Hairer, Lubich, and Wanner 2006

in 2D equivalent to area conservation in phase space  
(in higher dimensions implies volume conservation)
Variational Time Integrators

Discretize Lagrangian

Apply Variational Principle

Arrive at Discrete Equations of Motion

(as opposed to discretizing equations directly)
Discrete Noether’s Theorem

Discretize Lagrangian

Arrive at Discrete Equations of Motion

Continuous symmetries of the discrete Lagrangian imply conserved quantities throughout entire discrete motion.

(for not too large time steps)
Discrete Variational Integrators are Symplectic

... time is now discrete, so total energy is not conserved.

But, discrete symplectic structure guarantees **bounded oscillation** around true energy level
(for not too large time steps)
Discrete Variational Integrators are Symplectic

...time is now discrete, so total energy is not conserved.

But, discrete symplectic structure guarantees \textit{bounded oscillation} around true energy level

(for not too large time steps)
Part Two:
Why Use Variational Integrators?
Quick Recap

Physical paths are extremal amongst all paths from A to B of the action integral

Action is the integral of the Lagrangian, kinetic minus potential energy

Symmetries of Lagrangian and symplectic structure give rise to conservation laws
Variational Time Integrators

Discretize Action (integral of Lagrangian)

Apply Variational Principle

Arrive at Discrete Equations of Motion

(as opposed to discretizing equations directly)
Discrete Noether’s Theorem

Discretize Lagrangian

Arrive at Discrete Equations of Motion

Continuous symmetries of discrete Lagrangian imply conserved quantities throughout entire discrete motion, e.g., conservation of linear and angular momentum

(for not too large time steps)
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But, discrete symplectic structure guarantees **bounded oscillation** around true energy level (for not too large time steps).

Variational integrators are symplectic and vice versa. Both equivalent terms are used.
Discrete Variational Integrators are Symplectic

... time is now discrete, so total energy is not conserved.

But, discrete symplectic structure guarantees bounded oscillation around true energy level (for not too large time steps).

Variational integrators are symplectic and vice versa. Both equivalent terms are used.
Building a Variational Time Integrator

1. Choose a finite difference scheme for $\dot{q}$, e.g.,
Building a Variational Time Integrator

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- forward
- backward
- central
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2. Choose a quadrature rule to integrate action, e.g.,

- rectangular
- midpoint
- trapezoid
Building a Variational Time Integrator

1. Choose a finite difference scheme for $\dot{q}$, e.g.,

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- backward
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2. Choose a quadrature rule to integrate action, e.g.,

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3. Apply variational principle
Discrete Variational Principle Example

\[ \dot{q} \approx \dot{q}_k = \frac{q_{k+1} - q_k}{\Delta t} \]

\[ \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}) \, dt \approx \sum_{k=0}^{N} \mathcal{L}(q_k, \dot{q}_k) \Delta t \]
Discrete Variational Principle Example

\[ \dot{q} \approx \dot{q}_k = \frac{q_{k+1} - q_k}{\Delta t} \]

\[ \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}) \, dt \approx \int_{t}^{t+\Delta t} \mathcal{L}(q, \dot{q}) \, dt \approx \Delta t \mathcal{L}(q_k, \dot{q}_k) \]

\[ \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}) \, dt \approx \sum_{k=0}^{N} \mathcal{L}(q_k, \dot{q}_k) \Delta t \]
Choose a finite difference scheme and quadrature rule and write down the **discrete action sum**.

\[
\int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}) \, dt \approx \sum_{k=0}^{N} \mathcal{L}(q_k, \dot{q}_k) \Delta t
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Discrete Variational Principle Example

\[ S_{\Delta t} = \sum_{k=0}^{N} \left( \frac{m}{2} \dot{q}_k^2 - U(q_k) \right) \Delta t \]

\[ \delta_\eta S_{\Delta t} = \frac{d}{d\varepsilon} S_{\Delta t} (q_k + \varepsilon \eta_k) \bigg|_{\varepsilon=0} \]

\[ = \sum_{k=0}^{N} (m\dot{q}_k \dot{\eta}_k - U'(q_k) \eta_k) \Delta t \]

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\[ \delta_\eta S_{\Delta t} = \sum_{k=0}^{N} (m \dot{q}_k \dot{\eta}_k - U'(q_k) \eta_k) \Delta t \]
Discrete Variational Principle Example

\[\delta_\eta S_{\Delta t} = \sum_{k=0}^{N} \left( m \dot{q}_k \dot{\eta}_k - U'(q_k) \eta_k \right) \Delta t\]

get rid of derivatives of the offset
Discrete Variational Principle Example

\[ \delta \eta S_{\Delta t} = \sum_{k=0}^{N} \left( m \dot{q}_k \dot{\eta}_k - U'(q_k) \eta_k \right) \Delta t \]

get rid of derivates of the offset

Summation by Parts

\[ \sum_{k=0}^{N} \dot{q}_k \dot{\eta}_k \Delta t = bdy - \sum_{k=0}^{N} \ddot{q}_k \eta_{k+1} \Delta t \]
Discrete Variational Principle Example

\[ \delta \eta S_{\Delta t} = \sum_{k=0}^{N} \left( m \dot{q}_k \dot{\eta}_k - U'(q_k) \eta_k \right) \Delta t \]

get rid of derivates of the offset

Recall offset vanishes at boundary

\[ \eta_{N+1} = \eta_0 = 0 \]
Discrete Variational Principle Example

\[ \delta \eta S_{\Delta t} = - \sum_{k=0}^{N} m \frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} \eta_{k+1} \Delta t - \sum_{k=0}^{N} U'(q_k) \eta_k \Delta t \]

\[ = - \sum_{k=0}^{N} \left( m \frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} + U'(q_{k+1}) \right) \eta_{k+1} \Delta t \]
Discrete Variational Principle Example

\[
\delta_{\eta} S_{\Delta t} = - \sum_{k=0}^{N} m \ddot{q}_k \eta_{k+1} \Delta t - \sum_{k=0}^{N} U'(q_k) \eta_k \Delta t
\]

\[
= - \sum_{k=0}^{N} m \left( \frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} \right) \eta_{k+1} \Delta t - \sum_{k=0}^{N} U'(q_k) \eta_k \Delta t
\]

\[
= - \sum_{k=0}^{N} \left( m \frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} + U'(q_{k+1}) \right) \eta_{k+1} \Delta t
\]
Discrete Variational Principle Example

\[ \delta_{\eta} S_{\Delta t} = - \sum_{k=0}^{N} m \ddot{q}_k \eta_{k+1} \Delta t - \sum_{k=0}^{N} U'(q_k) \eta_k \Delta t \]

= \[- \sum_{k=0}^{N} m \left( \frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} \right) \eta_{k+1} \Delta t - \sum_{k=0}^{N} U'(q_k) \eta_k \Delta t \]

= \[- \sum_{k=0}^{N} \left( m \frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} + U'(q_{k+1}) \right) \eta_{k+1} \Delta t \]
Discrete Variational Principle Example

\[ \delta_{\eta} S_{\Delta t} = - \sum_{k=0}^{N} m \ddot{q}_k \eta_{k+1} \Delta t - \sum_{k=0}^{N} U'(q_k) \eta_k \Delta t \]

\[ = - \sum_{k=0}^{N} m \left( \frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} \right) \eta_{k+1} \Delta t - \sum_{k=0}^{N} U'(q_k) \eta_k \Delta t \]

\[ = - \sum_{k=0}^{N} \left( m \frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} + U'(q_{k+1}) \right) \eta_{k+1} \Delta t \]

(shift index)

\[ (\eta_{N+1} = \eta_0 = 0) \]
Discrete Variational Principle Example

\[ \delta_{\eta} S_{\Delta t} = - \sum_{k=0}^{N} \left( m \frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} + U' (q_{k+1}) \right) \eta_{k+1} \Delta t \]

(discrete) Fundamental Lemma of Calculus of Variations

\[ \delta S_{\Delta t} = 0 \iff -U' (q_{k+1}) = m \frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} \]

\[ \text{discrete Euler-Lagrange} \]

Recall:

\[ \delta S (q) = 0 \iff F = m \ddot{q} \]
Discrete Variational Integrator Scheme

\[ \dot{q}_k = \frac{q_{k+1} - q_k}{\Delta t} \]

\[ -U'(q_{k+1}) = m \frac{(\dot{q}_{k+1} - \dot{q}_k)}{\Delta t} \]

Symplectic (variational) Euler

\[ q_{k+1} = q_k + \Delta t \dot{q}_k \]

\[ \dot{q}_{k+1} = \dot{q}_k + \Delta t m^{-1} (-U'(q_{k+1})) \]

\[ (q_k, \dot{q}_k) \mapsto (q_{k+1}, \dot{q}_{k+1}) \]
Discrete Variational Integrator Scheme

\[
q_{k+1} = q_k + \Delta t \, \dot{q}_k
\]

\[
\dot{q}_{k+1} = \dot{q}_k + \Delta t \, m^{-1}(U'(q_{k+1}))
\]

Semi-implicit Euler

\[
(\dot{q}_k, q_k) \rightarrow (\dot{q}_{k+1}, q_{k+1})
\]
Discrete Variational Integrator Scheme

\[ \dot{q}_{k+1} = \dot{q}_k + \Delta t \ m^{-1}( -U'(q_k) ) \]

\[ q_{k+1} = q_k + \Delta t \dot{q}_{k+1} \]

Use Symplectic Euler Method B

\((q_k, \dot{q}_k) \mapsto (q_{k+1}, \dot{q}_{k+1})\)
Time Integration Schemes

Great... we know how to derive a variational integrator, but what other integrators are there?

Where do they come from?

Why are they used?

How do they compare?
First Order Integration Schemes

Explicit Euler

Use (forward) first order Taylor approximation of motion

\[
q(t + \Delta t) = q(t) + \dot{q}(t) \Delta t + \frac{\ddot{q}(t)}{2} \Delta t^2 + \ldots
\]

\[
\dot{q}(t + \Delta t) = \dot{q}(t) + \ddot{q}(t) \Delta t + \frac{\dddot{q}(t)}{2} \Delta t^2 + \ldots
\]
First Order Integration Schemes

Explicit Euler

\[ q(t + \Delta t) = q(t) + \dot{q}(t) \Delta t \]

\[ \dot{q}(t + \Delta t) = \dot{q}(t) + \ddot{q}(t) \Delta t \]
First Order Integration Schemes

Explicit Euler

\[ q(t + \Delta t) = q(t) + \dot{q}(t)\Delta t \]

\[ \dot{q}(t + \Delta t) = \dot{q}(t) + \ddot{q}(t)\Delta t \]

use Newton’s law

\[ F = -U'(q) = m\ddot{q} \]

\[ m\ddot{q}(t + \Delta t) = m\dot{q}(t) + \Delta t(-U'(q(t))) \]
First Order Integration Schemes

Explicit Euler

\[ q_{k+1} = q_k + \Delta t \dot{q}_k \]

\[ \dot{q}_{k+1} = \dot{q}_k + \Delta t m^{-1}(-U'(q_k)) \]

Cheap to compute -- explicit dependence of variables

but

“unstable” for large time steps

(dramatically deviates from true trajectories)
Explicit Euler

$2^{-6}$

step size in seconds
Explicit Euler

$2^{-6}$

step size in seconds
Explicit: Time Step Refinement

$2^{-6}$

step size in seconds

$2^{-9}$

$2^{-10}$

$2^{-11}$
First Order Integration Schemes

Explicit (forward) Euler

\[ q_{k+1} = q_k + \Delta t \, \dot{q}_k \]
\[ \dot{q}_{k+1} = \dot{q}_k + \Delta t \, m^{-1}(-U'(q_k)) \]

Implicit (backward) Euler

\[ q_{k+1} = q_k + \Delta t \, \dot{q}_{k+1} \]
\[ \dot{q}_{k+1} = \dot{q}_k + \Delta t \, m^{-1}(-U'(q_{k+1})) \]

motion “implicitly” depends on variables
First Order Integration Schemes

Implicit Euler

\[ q_{k+1} = q_k + \Delta t \dot{q}_{k+1} \]

\[ \dot{q}_{k+1} = \dot{q}_k + \Delta t m^{-1}(-U'(q_{k+1})) \]

“stable” for large time steps
(stays close to true trajectories)

but

adds artificial damping

more expensive -- nonlinear solve for implicit variables
Implicit Euler

\[ 2^{-6} \]

step size in seconds
Implicit Euler

$2^{-6}$

step size in seconds
Implicit: Time Step Refinement

$2^{-6}$

step size in seconds

$2^{-7}$

$2^{-8}$

$2^{-9}$

$2^{-10}$

$2^{-11}$
First Order Integration Schemes

Symplectic Euler Method A

\[ q_{k+1} = q_k + \Delta t \dot{q}_k \]
\[ \dot{q}_{k+1} = \dot{q}_k + \Delta t m^{-1}(-U'(q_{k+1})) \]

Symplectic Euler Method B

\[ q_{k+1} = q_k + \Delta t \dot{q}_{k+1} \]
\[ \dot{q}_{k+1} = \dot{q}_k + \Delta t m^{-1}(-U'(q_k)) \]

also called “semi-implicit” Euler methods
First Order Integration Schemes

Symplectic Euler Methods, e.g.,

\[ q_{k+1} = q_k + \Delta t \, \dot{q}_{k+1} \]
\[ \dot{q}_{k+1} = \dot{q}_k + \Delta t \, m^{-1}(-U'(q_k)) \]

as cheap as Explicit Euler

bounded energy oscillation (little artificial damping/driving)

conserved linear and angular momentum

also unstable for very large time steps
Symplectic Euler (Method B)

$2^{-6}$

step size in seconds
Symplectic Euler (Method B)

$2^{-6}$

step size in seconds
Symplectic: Time Step Refinement

$2^{-6}$
step size in seconds

$2^{-7}$

$2^{-8}$

$2^{-9}$

$2^{-10}$

$2^{-11}$
Phase Space (energy levels)

- momentum: \(\text{mass} \times \text{velocity}\)
- position

Methods:
- implicit
- symplectic
- explicit
Phase Space (energy levels)

Position

Momentum (mass x velocity)

Implicit symplectic
Explicit
Energy Landscape Under Step Refinement

- **Energy**
- **Time (s)**
- **2^{-6}**
- **2^{-11}**
- **2^{-6}**
- **2^{-11}**

Explicit and implicit methods are compared, with the true energy shown as a horizontal line. The graphs illustrate how the energy changes over time for different refinement steps.
Energy Landscape Near Time Zero

- explicit
- symplectic
- true energy
- implicit
Very Small Time Step

explicit

symplectic

implicit
Large Time Steps: Symplectic vs Implicit

Symplectic unstable region shown in largest time step

Implicit is stable, but damping is time step dependent
Three Integrators Summary

Explicit
cheap
artificial driving
unstable

Variational
cheap
good energy
unstable for large $\Delta t$
momenta conserved

Implicit
more expensive
artificial damping
stable
Three Integrators Summary

Explicit
cheap
artificial driving
unstable

Variational
cheap
good energy
unstable for large $\Delta t$
momenta conserved

Implicit
more expensive
artificial damping
stable
Three Integrators Summary

Variational Integrators

cheap
good energy
momenta conserved
but (can’t have it all!)
unstable for large $\Delta t$
Variational Integrators

cheap
good energy
momenta conserved
but (can’t have it all!)
unstable for large $\Delta t$
Damped Systems

Want to include non-conservative forces, too

\[ m \ddot{q} = -U'(q) + f(q, \dot{q}) \]

Systems with non-conservative forces satisfy the **Lagrange-D’Alembert Principle**

\[
\delta \eta \int_{t_1}^{t_2} \mathcal{L}(q(t), \dot{q}(t)) \, dt + \int_{t_1}^{t_2} f(q(t), \dot{q}(t)) \cdot \eta \, dt = 0
\]

variation of action in direction \( \eta \)  
integral of force in direction of variation, \( \eta \)

modification of Principle of Stationary Action
Damped Systems

Lagrange-D’Alembert Principle

\[ \delta \eta \int_{t_1}^{t_2} \mathcal{L}(q(t), \dot{q}(t)) \, dt + \int_{t_1}^{t_2} f(q(t), \dot{q}(t)) \cdot \eta \, dt = 0 \]

Discretize using Variational Principle with:

(Forced Symplectic Euler Method)
Discrete Lagrange-D’Alembert Principle

Forced Symplectic Euler Method B

\[
q_{k+1} = q_k + \Delta t \dot{q}_{k+1}
\]

\[
\dot{q}_{k+1} = \dot{q}_k + \Delta t m^{-1} \left( -U'(q_k) + \frac{f_{k-1} + f_k}{2} \right)
\]
Discrete Lagrange-D’Alembert Principle

Forced Symplectic Euler Method B

\[ q_{k+1} = q_k + \Delta t \dot{q}_{k+1} \]

\[ \dot{q}_{k+1} = \dot{q}_k + \Delta t m^{-1} \left( -U'(q_k) + \frac{f_{k-1} + f_k}{2} \right) \]

\[ f_k = -c \dot{q}_k \]

e.g., air resistance
Variational Damped Pendulum

30% damped

non-damped
Variational Damped Pendulum

30% damped

non-damped
Variational Damped Pendulum

30% damped behavior independent of step size (within stable region)
Variational Damped Pendulum

80% damped

behavior independent of step size (within stable region)

30% damped
Variational Damped Pendulum

- 80% damped
- 30% damped

behavior independent of step size (within stable region)
30% Damped Pendulum

**Variational**
step size independent

\[ \Delta t \]

**Implicit**
step size dependent

\[ 2^{-5} \]

\[ 2^{-10} \]
30% Damped Pendulum

Variational
step size
independent

\[ \Delta t \]

Implicit
step size
dependent

\[ 2^{-5} \quad 2^{-10} \]
30% Damped Pendulum

Forced Variational Integrators

- cheap
- good energy behavior
- behavior independent of step size (in stable region)

Essential for rough previews often done in Computer Graphics
Higher Order Variational Integrators

Recall: forward yields first order integration scheme
Higher Order Variational Integrators

Recall:

forward quadrature yields first order integration scheme

Generically:

\[ r^{th} \text{ order quadrature yields } (r + 1)^{st} \text{ order integrator} \]
Higher Order Variational Integrators

Recall:

\( r^{th} \) order quadrature yields \((r + 1)^{st}\) order integrator

Variational Integrators exist of all orders

\((r + 1)^{st}\) order integrator
Some Well Known Variational Integrators

(of second order)

Use: trapezoid

Derive: Störmer-Verlet Method
Some Well Known Variational Integrators

(of second order)

Use: forward

Derive: Implicit Midpoint Method

(algebraic miracle, zeroth yields second order)
Comparison of First and Second Order Integrators

![Comparison of First and Second Order Integrators](Image from Hairer, Lubich, and Wanner 2006)
Summary: Variational Time Integrators

No more difficult to implement

... but have many advantages ...
Summary: Variational Time Integrators

Discrete Principle of Stationary Action

Symplectic structure guarantees good energy behavior

Noether’s theorem guarantees conservation of momenta

Forced systems have behavior independent of step size (for stable time steps)
Questions?
Principle of Least Action
Feynman Lectures on Physics II.19
http://www.feynmanlectures.caltech.edu/II_19.html


Variational integrators.

Geometric, variational integrators for computer animation.

Speculative parallel asynchronous contact mechanics.
Samantha Ainsley, Etienne Vouga, Eitan Grinspun, and Rasmus Tamstorf. 2012. ACM Trans. Graph. 31, 6, Article 151 (November 2012), 8 pages. DOI=10.1145/2366145.2366170
Details of Movies Shown

Pendulum assumptions:

mass equals length equals one

$$-U'(q) = - \sin(q)$$

initial conditions

$$\dot{q}(0) = 0$$

$$q(0) = \pi/4$$

movies at 16 fps