Variational Time Integrators: the geometry of dynamics

Motivation

Time integration is essential!

Needs to be:
- efficient
- stable
- physical
Simple Example

Pendulum: \( \dot{q} = v, \dot{v} = -\sin q \)
- forward Euler
- backward Euler
- Runge-Kutta
- Newmark

\[ q_{k+1} = q_k + hv_k \\
\dot{v}_k = v_k - h\sin q_k \]
Simple Example

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  \[ v_{k+1} = v_k - h \sin q_k \]
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Simple Example

Pendulum: \( \dot{q} = v, \; \dot{v} = -\sin q \)
- forward Euler
- backward Euler
- Runge-Kutta
- Newmark
  - Störmer/Verlet
  - Variational!

\[ v_{k+1} = v_k - h \sin q_k \]
\[ q_{k+1} = q_k + hv_{k+1} \]

Geometric Integration

Usual approach
- numerical discretization of \( M\ddot{q} = F(q) \)

Variational integrators
- path has geometric properties
- use discrete geometric knowledge
- preserve invariants of the system
  - symplectic form preserved
Today’s Show

Variational Integrators
- overview of variational mechanics
- constructing an integrator
- fully variational update

Application
- non-linear elasticity
- improved damping model

Variational Mechanics

Hamilton’s Stationary Action Principle:

A dynamical system always finds an optimal course from one position to another

\[ \delta S(q) = \delta \int_{0}^{T} \left( L(q, \dot{q}) + K(q, \dot{q}) - W(q) \right) \, dt \]

Euler-Lagrange Equation
\[ \frac{\partial L}{\partial q} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) = 0 \]

Newton’s Second Law
\[ M\ddot{q} = F(q) \]
Hamilton’s Stationary Action Principle:

A dynamical system always finds an optimal course from one position to another.

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

\[ = \int_0^T \left[ \frac{\partial L}{\partial q} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) \right] \delta q \, dt + \left[ \frac{\partial L}{\partial \dot{q}} \cdot \delta \dot{q} \right]_0^T, \]

Discrete Mechanics

Discrete Euler-Lagrange Equations

\[ D_1 L_d(q_{k+1}, q_{k+2}) + D_2 L_d(q_k, q_{k+1}) = 0 \]

\[ \delta S_d(q) = \delta \sum_{k=0}^{N} L_d(q_k, q_{k+1}) = 0 \]
Discrete Mechanics

Hamilton’s Stationary Action Principle:

a dynamical system always finds an optimal course from one position to another

Discrete Euler-Lagrange Equations

\[ D_1L_d(q_{k+1}, q_{k+2}) + D_2L_d(q_k, q_{k+1}) = 0 \]

solve DEL for time integration: \((q_k, q_{k+1}) \rightarrow q_{k+2}\)

Discrete Lagrangian

Discrete: \( L(q, \dot{q}) = K(\dot{q}) - W(q) \)

\[ L_d(q_k, q_{k+1}) = h \left[ \frac{1}{2} \left( \frac{q_{k+1} - q_k}{h} \right)^T M(q_{k+1} - q_k) \right] - W((1 - \alpha)q_k + \alpha q_{k+1}) \]

- integral over timestep
- one point quadrature
- discretize potential
Elasticity Potential

Discrete elastic energy (FEM 101)
- function of Cauchy-Green strain tensor

\[ F = \frac{\partial \varphi(X)}{\partial X} \]
\[ C = F^T F \]

for each tet: \[ W^e(C) = \mu(tr(C) - 3) + \kappa(det(C) - 1)^2 \]
total: \[ W = \sum_{e=1}^{m} W^e(C)V^e \]

Advantages

Even with low accuracy/large steps
- results are qualitatively correct

Higher accuracy is easy
- high-order quadrature

Conservation laws
- momentum \textit{exactly}
- energy almost
Hamilton–Pontryagin

Continuous Hamilton–Pontryagin

\[ \delta \int_0^T (p(q - v) + L(q,v)) \, dt = 0 \]

- equivalent to Hamilton’s principle
- decouples velocity and position
- Lagrange multiplier = momentum
- used for variational update

Discrete:

\[ \delta \sum_{k=0}^{N} \left( h p_{k+1} \left( \frac{q_{k+1} - q_k}{h} - v_{k+1} \right) + L^d(q_k, v_{k+1}) \right) = 0 \]

taking variations with respect to all discrete variables

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Derivations

Take variations w.r.t. all variables

\[ \delta \sum_{k=0}^{N} \left( h p_{k+1} \frac{q_{k+1} - q_k}{h} - v_{k+1} + L^d(q_k, v_{k+1}) \right) = 0 \]

\[ \delta p : \quad q_{k+1} - q_k = h v_{k+1} \]

Discrete Integration

Algorithm

- set initial \( q_0 \) and \( p_0 \)
- solve for \( v_{k+1} \)

\[ D_2 L^d(q_k, v_{k+1}) - h D_1 L^d(q_k, v_{k+1}) - h p_k = 0 \]

- explicit update
  \[ q_{k+1} = q_k + hv_{k+1} \]
  \[ p_{k+1} = D_2 L^d(q_k, v_{k+1})/h \]
**Fully Variational Update**

**Algorithm**

- set initial $q_0$ and $p_0$
- solve for $v_{k+1}$
  
  \[
  L^d(q_k, v_{k+1}) - hP(q_k, v_{k+1}) - hp_kv_{k+1}
  \]
- explicit update
  
  \[
  q_{k+1} = q_k + hv_{k+1},\quad p_{k+1} = D_2L^d(q_k, v_{k+1})/h
  \]

where $D_2P(q_k, v_{k+1}) = D_1L^d(q_k, v_{k+1})$

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**Variational Update**

Next position can be found by solving a minimization problem

- **integrability condition**
  
  - quite general anyway
  - convex for small enough timesteps
  - more efficient solvers
  - 2–3 times speed-up on small examples
**Conservation Laws**

Energy

- Total
- Kinetic
- Potential

Momenta

- Linear X
- Angular X, Angular Y, Angular Z
- Linear Y, Z

Damping

Full control over dissipation forces

- Use d’Alembert principle
  - Add any external forces this way
- Simple damping model
  - Essentially independent of timestep
    - Damping not a side effect of bad numerics
    - Crucial requirement for coarse previews!
- Preserves angular momentum
Damping Model

Use existing potential functions
- penalize deformation w.r.t.
  positions at previous timestep
- kill high frequencies, not low ones

Example Of Damping

variational integrators
and damping
damped Newmark
Example Of Damping

Later on...

Variational integrators and damping

damped Newmark

Plots

Total Energy

Angular momentum (Z direction)

Legend

- Newmark (dt = 0.001)
- Newmark (dt = 0.002)
- Var. Integrator (0.001 and 0.002)
Bunny Movie

Conclusions

Geometric approach to integration:
- helps design simple schemes
- that are symplectic, momentum preserving, w/ well-behaved energy
- with any order of accuracy
- and can even lead to minimization-based updates