CS 101

Numerical Geometric Integration

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Today

Varying Time Steps

- we always assumed constant timesteps
  - no more
- messing up with time means messing up with energy
  - remember; conjugate momentum
    - $p_j = \partial \mathcal{L} / \partial \dot{q}_j$
  - we'll see a similar relationship btw E & t

Motivation

Adaptive time stepping useful for

- efficiency
- accuracy
- better energy behavior

No reason to take constant time steps

- so let's try adapting time steps

Automatic Time Step Control

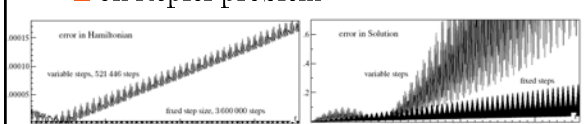
Take smaller time steps if too "off"

- how do you know the current error?
  - for instance, compare 2 integrators
- adapt timestep size based on error
  - integrate
  - adapt time step
  - repeat
- simple enough, right?

Alas...

For Störmer-Verlet

- on Kepler problem

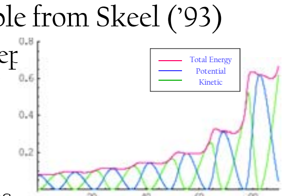


- changing time, even in order to reduce error, can have an adverse effect

Simple, Tailored Example

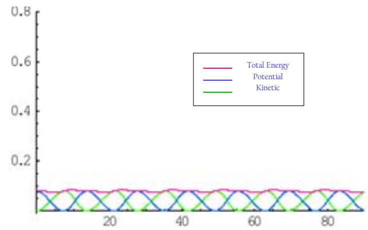
In some cases one can expect very, very bad energy behavior

- 1-D spring example from Skeel ('93)
  - changing timestep of a spring every quarter-period
  - hard to design similar behavior on complex cases



What We Ultimately Want

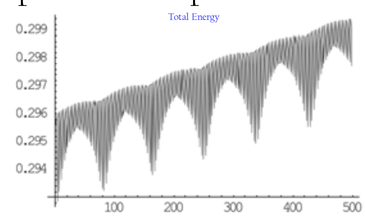
Variational time adaptation



Other (Naive) Time Adaptions

Simple pendulum

- explicit time adaption on velocity



How To Fix This?

- Hamiltonian point of view
  - adaptive Störmer-Verlet derived
- more recently, variational approach
  - very simple!
- symmetry can help too
  - another adaptive Störmer-Verlet

Hamiltonian Approach (I)

Naïve treatment of time adaption

- consider a Hamiltonian system

$$\dot{y} = J^{-1}\nabla H(y)$$

- and a function $\sigma(y)$ that scales time
  - it determines new step size $\Delta t = \sigma(y)\Delta\tau$

$$t' = \sigma(y)$$

  - so now: $y' = \sigma(y)J^{-1}\nabla H(y)$

Hamiltonian Approach (II)

Unfortunately...

- it is still Hamiltonian only when

$$\frac{d}{dt}\sigma(y(t)) = \nabla\sigma(y(t))^T J^{-1}\nabla H(y(t)) = 0$$

constant

- Proof?
  - Jacobian of $\sigma(y(t))\nabla H(y(t))$ symmetric...
  - iff $\nabla H \nabla\sigma^T$ symmetric

Hamiltonian Approach (III)

Fixed by Hairer '97, Reich '99

- consider new Hamiltonian

$$\widehat{H(y)} = \sigma(y)(H(y) - H_0)$$

- new Hamiltonian system is

$$y' = \sigma(y)J^{-1}\nabla H(y) + \underline{(H(y) - H_0)J^{-1}\nabla\sigma(y)}$$

  - adds "small" perturbation to original path
  - and makes the system Hamiltonian
- can be used as is for integrators!

Adaptive Störmer-Verlet

Adapted from Hamiltonian standpoint

$$p_{k+1/2} = p_k - \frac{h s_k}{2}\nabla W(q_k) - \frac{h}{2}(H(p_{k+1/2}, q_k) - H_0)\nabla\sigma(q_k)$$

$$q_{k+1} = q_k + h\frac{s_k + s_{k+1}}{2} M^{-1} p_{n+1/2}$$

$$p_{n+1} = p_{n+1/2} - \frac{h s_{k+1}}{2}\nabla W(q_{k+1}) - \frac{h}{2}(H(p_{k+1/2}, q_{k+1}) - H_0)\nabla\sigma(q_{k+1})$$

with $s_k = \sigma(q_k)$

- Note that $t_{k+1} = t_k + h\frac{s_k+s_{k+1}}{2}$.

Fictitious Constant Timestep

Variational Approach

Define timestep as fct of q_k and q_{k+1}

$$t_{k+1} - t_k = h\sigma(q_k, q_{k+1})$$

Fictitious Constant Timestep

Define new Lagrangian as:

$$\tilde{L}_d(q_k, q_{k+1}, h_{k+1}) = L_d(q_k, q_{k+1}, h\sigma(q_k, q_{k+1})) - E_0 h\sigma(q_k, q_{k+1})$$

- $E_0 h$ term is crucial in order for DEL equations to simulate nearby system
- without it, it ain't working

Alternative Formulation

Force timestep w/ Lagrange multipliers

$$\tilde{L}_d(q_k, q_{k+1}, t_k, t_{k+1}) =$$

$$L_d(q_k, q_{k+1}, t_k, t_{k+1}) + \lambda(t_{k+1} - t_k - h\sigma(q_k, q_{k+1}))$$

Take variations w.r.t. all the variables…

- notice that E_0 will show up

New DEL Equations

$$L_d(q_k, q_{k+1}, t_k, t_{k+1}) + \lambda_{k+1}(t_{k+1} - t_k - h\sigma(q_k, q_{k+1}))$$

- Variations wrt. λ_{k+1} give time update
- Variations wrt. t_k yield λ_{k+1} update as:

$$\boldsymbol{\lambda_{k+1} = E_{k+1} - E_k + \lambda_k} = E_{k+1} - E_0$$

  - where $E_k = \partial L_d(q_{k-1}, q_k, t_{k-1}, t_k)/\partial t_k$
- Usual DEL equations get extra term:

$$DEL + h\lambda_{k+1} D_1\sigma(q_k, q_{k+1}) + h\lambda_k D_2\sigma(q_{k-1}, q_k) = 0$$

Error Bounds

Both approaches are equivalent

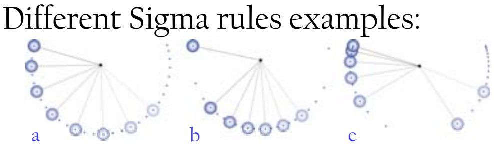
- They can be viewed as variational integrator with fictitious constant timestep $h = \tau_{k+1} - \tau_k$
- Discrete energy nearly preserved:

$$\widehat{E}_k = \lambda_k\, \sigma(q_k, q_{k+1}) = (E_k - E_0)\, \sigma(q_k, q_{k+1}).$$

- As λ stays bounded, the system simulated stays close to the original

Sigma Rules

Different Sigma rules examples:



- equispaced positions

$$\sigma(q_k, q_{k+1}) = 1/\sqrt{E_0 - W(q_k, q_{k+1}) + \varepsilon}$$

- or inverse of kinetic energy
- or 1/acceleration (similar to (p,q) equispaced)

But.... Symmetry Can Help Too

Near energy preservation over long simulations even with naive way

- with *time reversible* integrator & symmetric σ, you get time reversible adaptive integrator

$$\sigma(q_k, q_{k+1}) = \sigma(q_{k+1}, q_k)$$

- "thus", good energy behavior
  - more on "thus" next time

Adaptive Störmer-Verlet

Time symmetry simplifies things...

$$p_{k+1/2} = p_k - \frac{h s_k}{2} \nabla W(q_k)$$

$$q_{k+1} = q_k + h\frac{s_k + s_{k+1}}{2} M^{-1} p_{n+1/2}$$

$$p_{k+1} = p_{k+1/2} - \frac{h s_{k+1}}{2} \nabla W(q_{k+1})$$

with $s_k = \sigma(p_{k+1/2}, q_k), \quad s_{k+1} = \sigma(p_{k+1/2}, q_{k+1})$

- Note that $t_{k+1} = t_k + h\frac{s_k + s_{k+1}}{2}$.

Discussion on Numerics

Cost of symplectic time adaption:

- adds 2 new variables (λ_k and time)
  - for $\sigma(q_k, q_{k+1}) = \sigma(q_k)$, only λ_k is implicit
- but extra vars coupled to other dofs
- dense + nonsymmetric Jacobian of DEL
  - ouch, but it's the price to pay

Discussion on Numerics

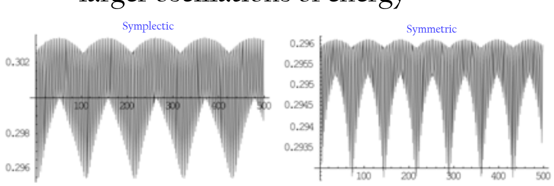
Cost of symmetric time adaption:

- adds a single new variable (time)
  - time always implicit because of symmetry
- time is coupled to all other dofs
  - nonsymmetric Jacobian of DEL
  - but sparse
- faster than symplectic time adaption

Energy oscillations

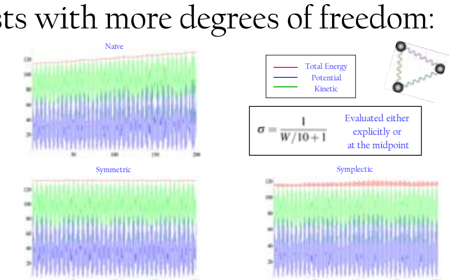
Both methods do not drift

- symplectic way introduces slightly larger oscillations of energy



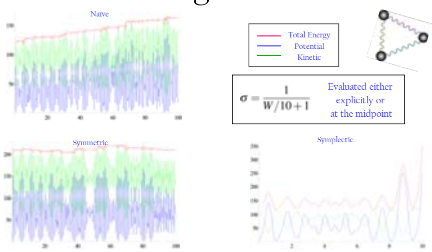
Time step size (max Δt=.1)

Tests with more degrees of freedom:



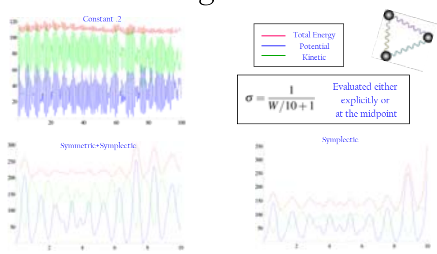
Time step size (max Δt=.2)

Tests with more degrees of freedom:



Time step size (max Δt=.2)

Tests with more degrees of freedom:



Symplectic + Energy-preserving?

Symplectic-energy-momentum preserving integrators (Kane '99)

- timestep is automatically updated to get energy preservation
  - special σ
- but no freedom on choosing it
- no free lunch…
  - very brittle near "turning points"

Explicit Reversible Integrators

Newer ways to deal with time adaption

- in particular Hairer's
- reversible, yet explicit!
- trick: update σ in time too