8A

Introduction to Numerical Methods for Hamiltonian Systems

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Numerical Methods for ODEs

to solve an initial value problem

one-step method: $\frac{x_{n+1} - x_n}{h} = \bar{f}(t_n, t_{n+1}; x_n, x_{n+1})$ where $t_n = t_0 + nh$, $x_n \approx x(t_n)$

as $h \to 0$, this becomes the vector field

Simplest: Euler method (explicit)

$x(t_0 + h) = x(t_0) + h f(t_0, x_0) + \mathcal{O}(h^2)$ repeat this for each time step

problem - for pendulum, explicit Euler, energy increases with time

Implicit Euler method

$x_{n+1} = x_n + h f(t_{n+1}, x_{n+1})$ x_{n+1} determined implicitly

have to solve a nonlinear system for each step - use Newton's method

much more expensive

for pendulum, energy decreases with time

Runge-Kutta Methods - higher order

use fundamental thm of calculus $x(t_{n+1}) = x(t_n) + \int_{t_n}^{t_{n+1}} \dot{x}(t)\, dt$

approx the integral by some quadrature rule

uses intermediate solutions between t_n & t_{n+1}

summarize coefficients in Butcher table - numerical analysis just from table.

RK4 - much less dissipation of energy, but it's still there - esp. for long times

Hamiltonian System

pendulum is a Hamiltonian system - there exists a symplectic structure

a symplectic map preserves this symplectic structure preserves phase space area.

└ or Jacobian of the map.

the integrators described before are not symplectic - don't preserve area.

instead, we should use integrators that preserve the symplectic structure.

Symplectic Euler - 1st order - but still stays close to one energy contour

energy is not exactly conserved, but error is bounded.

Structure-Preserving Integrators

we have some geometric structure preserved by the eqtns - should be preserved by integrator

standard methods minimize *local* truncation errors - but not global properties.

Why preserve this geometry?

affects stability - esp. long-time simulations

make integrator more robust - integrator works for more circumstances.

Symplectic Integrators

numerical one-step method for canonical Hamiltonian system

preserves symplectic structure

$\exists$ nearby Hamiltonian $\bar{H}$ that is exactly conserved

difference between $\bar{H}$ and actual stays bounded for exponentially long time

Symplectic Euler – 1st order
Runga-Kutta method can be made symplectic for any order
challenge - these are implicit – use partitioned RK for explicit method.

Poisson Integrators
works for non-canonical symplectic structures
Poisson structures – with Casimirs
no general methods that work for all systems
have to discretize on a system-by-system basis
you can convert to canonical coords, use symplectic integrator – often too hard
Poisson integrator
discrete flow is a Poisson map that preserves Casimirs
Splitting Methods
split Hamiltonian into explicitly solvable sub-Hamiltonians
composition of solutions of these is symplectic
higher order systems very hard

Integral-Preserving Method
conserves energy exactly
approximate ∇ and ∇H
↳ must maintain symmetry/anti-symmetry
multiple options for determining the discrete gradient
higher-order methods like RK – with continuous intermediate stages
these are usually implicit

For a canonical Hamiltonian system, which is better – symplectic vs. energy-preserving
it depends on your system, what you're looking at
integral-preserving methods are often conjugate to a symplectic integrator

Variational Integrators
to discretize Lagrangian system.
discretize Lagrangian & action principle
apply discretize action principle to discrete Lagrangian to get equations
solve approx system exactly
gives you exact conservation laws. From discrete Noether Thm.
leads to symplectic momentum eqtn ↳ discrete form of conservation law.
often obtain known integrators with good properties.

Action Principle: $A[q] = \int_0^T \mathcal{L}(q, \dot{q}, t)\, dt$

$$= \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} L(q(t), \dot{q}(t), t)\, dt$$ now approx this integral

$$\dot{q} \approx \frac{q_{n+1} - q_n}{h}, \quad \int_{t_n}^{t_{n+1}} L\, dt \approx h L\left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{h}, t_n + \frac{h}{2} \right)$$

Hamilton's Principle – vary this action. $\delta A_d = 0$.

set the result to zero → discrete Euler-Lagrange Eqtns.

can shift to discrete momentum-position space

discrete Lagrangian acts as generating function for Hamiltonian flow

Vlasov-Maxwell System

most of these techniques will also work for canonical Hamiltonian PDEs

but – most fluids & plasmas have non-canonical structure

need to approach them on a system-by-system basis

geometric structure in Vlasov-Maxwell:

Poisson structure, variational structure, de Bruijn complex structure

many conservation laws – Noether symmetries & Casimirs

4 things to go into discrete eqtns

fields f, E, B

Hamiltonian – functional

Poisson bracket – functional derivatives

time evolution

Maxwell's Eqtns should be thought of a differential forms – not vector calc.

ϕ – 0D point

E – 1D line

B – 2D surface

ρ – 3D volume

do not discretize these the same way

they are different differential forms

keep de Bruijn sequence properties in discretization

finite element exterior calculus

spline finite differences

] use one of these

Discretize fields

particle-like (or shape functions) for f

fields in terms of splines over finite basis functions

Discretize functionals

just restrict your input functions

Discretize functional derivatives

express them in terms of partial derivative for discrete functions

crutial step in discretization

then check if the semi-discrete bracket is still Poisson

needs: $\nabla \cdot B = 0$, curl of 1-form basis in 2-form basis.

Casimir Invariants

$C_s = \int h_s(f_s)\, dx\, dv$ automatically conserved by discretization
not Casimirs of semi-discrete brackets

Gauss's law & $\nabla \cdot B = 0$
are Casimirs of semi-discrete brackets

Time-Integration Splitting Methods

split Hamiltonian – 3 velocity directions, E, B.
solve each, then compose
almost explicit

split bracket
each piece should be antisymmetric, preserve Casimirs, satisfy Jacobi
use integral-preserving methods for each subsystem
implicit, but can use larger time steps
no Poisson structure, but conserves energy & Casimirs

① PIC Codes have noise problems,
these avoid grid heating, $\nabla \cdot B = 0$
but they still have problems with noise

② Why is Jacobi needed for semi-discrete Poisson bracket?
preserve symplectic structure & Poincaré invariants
could study by introducing a perturbation that breaks this

③ Constant time steps
usually, we do this
some subcycling – time step for particles shorter than for fields
adaptive time step for symplectic ODEs is hard.