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Outline

1. Why Use Symplectic Integrators?
2. Quick Review of Traditional Numerical Integrators: Euler and Runge-Kutta
3. Demonstrate the Phase Portrait and Energy Profile of a Harmonic Oscillator
4. Take Home Message

1. Why Use Symplectic Integrators?

1.1 Fundamental Difficulty with Numerical Integration for a Hamiltonian System

Numerical methods introduce the 'excitation' or 'damping'

Necessary conditions of a Hamiltonian system

1. $dp \wedge dq$ is a conserved quantity
2. $H = \text{Constant}$

- Weistein and Marsten (1988, Lie–Poisson Hamilton–Jacobi Theory and Lie–Poisson Integrators[1])
  - proof that there is no numerical methods to preserved the above two conditions
- piratical solutions
  - preserved energy
    - methods: discrete Lagrange...
    - loss the phase space information
      - if one interested in where the objector are, it is not a good option (e.g. many-body system)
  - preserved phase space volume (preserved the symplectic structure)
    - build the symplectic integrator

1.2 Comparison between Symplectic and Non-Symplectic Integrator

- **Preserve Structure:** Many dynamical systems (like planetary motion, molecular dynamics) are governed by Hamiltonian mechanics. These systems possess a geometric structure called the "symplectic structure," crucial for accurately capturing long-time behaviour.
- **Conservation Properties:** Symplectic integrators conserve quantities such as phase-space volume and, more importantly, tend to have good long-term energy behaviour. Non-symplectic methods often introduce artificial damping or energy drift over time.
- **Long-term Simulation:** For simulations over long timescales, symplectic integrators avoid the secular (systematic) drift in energy that standard integrators can introduce.

	Symplectic Integrators	Non-Symplectic Integrators
Energy Conservation	Approximately conserved (bounded oscillations)	Often drifts (grows or decays over time)
Phase Space Volume	Preserved (Liouville's theorem)	Not preserved
Long-term Stability	Excellent	Poor (error accumulates)
Global Error	Grows slowly (typically as √t)	Grows linearly with time
Examples	Leapfrog/Verlet, Symplectic Euler	Euler, Runge-Kutta
When to Use	Hamiltonian systems, long-term simulations	General ODEs, short-term simulations, stiff ODEs
Computational Cost	Often similar to non-symplectic (per step)	Can be lower or higher, depending on method
Complexity for High Order	Harder to construct	Easier (e.g. Runge-Kutta methods)

2. Quick review of Numerical integrators: Euler and Runge-Kutta

For an initial value problem,

$$\dot{\mathbf{x}} = f(\mathbf{x}, t); \quad \mathbf{x}(t_0) = \mathbf{x}_0 \in \mathbb{R}^n; \quad f : \mathbb{R}^n \times [t_0, \infty) \to \mathbb{R}^n$$

Find

$$\mathbf{x}(t); t \in [t_0, \pm\infty)$$

True solution is approximated by using Picard iteration,

$$\mathbf{x}(t_{k+1}) = \mathbf{x}(t_k) + \int_{t_k}^{t_{k+1}} f(x(t), t)\, dt$$

Expanding using Taylor's theorem:

$$
\begin{aligned}
x(t_{k+1}) &= x(t_k) + \int_{t_k}^{t_{k+1}} f(x(t), t)\, dt \\
&= x(t_k) + \underbrace{(t_{k+1} - t_k)}_{\Delta t} \frac{\partial x}{\partial t}(t_k) + \frac{\Delta t^2}{2} \frac{\partial^2 x}{\partial t^2}(t_k) + \mathcal{O}(\Delta t^3)
\end{aligned}
$$

2.1 Euler Methods: truncate at the first order (linearise it)

The explicit (forward) and implicit (backward) Euler methods are:

$$
\mathbf{x}_{k+1} = \begin{cases} \mathbf{x}_k + \Delta t\, f(\mathbf{x}_k, t_k) & \text{Forward Euler Method (explicit)} \\ \mathbf{x}_k + \Delta t\, f(\mathbf{x}_{k+1}, t_{k+1}) & \text{Backward Euler Method (implicit, need to interatively solve it sometimes)} \end{cases}
$$

2.2 Runge-Kutta: Use an additional point in the interval

The RK algorithms focus on reducing trucation error, but do not respect any inherantly conserved quantities.

$$
\mathbf{x}_{k+1} = \mathbf{x}_k + \Delta t \sum_{i=1}^{s} b_i g_i \begin{cases} g_1 = f(\mathbf{x}_k, t_k) \\ g_2 = f\left(\mathbf{x}_k + \Delta t(a_{21} g_1),\ t_k + c_2 \Delta t\right) \\ g_3 = f\left(\mathbf{x}_k + \Delta t(a_{31} g_1 + a_{32} g_2),\ t_k + c_3 \Delta t\right) \\ \vdots \\ g_i = f\left(\mathbf{x}_k + \Delta t \sum_{j=1}^{s} a_{ij} g_j,\ t_k + c_i \Delta t\right) \end{cases}
$$

Butcher tableau

$$
\begin{array}{c|cccc}
0 & & & & \\
c_2 & a_{21} & & & \\
c_3 & a_{31} & a_{32} & & \\
\vdots & \vdots & \vdots & \ddots & \\
c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} \\
\hline
 & b_1 & b_2 & \cdots & b_s
\end{array}
\qquad \Longrightarrow \qquad
\begin{array}{c|c}
\mathbf{c} & \mathbf{A} \\
\hline
 & \mathbf{b}^T
\end{array}
$$

Consistent when

$$
\sum_{j=1}^{s} a_{ij} = c_i \qquad i = 2 \ldots s.
$$

3. Demonstrate the Phase Portrait and Energy Profile of a Harmonic Oscillator

If the Hamiltonian can be written in separable form, $H(p, q) = T(p) + V(q)$, there exists an efficient class of explicit symplectic numerical integration methods. -> Harmonic Oscillator

Necessary conditions of a Hamiltonian system

1. $dp \wedge dq$ is a conserved quantity
2. $H = \text{Constant}$

3.1 Hamiltonian system: Simple Harmonic Oscillator

- example: 1D-SHO (One-dimensional simple harmonic oscillator)
  - Hamiltonian: $\mathcal{H} = \frac{1}{2}(p^2 + q^2)$
  - Hamiltonian version (c.f. Harmonic oscillator)
  -

$$
\begin{bmatrix} q \\ p \end{bmatrix}_{t+\Delta t} = \begin{bmatrix} \cos(\Delta t) & \sin(\Delta t) \\ -\sin(\Delta t) & \cos(\Delta t) \end{bmatrix} \begin{bmatrix} q \\ p \end{bmatrix}_t
$$

  - rotation matrix in 2D, Hamiltonian version of SHO is just purely a rotation in phase space.
  - Energy conservation: $\mathcal{E} = p^2 + q^2 = \text{const.}$
  - Linearisation (Euler)

$$
\begin{bmatrix} q \\ p \end{bmatrix}_{t+\Delta t} \approx \begin{bmatrix} 1 & \Delta t \\ -\Delta t & 1 \end{bmatrix} \begin{bmatrix} q \\ p \end{bmatrix}_t
$$

  - Energy is not conserved: $(p^2 + q^2)\big|_{t+\Delta t} = \left(1 + \Delta t^2\right)(p^2 + q^2)\big|_t$
  - source of error: Δt^2
  - Runge-Kutta
  - Energy is not conserved: $(p^2 + q^2)\big|_{t+\Delta t} = \left(1 - \frac{1}{2}\Delta t^6 + \ldots\right)(p^2 + q^2)\big|_t$

Since the numerical methods in general do not preserve the energy, we need the Liouville theorem

Optional: The Liouville Theorem

For a Hamiltonian system with coordinates q_i and conjugate momenta p_i, define a **phase space distribution function** ρ such that $\rho(\mathbf{q}, \mathbf{p})$ determines the probability that the system will be found in the infinitesimal phase space volume $\mathrm{d}^n\mathbf{q}, \mathrm{d}^n\mathbf{p}$.

The evolution of ρ is governed by:

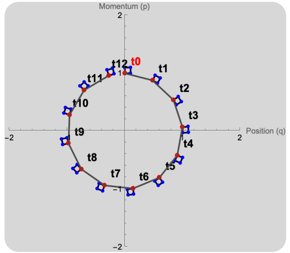
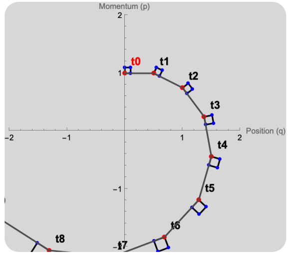
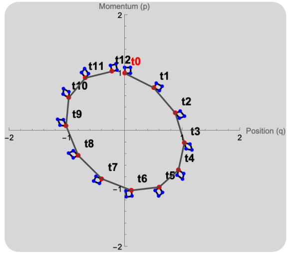
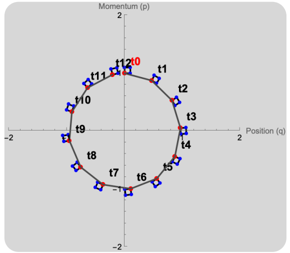
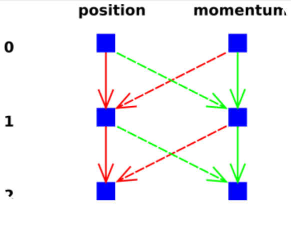
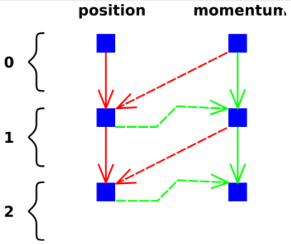
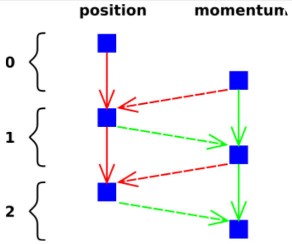
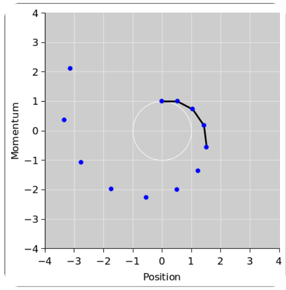
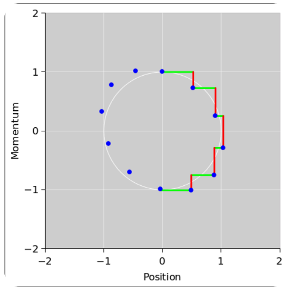
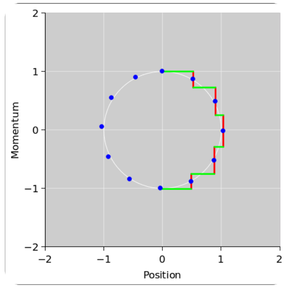
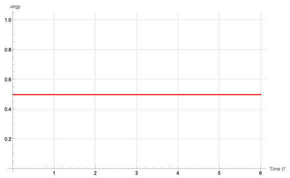
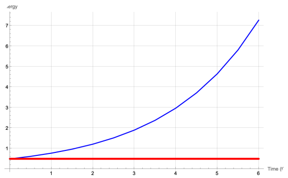
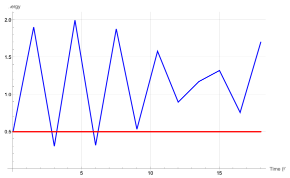
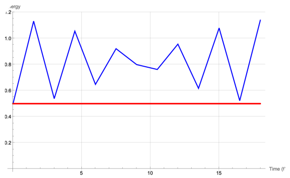
The Liouville Equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{\partial \rho}{\partial t} + \sum_{i=1}^{n}\left(\frac{\partial \rho}{\partial q_i}\dot{q}_i + \frac{\partial \rho}{\partial p_i}\dot{p}_i\right) = 0$$

Liouville's Theorem

The distribution function is constant along any trajectory in phase space.

3.2 Visualisation of a Harmonic Oscillator

	Exact	Forward Euler	Symplectic Euler; 1^{st} order	Leapfrog (Velocity Verlet); 2^{nd} order
	$\begin{bmatrix}q\\p\end{bmatrix}_{t+\Delta t} = \begin{bmatrix}\cos(\Delta t) & \sin(\Delta t)\\ -\sin(\Delta t) & \cos(\Delta t)\end{bmatrix}\begin{bmatrix}q\\p\end{bmatrix}_t$	$\begin{bmatrix}q\\p\end{bmatrix}_{t+\Delta t} \approx \begin{bmatrix}1 & \Delta t\\ -\Delta t & 1\end{bmatrix}\begin{bmatrix}q\\p\end{bmatrix}_t$	$q_{t+\Delta t} = q_t + \Delta t\, p_t$ $p_{t+\Delta t} = p_t - \Delta t\, q_{t+\Delta t}$	$p_{t+\frac{\Delta t}{2}} = p_t - \frac{\Delta t}{2} q_t$ $q_{t+\Delta t} = q_t + \Delta t\, p_{t+\frac{\Delta t}{2}}$ $p_{t+\Delta t} = p_{t+\frac{\Delta t}{2}} - \frac{\Delta t}{2} q_{t+\Delta t}$
phase portrait				
			1. The symplectic integrator conserves area in phase space exactly. 2. Area is conserved no matter how large or how small the step-size. 3. **Symplectic Euler**: The boxes change shape, but their area stays the same.	
Update rule				
				
Energy profile				

	Exact	Forward Euler	Symplectic Euler; 1^{st} order	Leapfrog (Velocity Verlet); 2^{nd} order
			The symplectic integrator conserves energy only approximately.	

4. Take Home Message

Take Home Message

- **Symplectic Integrators**:
  - A symplectic integrator conserves the area in phase space.
- **Benefits**:
  - Better long-term energy conservation.
  - Improved stability in simulations.

Reference

- Basic Properties of a Symplectic Integrator
- YT: RK4 and Symplectic Methods of Integration
  - GitHub: HigherOrderMethods
  - GitHub: Symplectic
- Mathematical Methods for Physicists: A Comprehensive Guide ch7, 8: general description, more on the application side and no connection to symplectic structure.
- Numerical Quantum Dynamics: my first numerical book
- Advanced astrodynamics - Numerical methods: systematic and good overview.
- Geometric numerical integration: more mathematical description, TU Munich lecture notes.
- Code
  - Numerical Solutions of Initial Value Problems Using Mathematica
  - Wolfram: SymplecticPartitionedRungeKutta" Method for NDSolve
- My permanent notes
  - SHO
  - Euler Integrator
  - Runge-Kutta Integrator
  - Leapfrog Integrator

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1. "Lie–Poisson Hamilton–Jacobi Theory and Lie–Poisson Integrators" by Jerrold E. Marsden and Alan Weinstein, published in 1988.
   This work discusses numerical integrators that preserve momentum maps and Poisson brackets, leading to integrators that maintain certain geometric structures in Hamiltonian systems.
   In this paper, Marsden and Weinstein explore the limitations of numerical methods in preserving specific properties of dynamical systems. They present results indicating that while certain integrators can preserve some structures (like momentum maps), they may fail to preserve others (such as energy), highlighting inherent trade-offs in numerical integration schemes. ↩