What did we see yesterday?

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Symplectic Integrator

- A solver (numerical integrator) for Hamiltonian dynamical systems

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial q} \qquad \frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial H}{\partial p}$$

- A variant of *geometric numerical integrator*
- Preserves the energy of the system

Solving differential equations

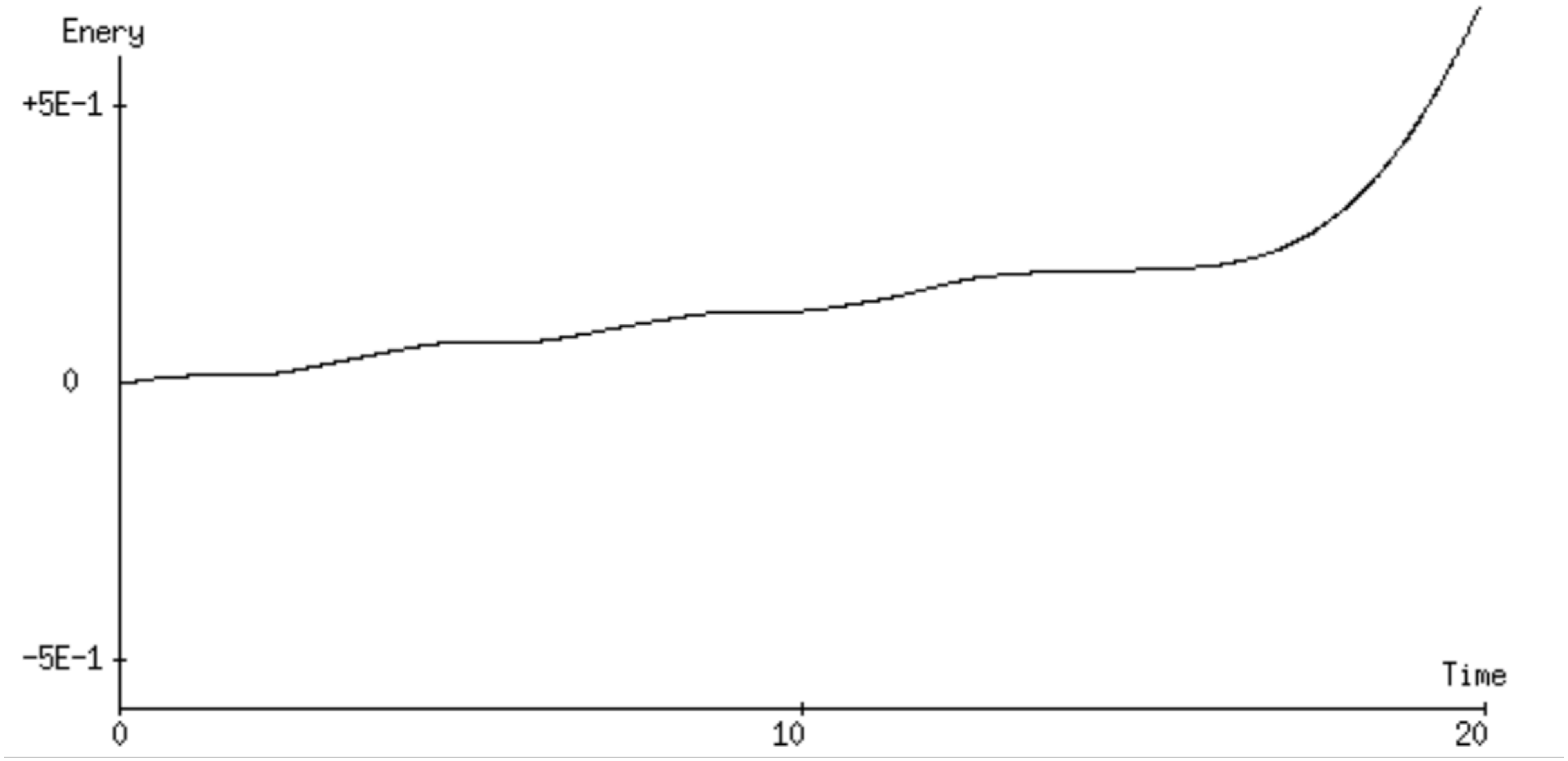
$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(t, y(t))$$

Euler method

$$y_{n+1} = y_n + hf'(t_n, y_n)$$

- Requires numerical integration (discretisation)
- General methods:
  → Broad applicability
  → Don't care about the structure of the system
- Discretisation could break the structure
  e.g. Conservation Laws

Example (first order Euler)



$$H = \frac{1}{2}(p_x^2 + p_y^2 + q_x^2 q_y^2) - 2$$

With $q_x = 2, q_y = 1,\ p_x = 0,\ p_y = 0$ for $t = 0$

Example (fourth order Runge-Kutta)

$$H = \frac{1}{2}(p_x^2 + p_y^2 + q_x^2 q_y^2) - 2$$

With $q_x = 2, q_y = 1,\ p_x = 0,\ p_y = 0$ for $t = 0$

Hamiltonian Mechanics

- Differential equations described by $H(p, q)$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial q}$$

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial H}{\partial p}$$

$$\mathbf{r}(t) = (p(t), q(t))$$

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = D_H\mathbf{r}$$

$$D_H f := \frac{\partial f}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial H}{\partial q}$$

- Solution

$$\mathbf{r}(\tau) = \exp(\tau D_H)\mathbf{r}(0)$$

$\exp(\tau D_H)$ =operator taking the system from 0 to τ

Solving a Hamiltonian system

- Assume

$$H(p,q) = \underbrace{T(p)}_{\textbf{kinetic}} + \underbrace{V(q)}_{\textbf{potential}}$$

- Then

$$\exp(\tau D_H) = \exp(\tau(D_T + D_V))$$

- If $\exp(\tau(D_T + D_V)) = \exp(\tau D_T)\exp(\tau D_V)$

  → solve two set of equations (can do exactly)

① $\dfrac{\mathrm{d}p}{\mathrm{d}t} = -\dfrac{\partial V}{\partial q}$ **&** $\dfrac{\mathrm{d}q}{\mathrm{d}t} = 0$

② $\dfrac{\mathrm{d}p}{\mathrm{d}t} = 0$ **&** $\dfrac{\mathrm{d}q}{\mathrm{d}t} = \dfrac{\partial V}{\partial p}$

Implicit Hamiltonian

But $\exp(\tau(D_T + D_V)) \neq \exp(\tau D_T)\exp(\tau D_V)$

How about I do anyway?

→ it actually makes sense (using Baker-Campbell-Hausdorff formula)

$$\exp(\tau D_T)\exp(\tau D_V) = \exp(\tau \tilde{H})$$

$$\begin{aligned}\tilde{H} &= T + V + \frac{\tau}{2}\{V, T\} + \frac{\tau^2}{12}\left(\{\{V, T\}, T\} + \{\{T, V\}, V\}\right) + \cdots \\ &= H + O(\tau)\end{aligned}$$

Using $\exp(\tau D_T)\exp(\tau D_V)$ ⟷ Solving about $\tilde{H}$ (we can do exactly)

Symplectic Integrator (SI)

First order Symplectic Integrator

- Update rule:

$$p_{n+1} = p_n - \tau \frac{\partial V}{\partial q}\bigg|_{q_n}$$

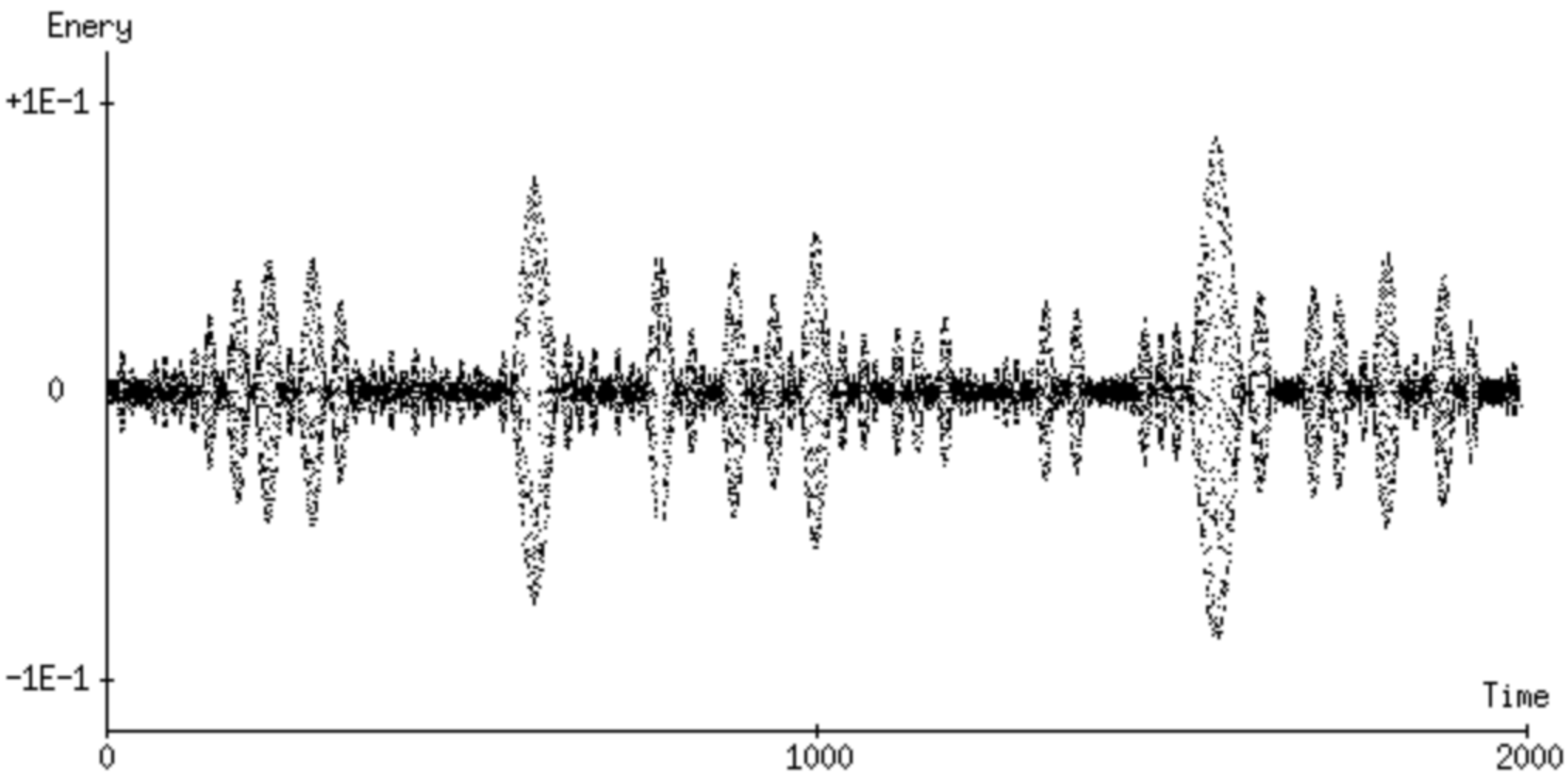
$$q_{n+1} = q_n + \tau \frac{\partial K}{\partial q}\bigg|_{p_{n+1}}$$

- Energy error

$$H = \tilde{H} + O(\tau)$$

- Benefit = long-term analysis with rough τ is okay

Example (first order symplectic)



$$H = \frac{1}{2}(p_x^2 + p_y^2 + q_x^2 q_y^2) - 2$$

With $q_x = 2, q_y = 1,\ p_x = 0,\ p_y = 0$ for $t = 0$

Symplectic Integrator (SI)

Higher order Symplectic Integrator

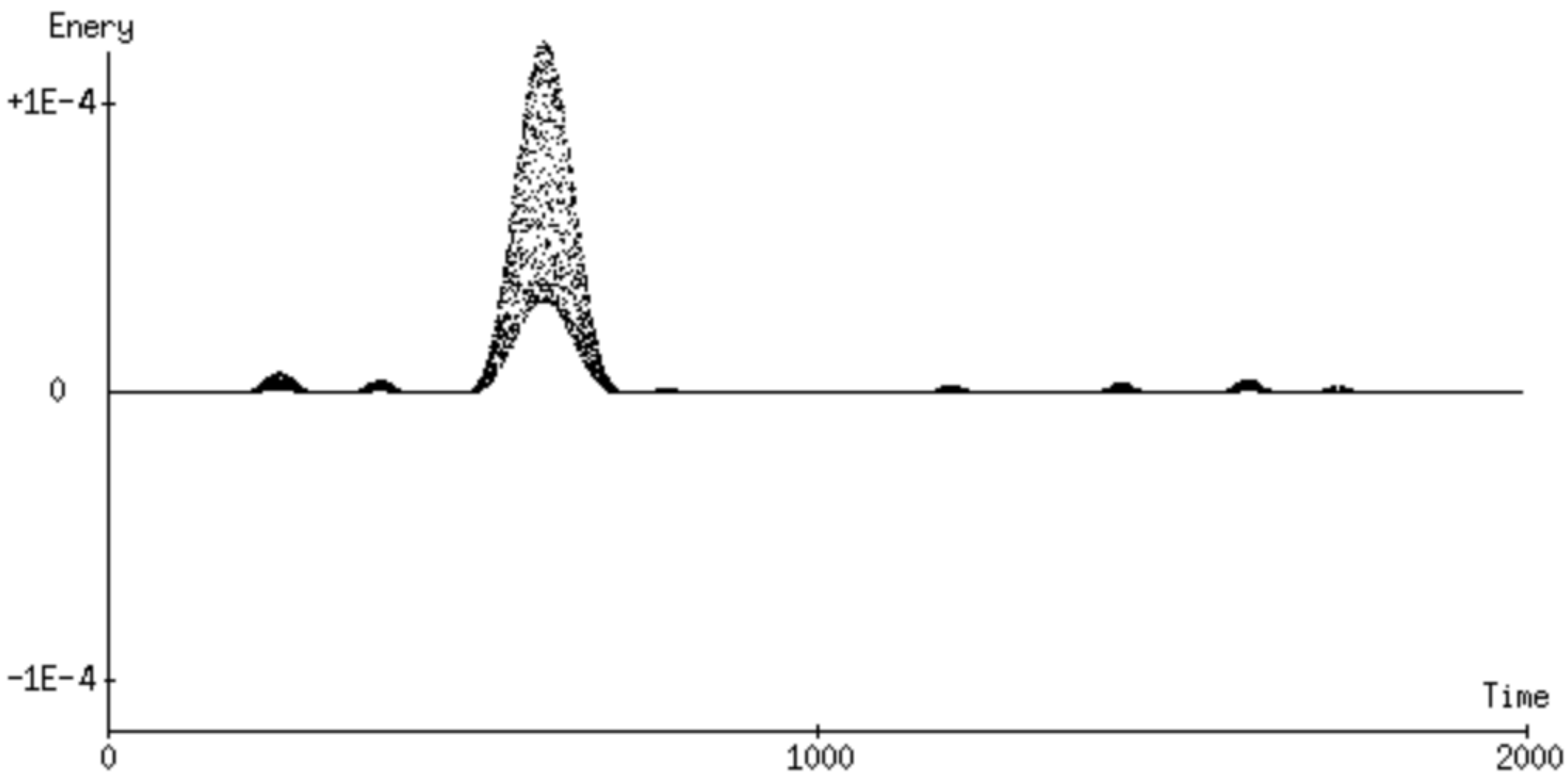
- Example:
  - Leap-frog method (2nd order)

  → People use for HMC
- Construction

$$\exp(\tau(D_T + D_V) = \prod_{k=1}^{K} \exp(\tau c_k D_T)\exp(\tau d_k D_V) + O(\tau^{K+1})$$

→Find c_k, d_k

Example (fourth order symplectic)



$$H = \frac{1}{2}(p_x^2 + p_y^2 + q_x^2 q_y^2) - 2$$

With $q_x = 2, q_y = 1, p_x = 0, p_y = 0$ for $t = 0$

What did I talk about?

- Introduced a numerical integrator that preserves a structure of the system
  → There is a field studying this kind of methods (geometric numerical integration)
- Symplectic Integrator is a method for Hamiltonian systems

Reference:

1. Wikipedia page on Symplectic Integrator
2. Application to optimisation: **On Symplectic Optimization**

   Michael Betancourt, Michael I. Jordan, Ashia C. Wilson

   (Submitted on 10 Feb 2018 (v1), last revised 15 Feb 2018 (this version