CSE 291 (SP24)
Physical Simulations: Variational Integrators

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Variational integrator

- Variational integrators are numerical integrators for conservative systems derived from ***discrete Hamilton's least action principle***.

- Variational integrators obey ***symplecticity*** and ***momentum conservation***.

Recall continuous theory

- Continuous theory
- Discrete theory

Recall continuous theory

- Let Q denotes the space of generalized positions (e.g. $Q = \mathbb{R}^m$)
- A **Lagrangian** is a function $L : \boxed{TQ} \to \mathbb{R}$

  each element takes the form $(\mathbf{q}, \mathbf{v})$ where $\mathbf{q} \in Q, \mathbf{v} \in T_{\mathbf{q}}Q$

- Define the **action** for each path $\mathbf{q} : [0, T] \to Q$

$$S(\mathbf{q}(\cdot)) := \int_0^T L(\mathbf{q}(t), \dot{\mathbf{q}}(t))\, dt$$

- Hamilton's least action principle $\frac{\delta S}{\delta \mathbf{q}} = 0$

$$\implies \frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{q}}} - \frac{\partial L}{\partial \mathbf{q}} = \mathbf{0}$$

Euler–Lagrange equation

Momentum

- In this Lagrangian framework we call $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$ the momentum
- Note that $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$ is its differential of $L(\mathbf{q}, \cdot)\colon T_{\mathbf{q}}Q \to \mathbb{R}$

  So the type of momentum is **covector** $\mathbf{p} \in T^*_{\mathbf{q}}Q$

- The map $f : TQ \to T^*Q$

  $$f : (\mathbf{q}, \dot{\mathbf{q}}) \mapsto (\mathbf{q}, \tfrac{\partial L}{\partial \dot{\mathbf{q}}}(\mathbf{q}, \dot{\mathbf{q}}))$$

  reads off momentum from velocity

- EL eq $\frac{d}{dt}\mathbf{p} = f_{\mathbf{q}}^{-1} \frac{\partial L}{\partial \mathbf{q}}$

Continuous Noether's theorem

- **Theorem**
  A continuous symmetry of the system induces a conservation law.
- Continuous symmetry: Suppose $\mathbf{X}$ is a vector field on Q so that

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} S(\mathbf{q}+\varepsilon\mathbf{X}\circ\mathbf{q}) = 0 \quad \text{for all } \mathbf{q}$$

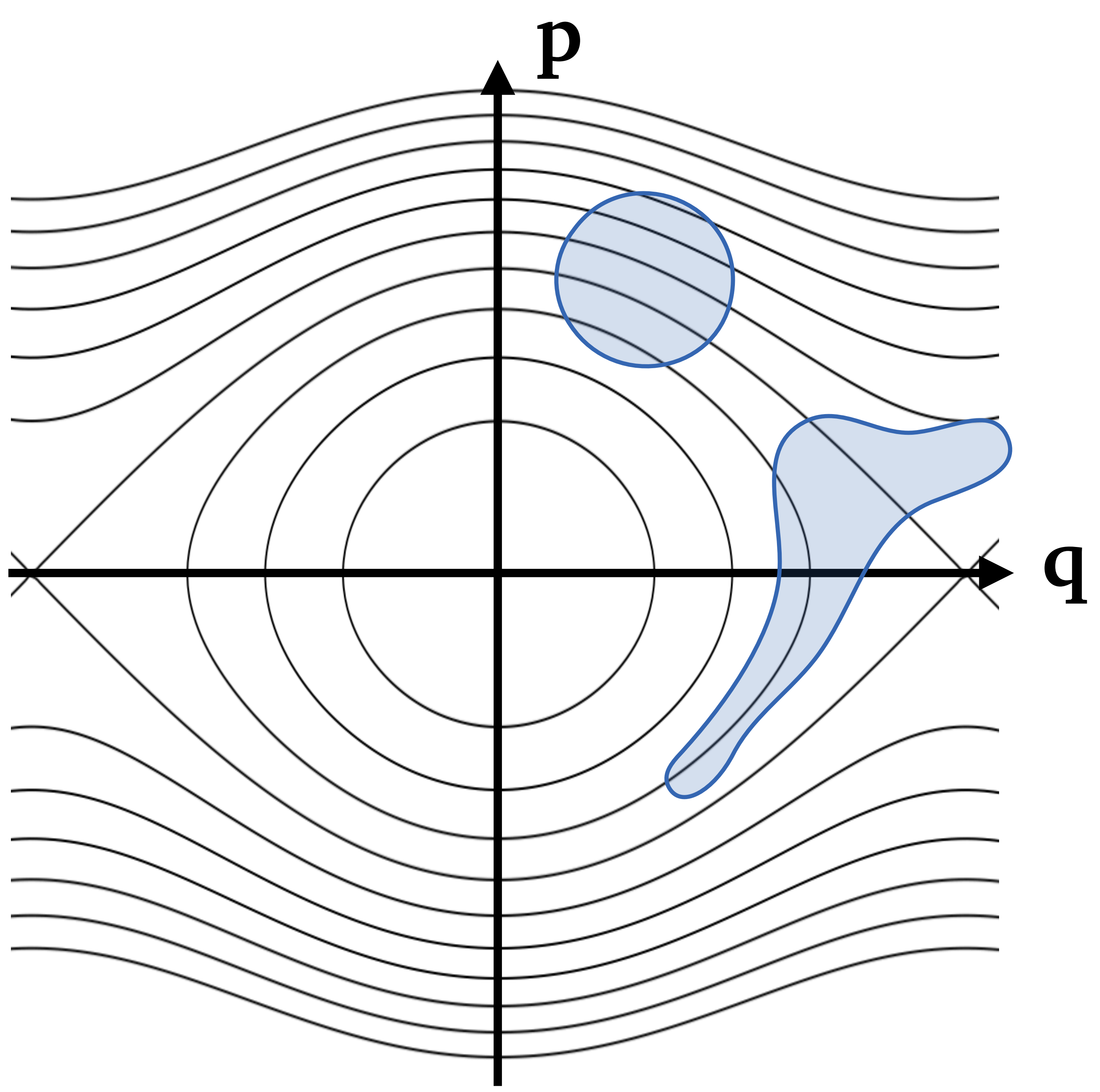
- This implies $\langle \frac{\partial L}{\partial \mathbf{q}} | \mathbf{X} \rangle + \langle \frac{\partial L}{\partial \dot{\mathbf{q}}} | \dot{\mathbf{X}} \rangle = 0$

$$\Longrightarrow \quad \langle \frac{\partial L}{\partial \mathbf{q}} | \mathbf{X} \rangle + \frac{d}{dt}\langle \frac{\partial L}{\partial \dot{\mathbf{q}}} | \mathbf{X} \rangle - \langle \frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{q}}} | \mathbf{X} \rangle = 0$$

$$\overset{\text{EL eq}}{\Longrightarrow} \quad \frac{d}{dt}\langle \frac{\partial L}{\partial \dot{\mathbf{q}}} | \mathbf{X} \rangle = 0$$

Liouville theorem (symplecticity)

- If there is a loop of initial conditions $(\mathbf{q}_\theta, \mathbf{p}_\theta)|_{t=0}, \ \theta \in [0, 2\pi)$
- The EL eq will evolve the loop over time $(\mathbf{q}_\theta(t), \mathbf{p}_\theta(t))$
- The loop has an "enclosed area" $\Omega(t) = \oint \langle \mathbf{p}_\theta | \frac{d\mathbf{q}_\theta}{d\theta} \rangle \, d\theta$
- **Theorem** $\frac{d}{dt}\Omega(t) = 0$



Discrete theory

- Continuous theory
- Discrete theory

Discrete Lagrangian

- Let h denotes discrete timestep.
- A discrete Lagrangian is a function $L_h : Q \times Q \to \mathbb{R}$ approximating the total action between two positions.
  - Example: trapezoidal rule. Suppose original problem is $L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{m}{2}|\dot{\mathbf{q}}|^2 - U(\mathbf{q})$

$$L_h(\mathbf{q}_0, \mathbf{q}_1) = \frac{h}{2}\left(L(\mathbf{q}_0, \tfrac{\mathbf{q}_1 - \mathbf{q}_0}{h}) + L(\mathbf{q}_1, \tfrac{\mathbf{q}_1 - \mathbf{q}_0}{h})\right)$$

$$= \frac{mh}{2}\left|\frac{\mathbf{q}_1 - \mathbf{q}_0}{h}\right|^2 - h\frac{U(\mathbf{q}_0) + U(\mathbf{q}_1)}{2}$$

- Discrete total action of a path

$$S_h(\mathbf{q}_0, \mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_N) = \sum_{k=0}^{N-1} L_h(\mathbf{q}_k, \mathbf{q}_{k+1})$$

Discrete Lagrangian

$$L_h(\mathbf{q}_0, \mathbf{q}_1) = \frac{mh}{2}|\frac{\mathbf{q}_1 - \mathbf{q}_0}{h}|^2 - h\frac{U(\mathbf{q}_0) + U(\mathbf{q}_1)}{2}$$

$$S_h(\mathbf{q}_0, \mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_N) = \sum_{k=0}^{N-1} L_h(\mathbf{q}_k, \mathbf{q}_{k+1})$$

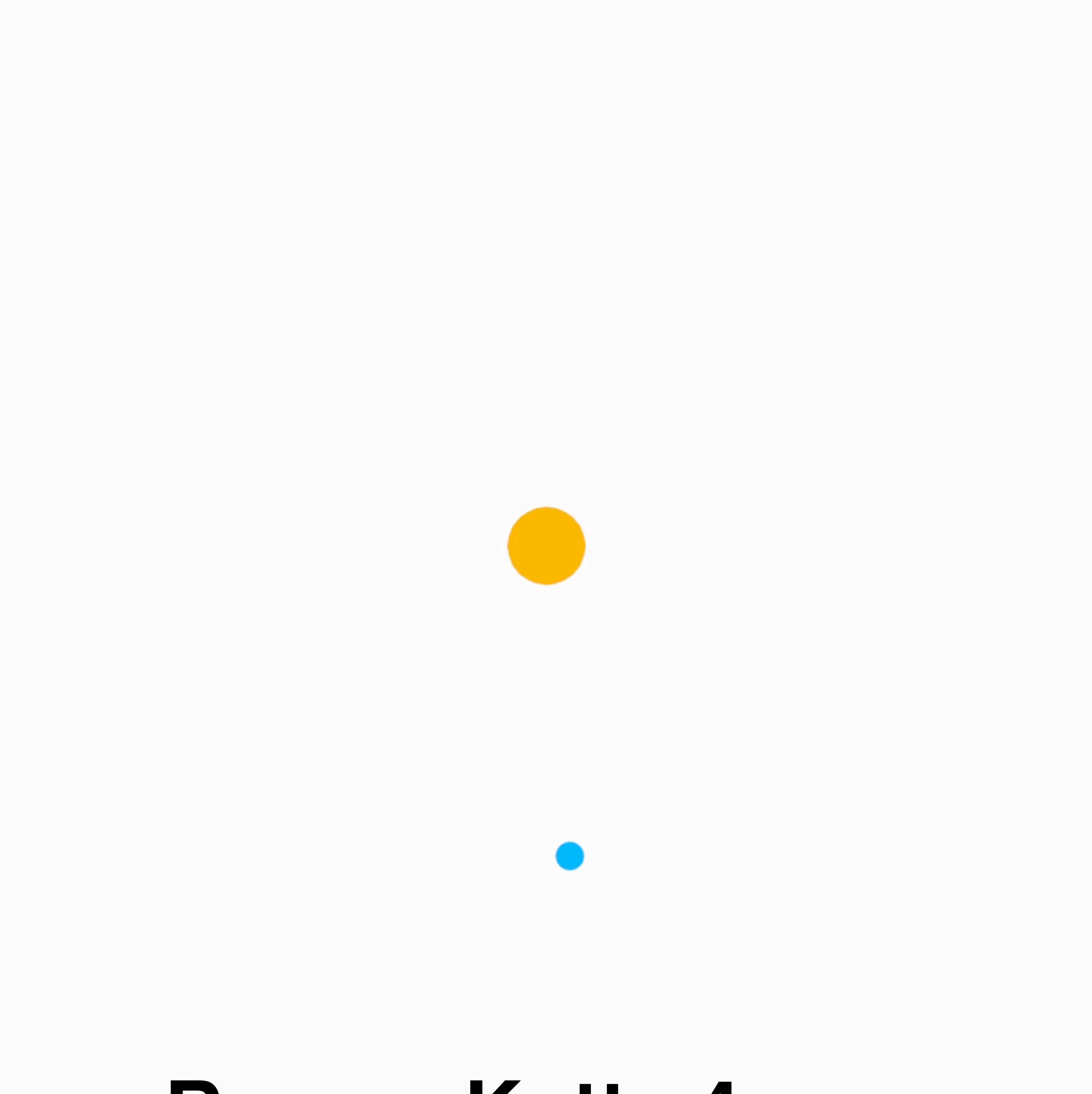
- Discrete Hamilton's principle $\frac{\partial S_h}{\partial \mathbf{q}_k} = \mathbf{0},\ \forall k$
- In the above example, we obtain

$$m\frac{\mathbf{q}_{k+1} - 2\mathbf{q}_k + \mathbf{q}_{k-1}}{h^2} = -dU(\mathbf{q}_k) =: \mathbf{F}(\mathbf{q}_k)$$

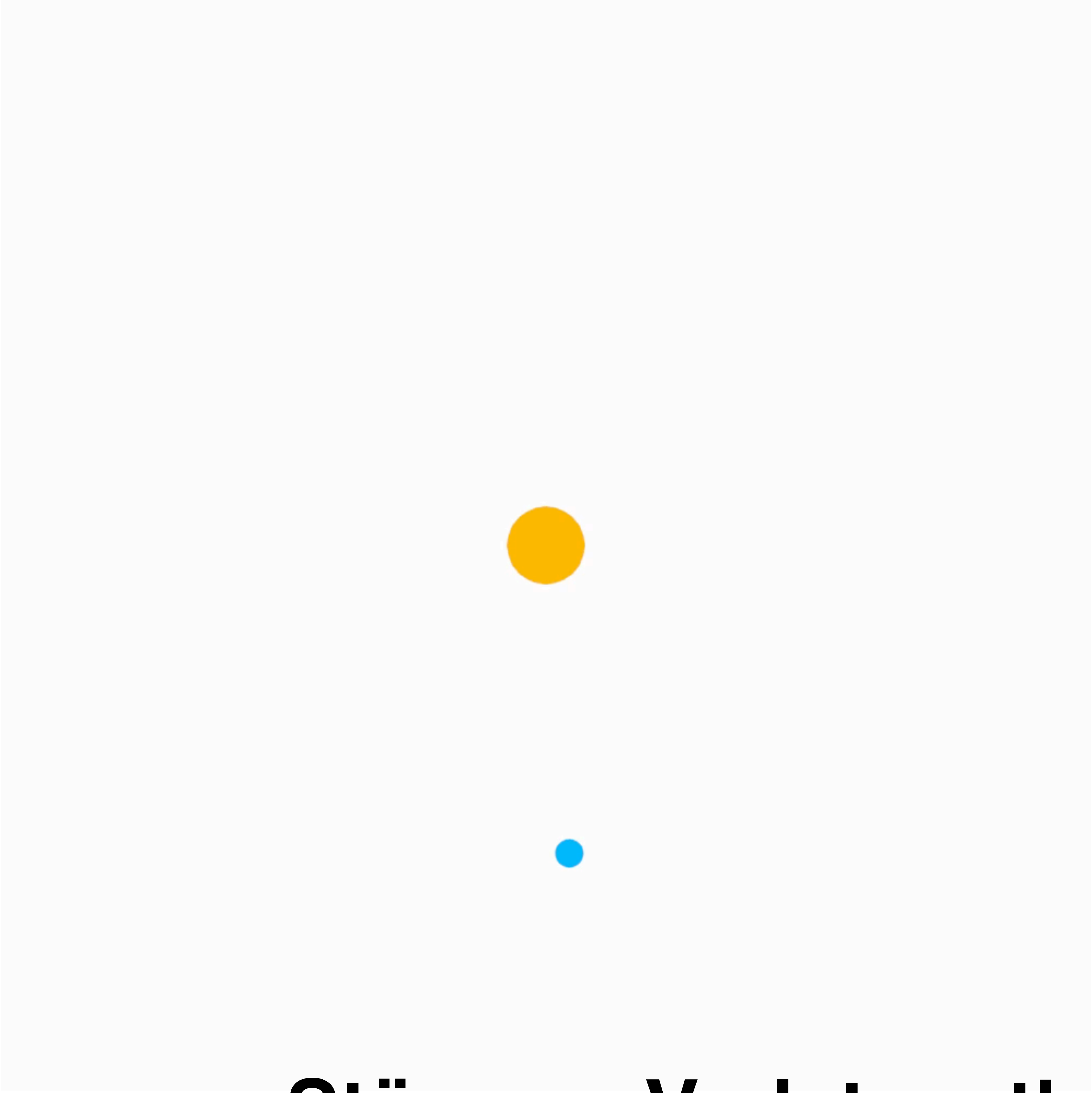
Explicit timestep marching: $(\mathbf{q}_{k-1}, \mathbf{q}_k) \mapsto (\mathbf{q}_k, \mathbf{q}_{k+1})$

$$\mathbf{q}_{k+1} = 2\mathbf{q}_k - \mathbf{q}_{k-1} + \frac{h^2}{m}\mathbf{F}(\mathbf{q}_k)$$ **Störmer–Verlet method**

RK4 vs Störmer–Verlet (2body problem)



Runge–Kutta 4



Störmer–Verlet method

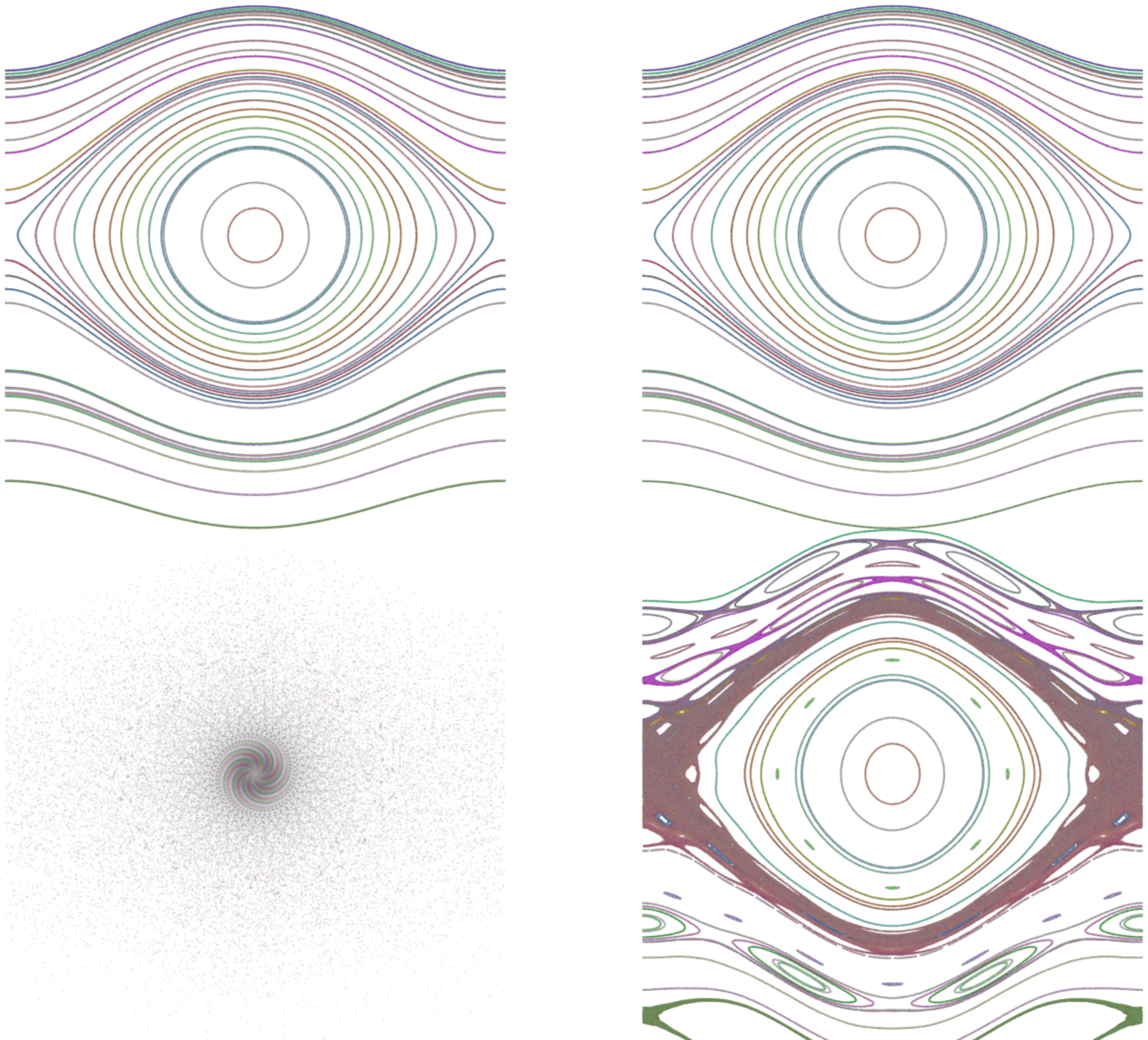
RK4 vs Störmer–Verlet (pendulum)

4th order Runge–Kutta

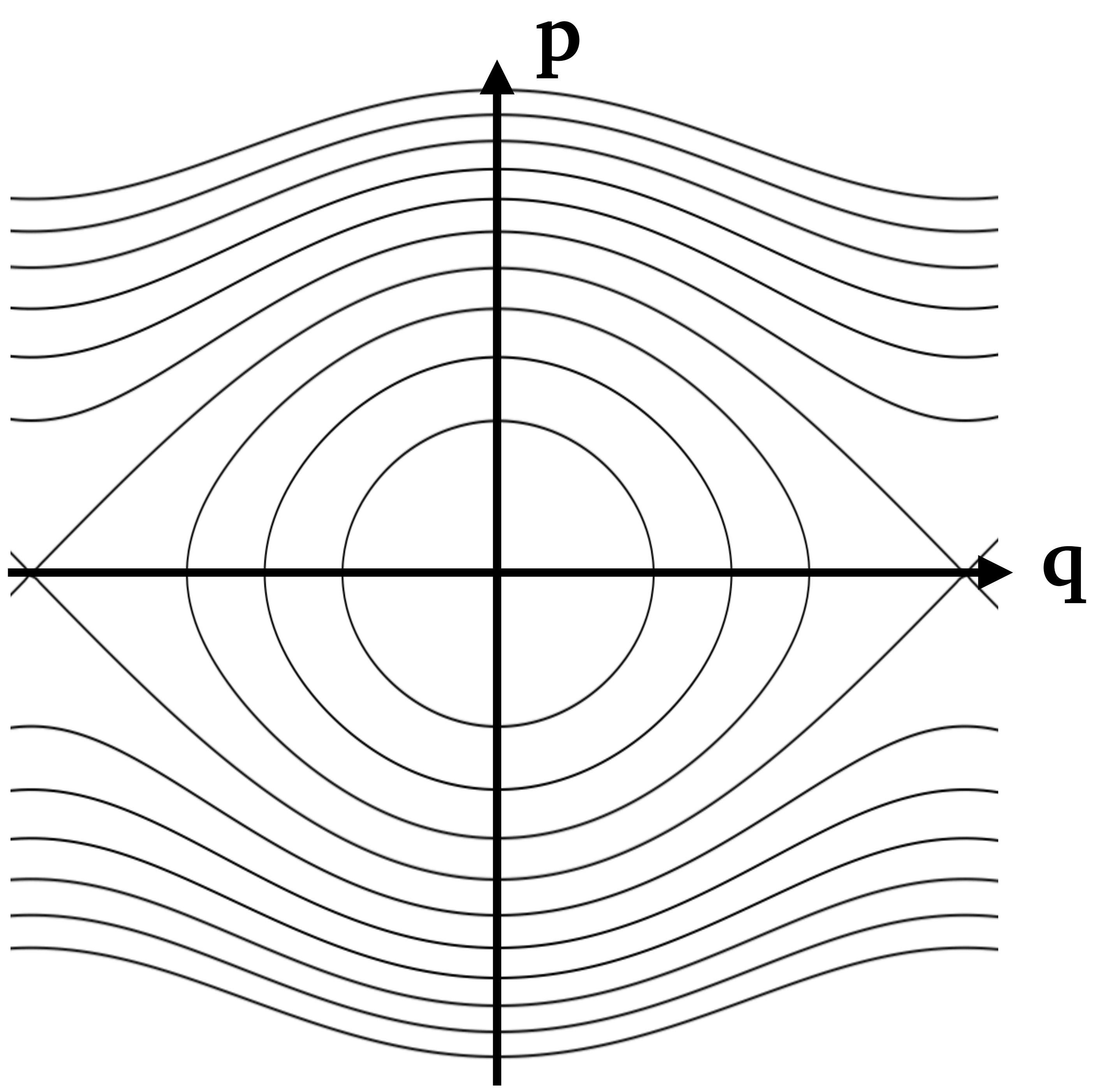
Variational integrator

$\Delta t = 0.1$

$\Delta t = 0.9$



exact trajectories on position–momentum plane



Theory on variational integrators

- Consider discrete Lagrangian and action $L_h : Q \times Q \to \mathbb{R}$

$$S_h(\mathbf{q}_0, \mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_N) = \sum_{k=0}^{N-1} L_h(\mathbf{q}_k, \mathbf{q}_{k+1})$$

- Discrete Euler–Lagrange equation:

$$D_2 L_h(\mathbf{q}_{k-1}, \mathbf{q}_k) + D_1 L_h(\mathbf{q}_k, \mathbf{q}_{k+1}) = \mathbf{0}$$

where D_i denotes partial differential on the *i*-th slot.

Theory on variational integrators

$$D_2 L_h(\mathbf{q}_{k-1}, \mathbf{q}_k) + D_1 L_h(\mathbf{q}_k, \mathbf{q}_{k+1}) = \mathbf{0}$$

- Think of “reading off momentum from velocity” $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$

$$f : (\mathbf{q}, \dot{\mathbf{q}}) \mapsto (\mathbf{q}, \frac{\partial L}{\partial \dot{\mathbf{q}}}(\mathbf{q}, \dot{\mathbf{q}}))$$

- Define $f_1, f_2 : Q \times Q \to T^*Q$

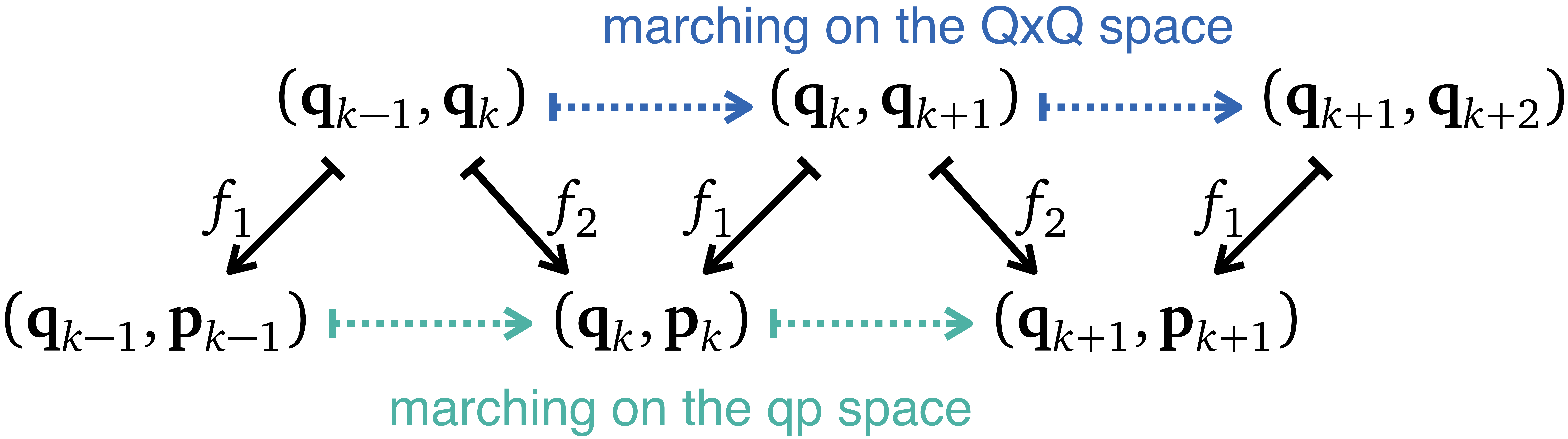
$$f_1 : (\mathbf{q}_1, \mathbf{q}_2) \mapsto (\mathbf{q}_1, -D_1 L(\mathbf{q}_1, \mathbf{q}_2))$$

$$f_2 : (\mathbf{q}_1, \mathbf{q}_2) \mapsto (\mathbf{q}_2, D_2 L(\mathbf{q}_1, \mathbf{q}_2))$$

- Then discrete EL is the marching:

$$(\mathbf{q}_k, \mathbf{q}_{k+1}) = f_1^{-1} \circ f_2(\mathbf{q}_{k-1}, \mathbf{q}_k)$$

Momentum variable



Another example: midpoint rule

- Midpoint rule approximation

$$L_h(\mathbf{q}_0, \mathbf{q}_1) = hL\left(\frac{\mathbf{q}_0+\mathbf{q}_1}{2}, \frac{\mathbf{q}_1-\mathbf{q}_0}{h}\right) = \frac{mh}{2}\left|\frac{\mathbf{q}_1-\mathbf{q}_0}{h}\right|^2 - hU\left(\frac{\mathbf{q}_0+\mathbf{q}_1}{2}\right)$$

- EL eq $\quad m\dfrac{\mathbf{q}_{k+1} - 2\mathbf{q}_k + \mathbf{q}_{k-1}}{h^2} = \frac{1}{2}\left(\mathbf{f}\left(\frac{\mathbf{q}_{k-1}+\mathbf{q}_k}{2}\right) + \mathbf{f}\left(\frac{\mathbf{q}_k+\mathbf{q}_{k+1}}{2}\right)\right)$

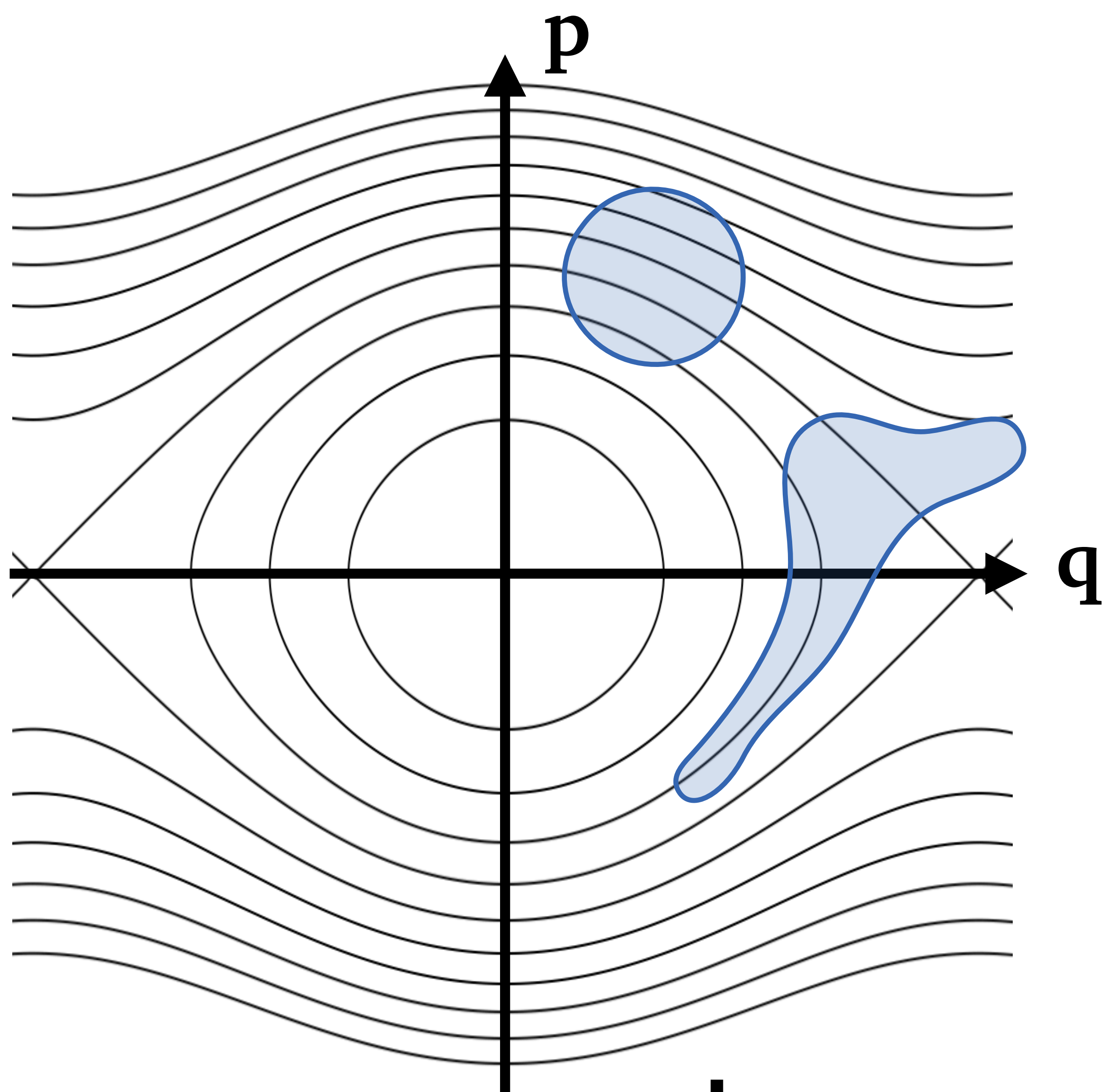
- Equivalently

$$\begin{cases} m\dfrac{\mathbf{q}_{k+1}-\mathbf{q}_k}{h} = \dfrac{\mathbf{p}_{k+1}+\mathbf{p}_k}{2} \\ \dfrac{\mathbf{p}_{k+1}-\mathbf{p}_k}{h} = \mathbf{f}\left(\dfrac{\mathbf{q}_{k+1}+\mathbf{q}_k}{2}\right) \end{cases}$$

implicit midpoint method

Theorems of variational integrators

- **Discrete Liouville theorem**
  Marching on the qp space preserves the enclosed area of marched loop.



- **Discrete Noether theorem**

  If the discrete Lagrangian has a continuous symmetry

$$\langle D_1 L(\mathbf{q}_1, \mathbf{q}_2) | \mathbf{X} \rangle + \langle D_2 L(\mathbf{q}_1, \mathbf{q}_2) | \mathbf{X} \rangle = 0 \quad \forall \mathbf{q}_1, \mathbf{q}_2 \in Q$$

  then $\langle \mathbf{p}_k | \mathbf{X} \rangle$ is conserved (constant independent of *k*).

- **Time reversal symmetry** If $L(\mathbf{q}_1, \mathbf{q}_2) = -L(\mathbf{q}_2, \mathbf{q}_1)$
  then the integrator is time-reversal symmetric.