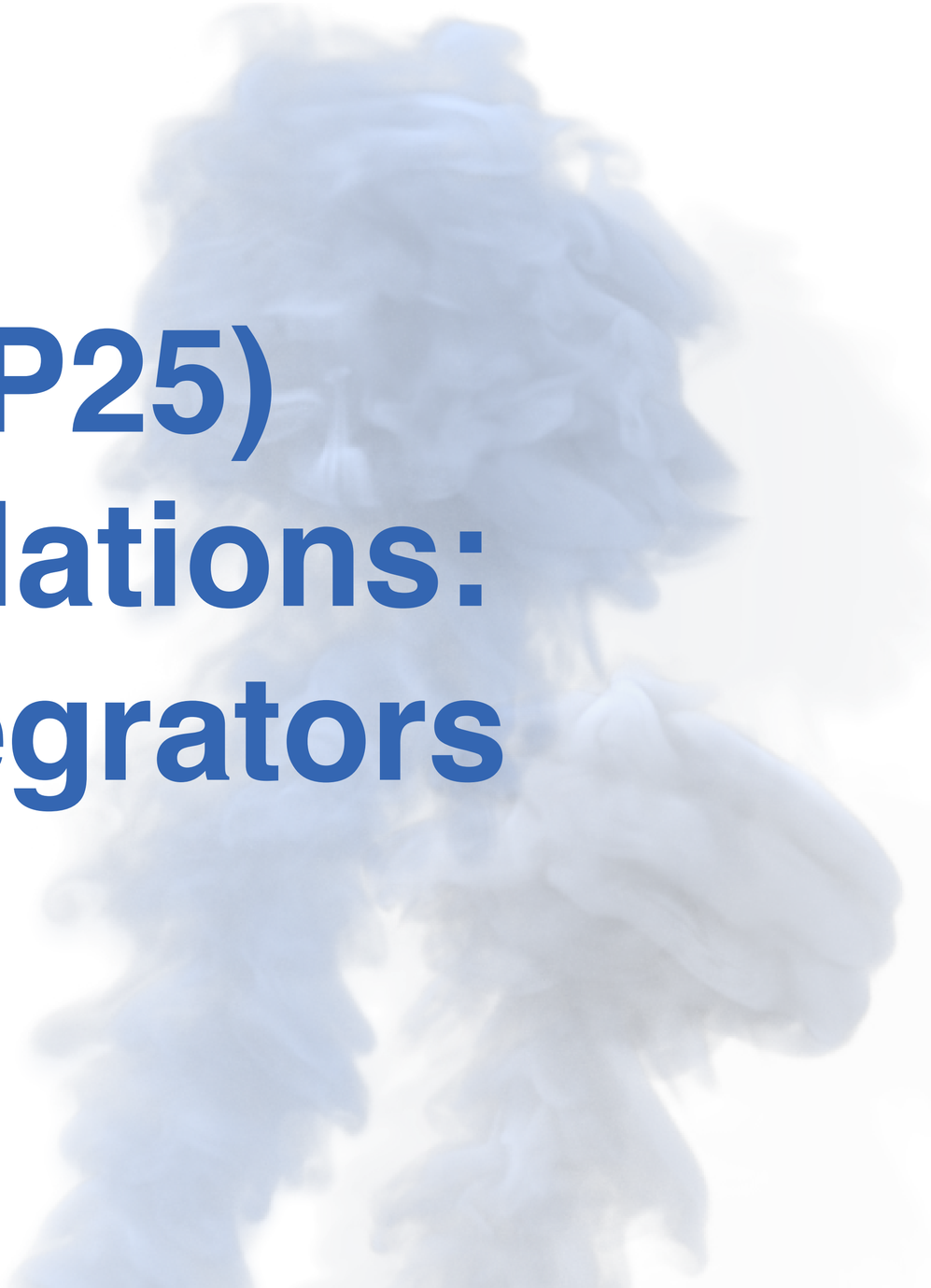
CSE 291 (SP25)
Physical Simulations:
Variational Integrators

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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

$$L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{m}{2}|\dot{\mathbf{q}}|^2 - U(\mathbf{q})$$

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

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

- 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

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

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

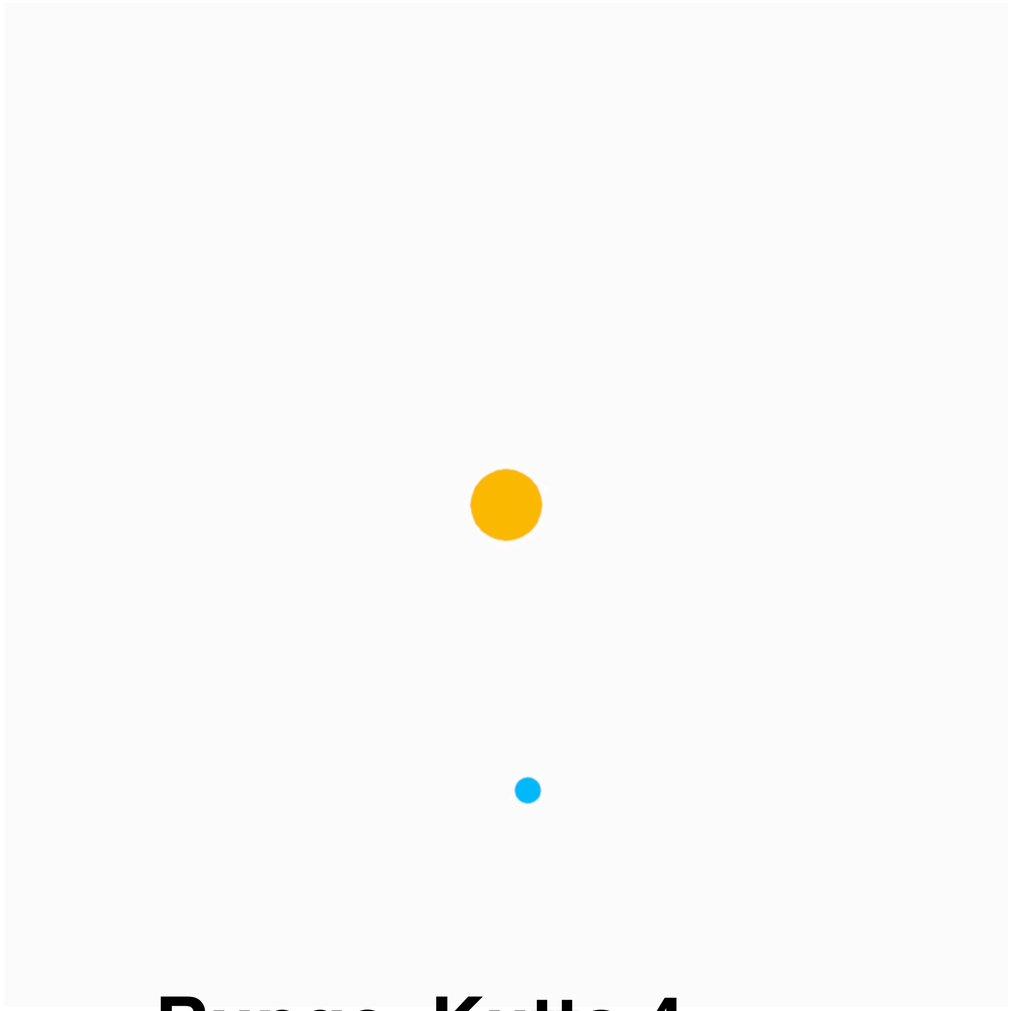
- Discrete least action principle $\frac{\partial S_h}{\partial \mathbf{q}_k} = \mathbf{0},\ \forall k$
- In the above example, we obtain

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

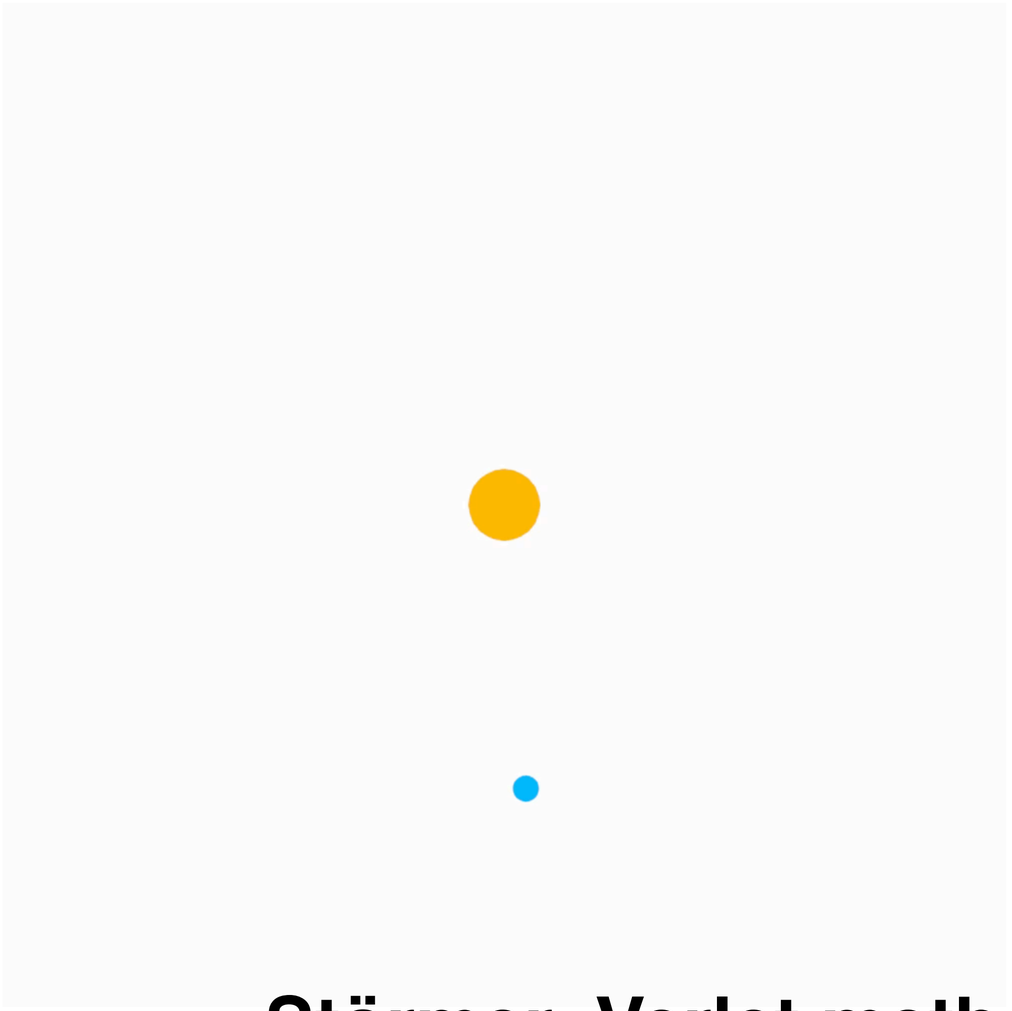
Explicit timestep marching: $(\mathbf{q}_{k-1}, \mathbf{q}_k) \mapsto (\mathbf{q}_k, \mathbf{q}_{k+1})$

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

RK4 vs Störmer–Verlet (2body problem)



Runge–Kutta 4



Störmer–Verlet method

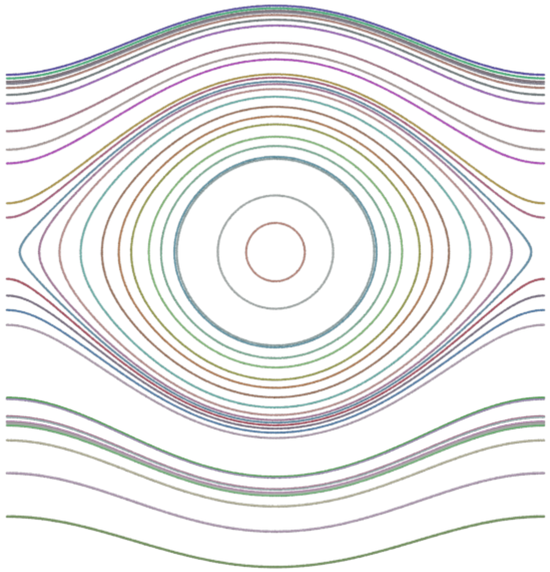
RK4 vs Störmer–Verlet (pendulum)

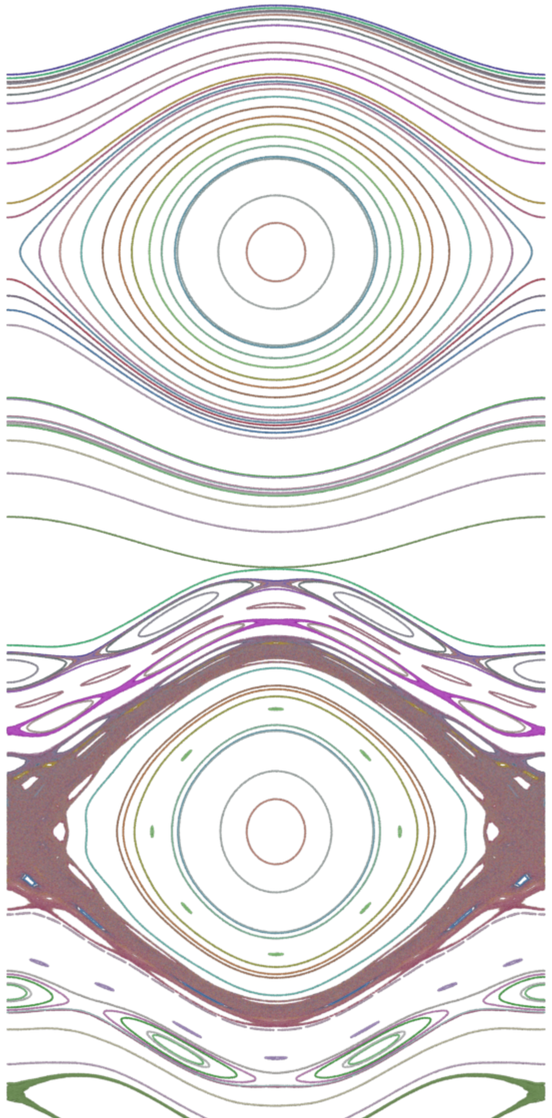
4th order Runge–Kutta

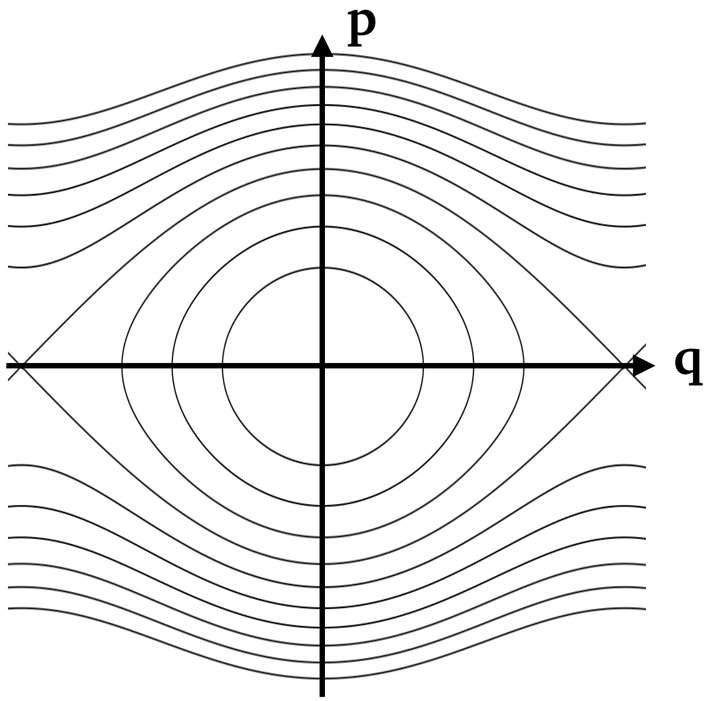
Variational integrator

exact trajectories on
position–momentum plane

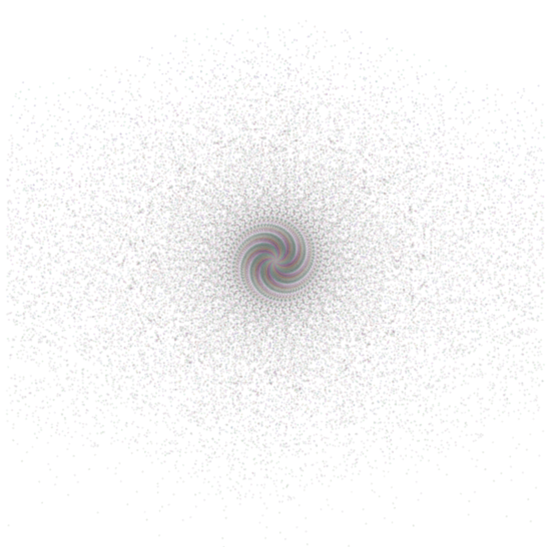
$\Delta t = 0.1$







$\Delta t = 0.9$



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

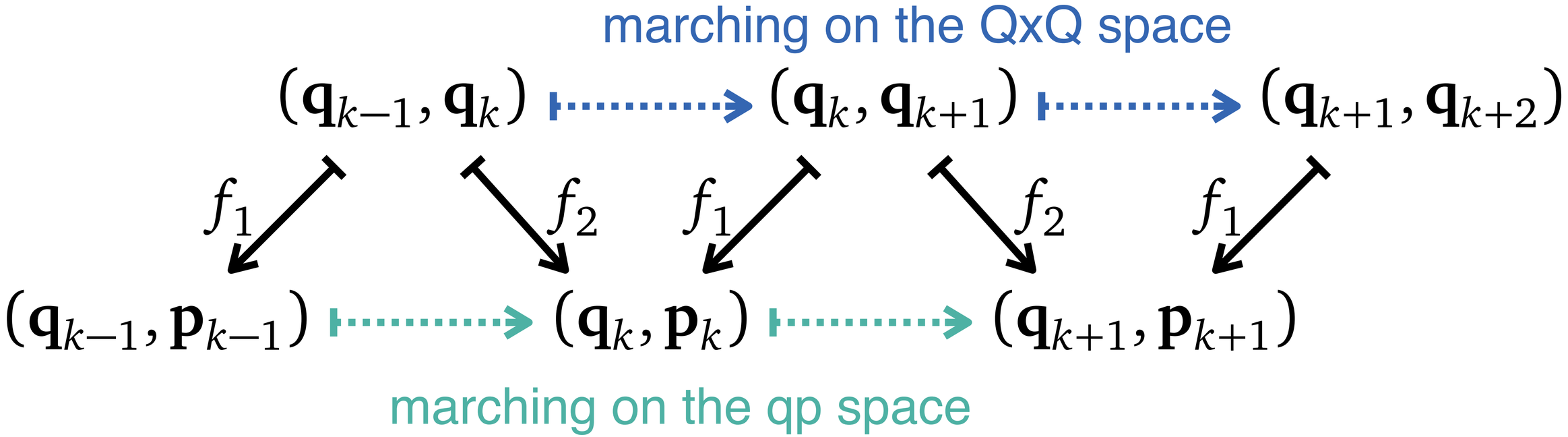
$$f_1 : (\mathbf{q}_1, \mathbf{q}_2) \mapsto (\mathbf{q}_1, -D_1 L(\mathbf{q}_1, \mathbf{q}_2))$$

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

- 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

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

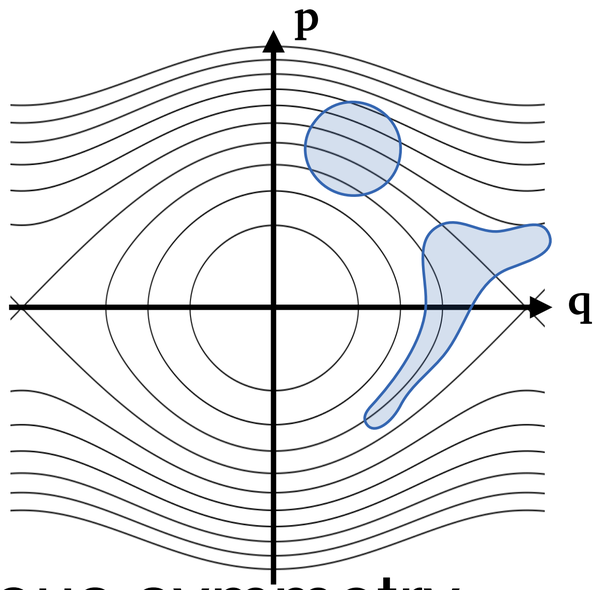
- EL eq $$m\frac{\mathbf{q}_{k+1}-2\mathbf{q}_k+\mathbf{q}_{k-1}}{h^2} = \frac{1}{2}\left(\mathbf{f}\left(\frac{\mathbf{q}_{k-1}+\mathbf{q}_k}{2}\right)+\mathbf{f}\left(\frac{\mathbf{q}_k+\mathbf{q}_{k+1}}{2}\right)\right)$$

- Equivalently

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

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.