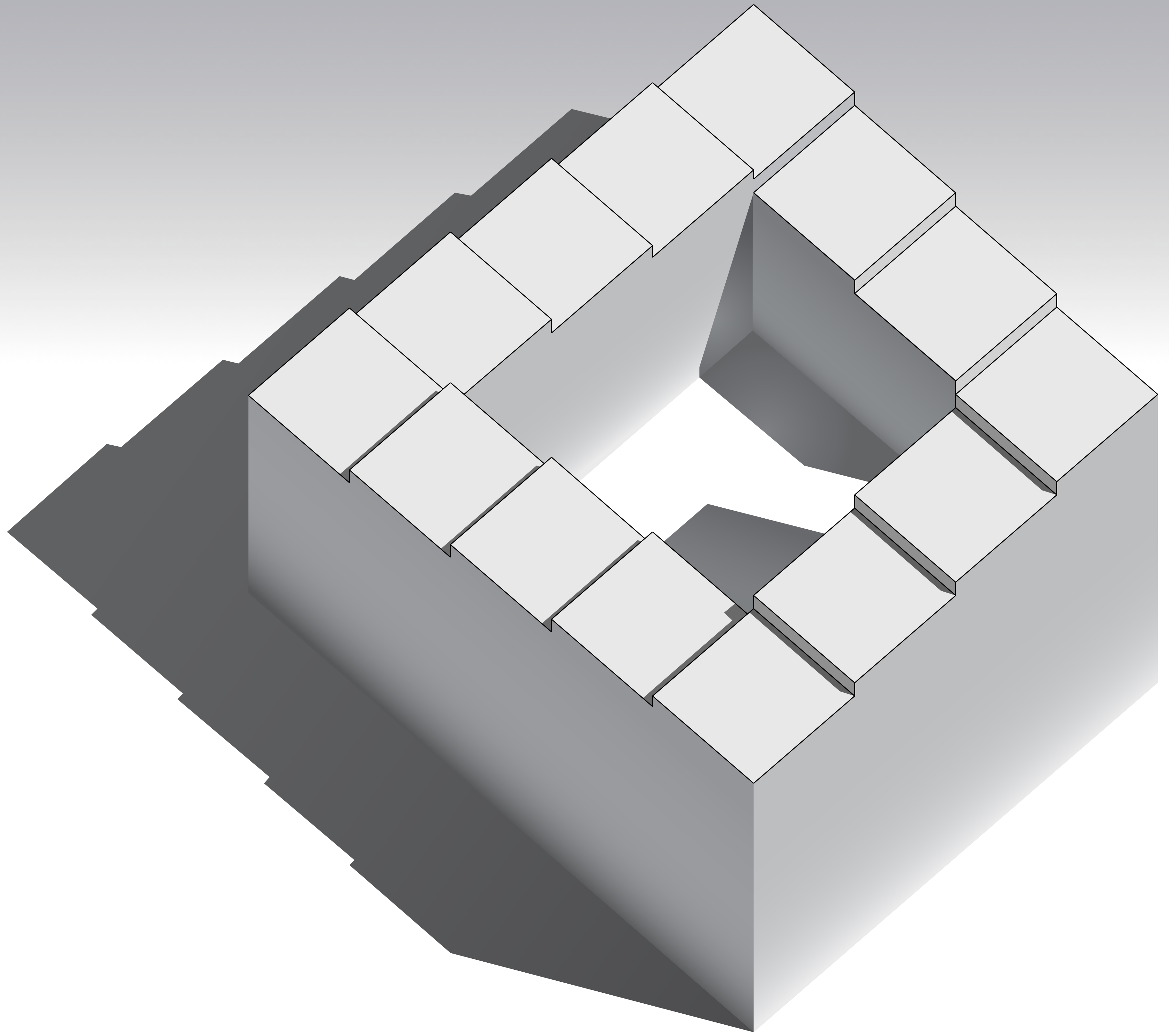

Discrete Differential Geometry: An Applied Introduction

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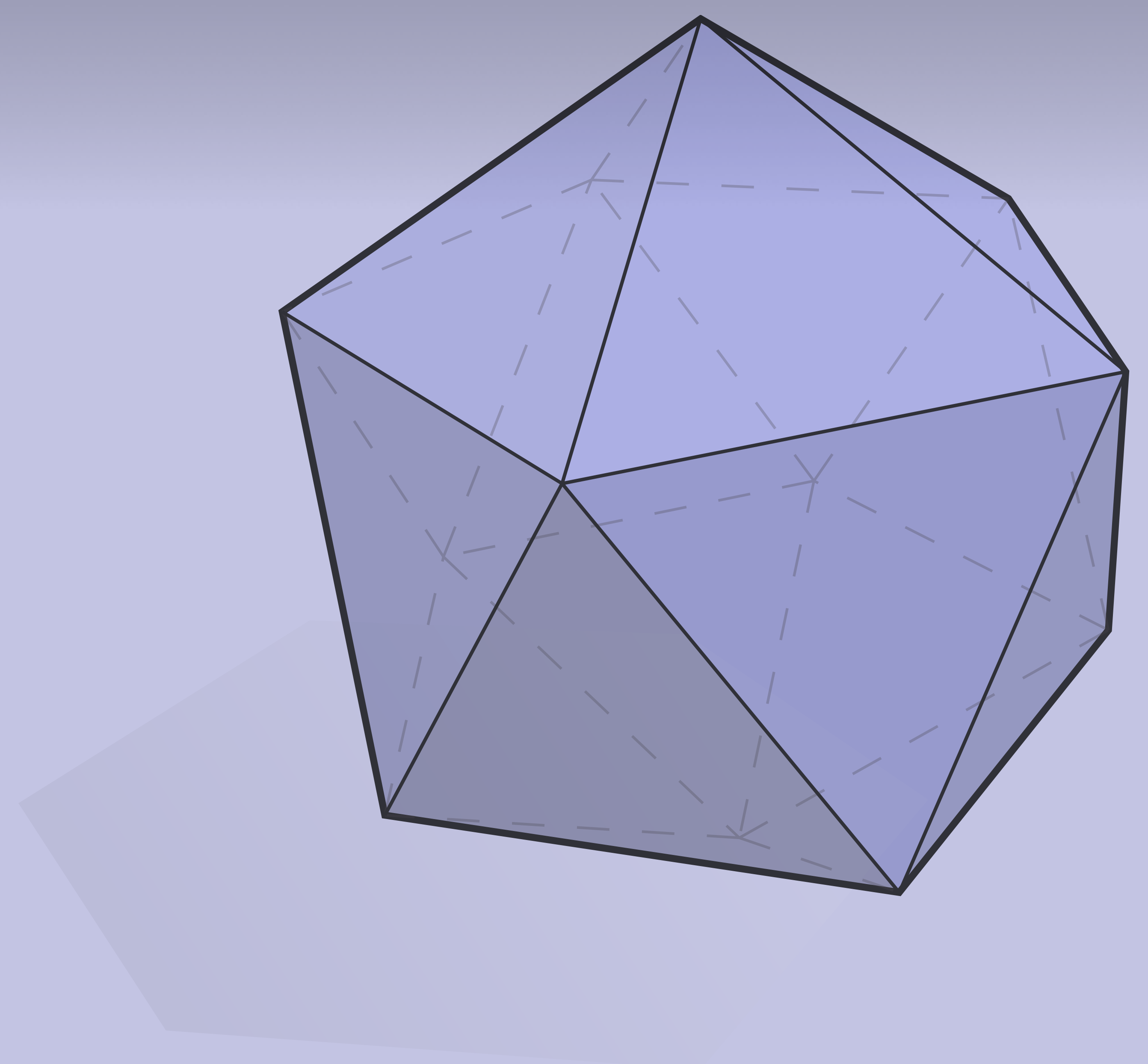
Lecture 20:
Simulation and Geometry



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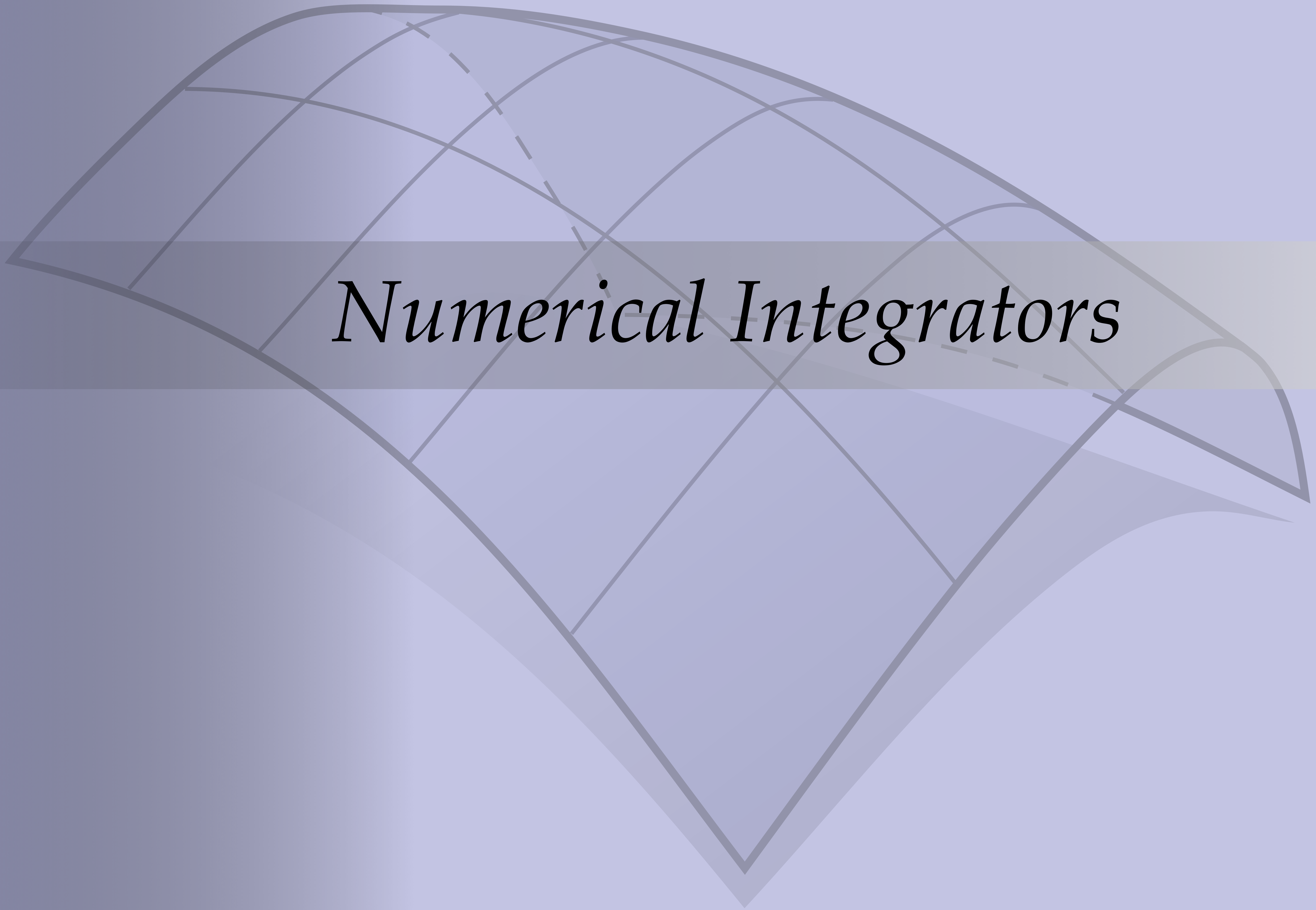
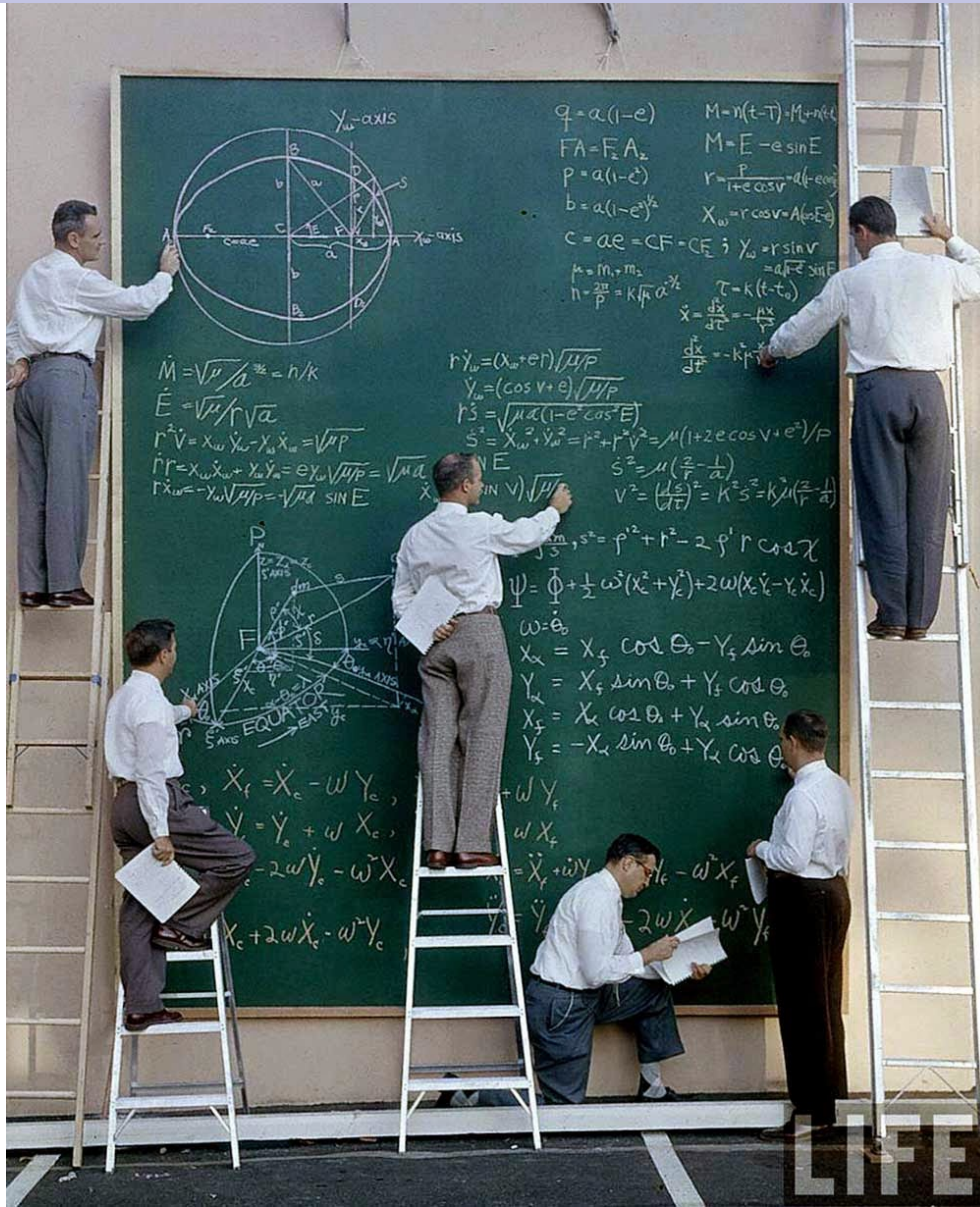
Numerical Integrators



Solving Differential Equations

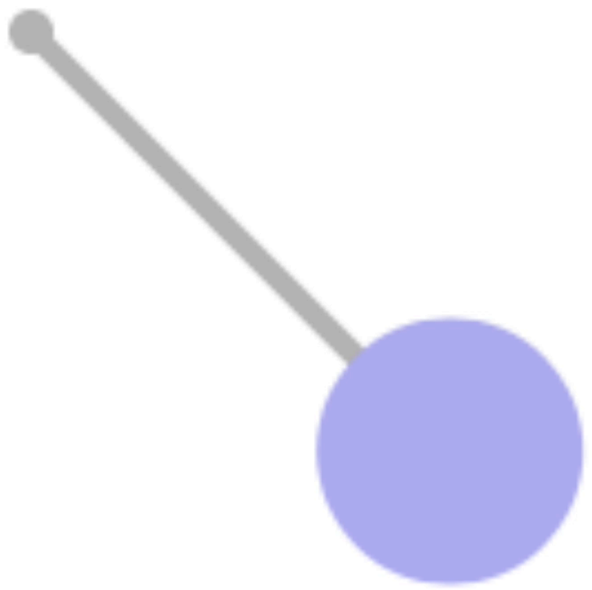
- People model all sorts of systems using differential equations
- Solving these equations is usually hard
- Sometimes you can do it by hand



https://rarehistoricalphotos.com/nasa-scientists-board-calculations-1961/

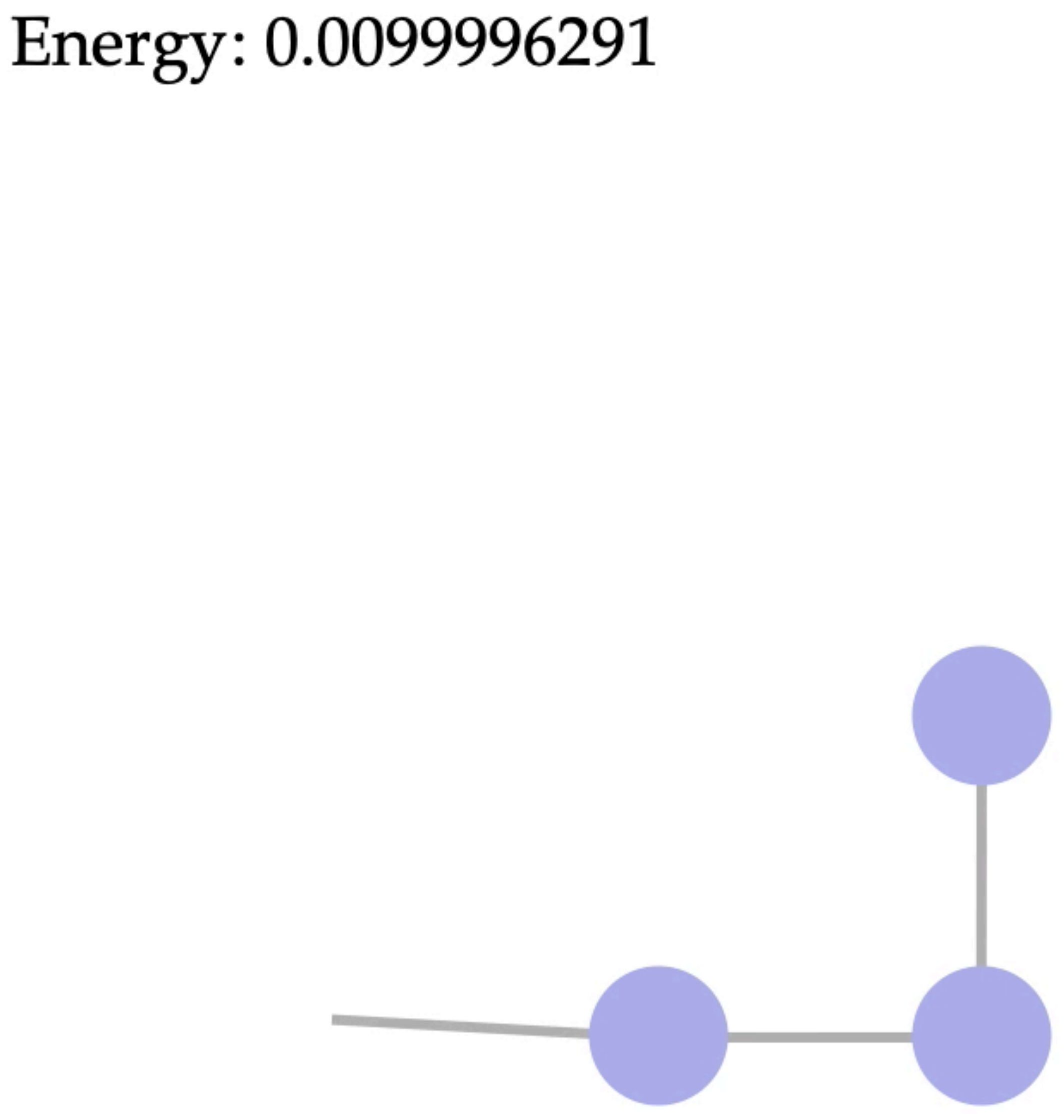
Solving Differential Equations

- Many differential equations don't have solutions that you can write down with elementary functions
- Even surprisingly-simple differential equations don't have analytical solutions



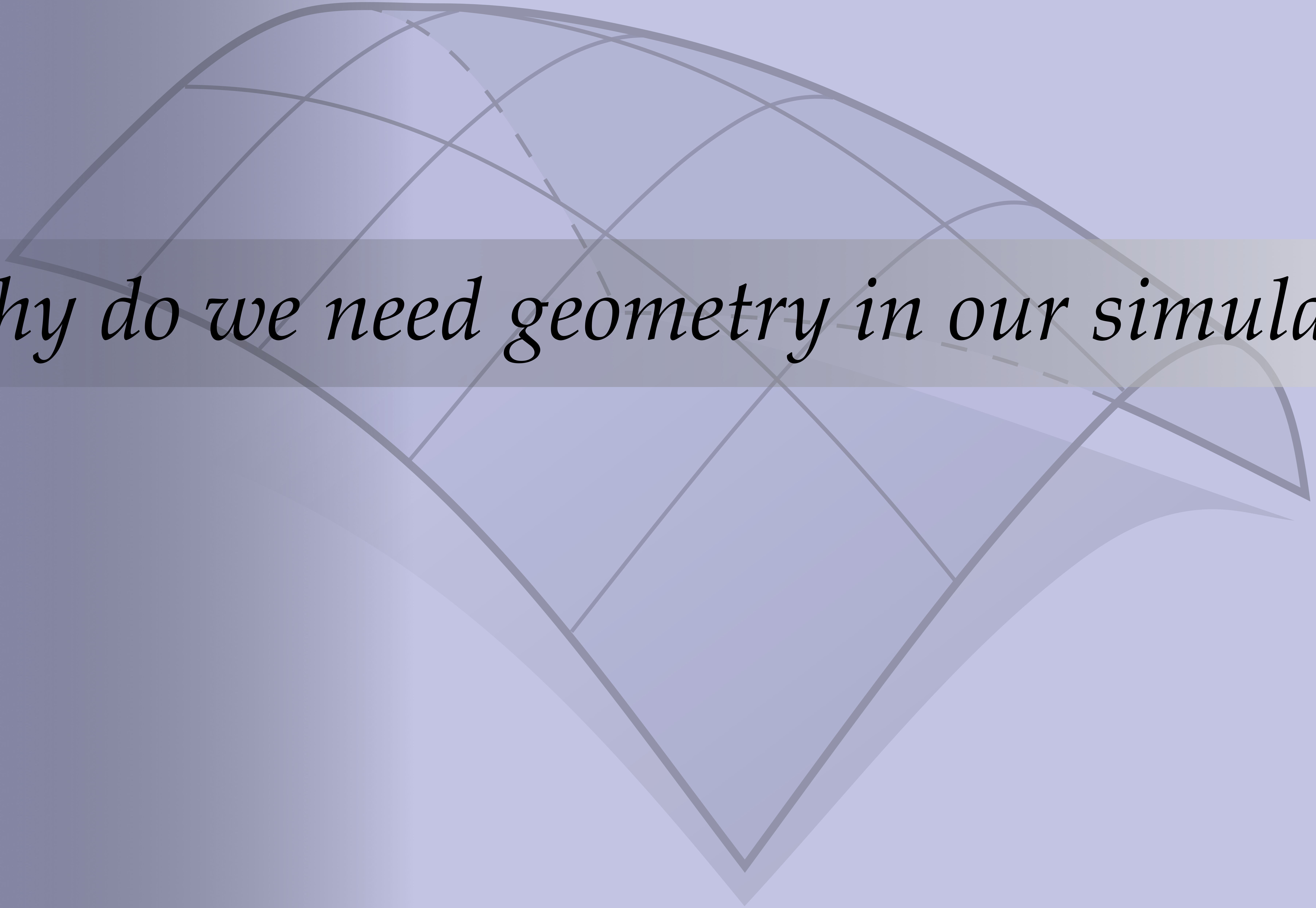
Why Do We Need Numerical Solutions?

- Many systems are too complicated to solve or approximate by hand



Journal of Statistical Mechanics, p. L09001-L09010 (2009) Tetsuro Konishi and Tatsuo Yanagita, https://www.youtube.com/watch?v=cHdZMXxnQIM

Why do we need geometry in our simulations?



Example: The Pendulum

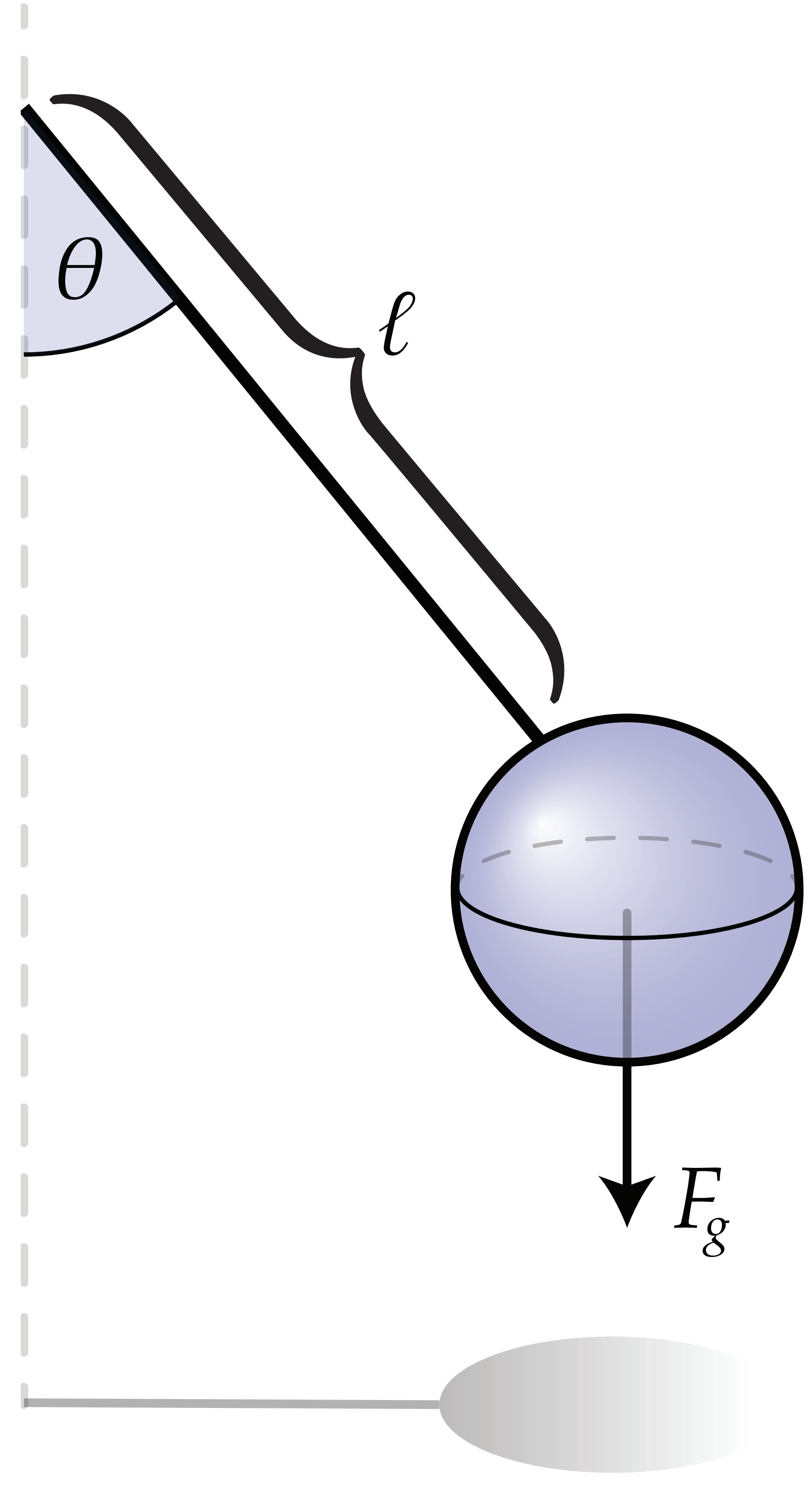
- A pendulum's behavior is governed by Newton's second law $F = ma$
- In this case, Newton's law tells us that

$$\ddot{\theta} = -\frac{g}{\ell} \sin \theta$$

- If we introduce the angular velocity variable $\omega := \dot{\theta}$ we can rewrite the equation as two first-order differential equations

$$\dot{\theta} = \omega$$

$$\dot{\omega} = -\frac{g}{\ell} \sin \theta$$



Example: The Pendulum

- There are 3 common techniques for simulating this system

$$\theta_{t+1} = \theta_t + h\omega_t$$
$$\omega_{t+1} = \omega_t - \tfrac{g}{\ell}\sin\theta_t$$

Explicit Euler

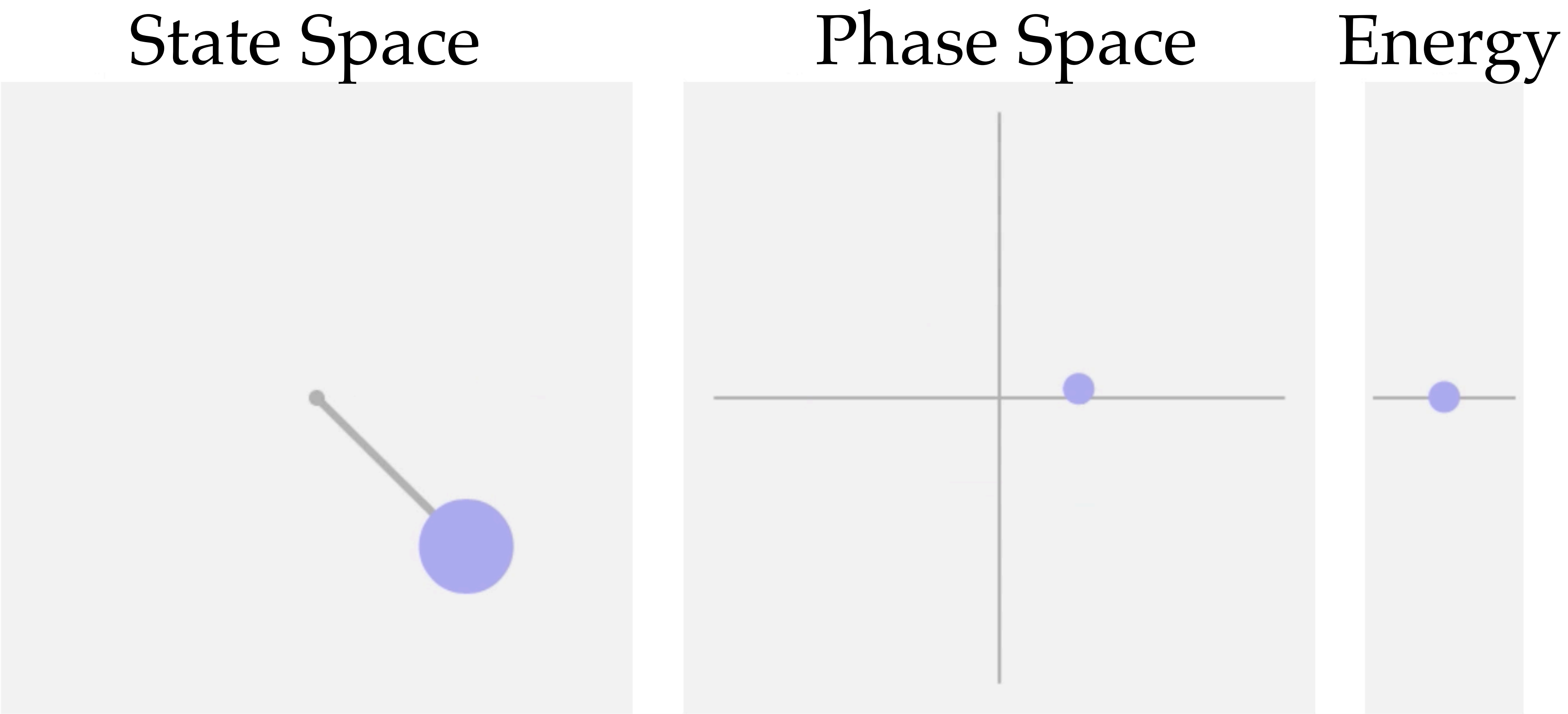
$$\theta_{t+1} = \theta_t + h\omega_{t+1}$$
$$\omega_{t+1} = \omega_t - \tfrac{g}{\ell}\sin\theta_{t+1}$$

Implicit Euler

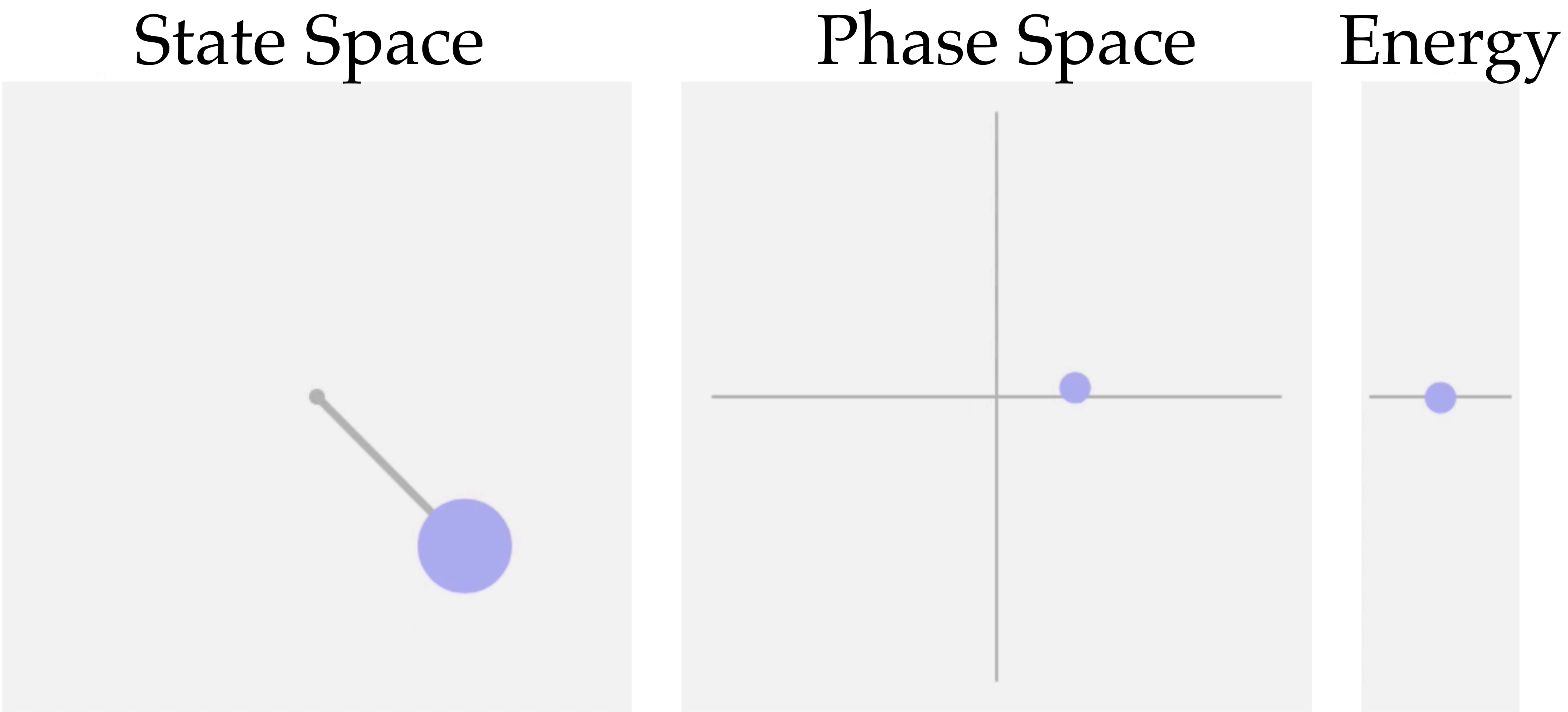
$$\theta_{t+1} = \theta_t + h\omega_{t+1}$$
$$\omega_{t+1} = \omega_t - \tfrac{g}{\ell}\sin\theta_t$$

Symplectic Euler

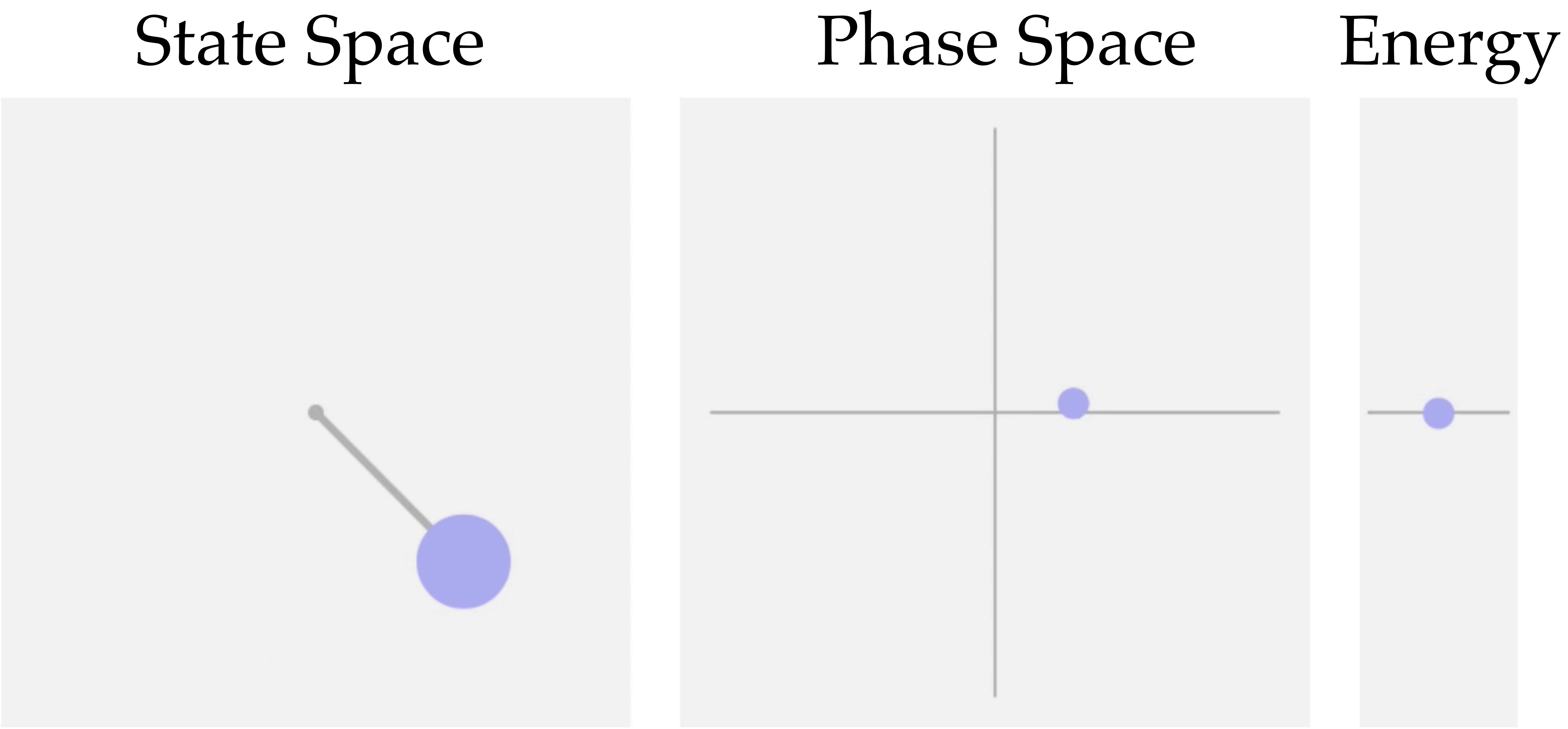
Example: The Pendulum



Explicit Euler



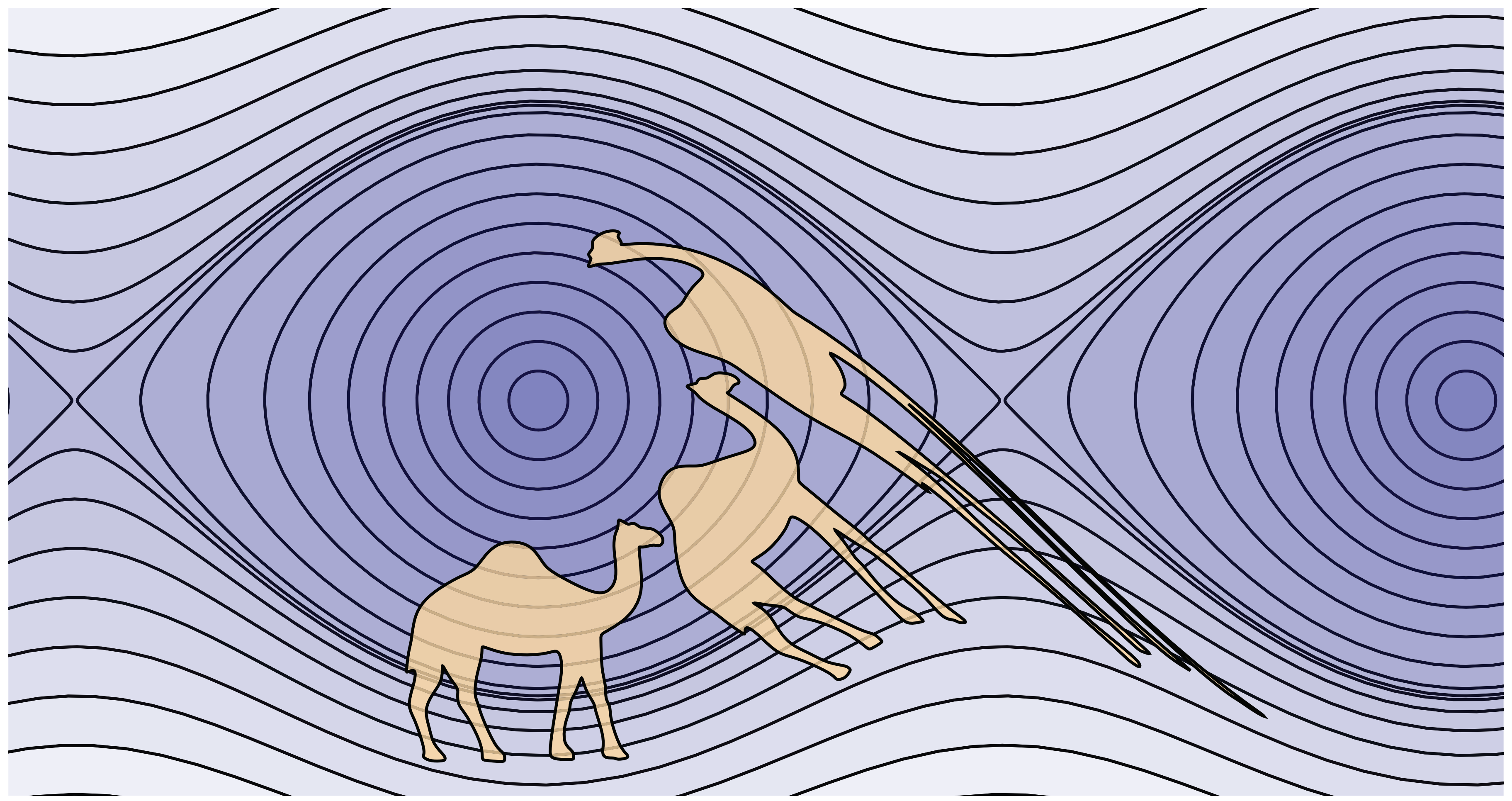
Implicit Euler

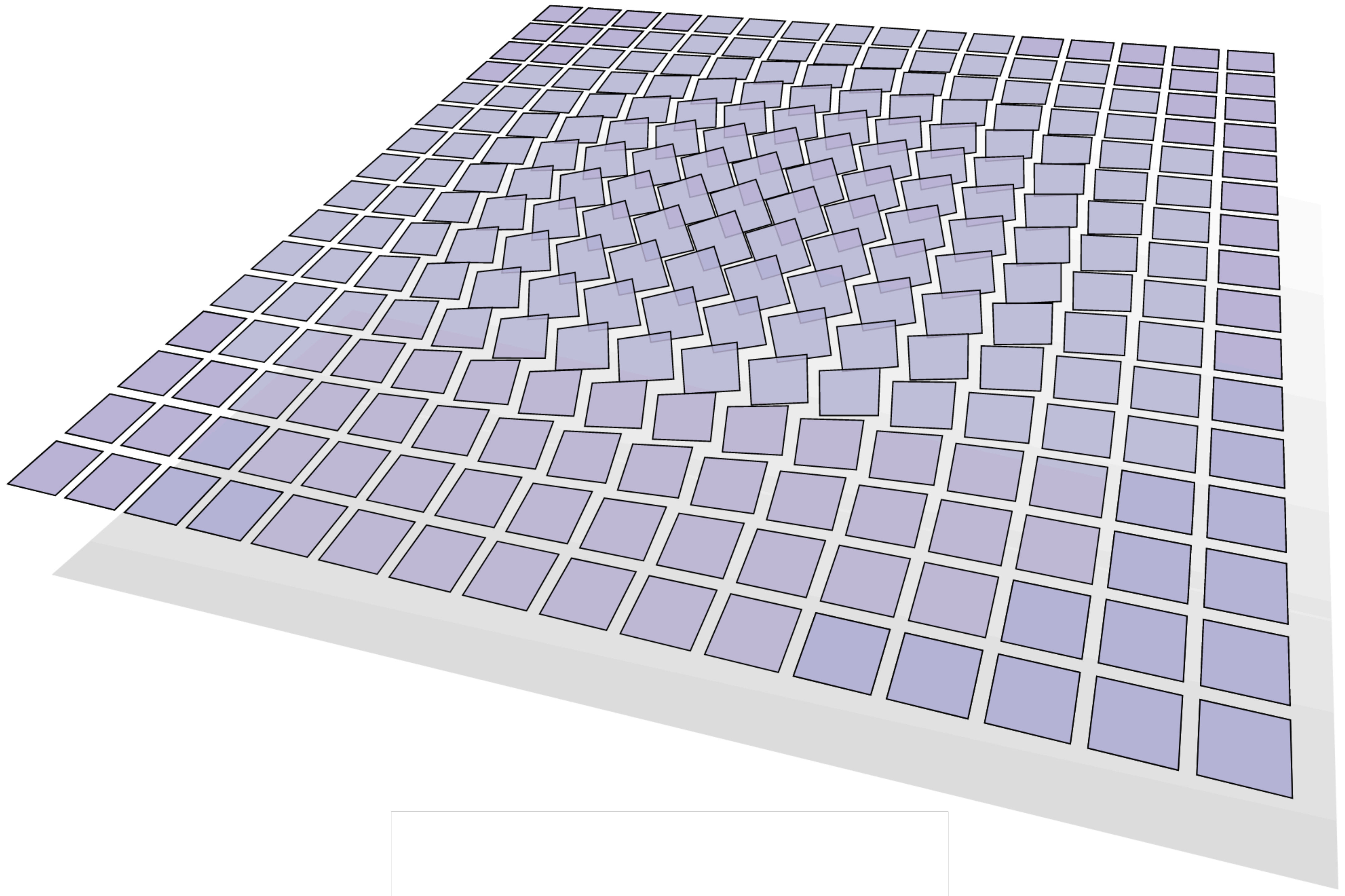


Symplectic Euler

What Makes Symplectic Euler Good?

- There is a lot of deep geometric structure underlying classical mechanics
- Symplectic Euler faithfully preserves some of this geometric structure
- *e.g.* Liouville's Theorem - time evolution of physical systems preserves area in phase space

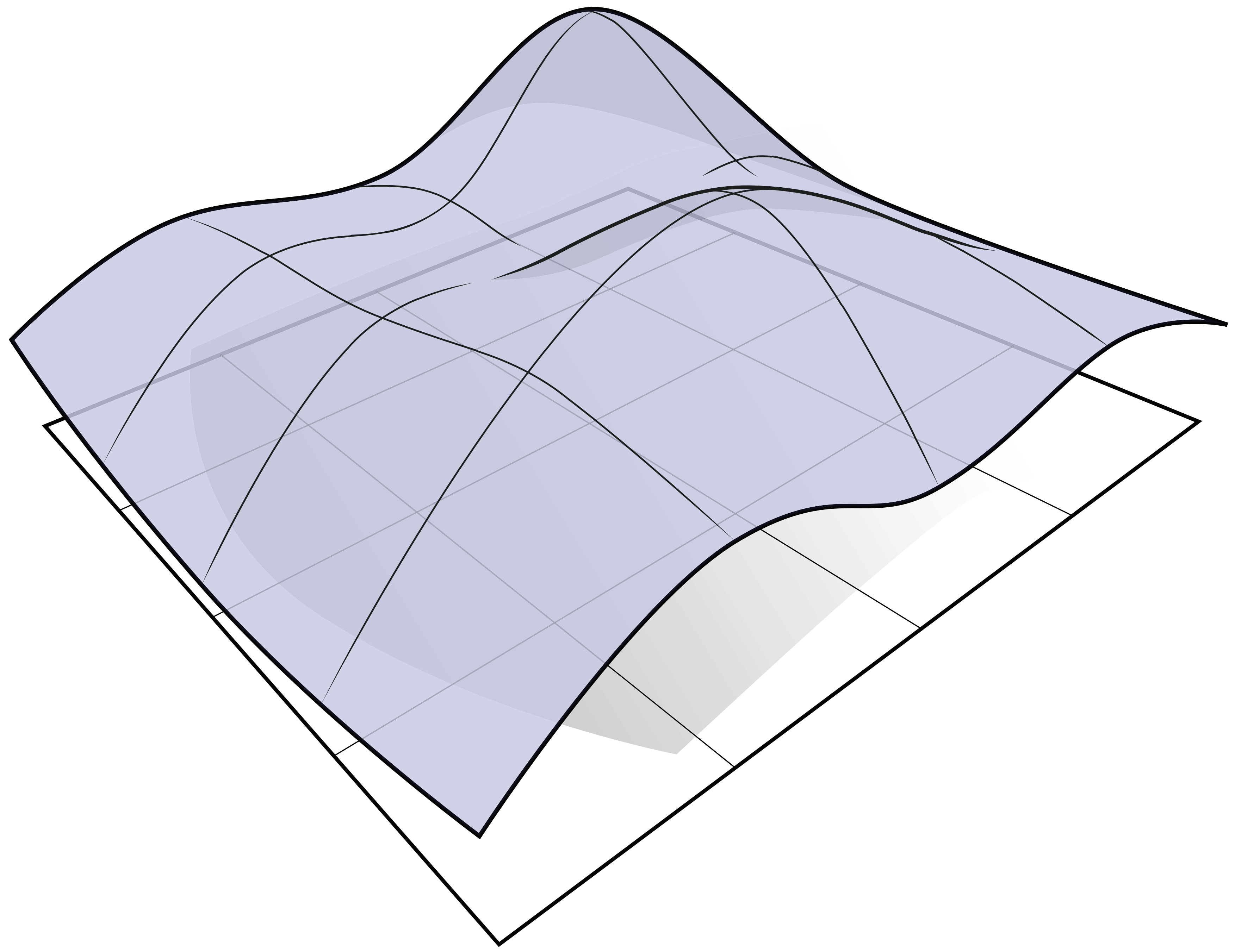




Lagrangian Mechanics

Physics is Optimization

- Newton gave us an equation that describes how things move in response to forces.
- Lagrange reformulated mechanics as an *optimization problem.*
    - Particles follow the *optimal path* according to some objective function (the *action*)
- Useful for proving theorems



Energy and the Lagrangian

- Recall that the *kinetic energy* K measures how much something is moving around. Usually $K(q, \dot{q}) = \frac{1}{2}k\dot{q}^2$
- The *potential energy* V measures how much energy is stored for future use. For a spring, $V(q, \dot{q}) = \frac{1}{2}kq^2$
- Next, we define a function $\mathcal{L}$ called the *Lagrangian*. Usually

$$\mathcal{L}(q, \dot{q}) = K(q, \dot{q}) - V(q, \dot{q})$$

- Note that all of these functions take a position and velocity as arguments. Equivalently, we can say that at each position, $\mathcal{L}$ takes in a vector and returns a scalar. So we can think of $\mathcal{L}$ as a 1-form

Action

- We define the *action* of a trajectory $q(t)$ to be the integral of $\mathcal{L}$ along $q(t)$

$$\mathcal{S}[q] := \int_{t_0}^{t_1} \mathcal{L}(q(t), \dot{q}(t)) \; dt$$

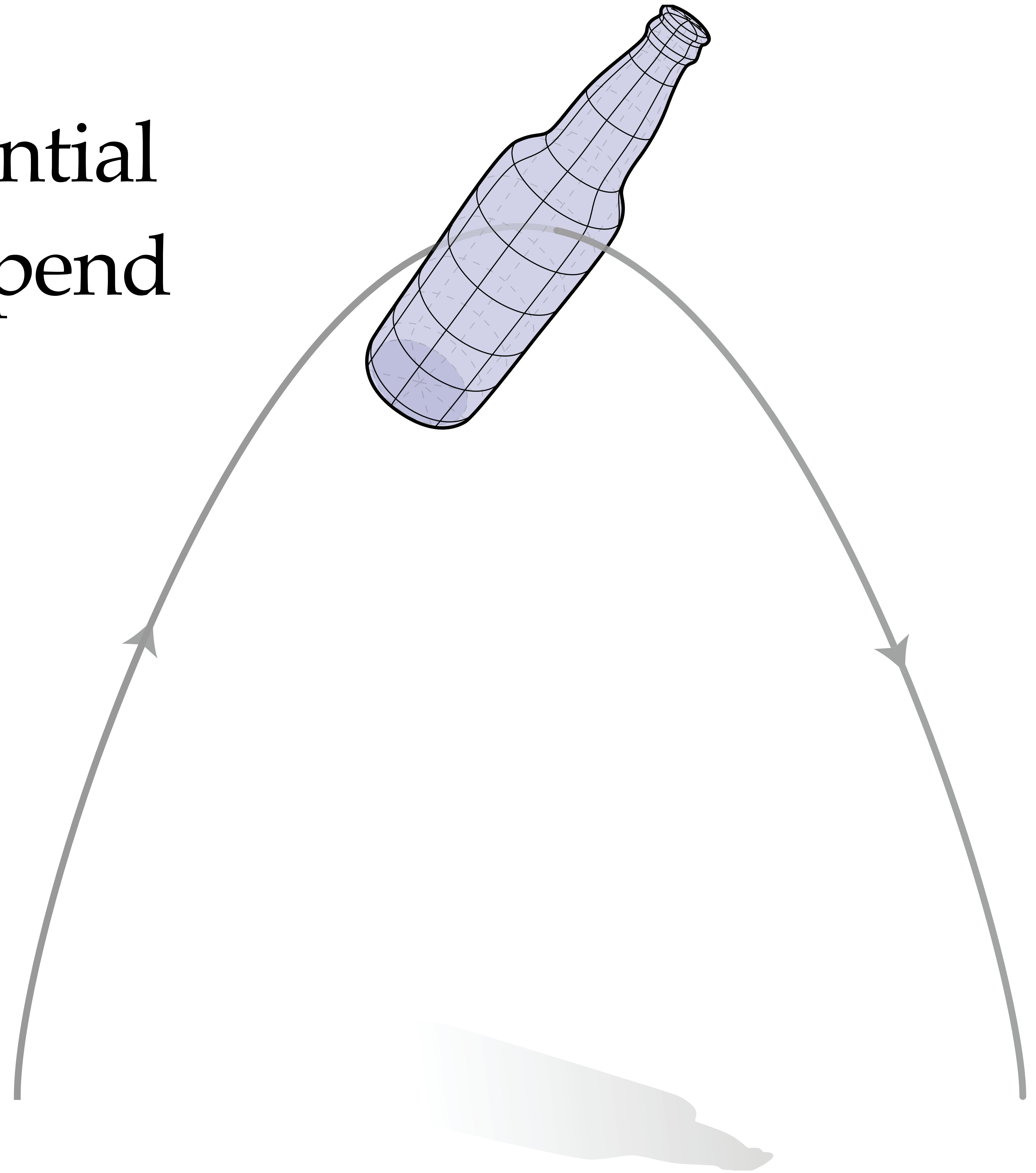
- The *principle of 'least' action* says that the trajectories taken by physical systems are *stationary points* of the action
    - These are often (but not always) minima

The Lagrangian Measures "Liveliness"

- The Lagrangian looks strange at first glance. Why is it meaningful to subtract energies like this?
- Kinetic energy measures how much is going on in our system at the moment.
- Potential energy measures how much could happen in the future.
- Minimizing the action means that the system never wants to do much at the moment - it prefers to save its energy for later
- "Nature is as lazy as possible" -John Baez

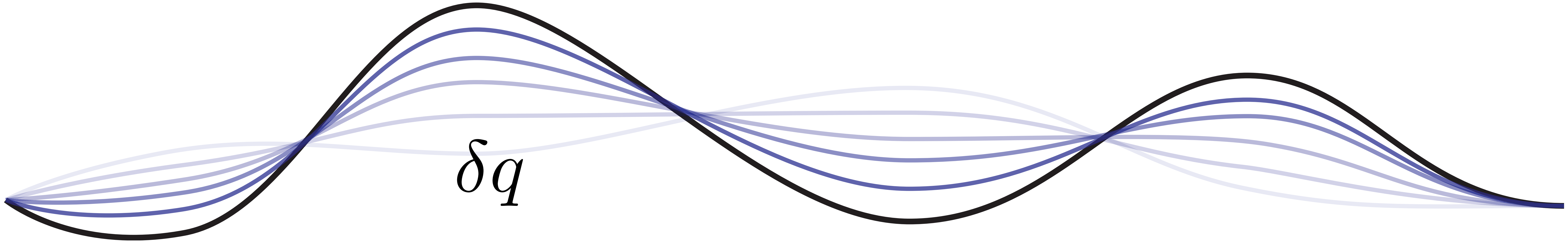
Example - Projectiles

- Consider the trajectory of a thrown object
- At the top of the arc, the object has high potential energy and low kinetic energy - it wants to spend time here
- At the bottom of the arc, the object has low potential energy and high kinetic energy - it does not want to spend much time here



The Euler-Lagrange Equation

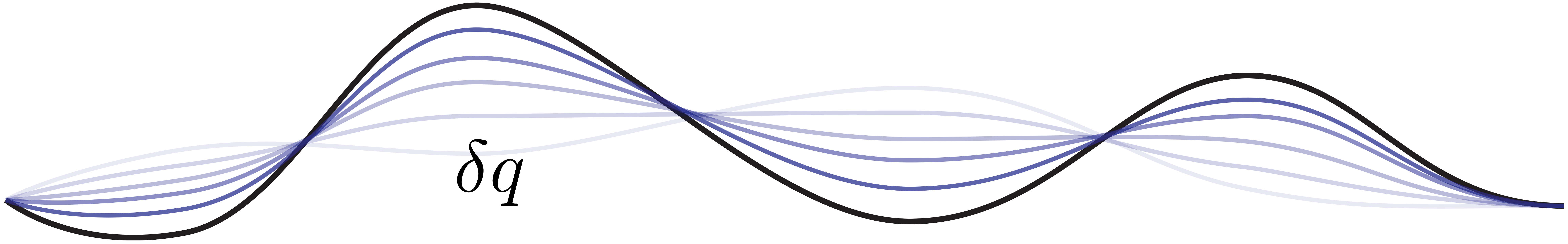
- To find stationary points of the action, we essentially set its derivative equal to 0
- The derivative of the action at a path should tell us how the action changes as we vary the path a little bit
- We restrict our attention to nearby paths which have the same endpoints



The Euler-Lagrange Equation

- Setting the variation to 0 yields the *Euler-Lagrange* equation

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



The Euler-Lagrange Equation

$$
\begin{aligned}
\delta S &= \delta \int_{t_0}^{t_1} L(q, \dot{q})\ dt \\
&= \int_{t_0}^{t_1} \frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta \dot{q}\ dt \\
&= \int_{t_0}^{t_1} \frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\frac{d}{dt}\delta q\ dt \\
&= \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\right)\delta q\ dt + \left.\frac{\partial L}{\partial \dot{q}}\delta q\right|_{t_0}^{t_1} \\
&= \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\right)\delta q\ dt
\end{aligned}
$$

Example - Newton's Law

- To get a feel for the Euler-Lagrange equation, let's look at an example
- Consider the Lagrangian of a particle with potential energy *V(q)*

$$\mathcal{L}(q,\dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q)$$

- We can differentiate the Lagrangian to find

$$\frac{\partial \mathcal{L}}{\partial q} = -\frac{\partial V}{\partial q} \qquad \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} = m\ddot{q}$$

Example - Newton's Second Law

- Now, the Euler-Lagrange equation tells us

$$\boxed{-\frac{\partial V}{\partial q} = m\ddot{q}}$$

- This is Newton's second law!

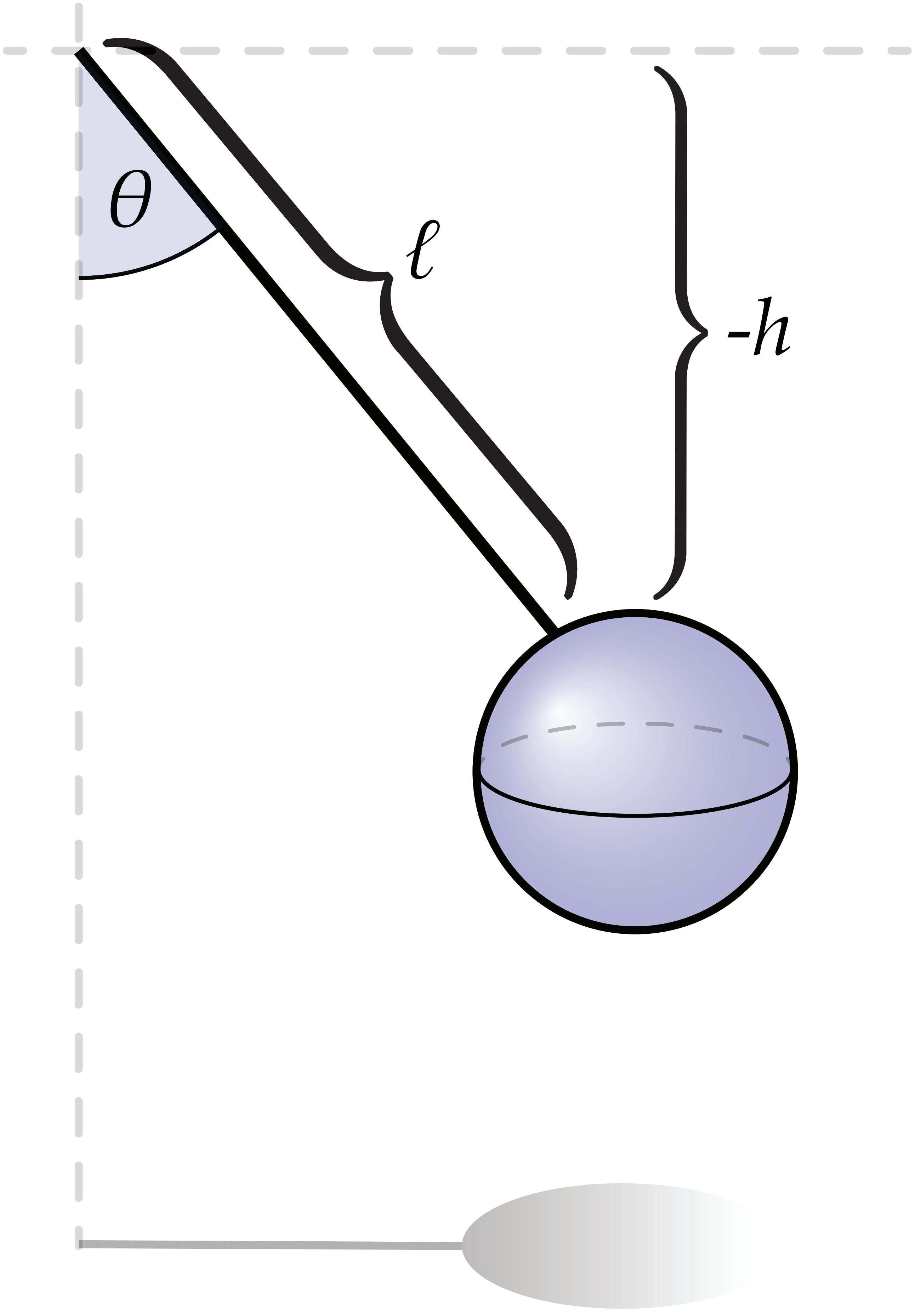
$$\boxed{F = ma}$$

More Specific Example: The Pendulum

- The kinetic energy of a pendulum is given by $K = \frac{1}{2}v^2 = \frac{1}{2}\ell^2\omega^2$
- The potential energy is given by $V = gh = -g\ell\cos\theta$
- Thus, our Lagrangian is

$$\mathcal{L}(\theta, \omega) = \frac{1}{2}\ell^2\omega^2 + g\ell\cos\theta$$

- This will be useful later



Momentum

- Hamilton noticed that it's very convenient to define *momentum* associated to the Lagrangian. We set

$$p := \frac{\partial \mathcal{L}}{\partial \dot{q}}$$

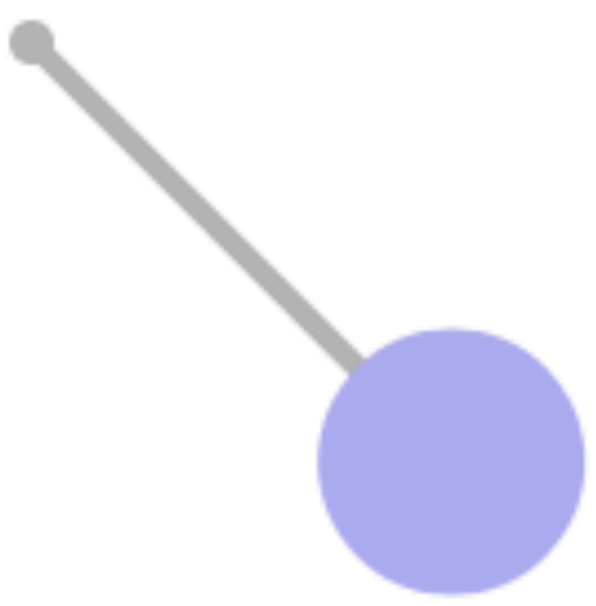
- Note that if $\mathcal{L} = \frac{1}{2}m\dot{q}^2 - V(q)$, then $p = m\dot{q}$ as usual
- Using momentum, the Euler-Lagrange equations can be written

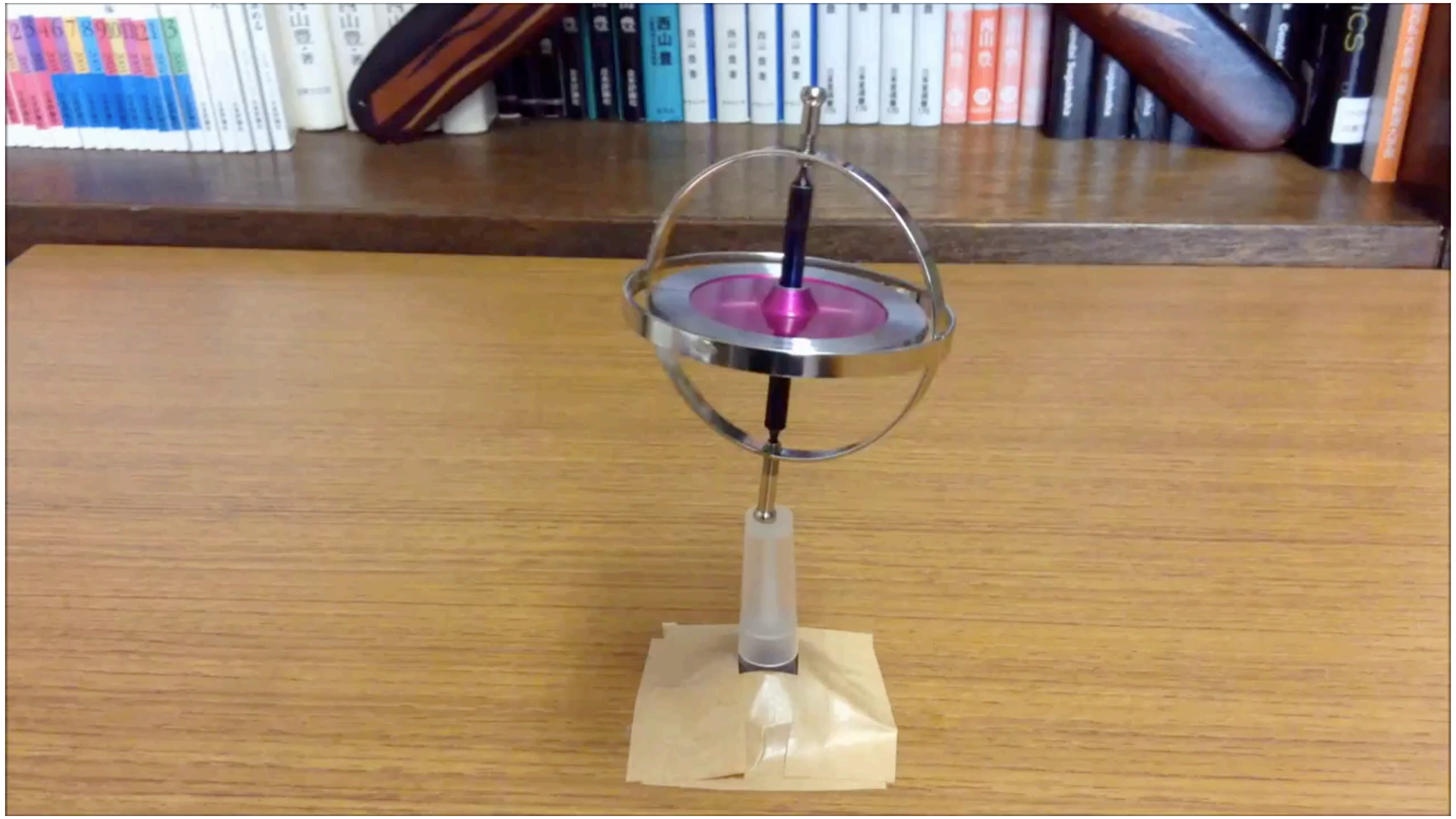
$$\dot{p} = \frac{\partial \mathcal{L}}{\partial q}$$

Conservation Laws & Constraints

Conservation Laws

- Many physical systems obey conservation laws





https://www.youtube.com/watch?v=sHnDzGWcqlQ

Noether's Theorem

- Symmetries give rise to conserved quantities
- Rotational symmetry $\iff$ angular momentum
- Translational symmetry $\iff$ momentum
- Temporal symmetry $\iff$ energy
- There's a slick proof using Lagrangian mechanics

https://en.wikipedia.org/wiki/File:Noether.jpg

Noether's Theorem

- Suppose W is a vector field, and flowing along W does not change our Lagrangian (e.g. $W = \frac{\partial}{\partial x}$)
- What does this do to the action? Well, nothing, since it doesn't change the Lagrangian
- On the other hand, it *does* induce a variation in action. Recall that

$$\delta S = \int_{t_0}^{t_1} \left(\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} \right) \cdot W \; dt + \frac{\partial \mathcal{L}}{\partial \dot{q}} \cdot W \bigg|_{t_0}^{t_1}$$

- Since we know that the action does not change, the left hand side is 0. And the Euler-Lagrange equations tell us that the first term is 0. So the quantity $\frac{\partial \mathcal{L}}{\partial \dot{q}} \cdot W$ does not change over time!

Lagrange Multipliers

- Lagrange multipliers are a neat way of turning *constrained* optimization problems into *unconstrained* optimization problems
- For example,

$$\max xy \quad \text{s.t. } x^2 + y^2 = 1 \quad \rightsquigarrow \quad \max xy + \lambda(1 - x^2 - y^2)$$

Lagrange Multipliers

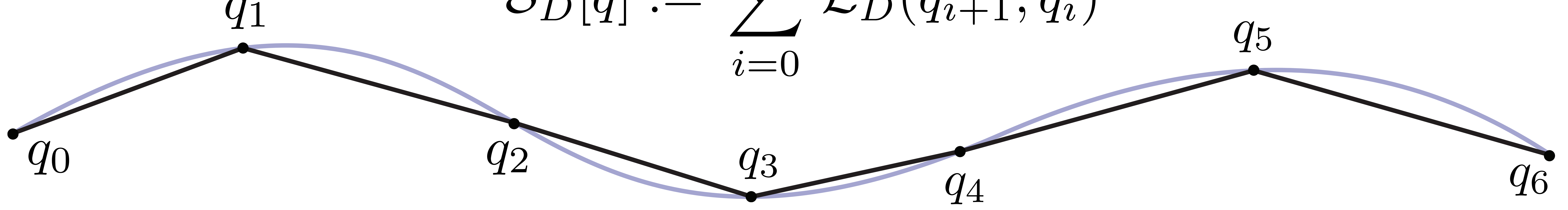
- Lagrangian mechanics casts physics as an optimization problem
- It turns out the we can use Lagrange multipliers to enforce constraints on our physical system!
- *e.g.* a pendulum is a free particle which is constrained to be a distance ℓ from the origin

Discrete Lagrangian Mechanics

Discrete Mechanics

- In classical mechanics, we compute trajectories $q(t)$
- In discrete mechanics, we compute discrete trajectories $q_0, q_1, \ldots, q_K$
- A discrete Lagrangian is a function $\mathcal{L}_D(q_k, q_{k+1})$
- The discrete action of a discrete trajectory is

$$\mathcal{S}_D[q] := \sum_{i=0}^{K-1} \mathcal{L}_D(q_{i+1}, q_i)$$



Note that the discrete Lagrangian is an *integrated* quantity. It's basically a discrete 1-form

Stationary Action for Discrete Mechanics

- Again, we want to find paths which are stationary points of the action.
- Now, everything is finite-dimensional, so we can just take regular derivatives
- At a stationary point, we must have $\frac{\partial \mathcal{S}_D}{\partial q_i} = 0$ for each q_i. Thus,

$$\frac{\partial \mathcal{L}_D(q_{i-1}, q_i)}{\partial q_i} + \frac{\partial \mathcal{L}_D(q_i, q_{i+1})}{\partial q_i} = 0$$

- People often write

$$D_2\mathcal{L}_D(q_{i-1}, q_i) + D_1\mathcal{L}_D(q_i, q_{i+1}) = 0$$

Stationary Action for Discrete Mechanics

- We call this equation the *discrete Euler-Lagrange equation*

$$\boxed{D_2\mathcal{L}_D(q_{i-1}, q_i) + D_1\mathcal{L}_D(q_i, q_{i+1}) = 0}$$

- If we know q_{i-1} and q_i, we can use the discrete Euler-Lagrange equation to solve for q_{i+1}
- To represent our state, we store *pairs* of positions (q_{i-1}, q_i)

Discrete Momentum

- It's often inconvenient to store our state as a pair of positions
- For convenience, we can define the *discrete momentum*

$$p_i = D_2\mathcal{L}_D(q_{i-1}, q_i)$$

- Now we can store pairs (q_i, p_i) and our implicit update rule is given by

$$D_1\mathcal{L}_D(q_i, q_{i+1}) = -p_i$$
$$D_2\mathcal{L}_D(q_i, q_{i+1}) = p_{i+1}$$

Example: The Pendulum

- We can define the discrete Lagrangian of a pendulum to be

$$\mathcal{L}_D(q_i, q_{i+1}) = h\left(\frac{1}{2}\ell^2\left(\frac{q_{i+1} - q_i}{h}\right)^2 + g\ell\cos q_i\right)$$

Integrated quantity

Kinetic energy

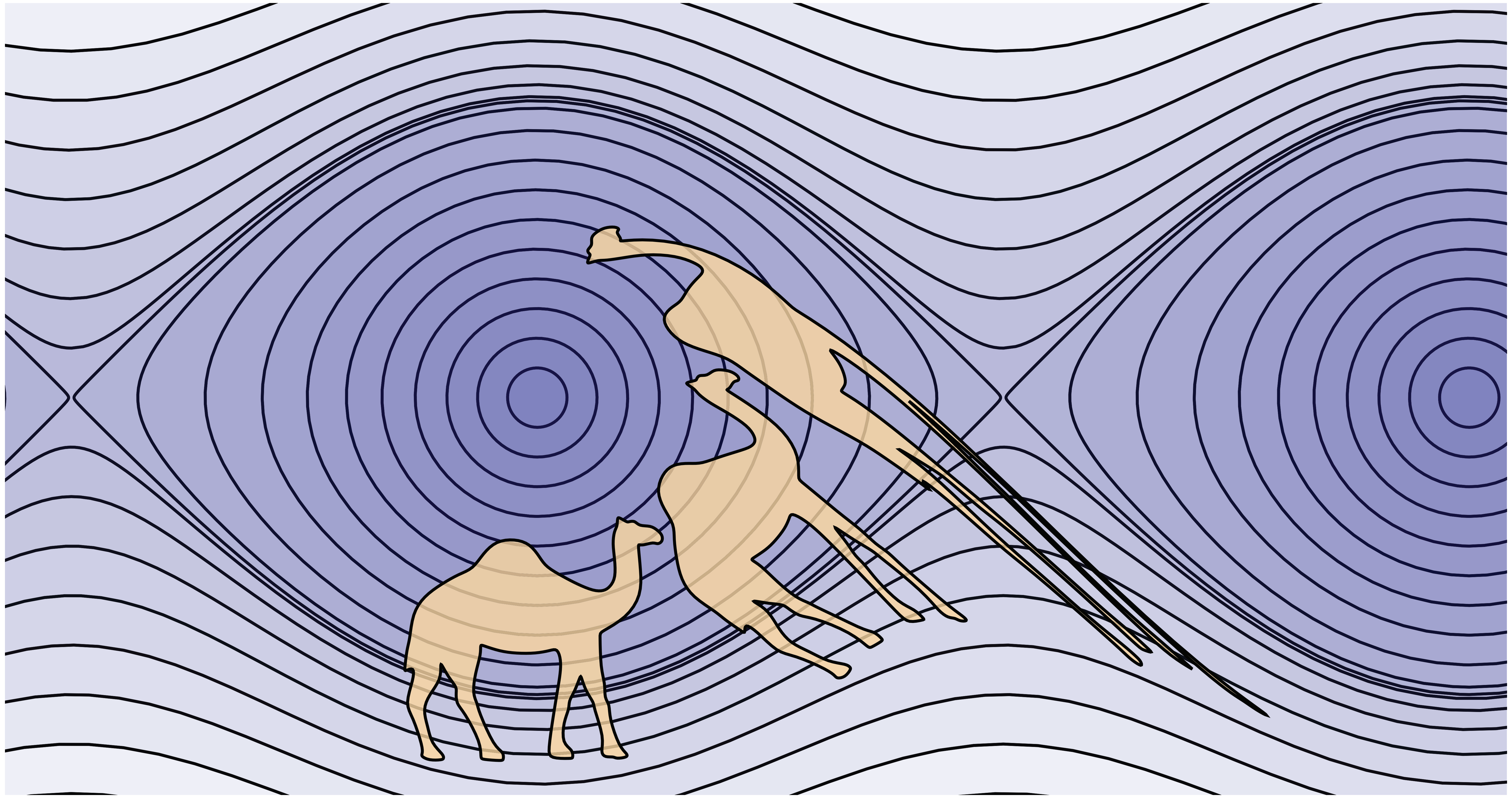
Potential energy

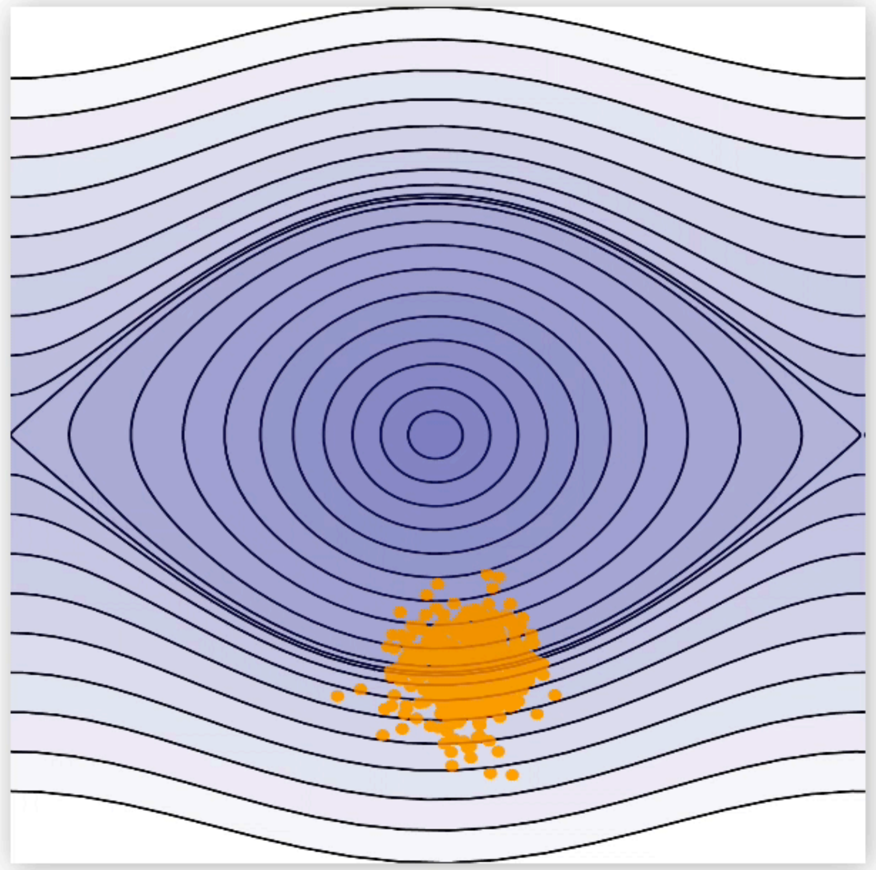
- Then the discrete Euler-Lagrange equations give us symplectic Euler!

What does it mean to be symplectic?

Physical Systems Conserve Area in Phase Space

- The motion of a pendulum preserves area in p





The Lagrangian 1-form

- Recall that in our derivation of the Euler-Lagrange equation, we saw that the change in action due to a variation δq is given by

$$\delta \mathcal{S} = \int_{t_0}^{t_1} \left(\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} \right) \delta q \; dt + \left. \frac{\partial \mathcal{L}}{\partial \dot{q}} \delta q \right|_{t_0}^{t_1}$$

$$\delta \mathcal{S} = \left. \frac{\partial \mathcal{L}}{\partial \dot{q}} \delta q \right|_{t_0}^{t_1} =: \left. \theta(\delta q) \right|_{t_0}^{t_1}$$

- We call θ the *Lagrangian 1-form*. In coordinates, $\theta = p \; dq$

The Lagrangian Symplectic Form

- The change in action due to a variation is essentially a directional derivative. We can think of it like applying a 1-form to a vector

$$\text{“}\delta S = d\mathcal{S}(\delta q)''$$

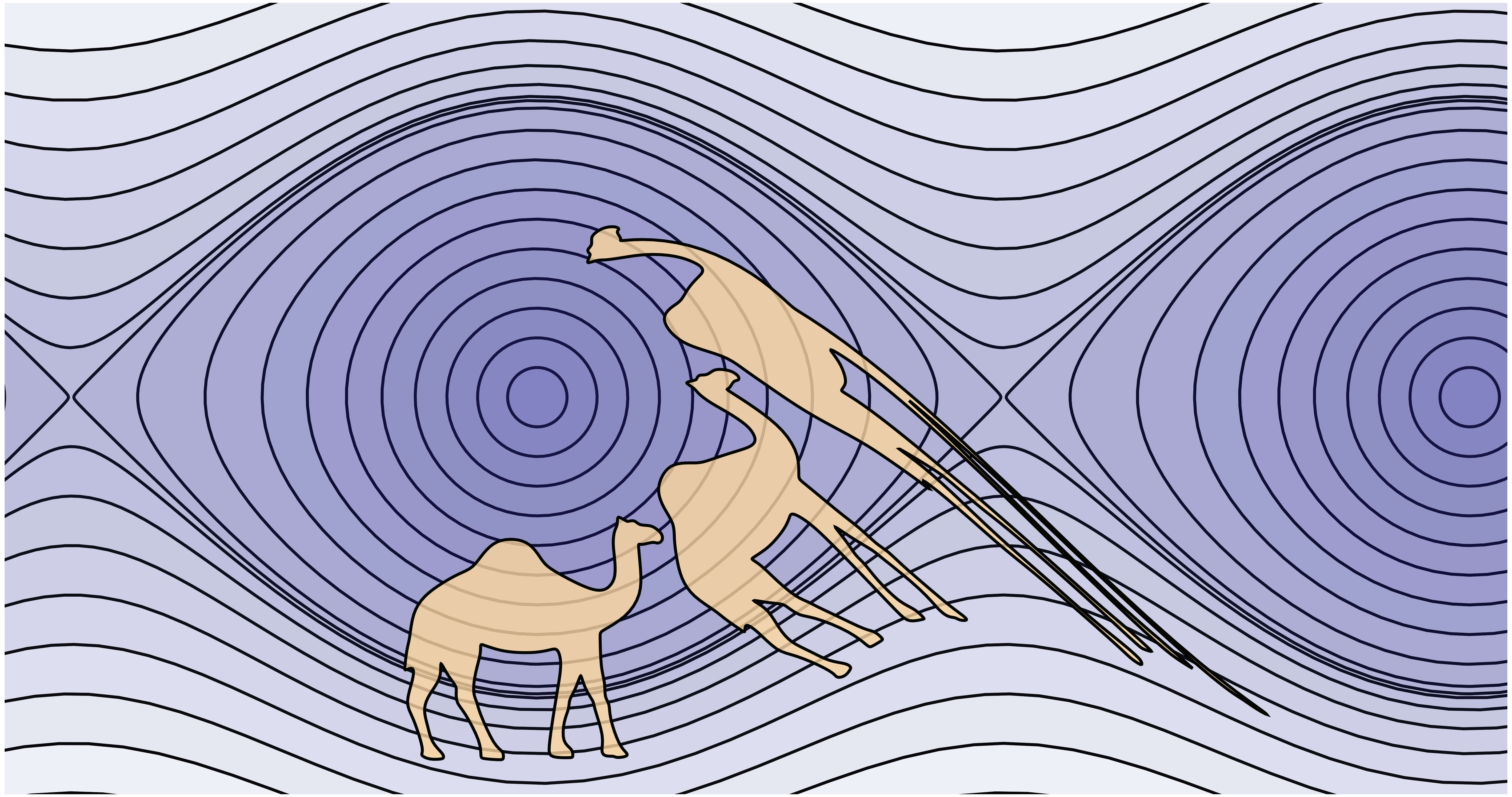
- So if we take the exterior derivative of δS, we should get 0. Recall that

$$\delta S = \theta(\delta q)\Big|_{t_0}^{t_1}$$

- Therefore, $d\theta$ is conserved, i.e. $d\theta\Big|_{t_0}^{t_1} = 0$

The Lagrangian Symplectic Form

- Note that $d\theta = d\big(p\ dq\big) = dp \wedge dq$
- In 2D, this is just area!



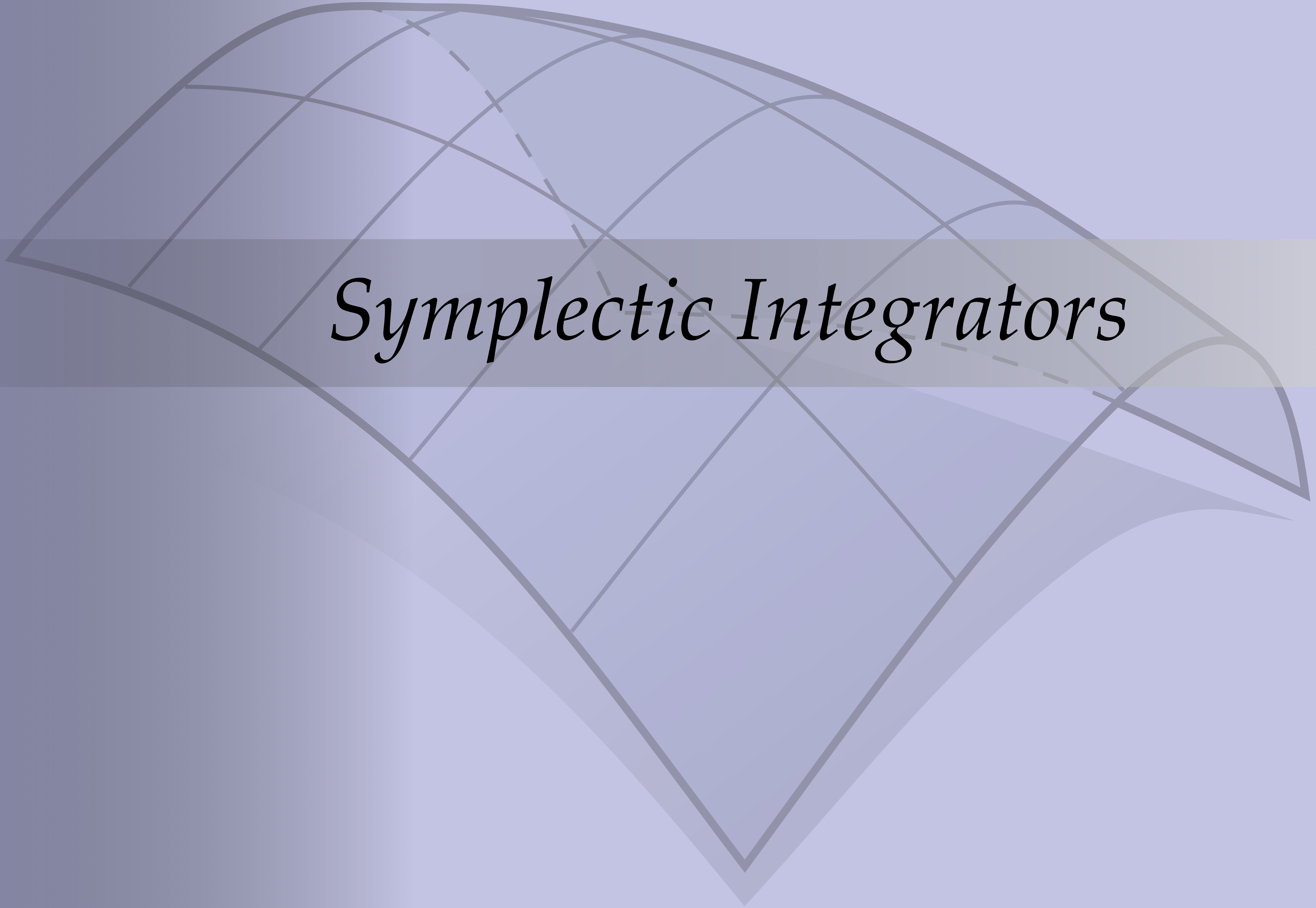
Higher Dimensions

- For higher-dimensional systems, $\theta = \sum_i p_i dq_i$
- The symplectic form is $d\theta = d\left(\sum_i p_i dq_i\right) = \sum_i dp_i \wedge dq_i$
- Preservation of the symplectic form implies preservation of volume
- For a 2*n*-dimensional system, the basis 1-forms are

$$\{dq_1, \ldots, dq_n, dp_1, \ldots, dp_n\}$$

- The *n*-fold wedge product of the symplectic form is the volume form!

Symplectic Integrators



So What's So Good About Symplectic Euler?

- We can view any simulation method as a function on phase space

$$F : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$$

- Now, we can ask if this function preserves area
- To check this, we can just compute the Jacobian
- In the case of symplectic Euler, we have

$$F : (q_k, p_k) \mapsto (q_k + hp_k - h^2 \sin q_k, p_k + h \sin q_k)$$

So What's So Good About Symplectic Euler?

$$F : (q_k, p_k) \mapsto (q_k + hp_k - h^2 \sin q_k, p_k - h \sin q_k)$$

- Taking the Jacobian, we find that

$$dF = \begin{pmatrix} 1 - h^2 \cos q_k & -h \cos q_k \\ h & 1 \end{pmatrix}$$

- Observe that $\det(dF) = 1$
- So symplectic Euler preserves area in phase space (*i.e.* symplectic Euler is symplectic)

What About Explicit Euler?

$$F : (q_k, p_k) \mapsto (q_k + hp_k, p_k - h \sin q_k)$$

$$dF = \begin{pmatrix} 1 & -h \cos q_k \\ h & 1 \end{pmatrix}$$

$$\det(dF) = 1 + h^2 \cos q_k$$

- For small angles, this is greater than 1.
- For small h, this is approximately 1

What About Implicit Euler?

$$q_{k+1} = q_k + hp_{k+1}$$
$$p_{k+1} = p_k - h\sin q_{k+1}$$

$$F^{-1} : (q_{k+1}, p_{k+1}) \mapsto \left(q_{k+1} - hp_{k+1}, p_{k+1} + h\sin q_{k+1}\right)$$

$$dF^{-1} = \begin{pmatrix} 1 & h\cos q_{k+1} \\ h & 1 \end{pmatrix}$$

$$\det dF = \frac{1}{1 + h^2 \cos q_{k+1}}$$

Why is Symplectic Euler Symplectic?

- Simulation methods based on discrete Lagrangian mechanics must be symplectic.
- The proof is (almost) exactly the same as the continuous proof!
- Recall that $p_i = D_2\mathcal{L}_D(q_{i-1}, q_i)$
- And for trajectories satisfying the discrete Euler-Lagrange equations,

$$D_2\mathcal{L}_D(q_{i-1}, q_i) = -D_1\mathcal{L}_D(q_i, q_{i+1})$$

Why is Symplectic Euler Symplectic?

$$
\begin{aligned}
d\mathcal{S}_D &= \sum_{i=1}^{n} \lceil L_D(q_{i-1}, q_i) \\
&= \sum_{i=1}^{n} D_1\mathcal{L}_D(q_{i-1}, q_i)dq_{i-1} + D_2\mathcal{L}_D(q_{i-1}, q_i)dq_i \\
&= D_1\mathcal{L}_D(q_0, q_1)dq_0 + \sum_{i=1}^{n-1} \left(D_2\mathcal{L}_D(q_{i-1}, q_i) + D_2\mathcal{L}_D(q_i, q_{i+1})\right) dq_i + D_2\mathcal{L}_D(q_{n-1}, q_n)dq_n \\
&= D_1\mathcal{L}_D(q_0, q_1)dq_0 + D_2\mathcal{L}_D(q_{n-1}, q_n)dq_n \\
&= -p_0 dq_0 + p_n dq_n
\end{aligned}
$$

$$
0 = d(d\mathcal{S}_D) = -dp_0 \wedge dq_0 + dp_n \wedge dq_n
$$

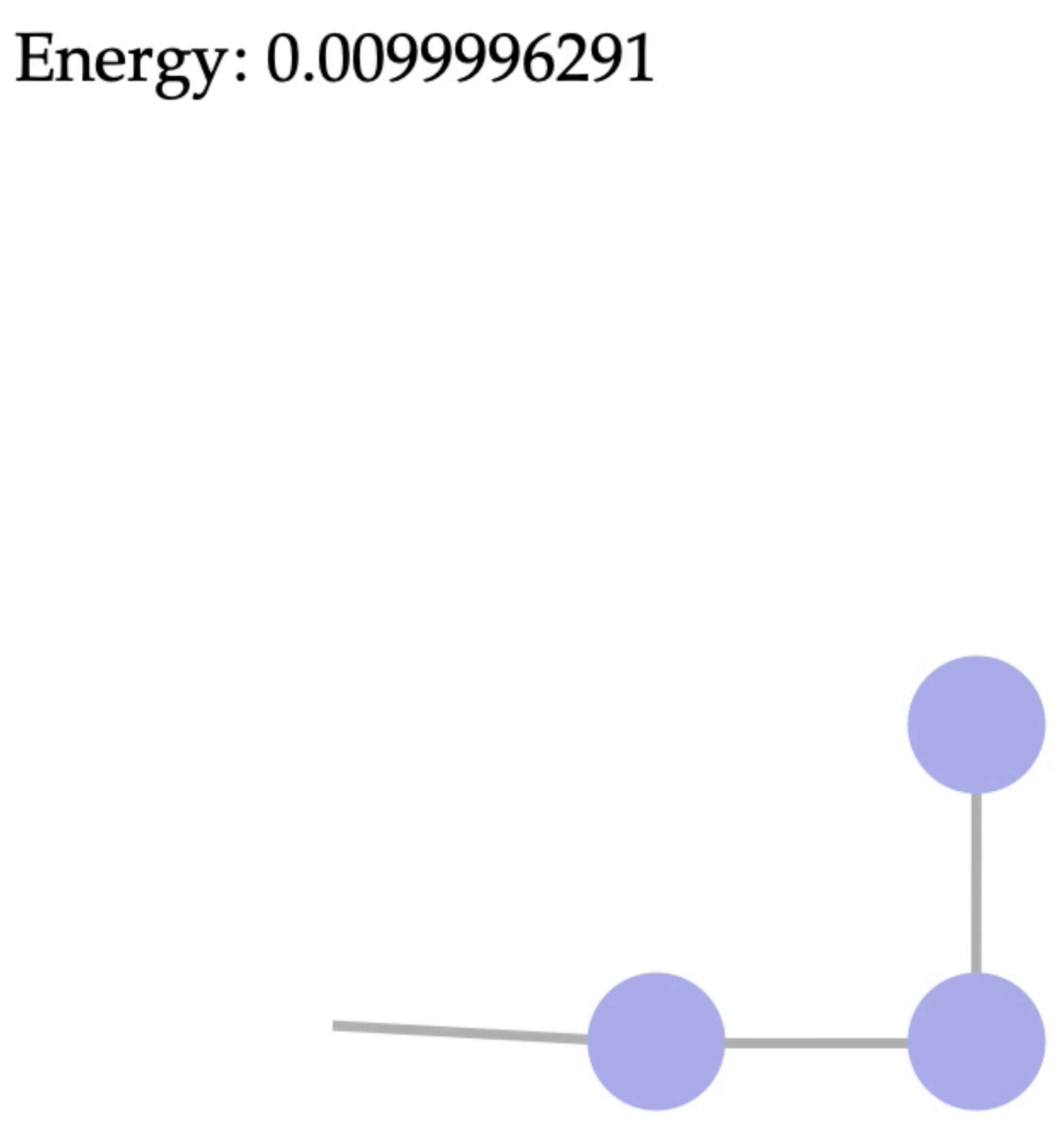
Discrete Conservation Laws & Constraints

Discrete Noether's Theorem

- Using the same tricks, we can prove a discrete version of Noether's theorem
- This proves, *e.g.* that the discrete momentum p_i is conserved for systems with translation-invariant discrete Lagrangians

Lagrange Multipliers

- We can also use Lagrange multipliers to enforce constraints on our simulation
- This make it a lot easier to simulate things like triple pendular



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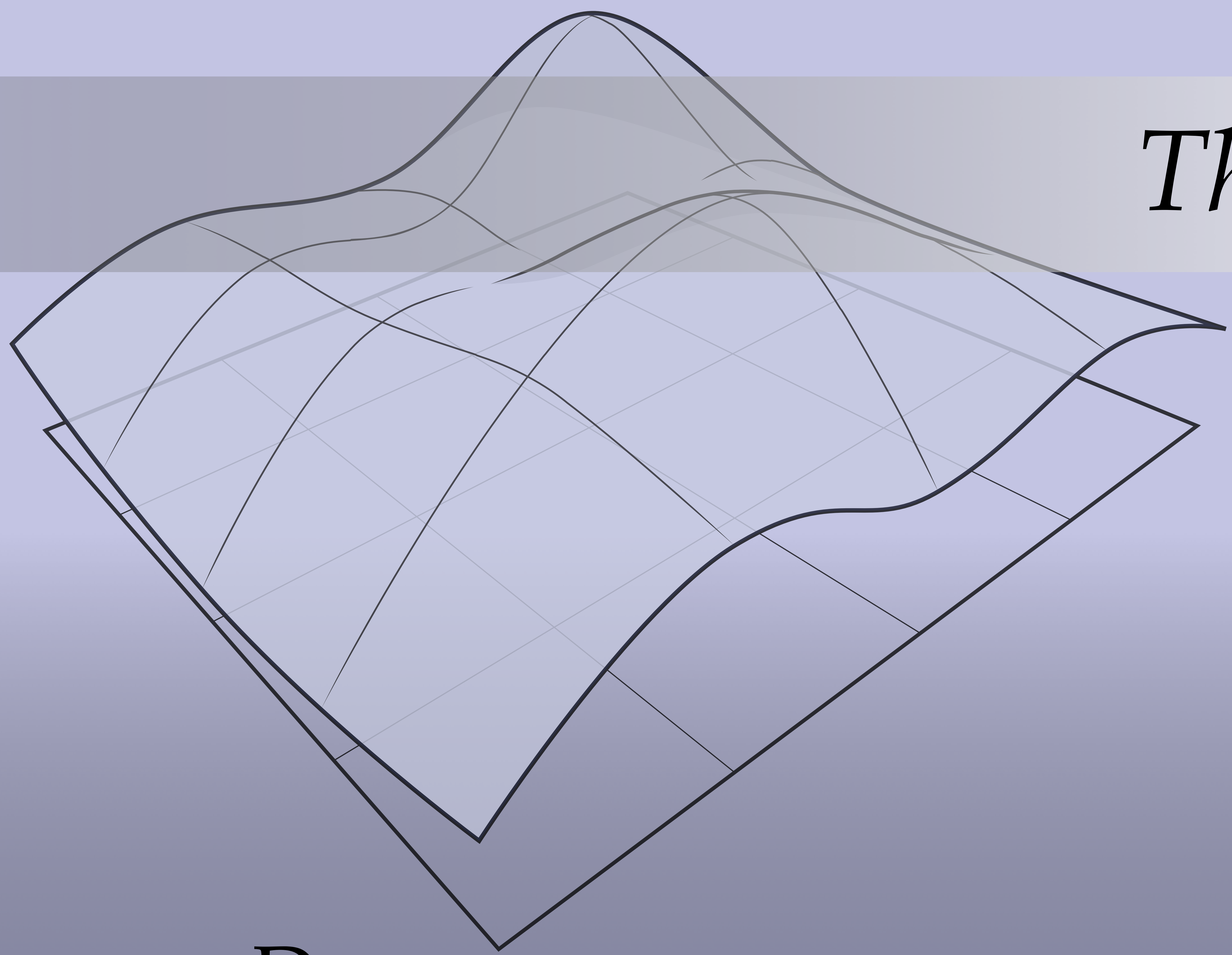

DISCRETE DIFFERENTIAL GEOMETRY:
AN APPLIED INTRODUCTION

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