Variational Time Integrators

Symposium on Geometry Processing Course 2015

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Time Integrator

Differential equations in time describe physical paths

Solve for these paths on the computer

Non-damped, Non-Driven Pendulum

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Differential equations in time describe physical paths

Solve for these paths on the computer

Non-damped, Non-Driven Pendulum

Methods of Time Integration

Non-damped, Non-Driven Pendulum

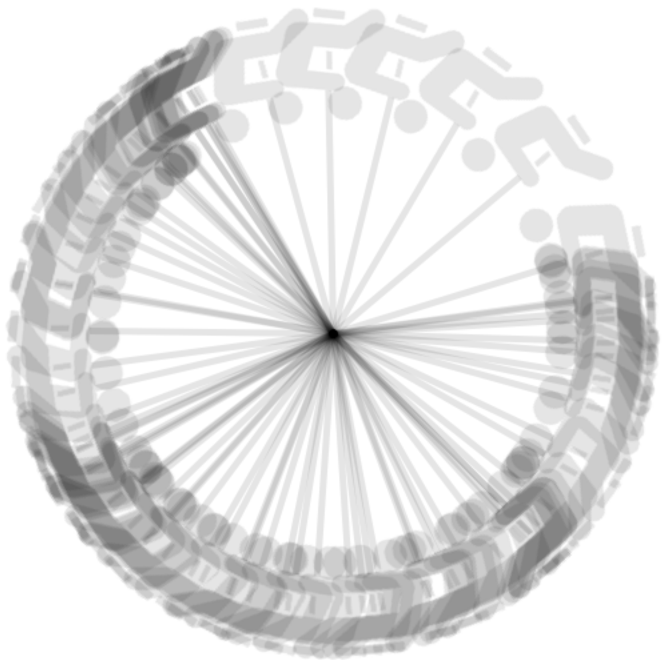
Explicit — "artificial driving"

Variational — "reasonable"

Implicit — "artificial damping"

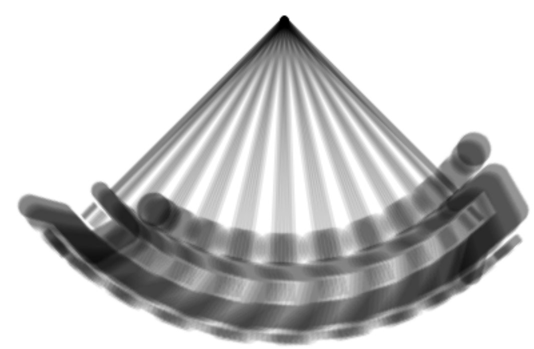
Methods of Time Integration

Non-damped, Non-Driven Pendulum



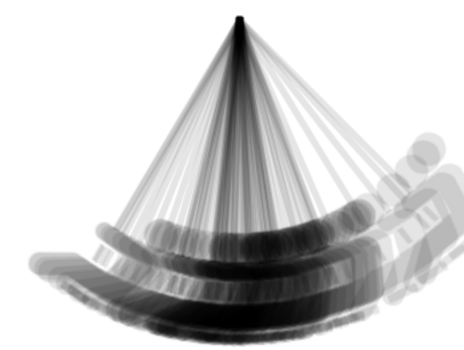
Explicit

“artificial driving”



Variational

“reasonable”



Implicit

“artificial damping”

Part One:
Reinterpreting Newtonian Mechanics
(what does "variational" mean?)

Part Two:
Why Use Variational Integrators?

A Butchering of Feynman's Lecture

http://www.nobelprize.org/nobel_prizes/physics/laureates/1965/feynman-bio.html

Principle of Least Action
(Feynman Lectures on Physics Volume II.19)

Newtonian Mechanics

Closed mechanical system $$q(t), \dot{q}(t)$$

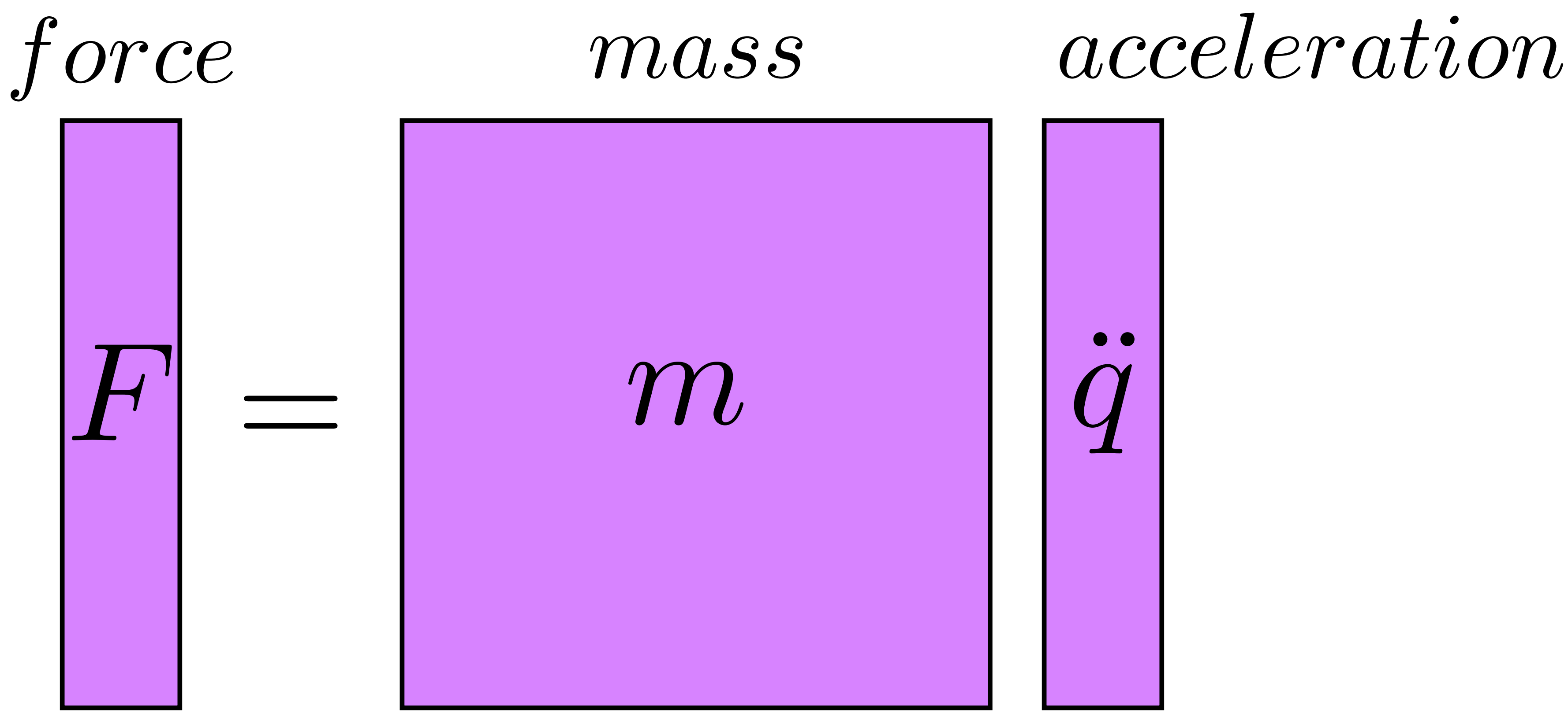
Kinetic energy $$T(\dot{q}) = \frac{1}{2} m \dot{q}^2$$

Potential energy $$U(q)$$

Total energy $$T(\dot{q}) + U(q)$$

Newtonian Mechanics

A physical path satisfies the vector equation



Worked out using force balancing

Difficult to compute with Cartesian coordinates

Lagrangian Reformulation

Goal:

Derive Newton's equations from a scalar equation

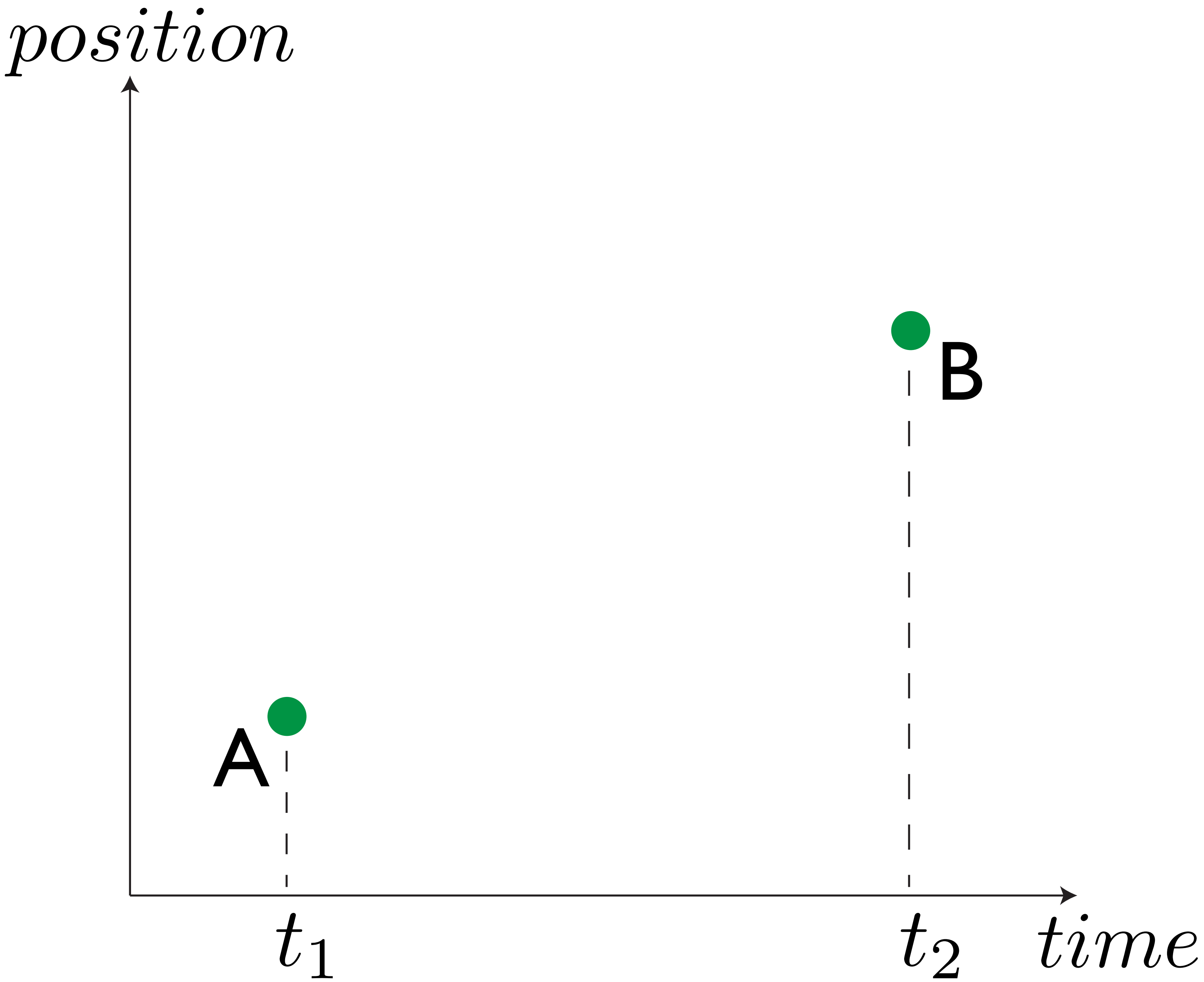
Why?

Works in every choice of coordinates

Highlights variational structure of mechanics

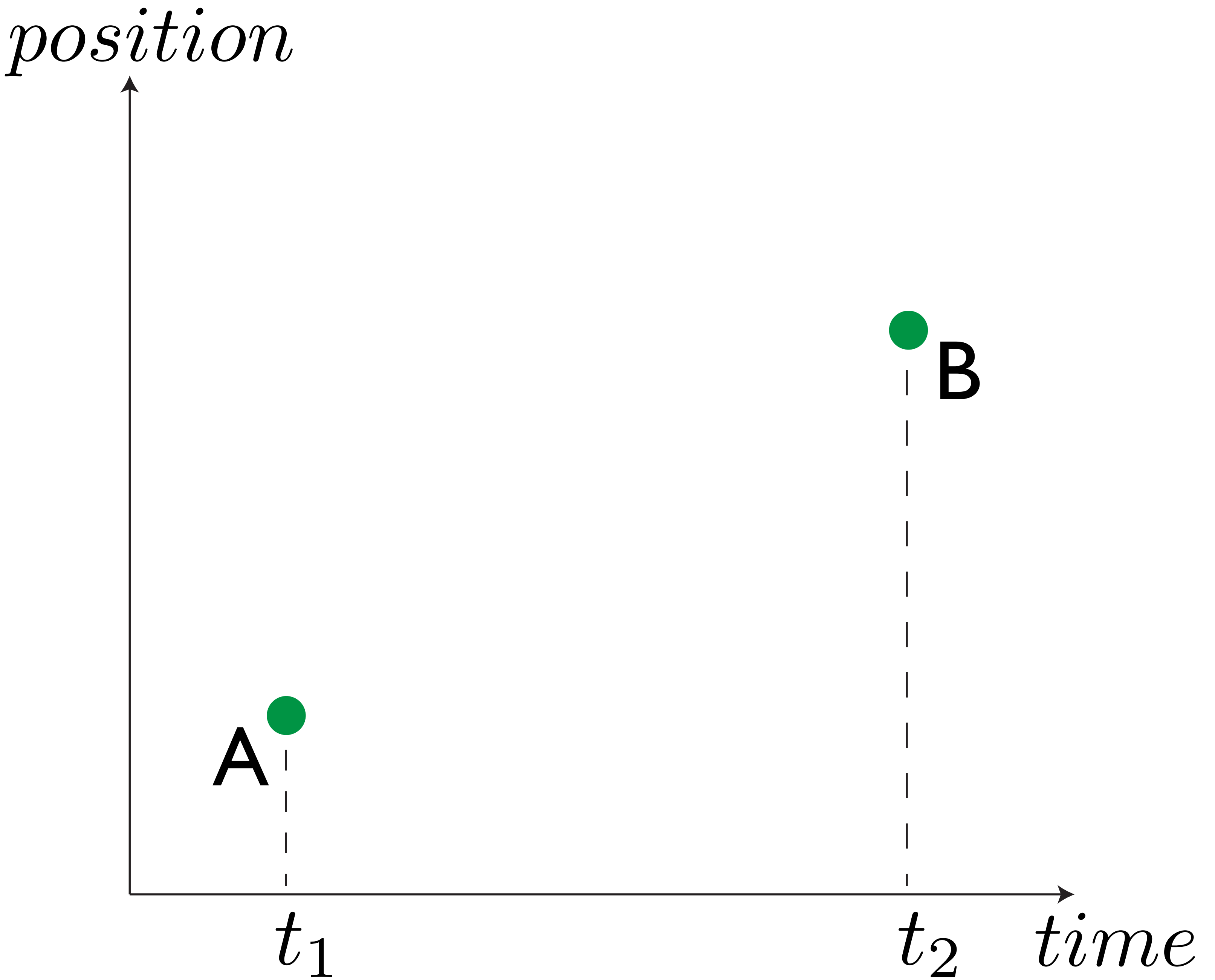
Energy is easy to write down

Particle in a Gravitational Field



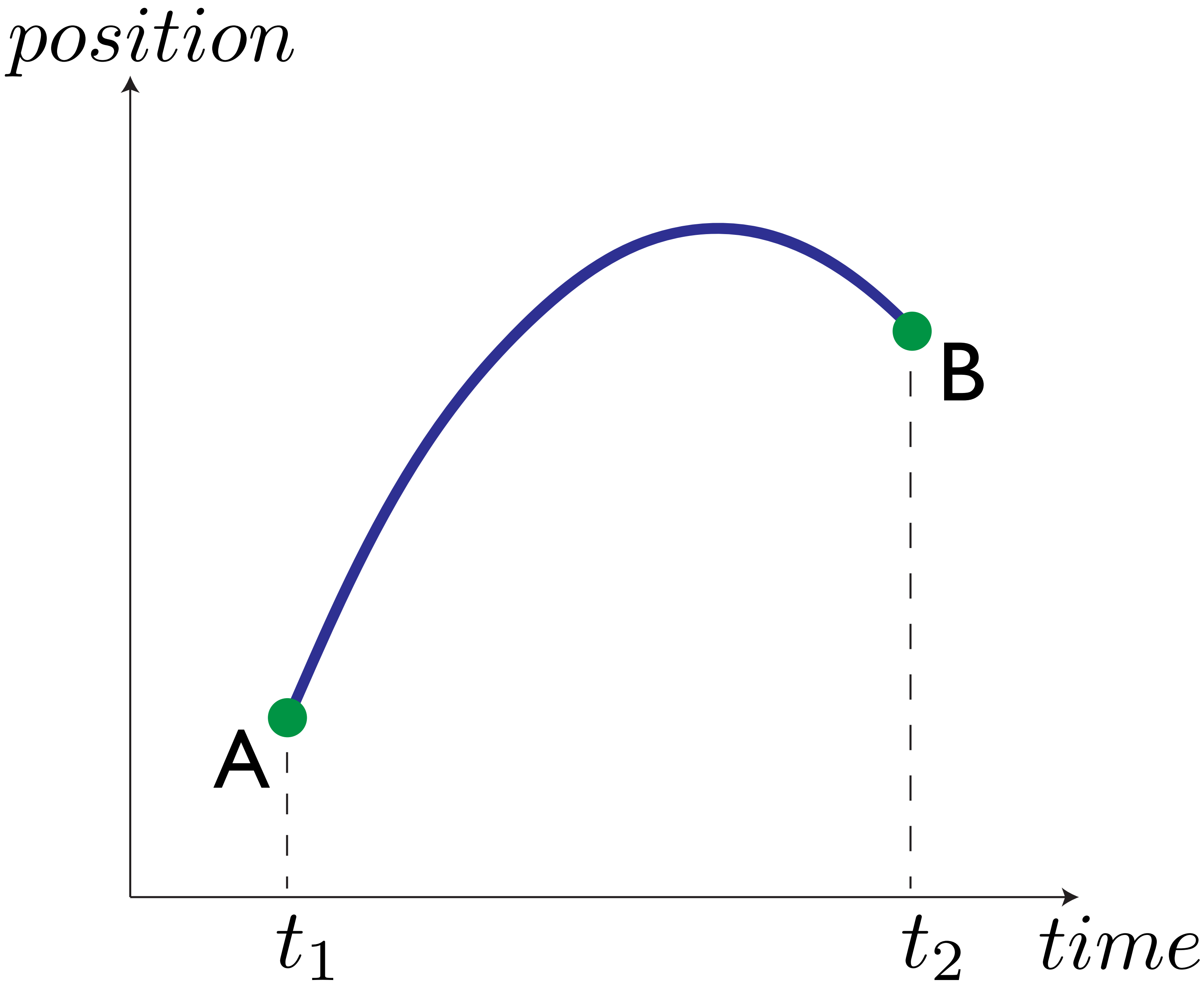
"Throw a ball in the air from (t_1, A) catch at (t_2, B)"

Particle in a Gravitational Field



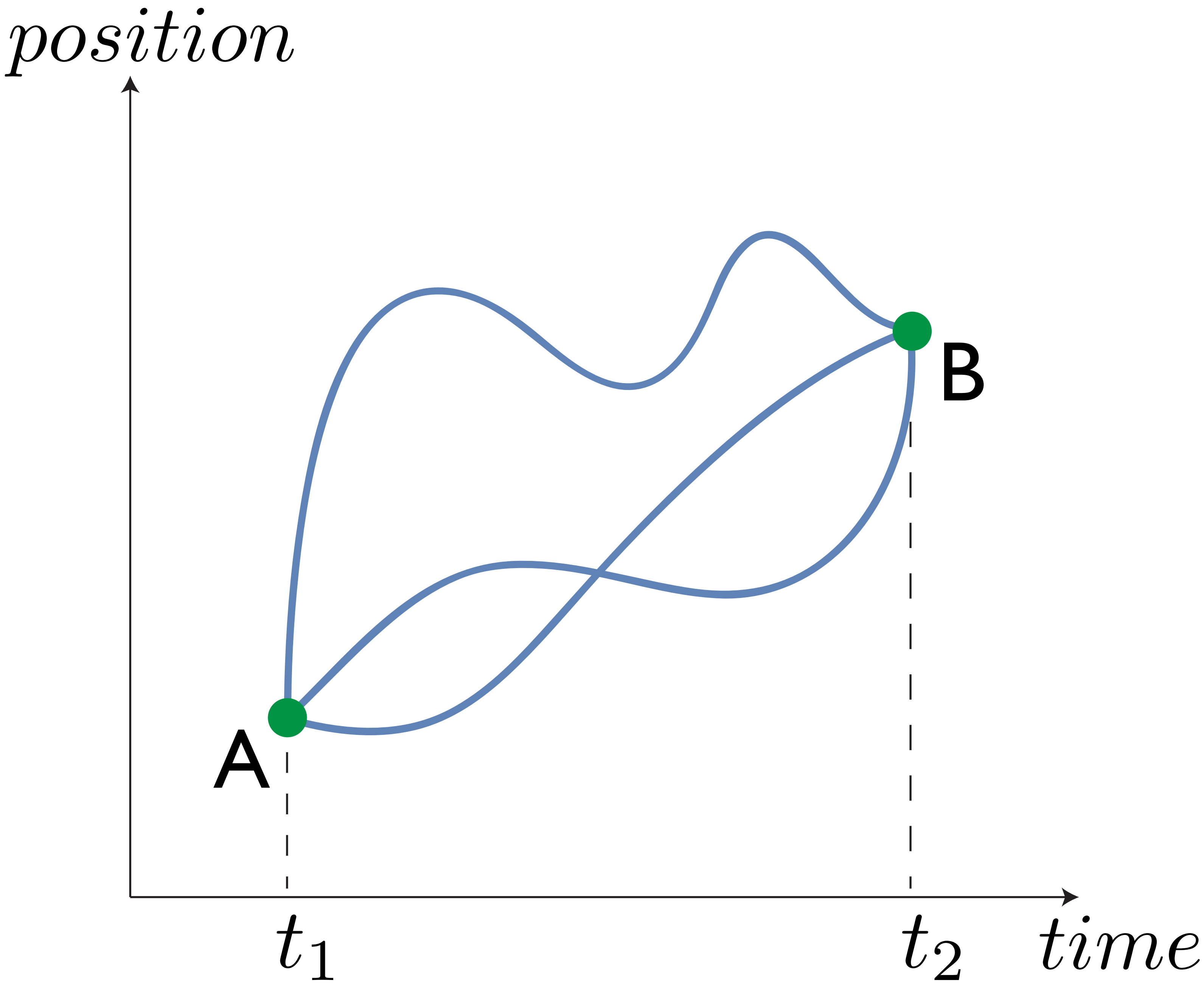
What path does the ball take to get from A to B in a given amount of time?

Particle in a Gravitational Field



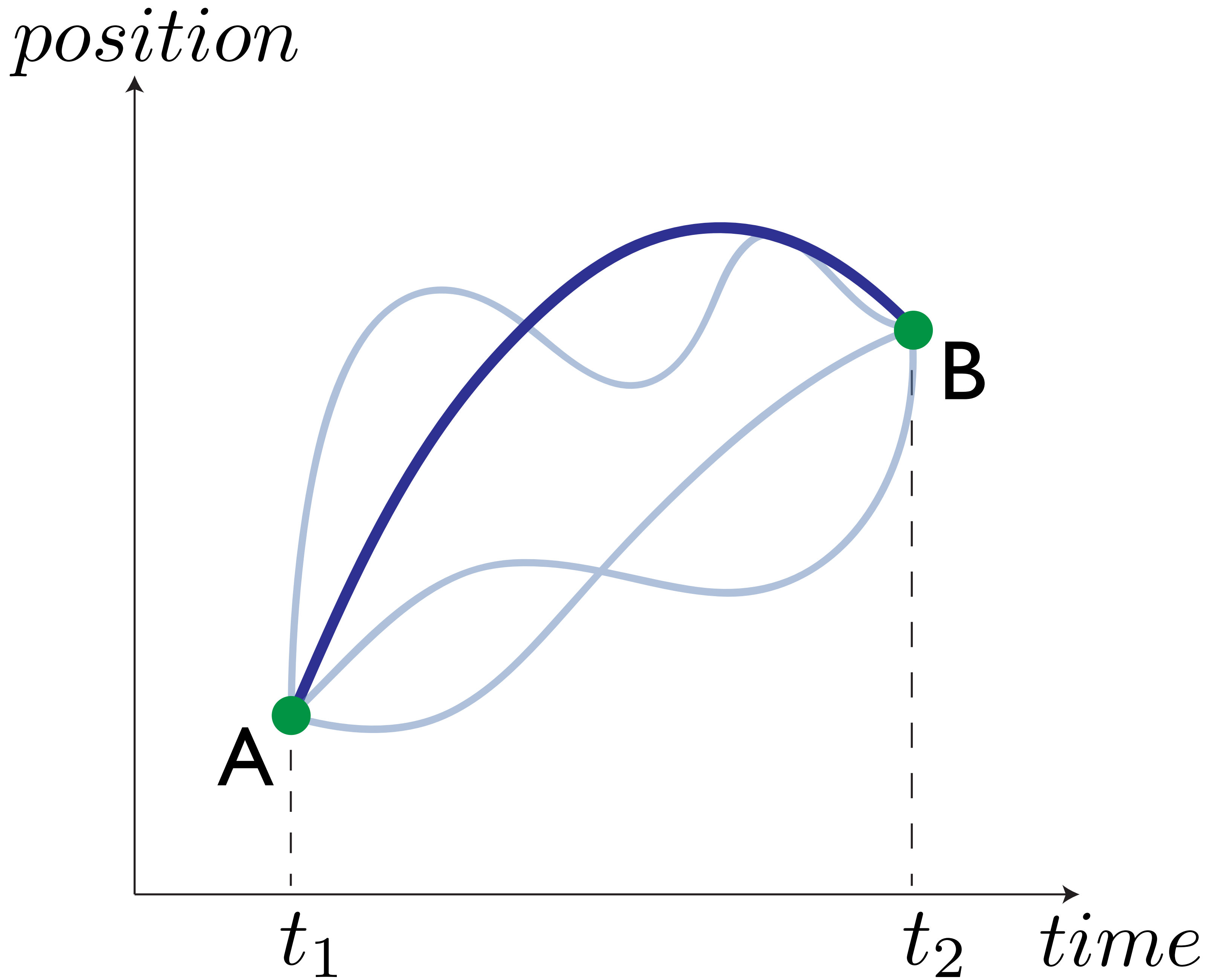
Physical path is unique and a parabola

Particle in a Gravitational Field



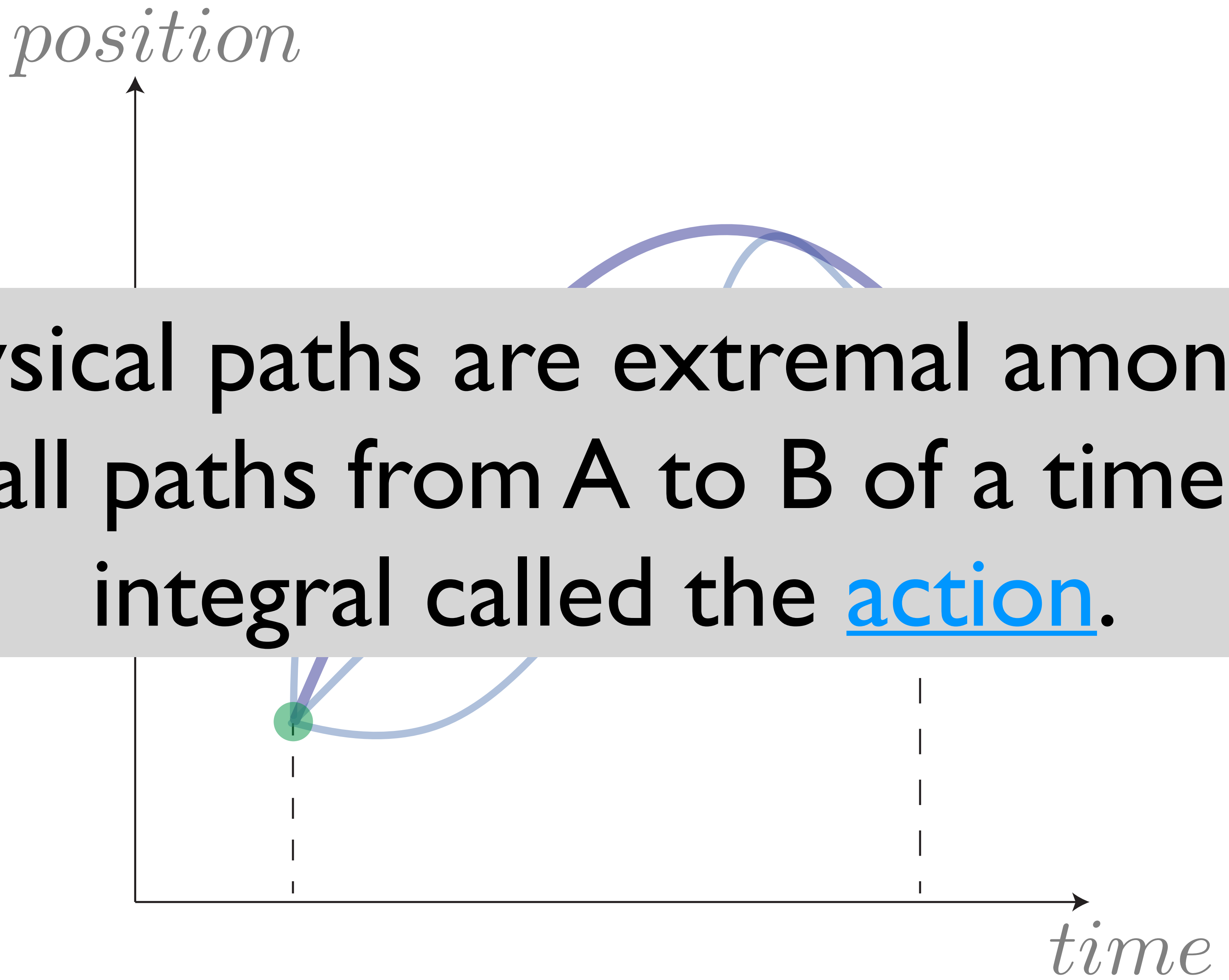
...but there are many possible paths

Particle in a Gravitational Field



How are physical paths special among all paths from A to B?

Hamilton's Principle of Stationary Action



Physical paths are extremal amongst all paths from A to B of a time integral called the action.

Hamilton's Principle of Stationary Action

Physical paths are extrema of a time integral called the action

$$\int_{t_1}^{t_2} \underbrace{T(\dot{q}) - U(q)}_{\substack{\text{Lagrangian} \\ \mathcal{L}(q,\dot{q})}} \, dt$$

(Lagrangian is not the total energy $T(\dot{q}) + U(q)$)

Hamilton's Principle of Stationary Action

Physical paths extremize the action

$$S = \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q})\, dt$$

$$\mathcal{L}(q, \dot{q}) = T(\dot{q}) - U(q)$$

...but how we find an extremal path in the space of all paths?

Use Lagrange's variational calculus

Finding an Extremal Path

1. Action of path

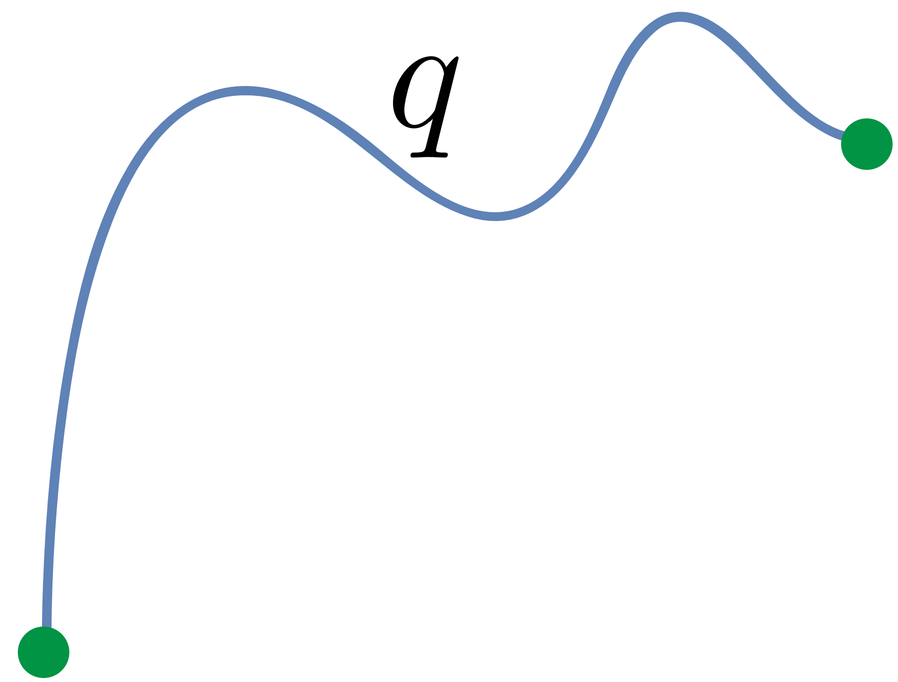
$$S(q)$$

2. Differentiate action

$$\delta S(q)$$

3. Study when

$$\delta S(q) = 0$$



Analogous to regular calculus

Defining the Variation of an Action

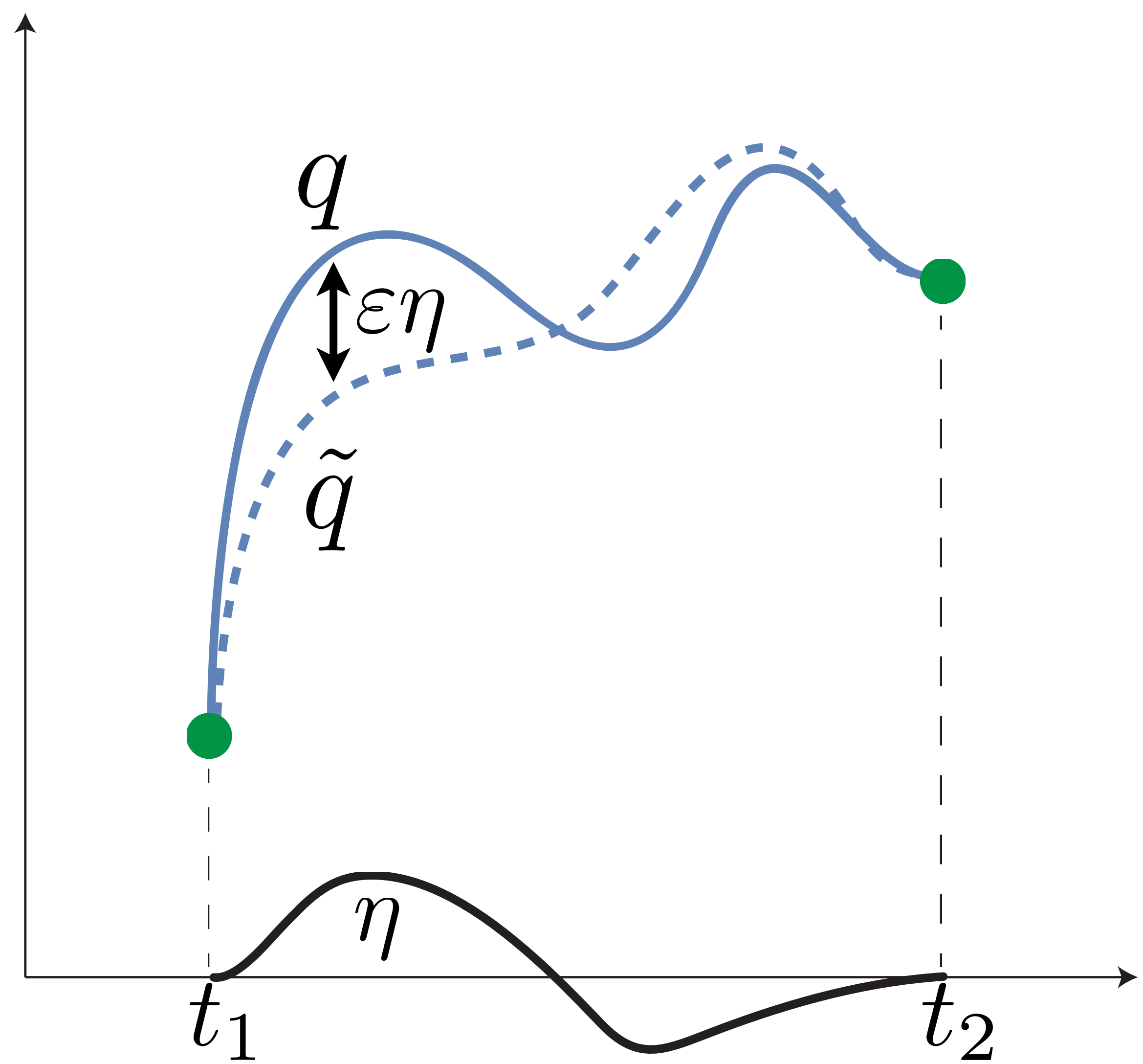
Arbitrary smooth offset $\eta(t)$

Perturbed curve

$$\tilde{q}(t) = q(t) + \varepsilon\eta(t)$$

Curves share endpoints

$$\eta(t_1) = \eta(t_2) = 0$$

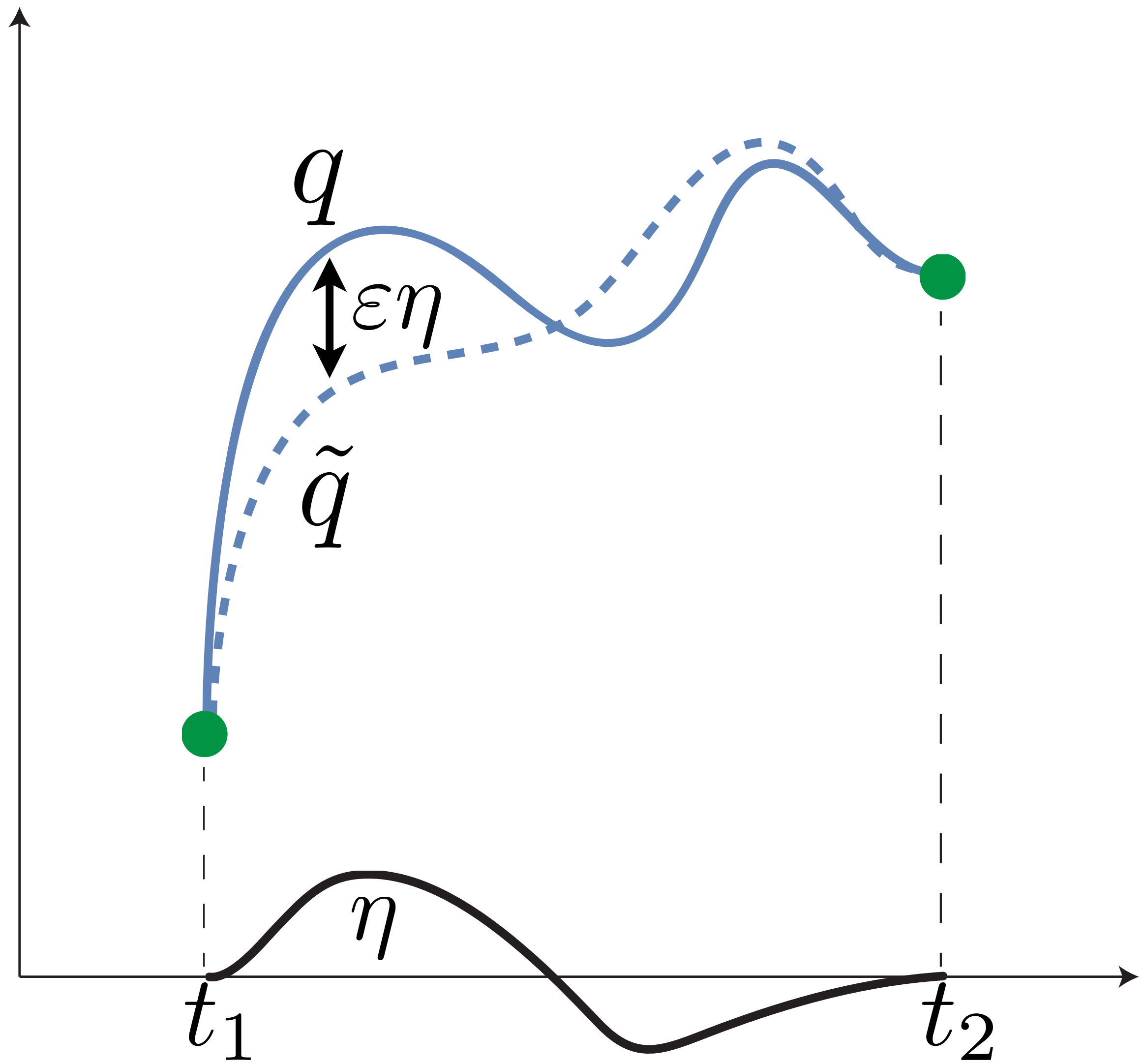


Defining the Variation of an Action

First Variation of the Action (in direction eta)

$$\delta_\eta S(q) := \frac{d}{d\varepsilon} S(q + \varepsilon\eta)\Big|_{\varepsilon=0}$$

Reduce to single variable calculus!



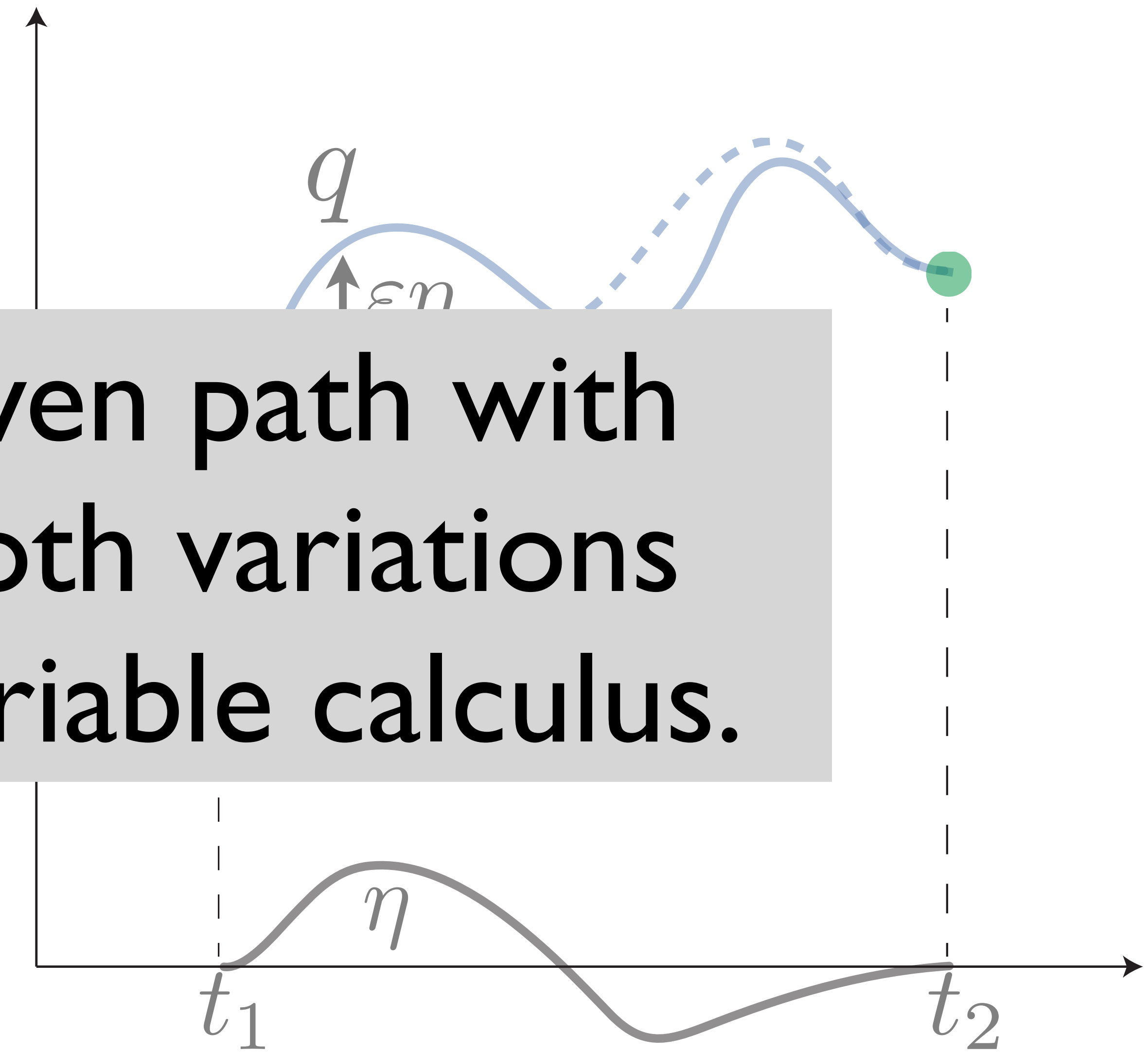
Defining the Variation of an Action

First Variation of the Action (in direction eta)

$\delta_\eta S(q$

Differentiating a given path with respect to all smooth variations reduces to single variable calculus.

Reduce to single variable calculus!

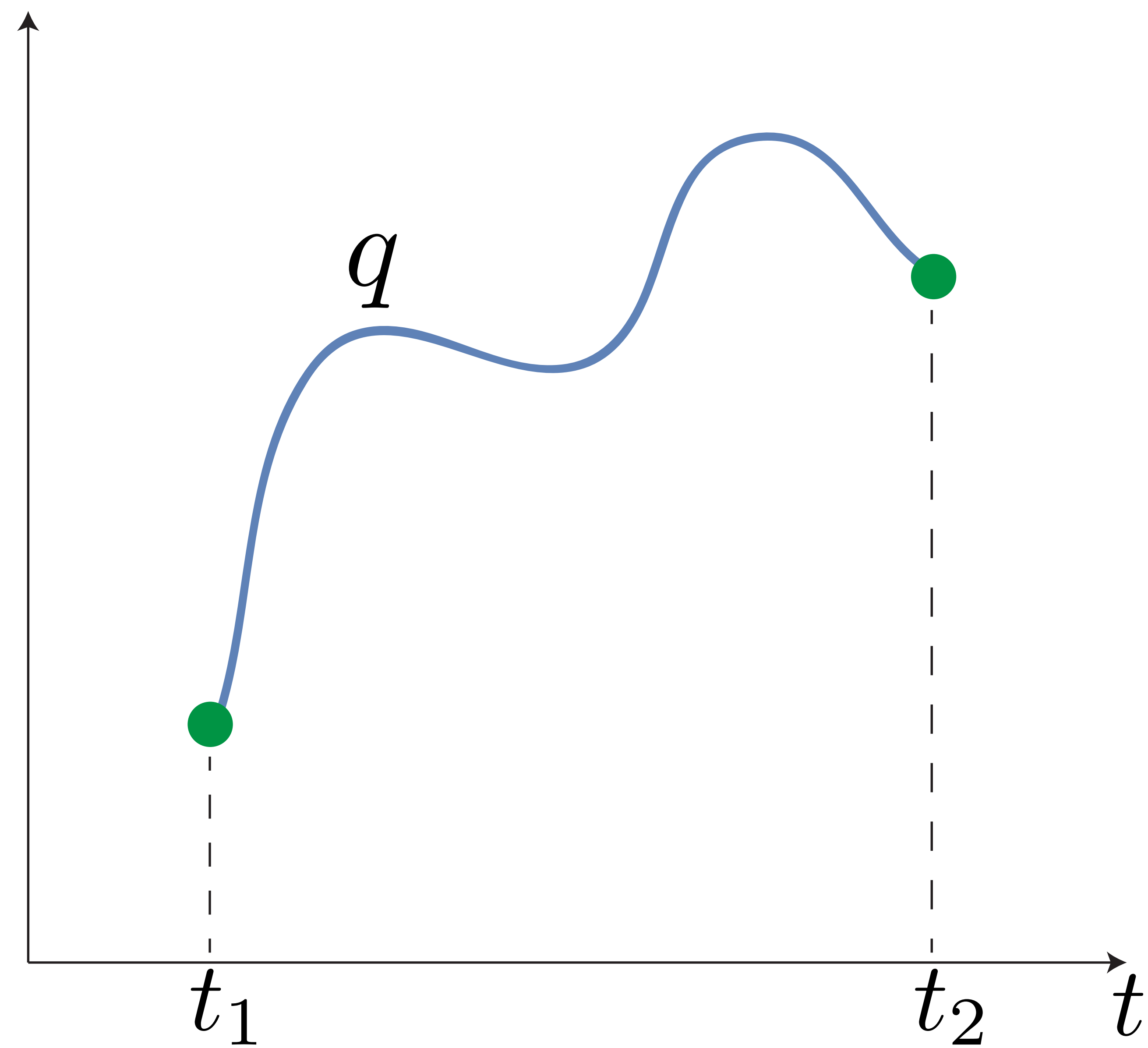


Particle Example: Setup

$$mass = 1$$

$$T(\dot{q}) = \frac{\dot{q}^2}{2}$$

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



$$S(q) = \int_{t_1}^{t_2} \frac{\dot{q}(t)^2}{2} - U(q(t))\, dt$$

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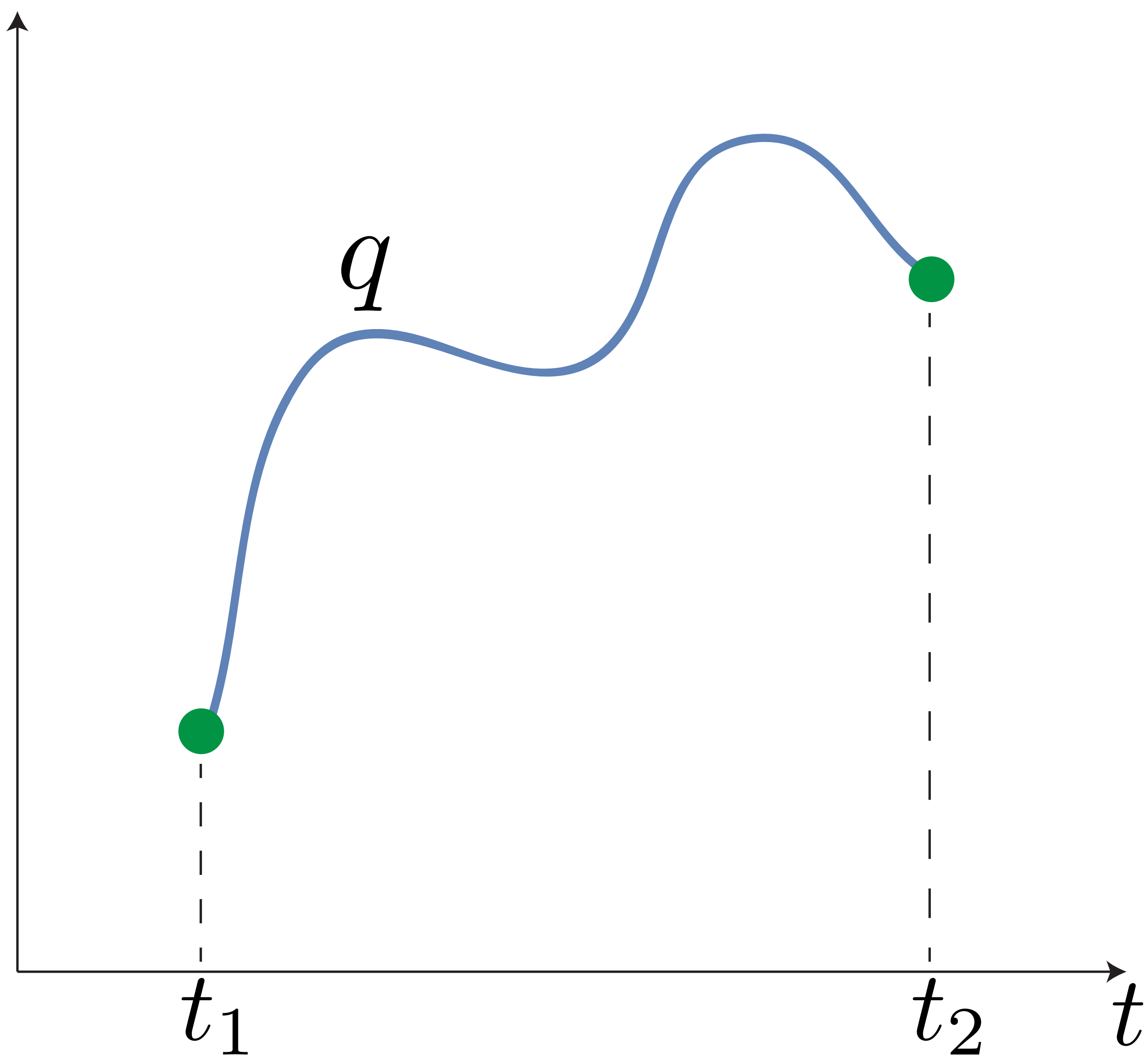

$$S(q) = \int_{t_1}^{t_2} \frac{\dot{q}(t)^2}{2} - U(q(t))\,dt$$

Particle Example: Investigating the Variation

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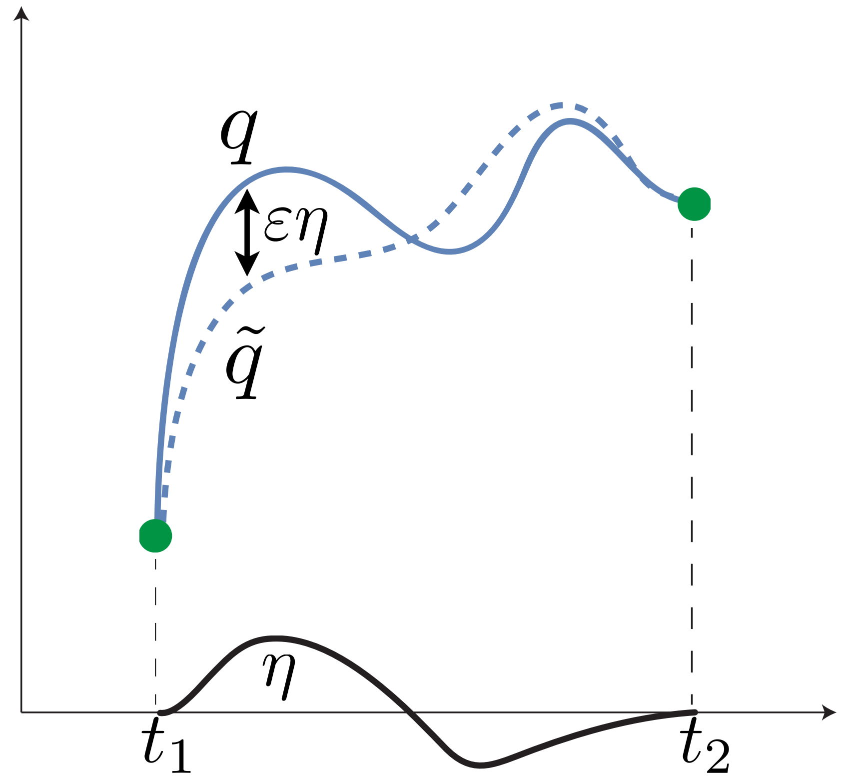

$$\delta_\eta S(q) = \frac{d}{d\varepsilon} S(q + \varepsilon\eta)\Big|_{\varepsilon=0}$$

$$= \int_{t_1}^{t_2} \frac{d}{d\varepsilon} \left(\frac{(\dot{q} + \varepsilon\dot{\eta})^2}{2} - U(q + \varepsilon\eta) \right) \Big|_{\varepsilon=0} dt$$

$$= \int_{t_1}^{t_2} (\dot{q} + \varepsilon\dot{\eta})\dot{\eta} - U'(q + \varepsilon\eta)\eta \Big|_{\varepsilon=0} dt$$

$$= \int_{t_1}^{t_2} \dot{q}(t)\dot{\eta}(t) - U'(q(t))\eta(t)\, dt$$

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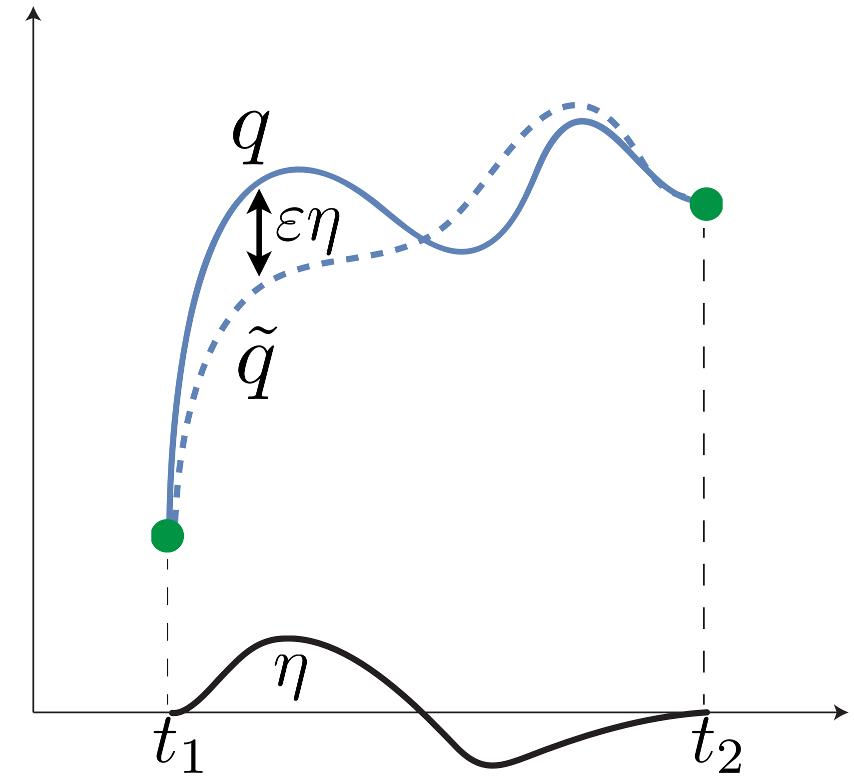

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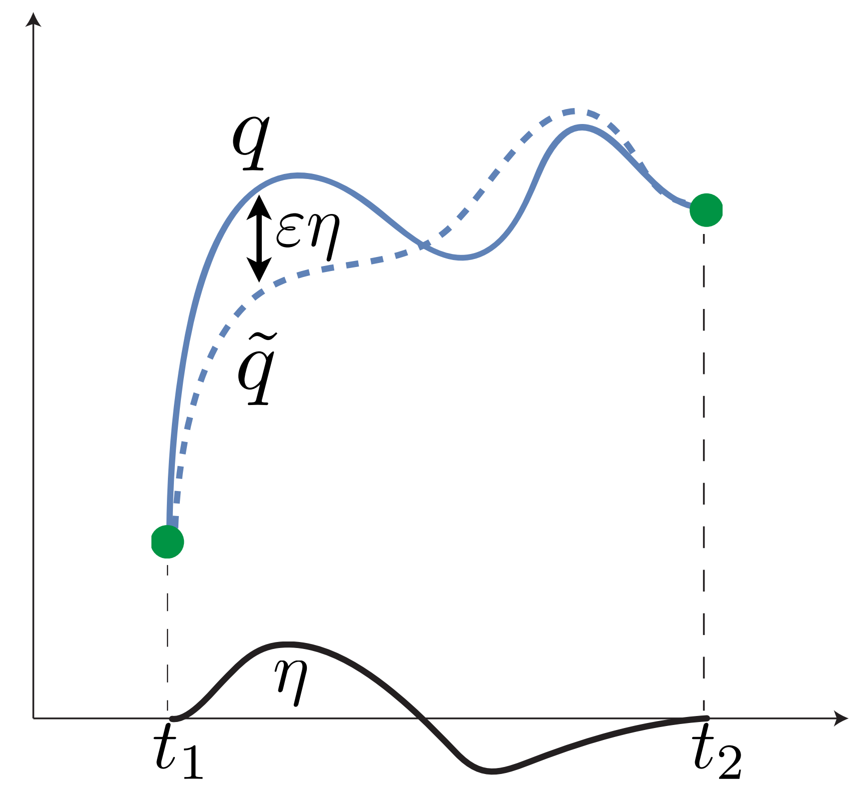

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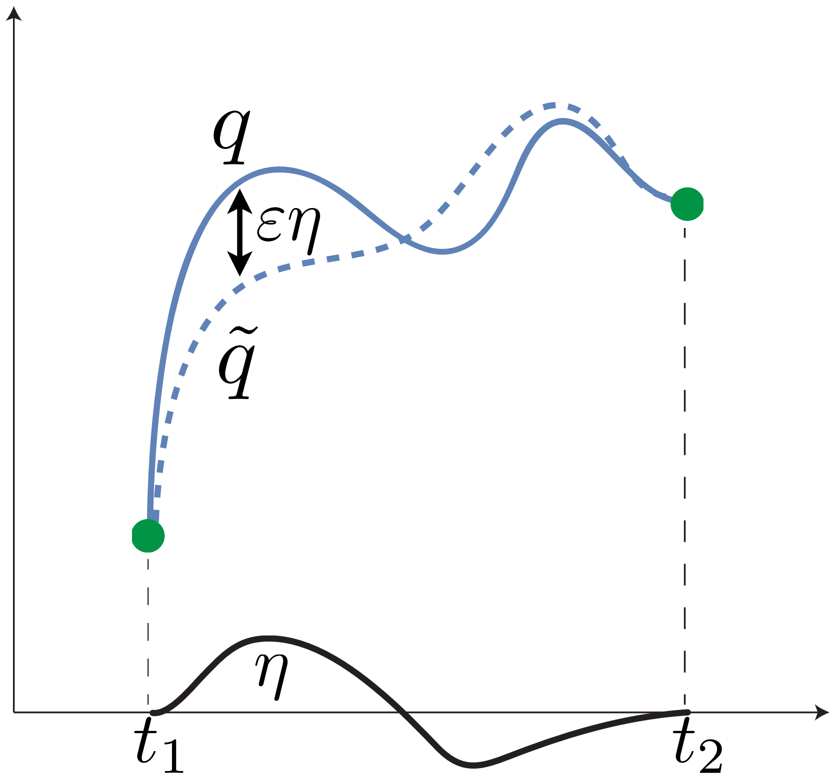

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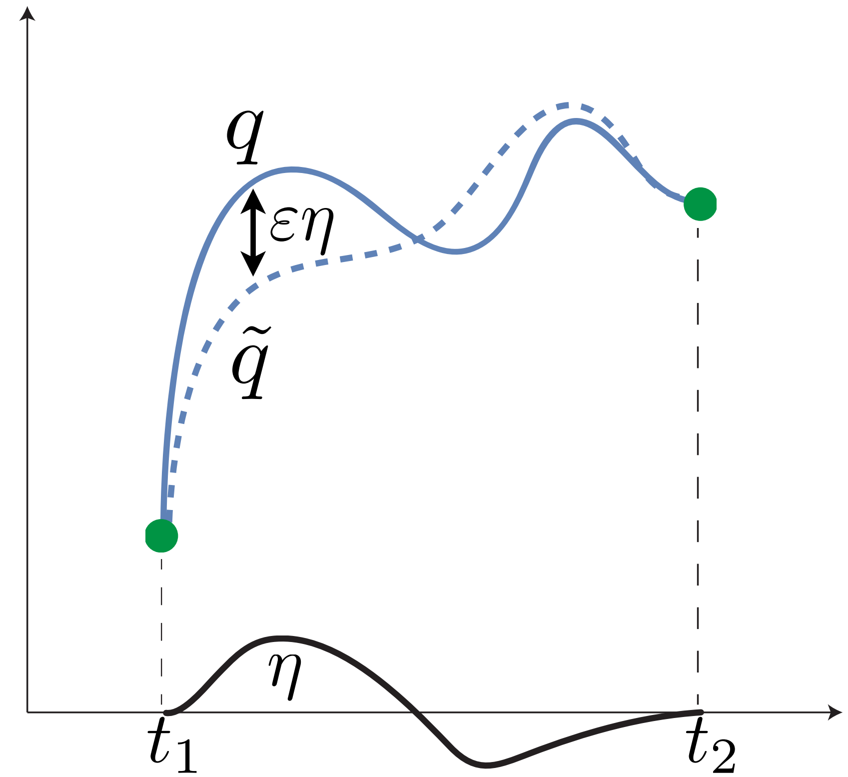

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Variational Trick: Essential Integration by Parts

$$\delta_\eta S(q) = \int_{t_1}^{t_2} \dot{q}(t)\dot{\eta}(t) - U'(q(t))\eta(t)\, dt$$

$$\int_{t_1}^{t_2} \dot{q}(t)\dot{\eta}(t)dt = \dot{q}(t)\eta(t)\Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \ddot{q}(t)\eta(t)\, dt$$

$$\delta_\eta S(q) = -\int_{t_1}^{t_2} (\ddot{q}(t) + U'(t))\eta(t)dt$$

Variational Trick: Essential Integration by Parts

$$\delta_\eta S(q) = \int_{t_1}^{t_2} \dot{q}(t)\dot{\eta}(t) - U'(q(t))\eta(t)\,dt$$

get rid of derivates of the offset

$$\int_{t_1}^{t_2} \dot{q}(t)\dot{\eta}(t)dt = \dot{q}(t)\eta(t)\Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \ddot{q}(t)\eta(t)\,dt$$

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0

recall offset vanishes at endpoints

$$\delta_\eta S(q) = -\int_{t_1}^{t_2} (\ddot{q}(t) + U'(t))\eta(t)dt$$

Variational Trick: Essential Integration by Parts

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$$\int_{t_1}^{t_2} \dot{q}(t)\dot{\eta}(t) dt = \dot{q}(t)\eta(t)\Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \ddot{q}(t)\eta(t)\, dt$$

$$\dot{q}(t)\eta(t)\Big|_{t_1}^{t_2} \rightarrow 0$$

recall offset vanishes at endpoints

$$\delta_\eta S(q) = -\int_{t_1}^{t_2} (\ddot{q}(t) + U'(t))\eta(t) dt$$

Variational Trick: Essential Integration by Parts

$$\delta_\eta S(q) = \int_{t_1}^{t_2} \dot{q}(t)\dot{\eta}(t) - U'(q(t))\eta(t)\, dt$$

Integrate by parts to get rid of the derivatives of the smooth offset. This requires the offset to vanish at the boundary.

$$\delta_\eta S(q) = -\int_{t_1}^{t_2} (\ddot{q}(t) + U'(t))\eta(t) dt$$

Particle Example: Investigating the Variation

$$\delta_\eta S(q) = -\int_{t_1}^{t_2} (\ddot{q}(t) + U'(q(t)))\eta(t)\, dt$$

When is $\delta_\eta S(q) = 0$ for all offsets η?

Fundamental Lemma of Variational Calculus

For a continuous function G if

$$\int_{t_1}^{t_2} G(t)\eta(t)\,dt = 0$$

for all smooth functions $\eta(t)$ with $\eta(t_1) = \eta(t_2) = 0$,

then G vanishes everywhere in the interval.

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then G vanishes everywhere in the interval.

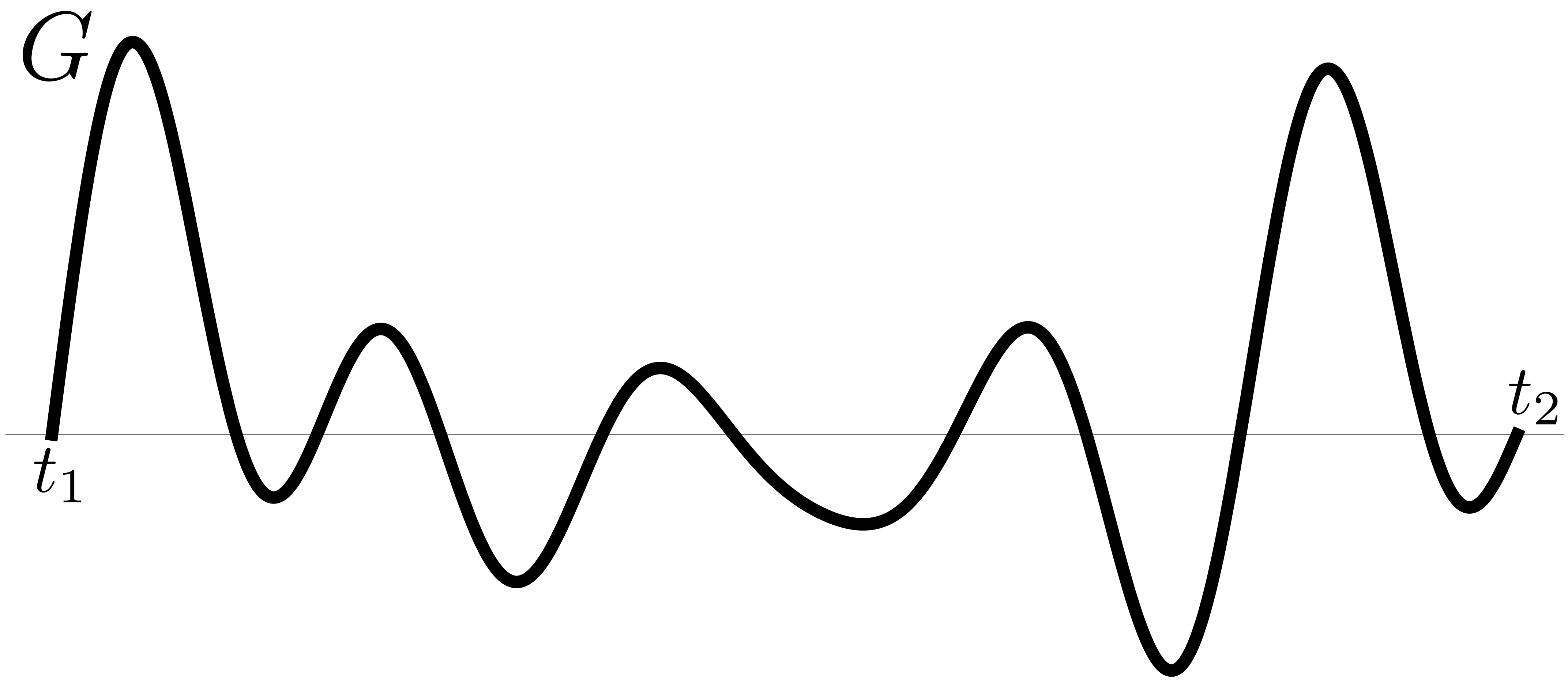
...believable, but why?

Fundamental Lemma of Variational Calculus

If $\int_{t_1}^{t_2} G(t)\eta(t)\, dt = 0$ for all offsets $\eta(t)$ zero at t_1, t_2

then G vanishes on the interval.

Assume



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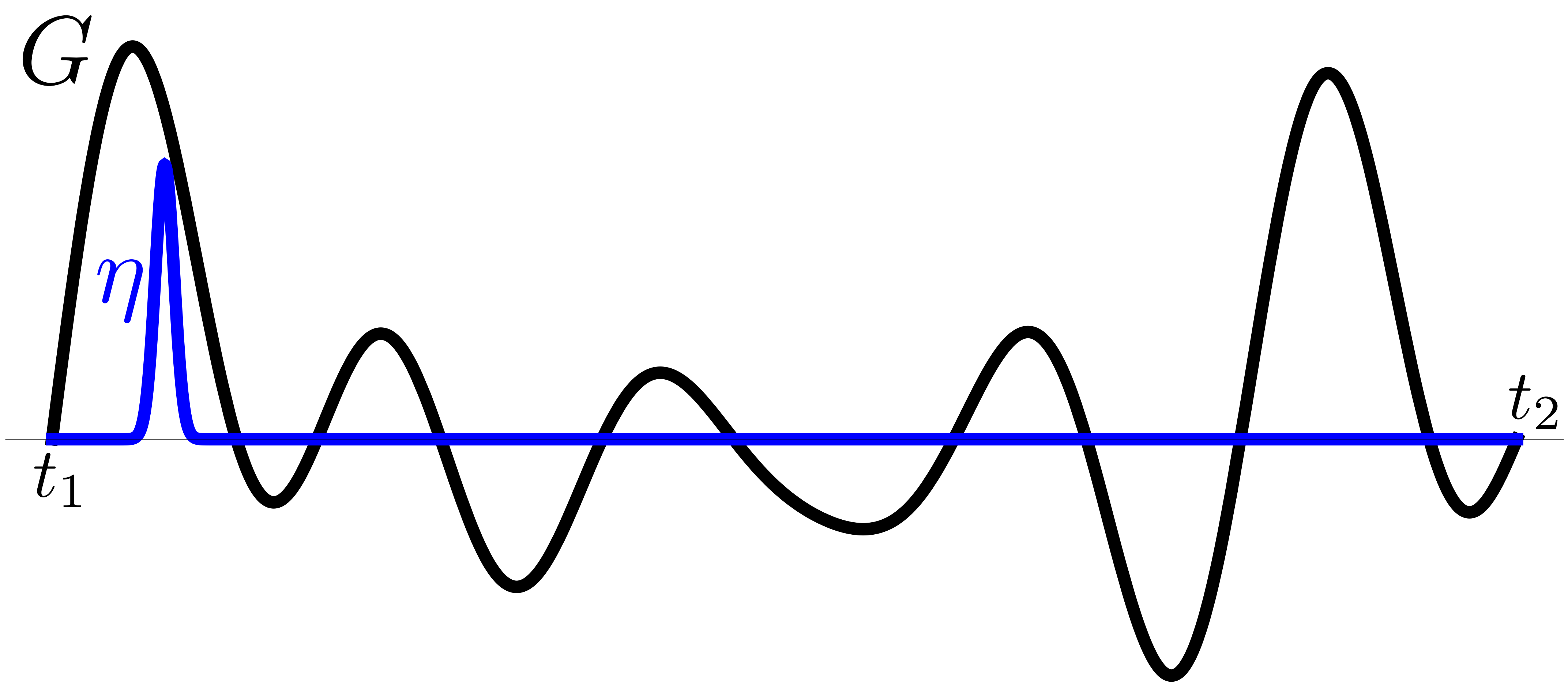

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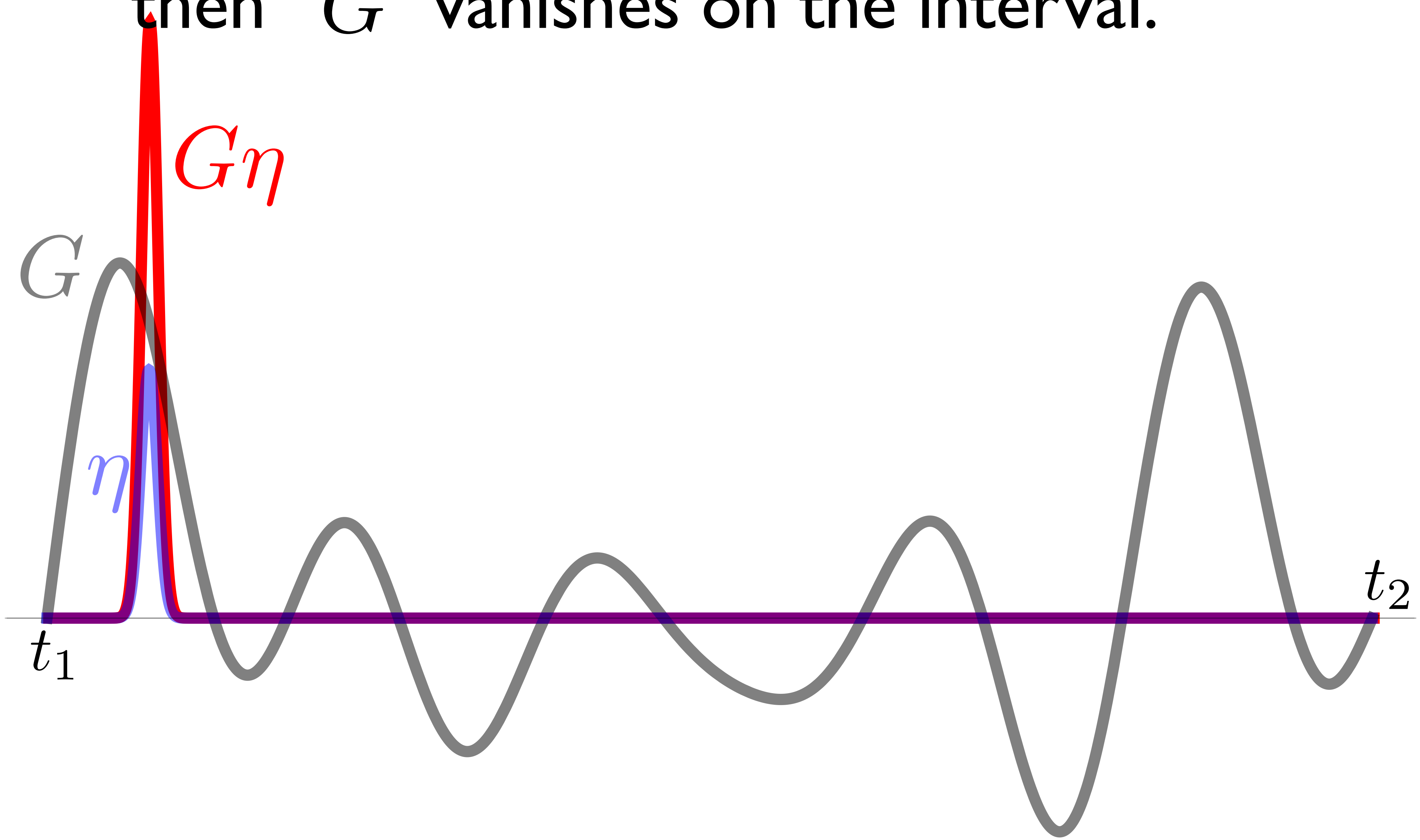

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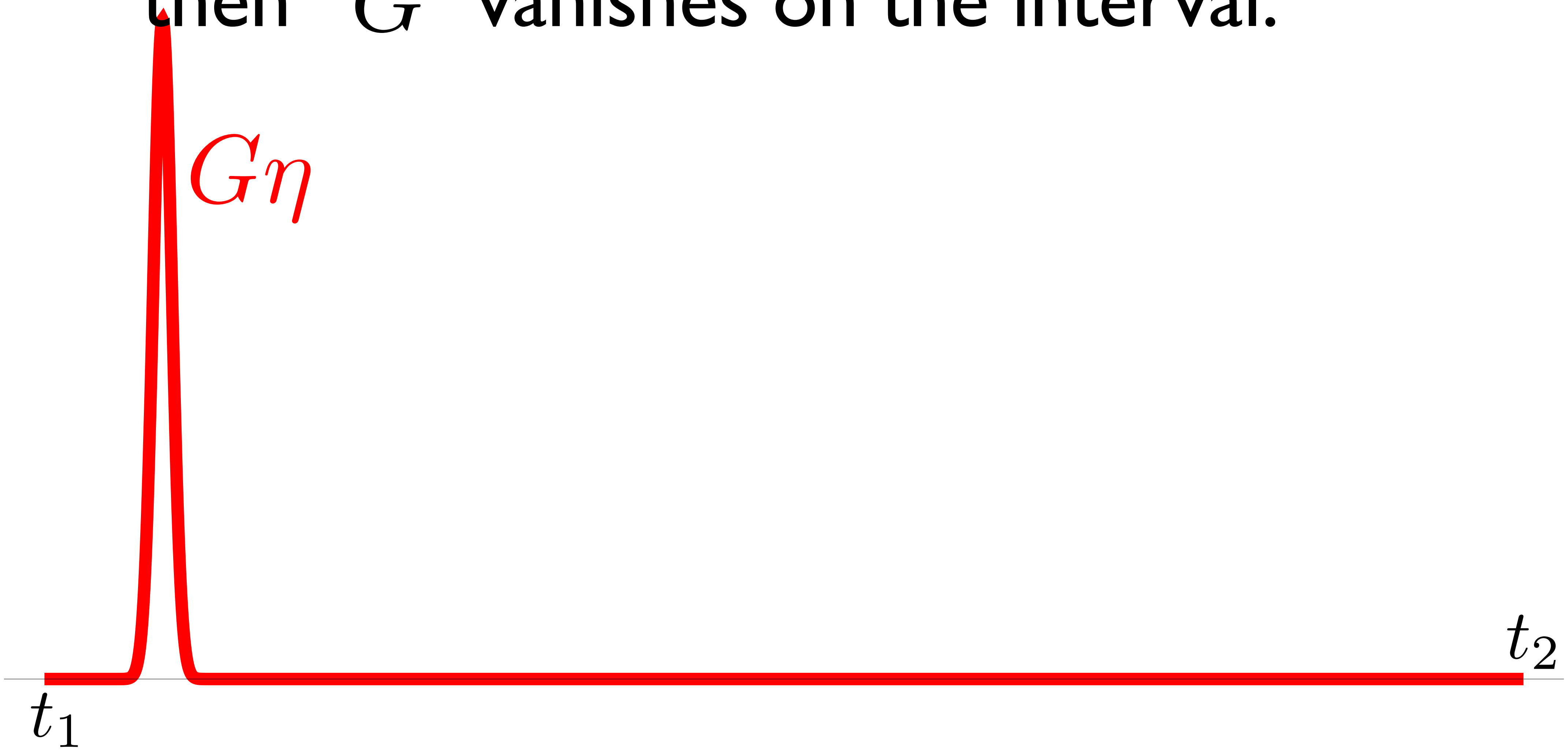

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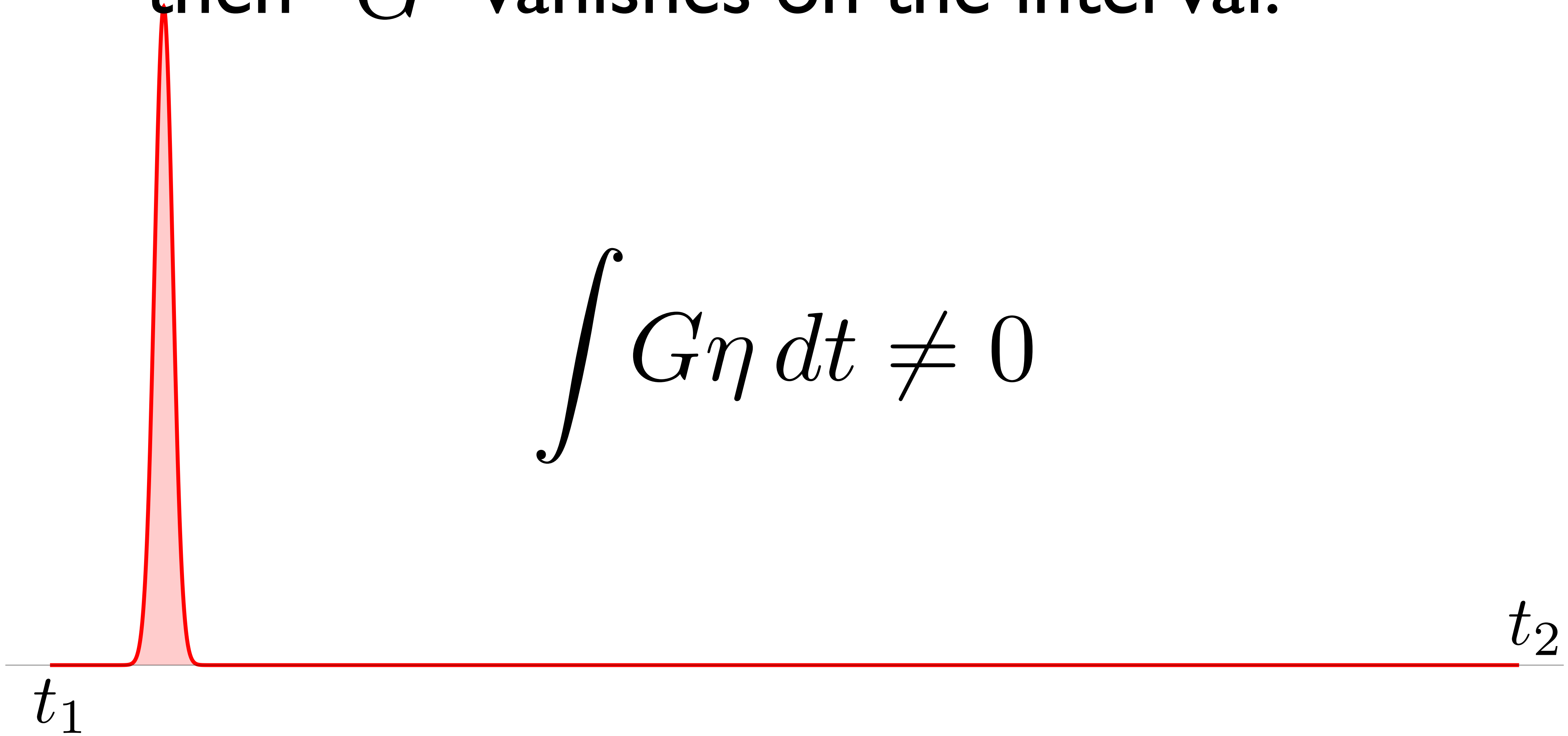


$$\int G\eta\,dt \neq 0$$

Fundamental Lemma of Variational Calculus

If $\displaystyle\int_{t_1}^{t_2} G(t)\eta(t)\, dt = 0$ for all offsets $\eta(t)$ zero at t_1, t_2

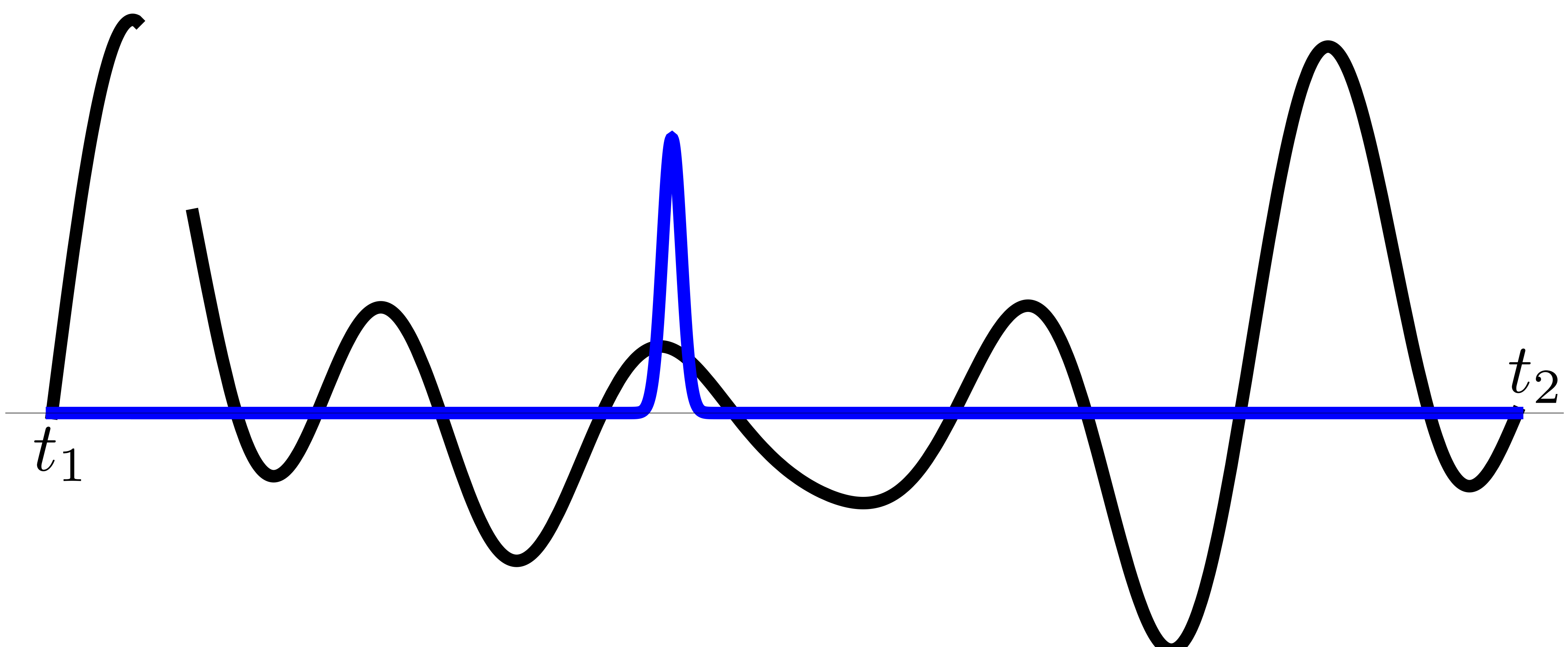
then G vanishes on the interval.

G must be zero where η is nonzero

Fundamental Lemma of Variational Calculus

If $\int_{t_1}^{t_2} G(t)\eta(t)\,dt = 0$ for all offsets $\eta(t)$ zero at t_1, t_2

then G vanishes on the interval.



must hold for every choice of η

Fundamental Lemma of Variational Calculus

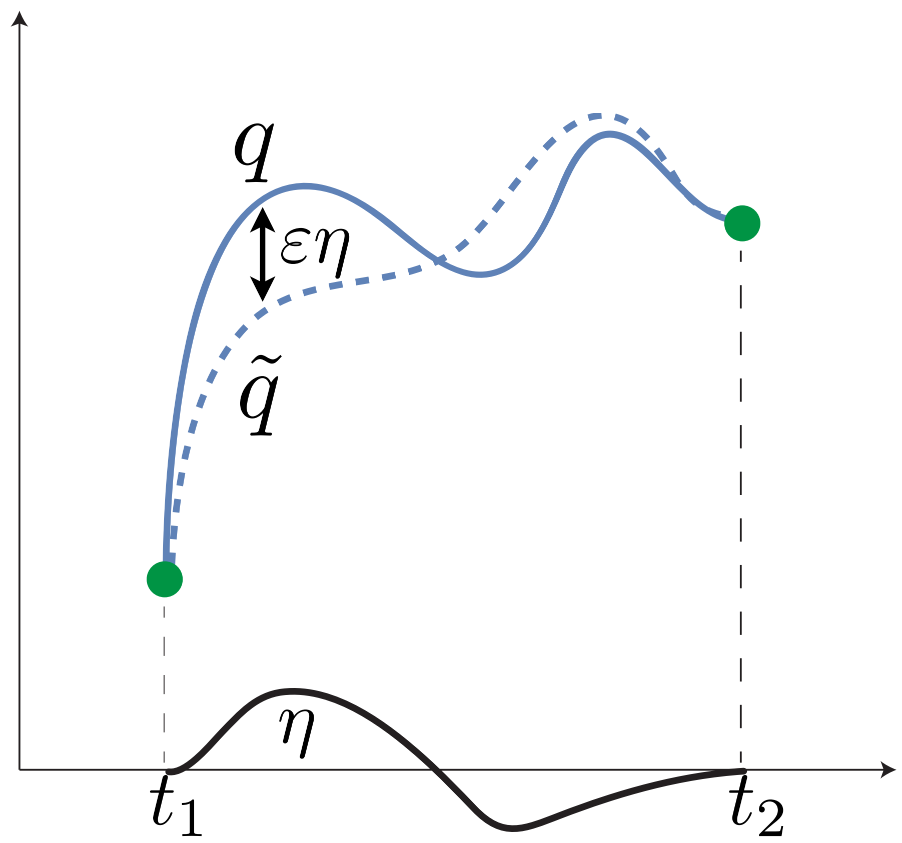
If $\int_{t_1}^{t_2} G(t)\eta(t)\,dt = 0$ for <u>all</u> offsets $\eta(t)$ zero at t_1, t_2

then G vanishes on the interval.

So G vanishes everywhere in the interval.

Particle Example: Deriving Euler-Lagrange Equations

Where were we?



$$\delta_\eta S(q) = -\int_{t_1}^{t_2} (\ddot{q}(t) + U'(q(t)))\eta(t)\, dt$$

When is $\delta_\eta S(q) = 0$ for all offsets η?

Particle Example: Deriving Euler-Lagrange Equations

$$\delta_\eta S(q) = -\int_{t_1}^{t_2} (\ddot{q}(t) + U'(q(t)))\eta(t)\,dt$$

Apply Fundamental Lemma

$$\delta_\eta S(q) = 0 \iff \underbrace{\ddot{q}(t) + U'(q(t)) = 0}$$

Euler-Lagrange equations

Particle Example: Deriving Euler-Lagrange Equations

$$\delta_\eta S(q) = -\int^{t_2} (\ddot{q}(t) + U'(q(t)))\eta(t)\, dt$$

Apply the Fundamental Lemma to see when the derivative vanishes

$$\delta_\eta S(q) = \int G(q, \dot{q}, \ddot{q})\eta\, dt = 0$$

and recover the Euler-Lagrange equations.

Euler-Lagrange Equations

Particle Example: Lagrangian Reformulation

$$\delta S(q) = 0 \iff \underbrace{\ddot{q}(t) + U'(q(t)) = 0}$$

Euler-Lagrange equations

Particle Example: Lagrangian Reformulation

$$\delta S(q) = 0 \iff \underbrace{\ddot{q}(t) + U'(q(t)) = 0}_{\text{Euler-Lagrange equations}}$$

Wait... this looks familiar!

Particle Example: Lagrangian Reformulation

$$\delta S(q) = 0 \iff \underbrace{\ddot{q}(t) + U'(q(t)) = 0}$$

Euler-Lagrange equations

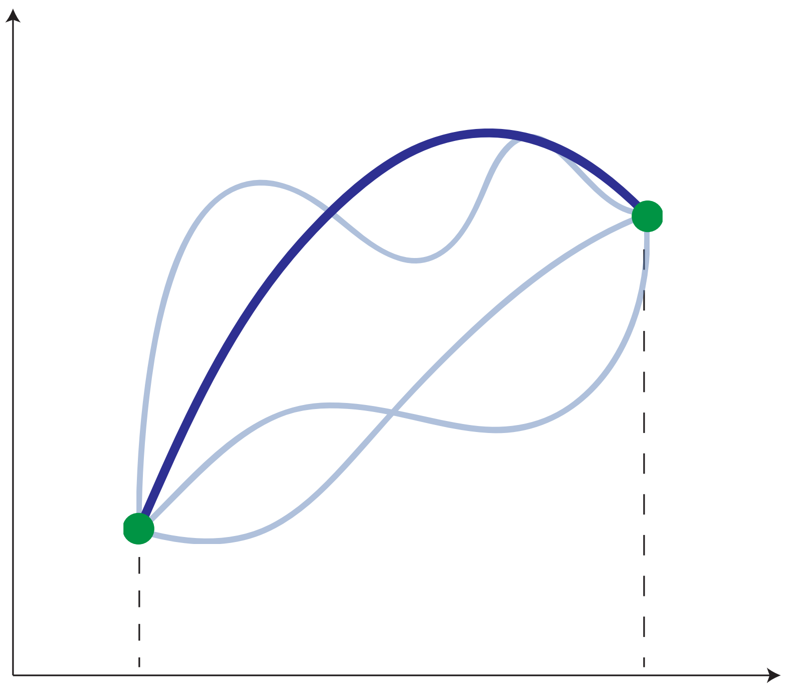
Wait... this looks familiar!

$m\,\ddot{q}(t) + U'(q(t)) = 0$ is Newton's law

(reinserting mass)

(force is derivative of potential energy)

Lagrangian Reformulation Summary



Principle of Stationary Action

A path connecting two points is a physical path precisely when the first derivative of the action is zero.

Lagrangian

$$\mathcal{L}(q, \dot{q}) = T(\dot{q}) - U(q)$$

Action

$$S = \int_{t_1}^{t_2} \mathcal{L}(q(t), \dot{q}(t))\, dt$$

Euler-Lagrange Equations

$$\delta S(q) = 0 \iff F = m\ddot{q}$$

Fundamental Lemma

(general) Principle of Stationary Action

"Variational principles" apply to many systems, e.g., special relativity, quantum mechanics, geodesics, etc.

Key is to find Lagrangian $\mathcal{L}(t, q(t), \dot{q}(t))$

$$\delta S(q) = 0 \iff \frac{d\mathcal{L}(t,q,\dot{q})}{dq} - \frac{d}{dt}(\frac{d\mathcal{L}(t,q,\dot{q})}{d\dot{q}}) = 0$$

Fundamental Lemma

so general Euler-Lagrange equations are the equations of interest

(general) Principle of Stationary Action

"Variational principles" apply to many systems, e.g., special relativity, quantum mechanics, geodesics, etc.

The Euler-Lagrange equations for a general Lagrangian $\mathcal{L}(t, q(t), \dot{q}(t))$ are

$$\frac{d\mathcal{L}(t,q,\dot{q})}{dq} - \frac{d}{dt}\left(\frac{d\mathcal{L}(t,q,\dot{q})}{d\dot{q}}\right) = 0$$

δS … 0

Lemma

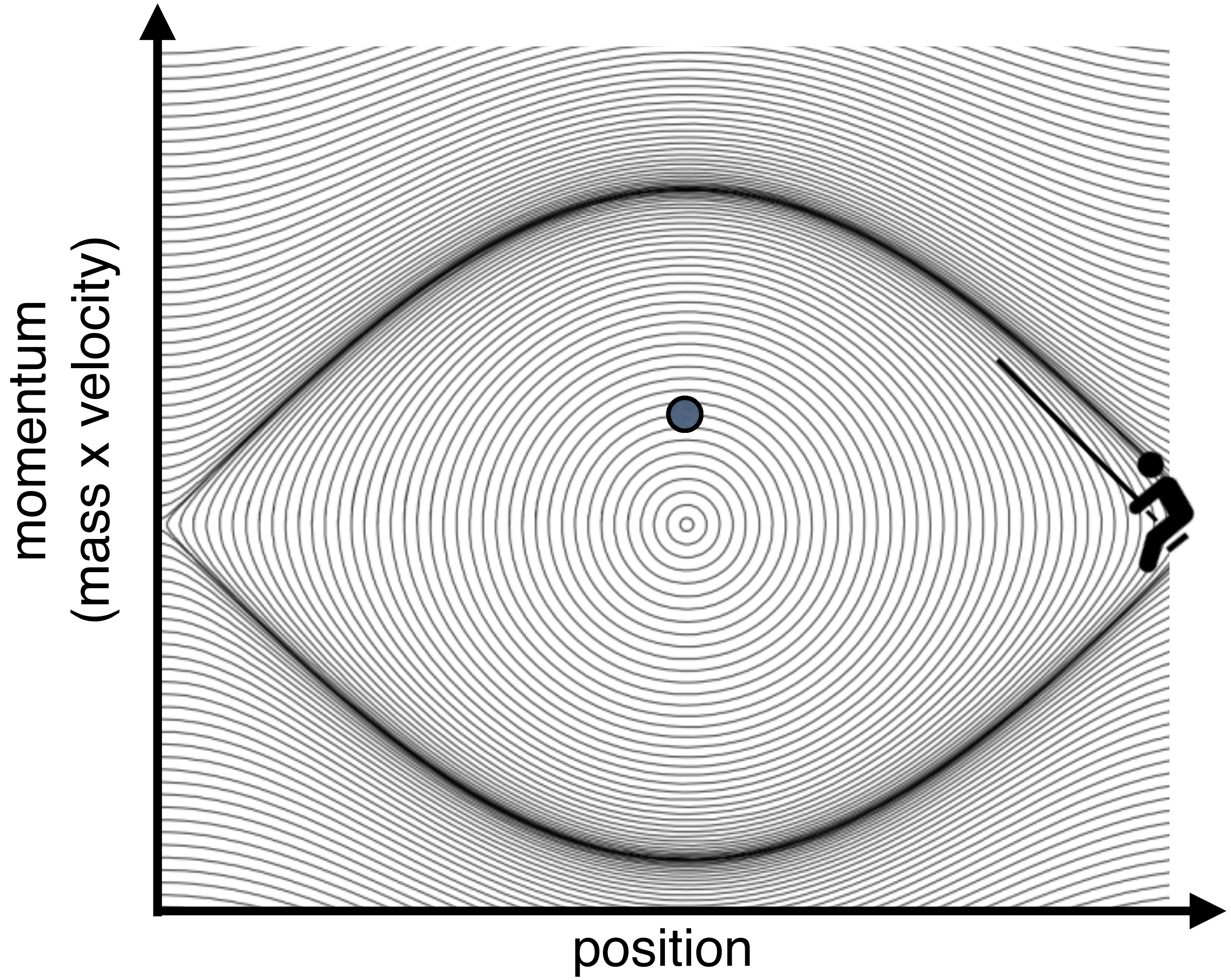
so general Euler-Lagrange equations are the equations of interest

Noether's Theorem

Continuous symmetries of the Lagrangian imply conservation laws for the physical system.

Continuous Symmetry	Conserved Quantity
Translational	Linear momentum
Rotational (one dimensional)	Angular momentum
Time	Total energy

Lagrangian Paths are Symplectic



energy levels

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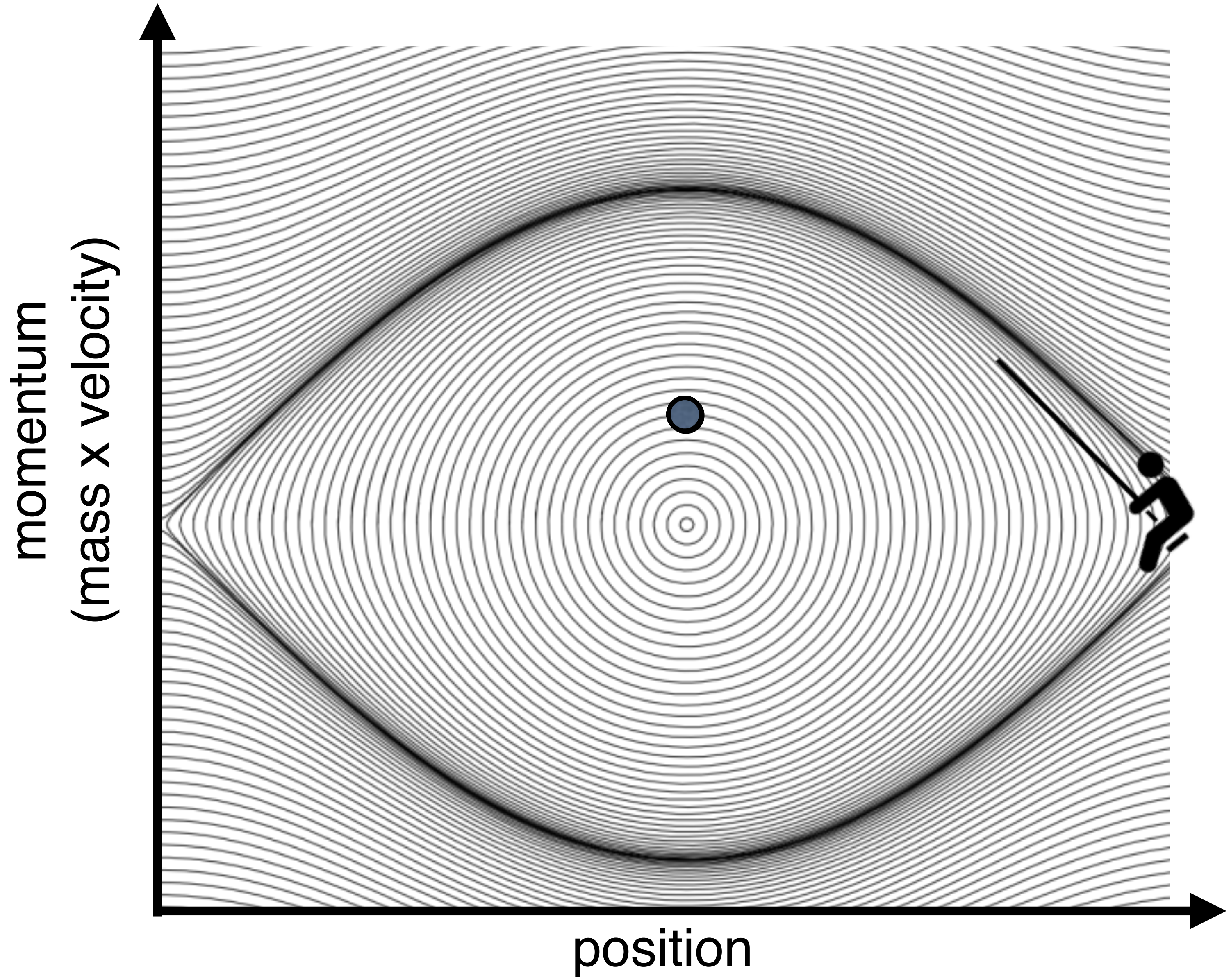

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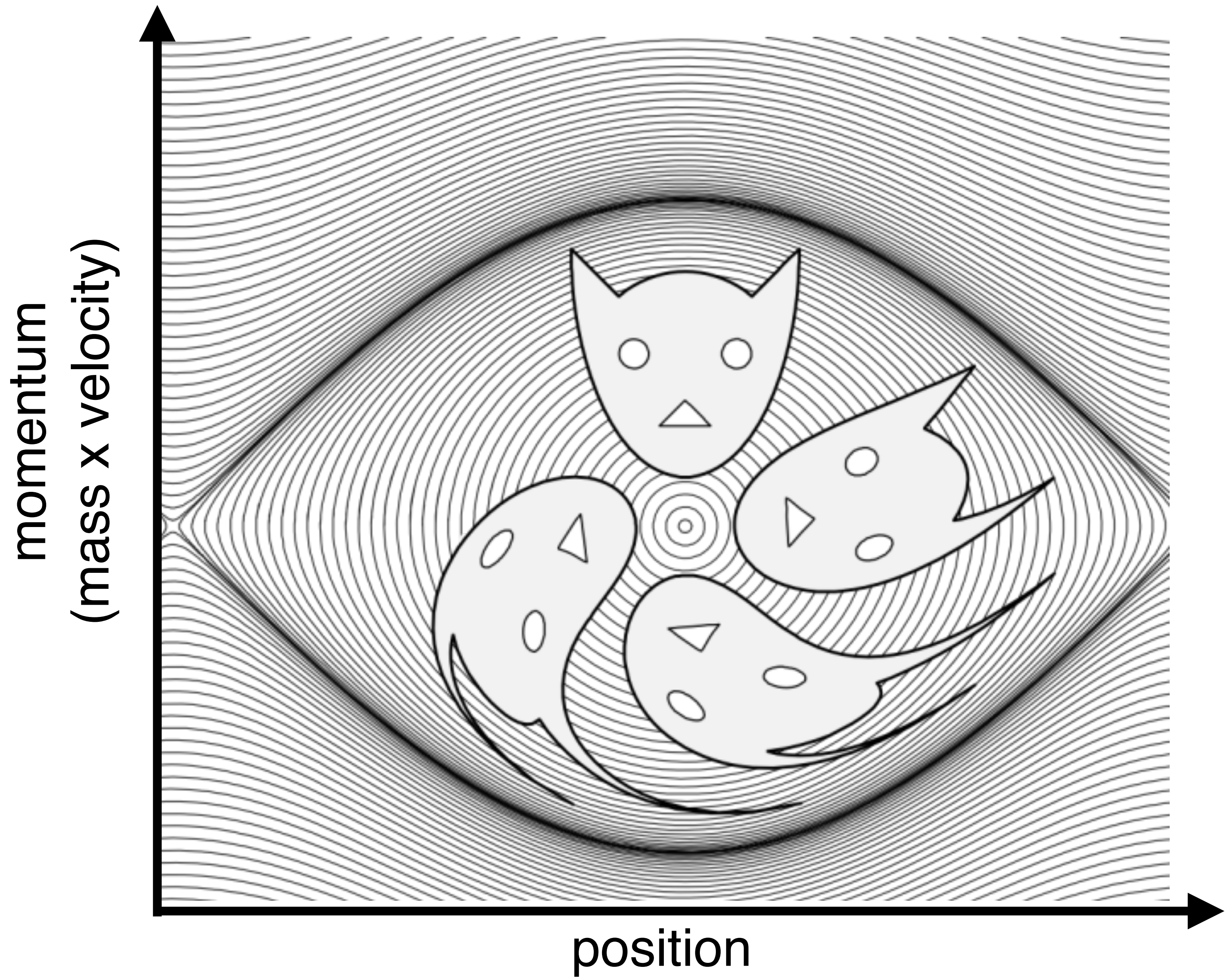
Lagrangian Paths are Symplectic

Image from Hairer, Lubich, and Wanner 2006



energy levels

in 2D equivalent to area conservation in phase space

(in higher dimensions implies volume conservation)

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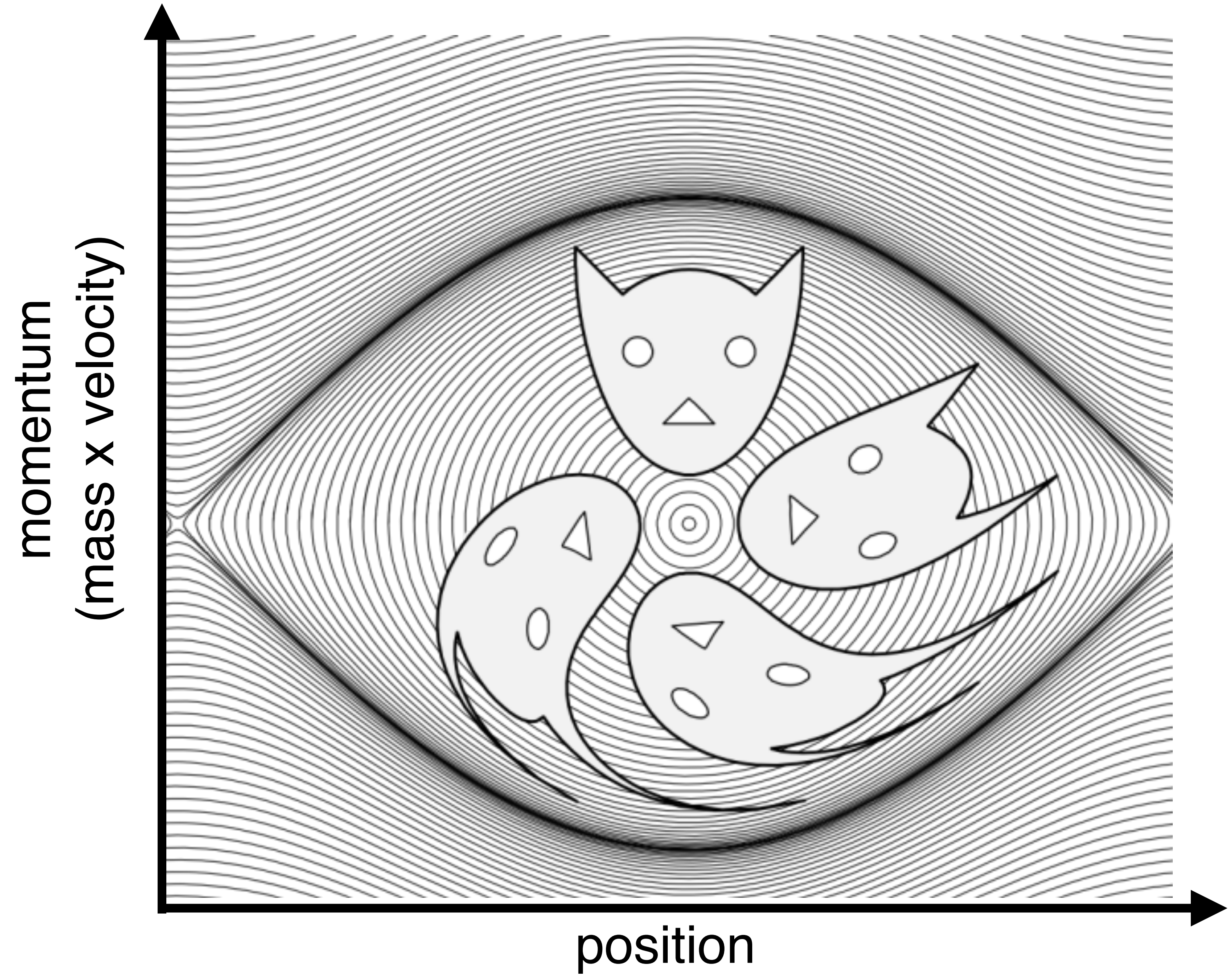

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Variational Time Integrators

Discrete Hamilton’s Principle

Discretize Lagrangian

↓

Apply Variational Principle

↓

Arrive at Discrete Equations of Motion

(as opposed to discretizing equations directly)

Discrete Noether's Theorem

Discretize Lagrangian

Arrive at Discrete Equations of Motion

Continuous symmetries of the discrete Lagrangian imply conserved quantities throughout entire discrete motion.

(for not too large time steps)

Discrete Variational Integrators are Symplectic

... time is now discrete, so total energy is not conserved.

But, discrete symplectic structure guarantees bounded oscillation around true energy level

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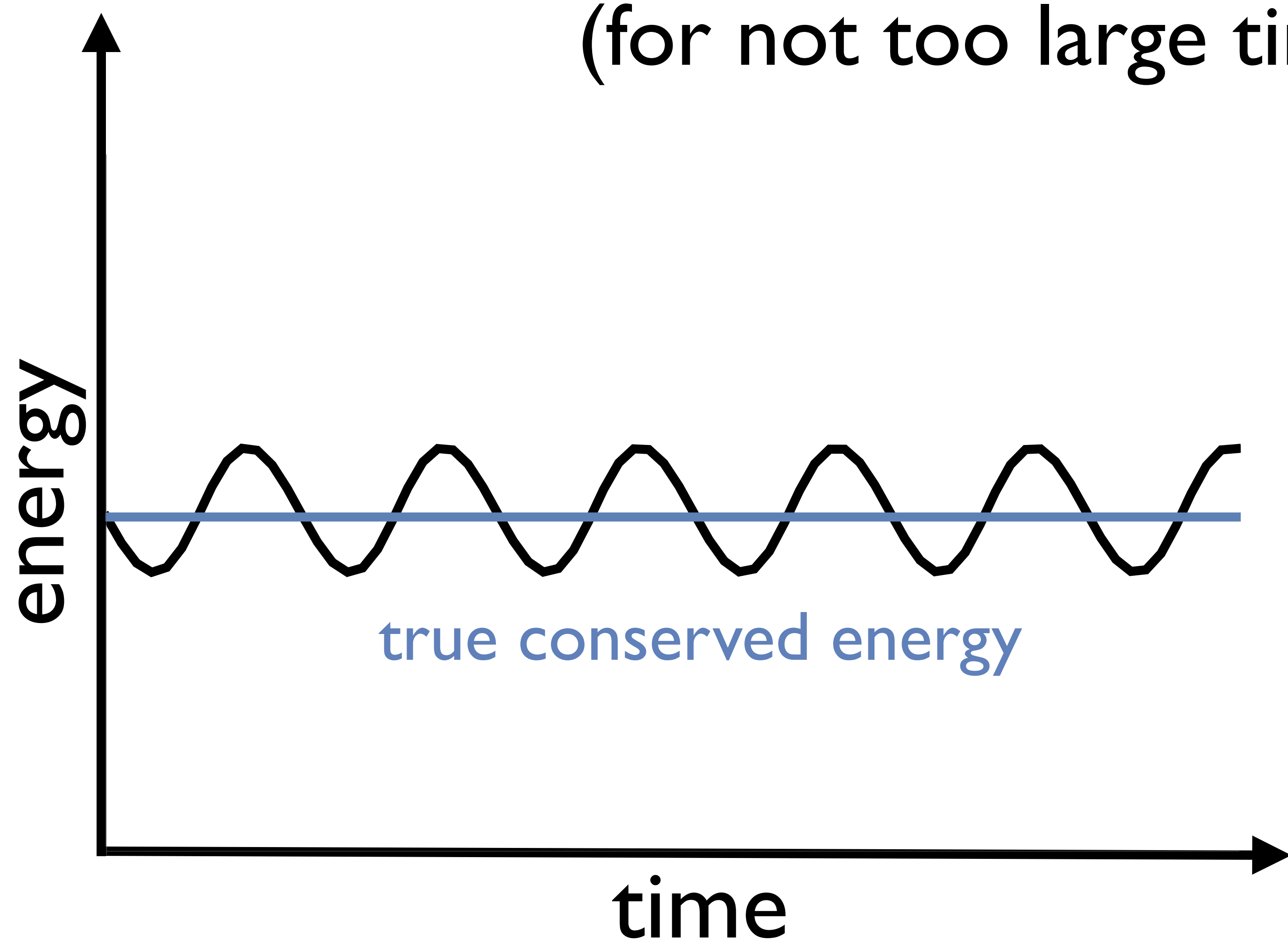

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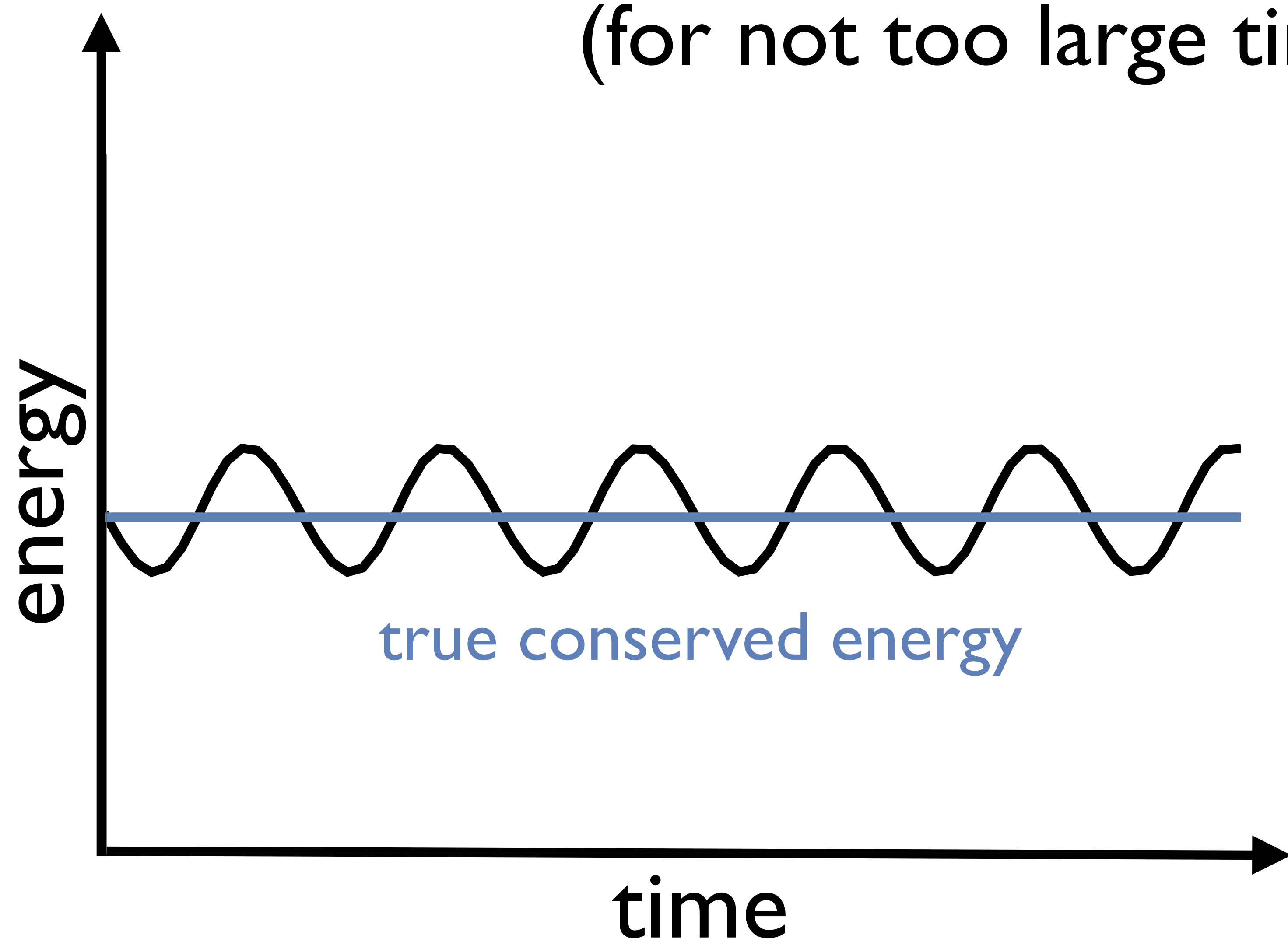


LUNCH

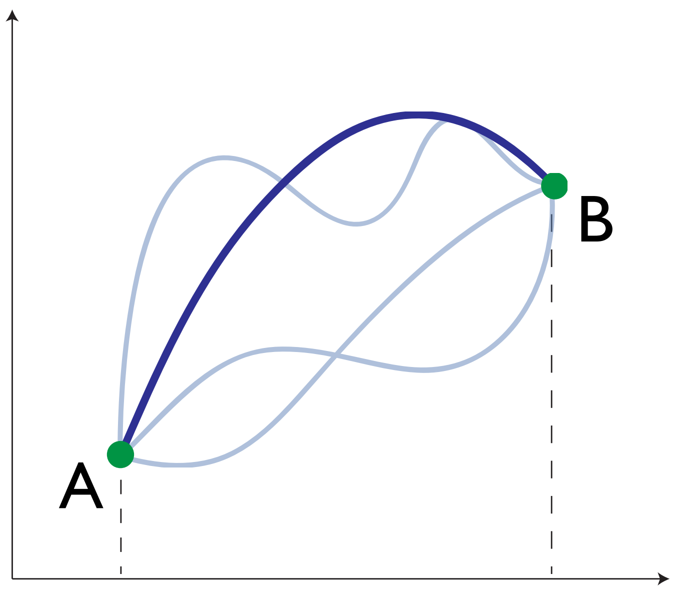
BREAK

image from openclipart.org

Part Two:
Why Use Variational Integrators?

Quick Recap

Physical paths are extremal amongst all paths from A to B of the action integral



Action is the integral of the Lagrangian, kinetic minus potential energy

Symmetries of Lagrangian and symplectic structure give rise to conservation laws

Variational Time Integrators

Discrete Hamilton's Principle

Discretize Action (integral of Lagrangian)

Apply Variational Principle

Arrive at Discrete Equations of Motion

(as opposed to discretizing equations directly)

Discrete Noether's Theorem

Discretize Lagrangian

↓

Arrive at Discrete Equations of Motion

Continuous symmetries of discrete Lagrangian imply conserved quantities throughout entire discrete motion,

e.g., conservation of linear and angular momentum

(for not too large time steps)

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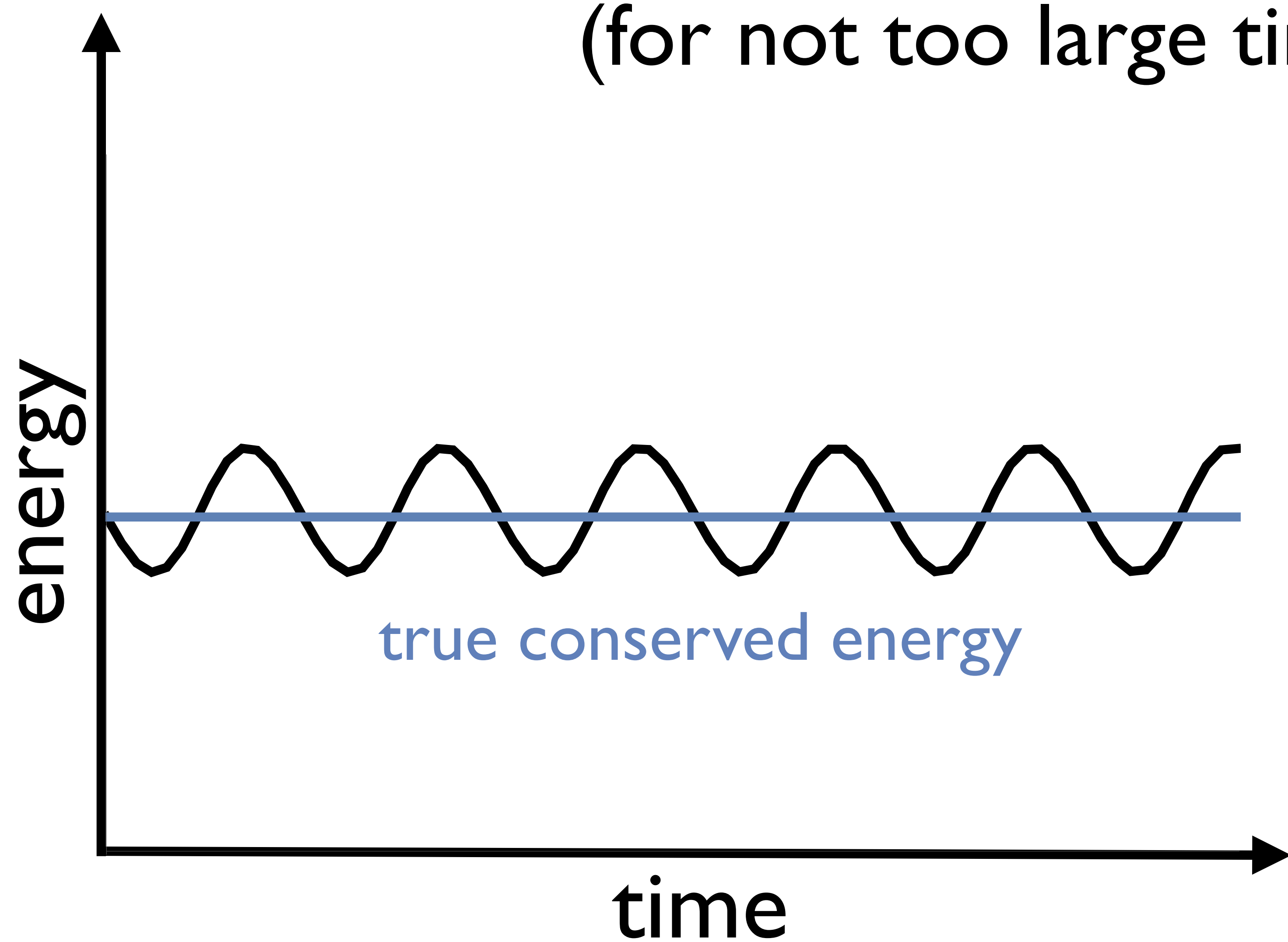

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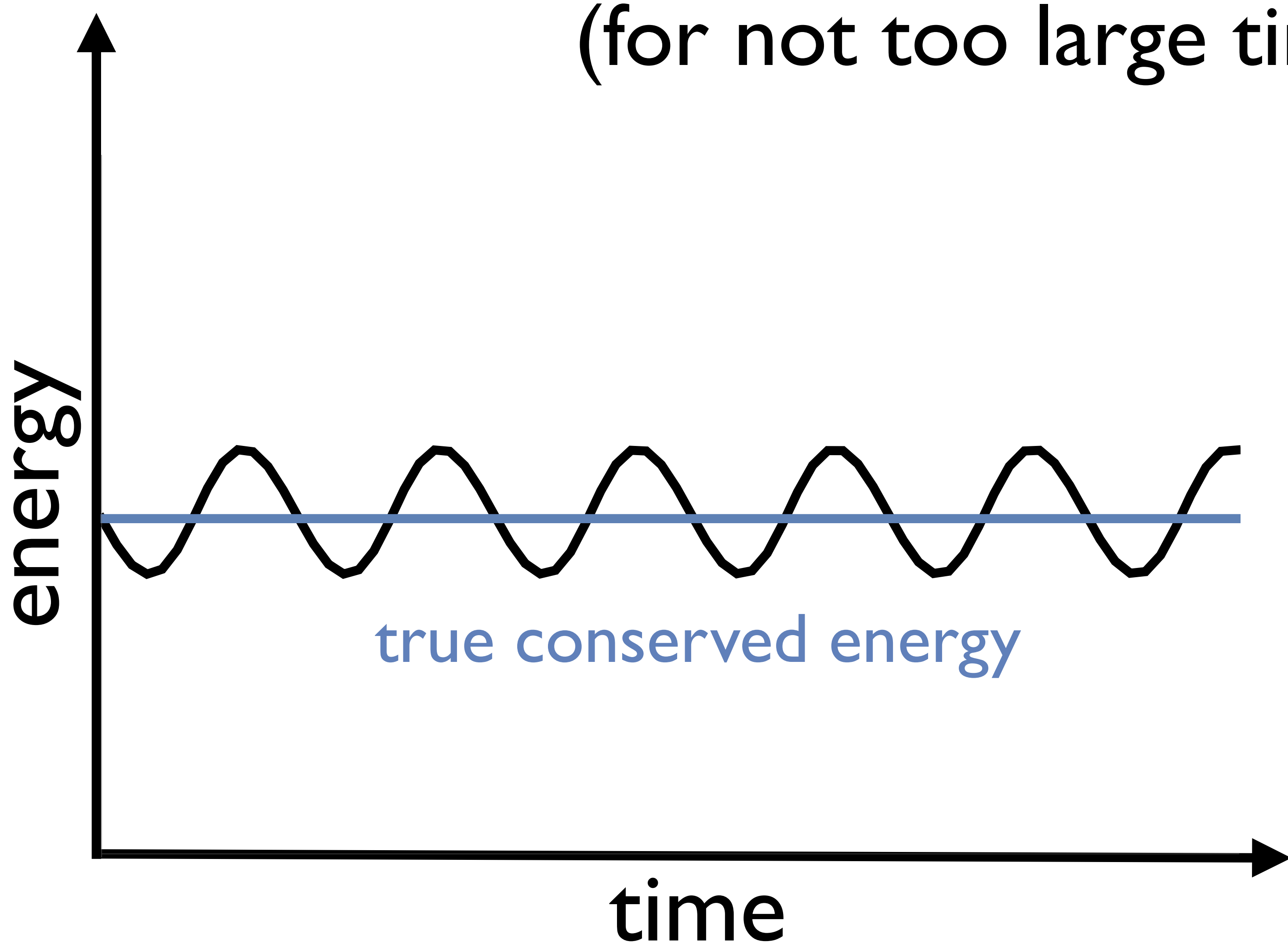

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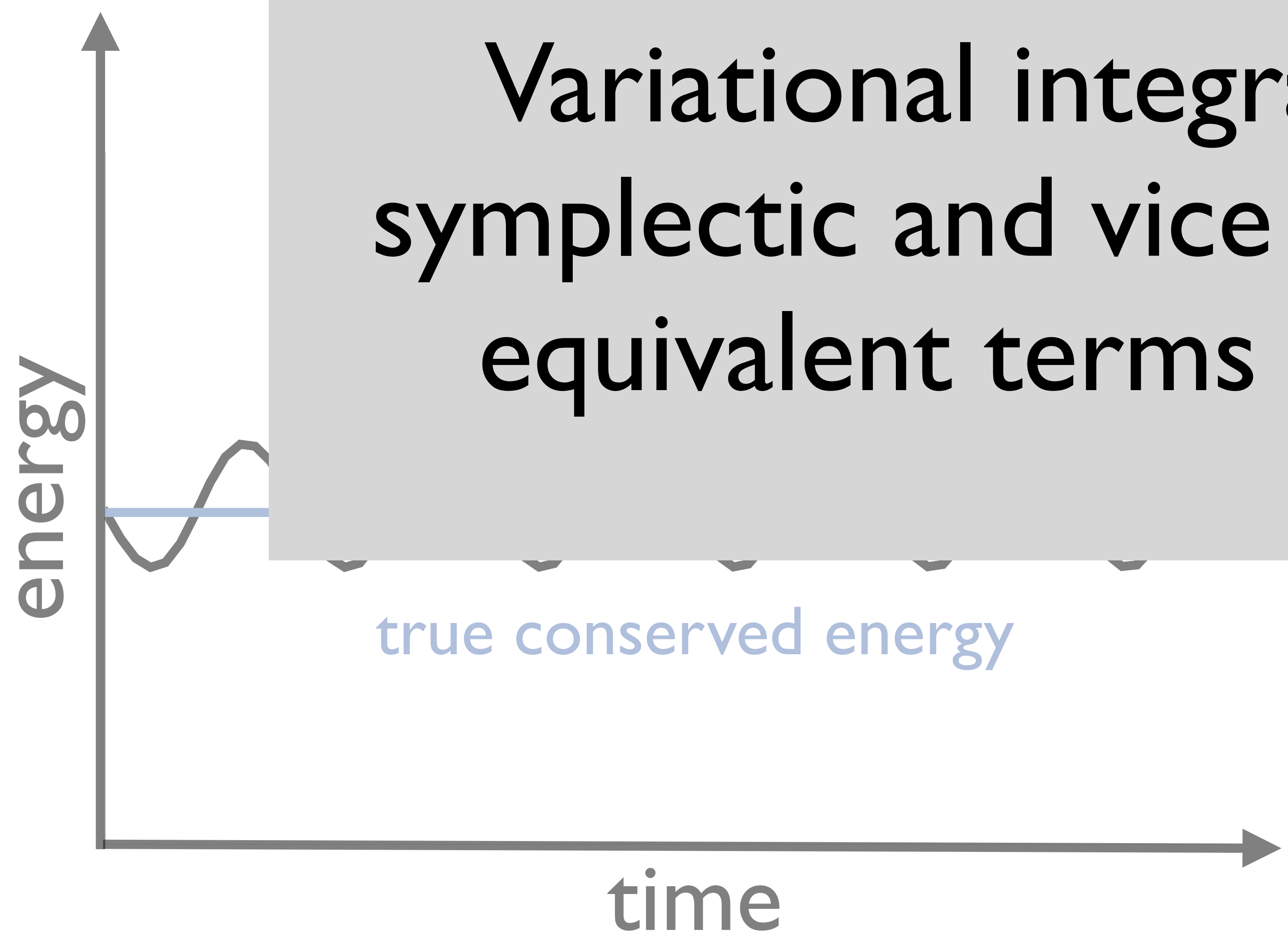

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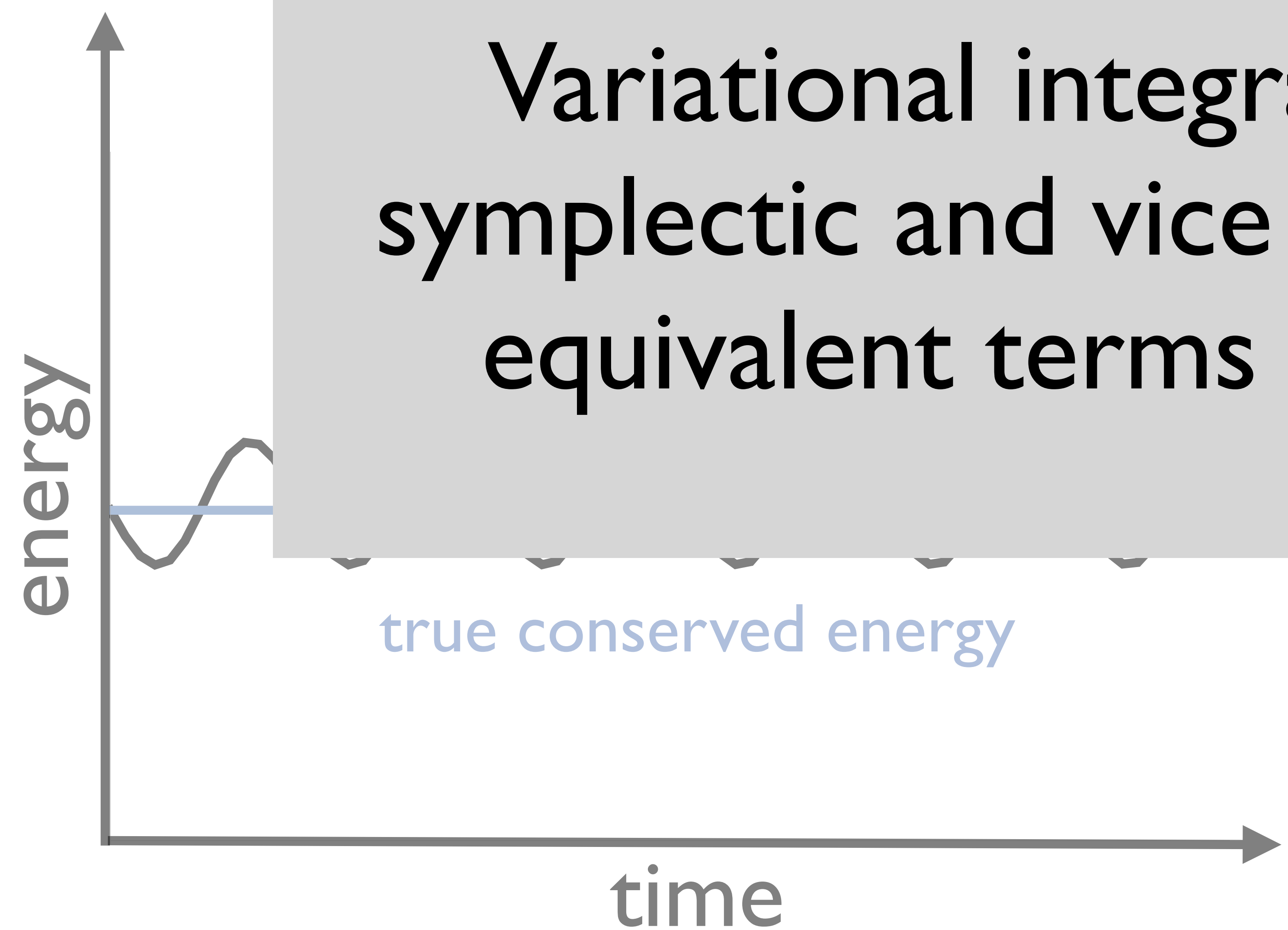

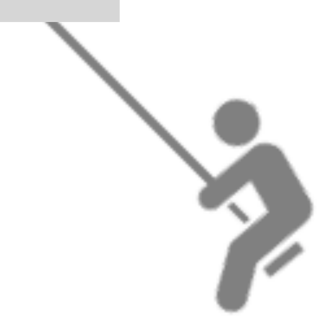

Building a Variational Time Integrator

1. Choose a finite difference scheme for $\dot{q}$, e.g.,

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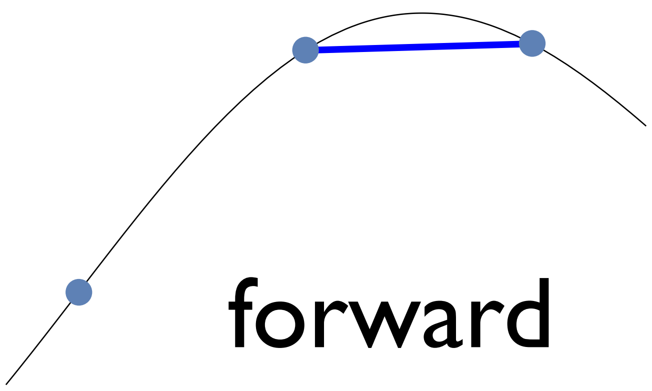

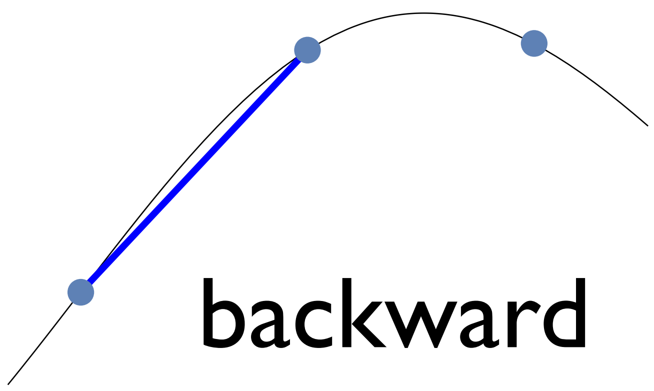

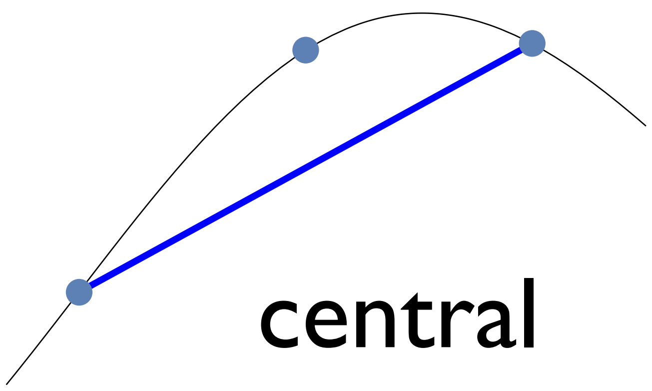

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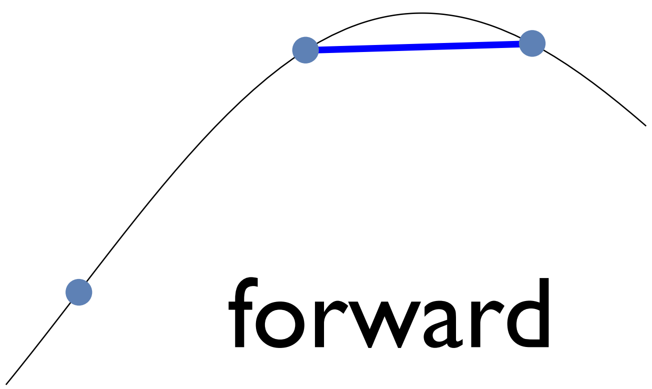

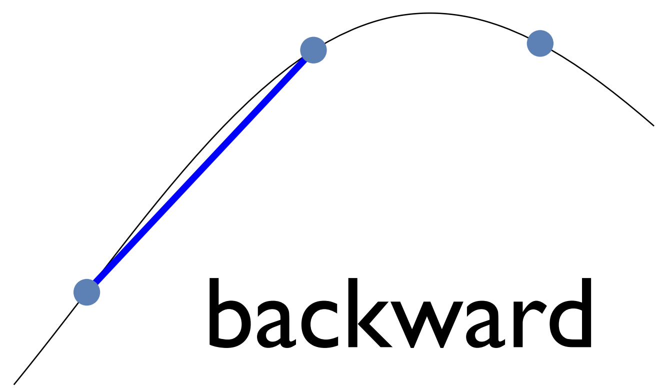

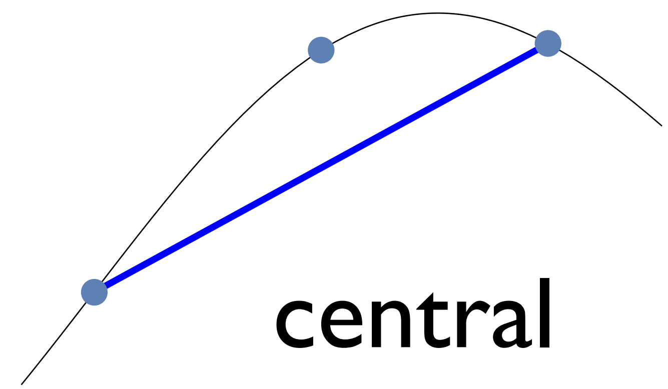

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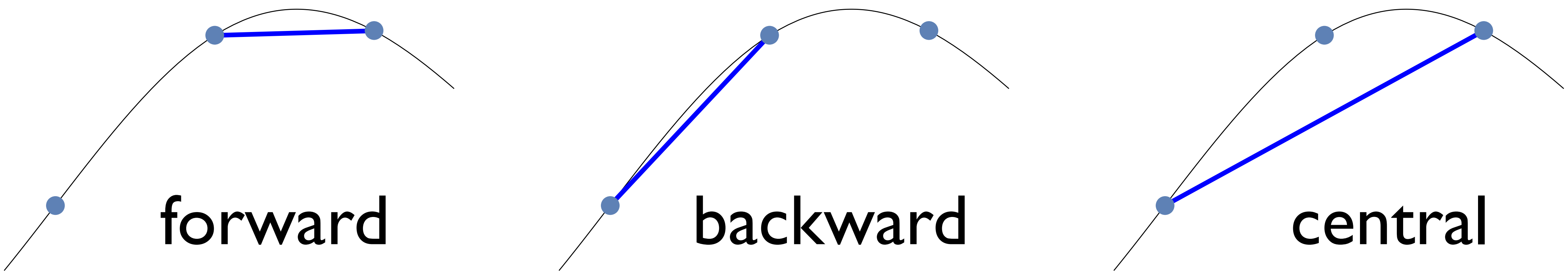

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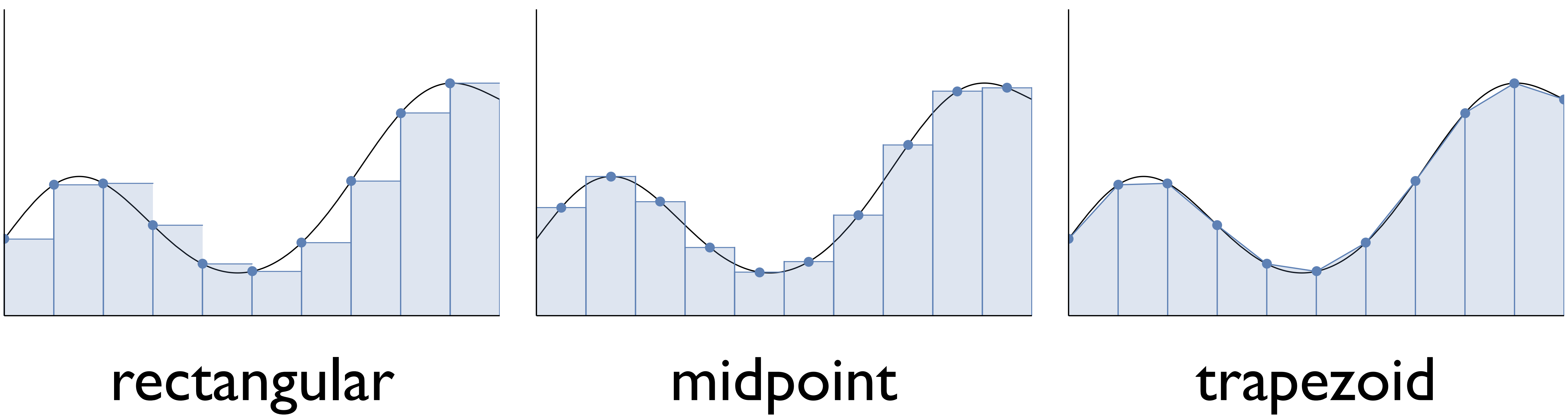

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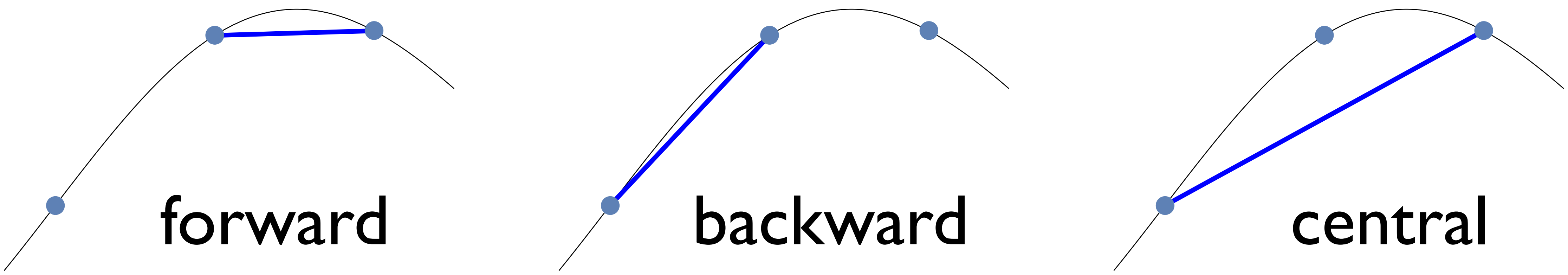

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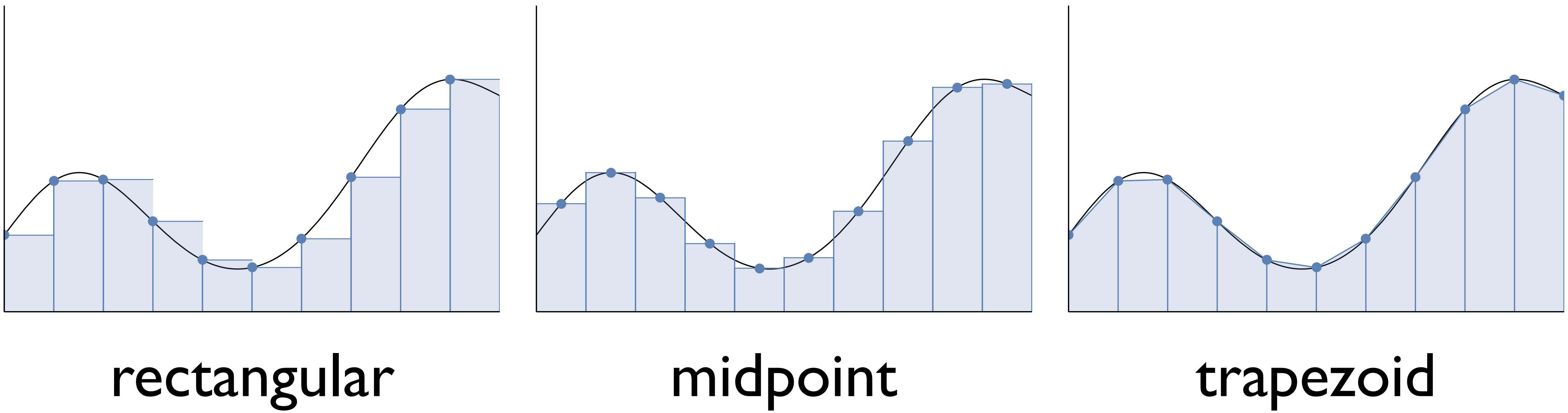
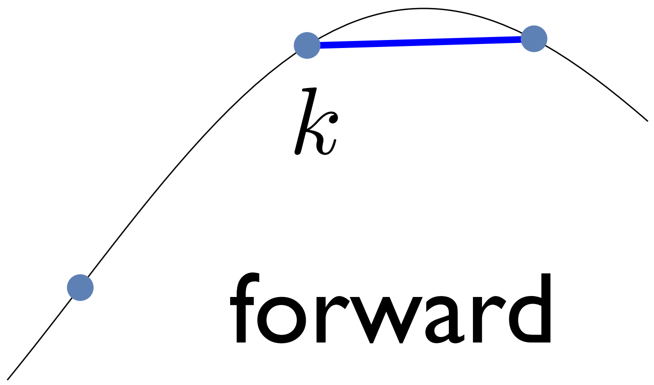


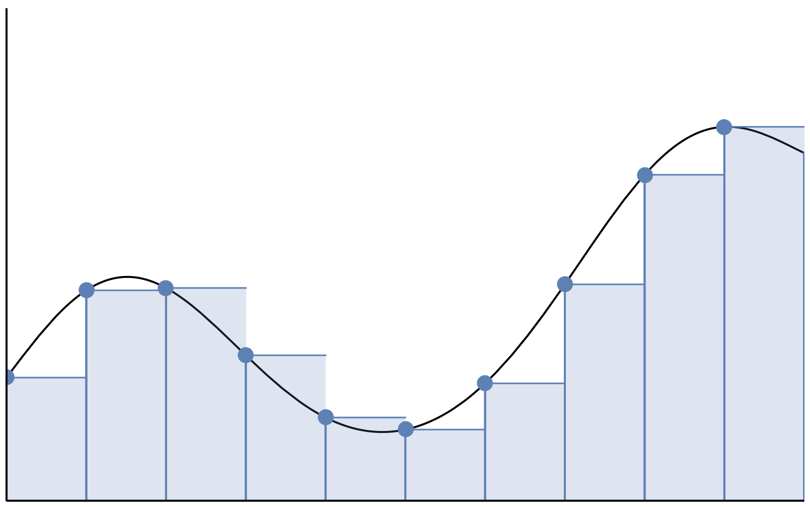
3. Apply variational principle

Discrete Variational Principle Example



forward

$$\dot{q} \approx \dot{q}_k = \frac{q_{k+1} - q_k}{\Delta t}$$

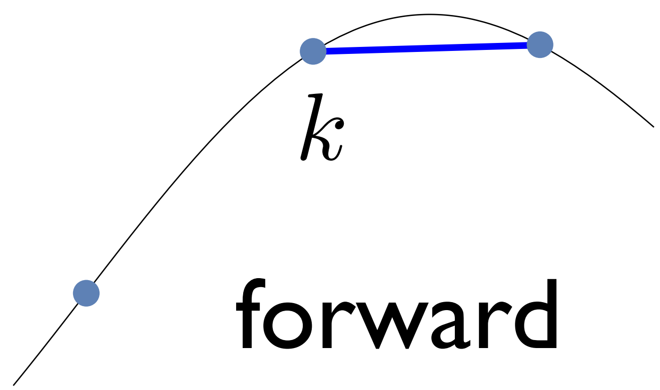


rectangular

$$\int_t^{t+\Delta t} \mathcal{L}(q, \dot{q})\, dt \approx \Delta t\, \mathcal{L}(q_k, \dot{q}_k)$$

$$\int_{t_1}^{t_2} \mathcal{L}(q, \dot{q})\, dt \approx \sum_{k=0}^{N} \mathcal{L}(q_k, \dot{q}_k)\, \Delta t$$

Discrete Variational Principle Example



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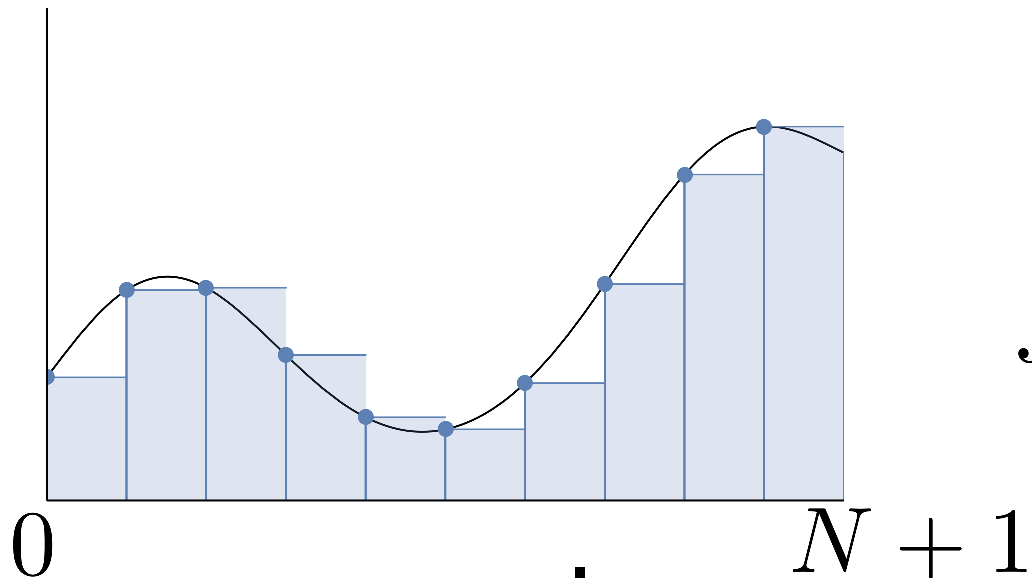

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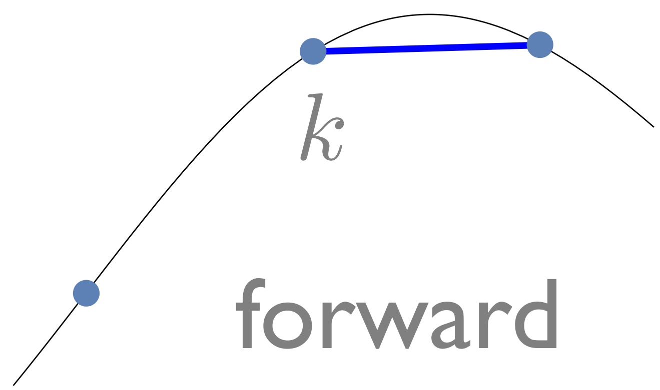

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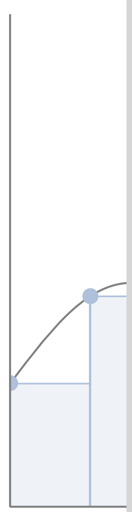
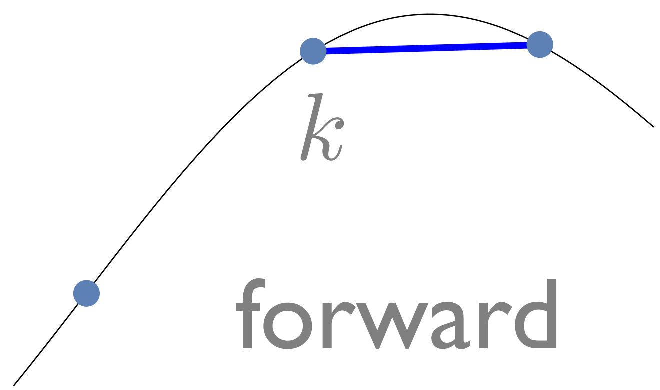


$(q_k, \dot q_k)$

Choose a finite difference scheme and quadrature rule and write down the discrete action sum.

$$\int_{t_1}^{t_2} \mathcal{L}(q, \dot q)\, dt \approx \sum_{k=0}^{N} \mathcal{L}(q_k, \dot q_k)\, \Delta t$$

Discrete Variational Principle Example



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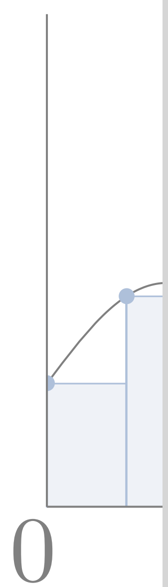

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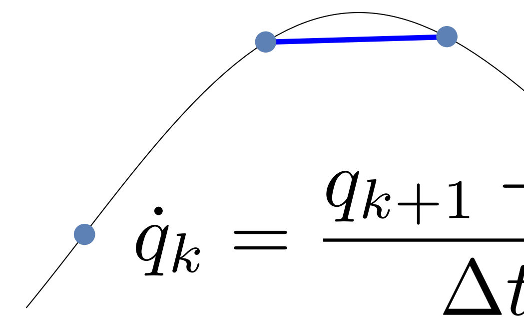
Discrete Variational Principle Example

$$S_{\Delta t} = \sum_{k=0}^{N} \left(\frac{m}{2} \dot{q}_k^2 - U(q_k) \right) \Delta t$$



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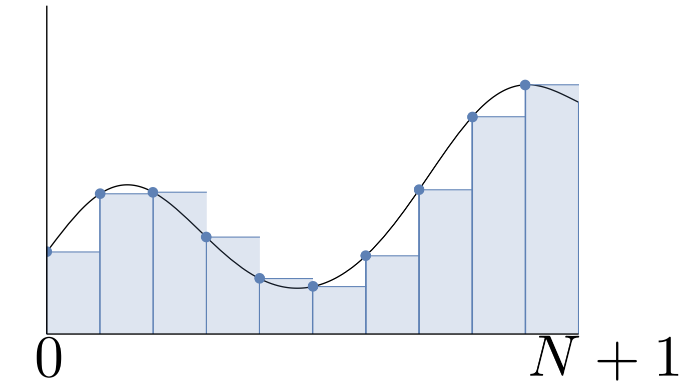

$$\delta_\eta S_{\Delta t} = \frac{d}{d\varepsilon} S_{\Delta t}(q_k + \varepsilon \eta_k) \Big|_{\varepsilon=0}$$

$$= \sum_{k=0}^{N} \left(m \dot{q}_k \dot{\eta}_k - U'(q_k) \eta_k \right) \Delta t$$

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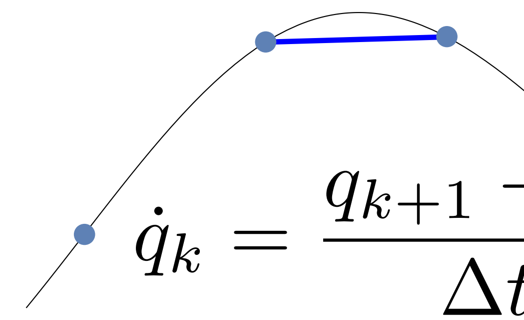

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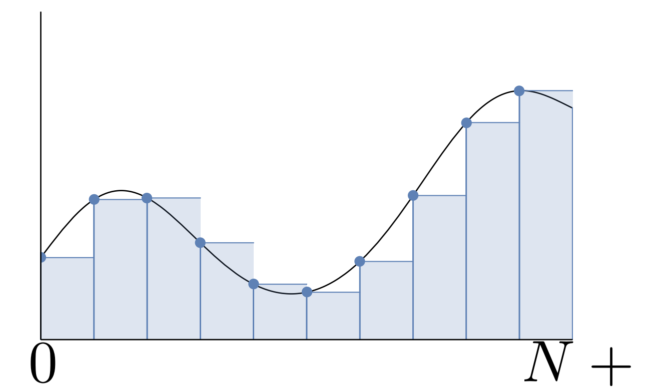

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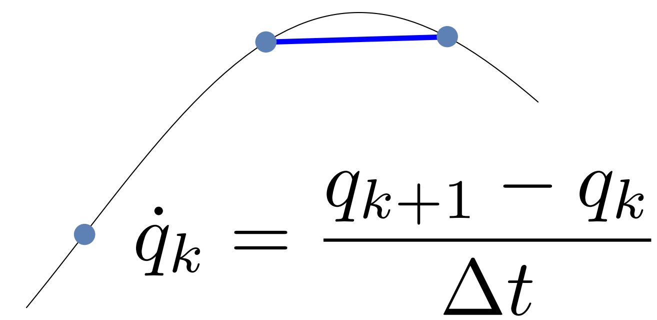

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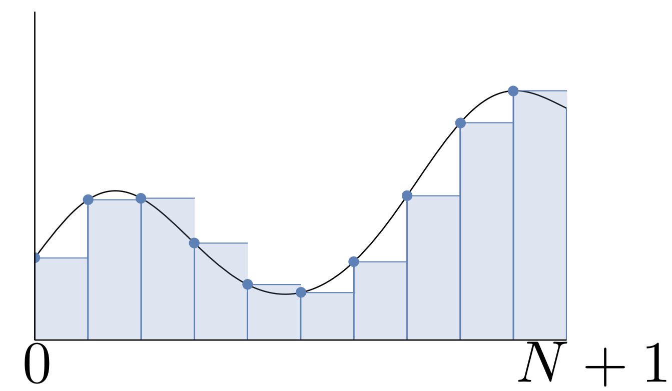

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get rid of derivates of the offset

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get rid of derivates of the offset

Summation by Parts

$$\sum_{k=0}^{N} \dot{q}_k \dot{\eta}_k\, \Delta t = bdry - \sum_{k=0}^{N} \ddot{q}_k \eta_{k+1}\, \Delta t$$

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$bdry \to 0$

recall offset vanishes at boundary

$$\eta_{N+1} = \eta_0 = 0$$

Discrete Variational Principle Example

$$\delta_\eta S_{\Delta t} = -\sum_{k=0}^{N} m\,\ddot{q}_k \eta_{k+1}\,\Delta t - \sum_{k=0}^{N} U'(q_k)\eta_k\,\Delta t$$

$$= -\sum_{k=0}^{N} m\,(\frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t})\eta_{k+1}\Delta t - \sum_{k=0}^{N} U'(q_k)\eta_k\,\Delta t$$

$$= -\sum_{k=0}^{N} \left(m\frac{\dot{q}_{k+1} - \dot{q}_k}{\Delta t} + U'(q_{k+1}) \right) \eta_{k+1}\Delta t$$

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shift index

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Discrete Variational Principle Example

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(discrete) Fundamental Lemma of Calculus of Variations

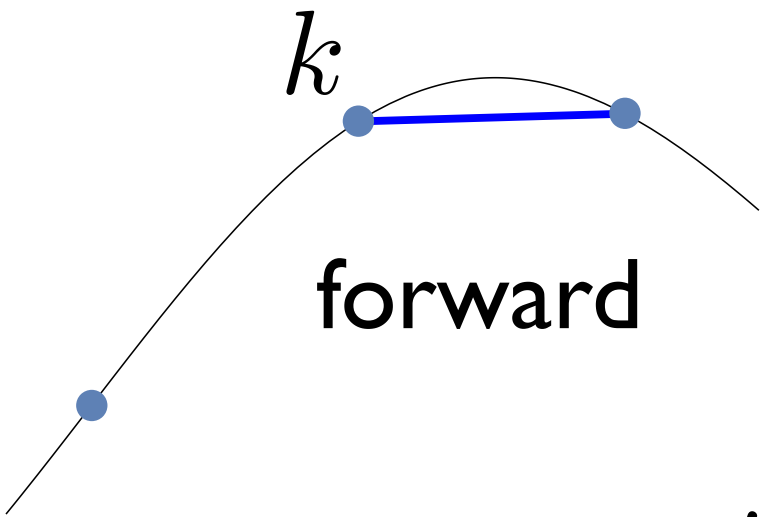
$$\delta S_{\Delta t} = 0 \iff \underbrace{-U'(q_{k+1}) = m \frac{(\dot{q}_{k+1} - \dot{q}_k)}{\Delta t}}$$

discrete Euler-Lagrange

Recall:

$$\delta S(q) = 0 \iff F = m\ddot{q}$$

Discrete Variational Integrator Scheme



$$\dot{q}_k = \frac{q_{k+1} - q_k}{\Delta t}$$

$$-U'(q_{k+1}) = m \frac{(\dot{q}_{k+1} - \dot{q}_k)}{\Delta t}$$

Symplectic (variational) Euler

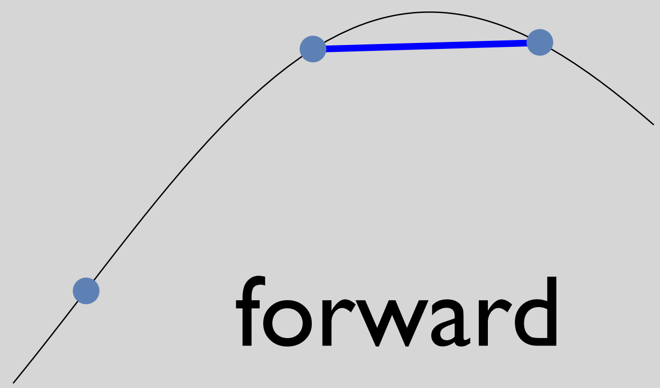
$$q_{k+1} = q_k + \Delta t \, \dot{q}_k$$

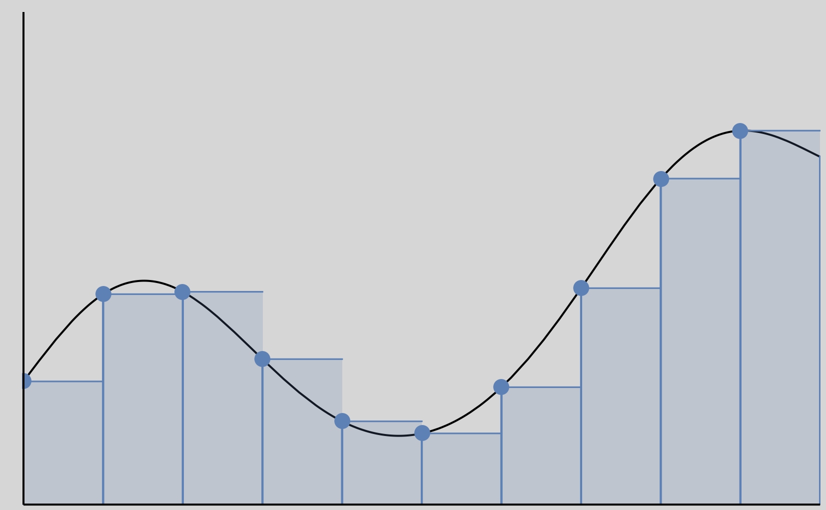
$$\dot{q}_{k+1} = \dot{q}_k + \Delta t \, m^{-1}(-U'(q_{k+1}))$$

$$(q_k, \dot{q}_k) \mapsto (q_{k+1}, \dot{q}_{k+1})$$

Discrete Variational Integrator Scheme

Use





(left) rectangular

Symplectic Euler Method A

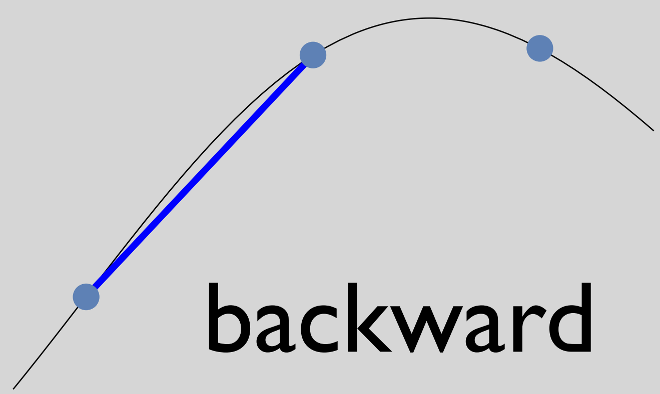
$$q_{k+1} = q_k + \Delta t\, \dot{q}_k$$

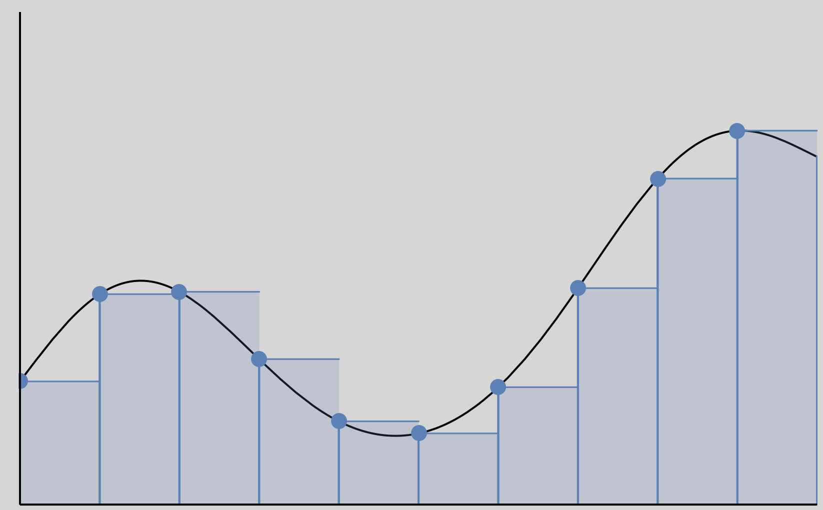
$$\dot{q}_{k+1} = \dot{q}_k + \Delta t\, m^{-1}(-U'(q_{k+1}))$$

$$(q_k, \dot{q}_k) \mapsto (q_{k+1}, \dot{q}_{k+1})$$

Discrete Variational Integrator Scheme

Use





(left) rectangular

Symplectic Euler Method B

$$\dot{q}_{k+1} = \dot{q}_k + \Delta t \, m^{-1} (-U'(q_{k}))$$

$$q_{k+1} = q_k + \Delta t \, \dot{q}_{k+1}$$

$$(q_k, q_k) \mapsto (q_{k+1}, q_{k+1})$$

Time Integration Schemes

Great... we know how to derive a variational integrator, but what other integrators are there?

Where do they come from?

Why are they used?

How do they compare?

First Order Integration Schemes

Explicit Euler

Use (forward) first order Taylor approximation of motion

$$q(t+\Delta t) = q(t) + \dot{q}(t)\Delta t + \frac{\ddot{q}(t)}{2}\Delta t^{2} + \ldots$$

$$\dot{q}(t+\Delta t) = \dot{q}(t) + \ddot{q}(t)\Delta t + \frac{\dddot{q}(t)}{2}\Delta t^{2} + \ldots$$

First Order Integration Schemes

Explicit Euler

$$q(t + \Delta t) = q(t) + \dot{q}(t)\Delta t$$

$$\dot{q}(t + \Delta t) = \dot{q}(t) + \ddot{q}(t)\Delta t$$

First Order Integration Schemes

Explicit Euler

$$q(t + \Delta t) = q(t) + \dot{q}(t)\Delta t$$

$$\dot{q}(t + \Delta t) = \dot{q}(t) + \ddot{q}(t)\Delta t$$

use Newton's law

$$F = -U'(q) = m\ddot{q}$$

$$m\dot{q}(t + \Delta t) = m\dot{q}(t) + \Delta t(-U'(q(t))$$

First Order Integration Schemes

Explicit Euler

$$q_{k+1} = q_k + \Delta t\,\dot{q}_k$$

$$\dot{q}_{k+1} = \dot{q}_k + \Delta t\,m^{-1}(-U'(q_k))$$

Cheap to compute -- explicit dependence of variables

but

adds artificial driving

“unstable” for large time steps
(drastically deviates from true trajectories)

Explicit Euler

2^{-6}

step size in seconds

Explicit Euler

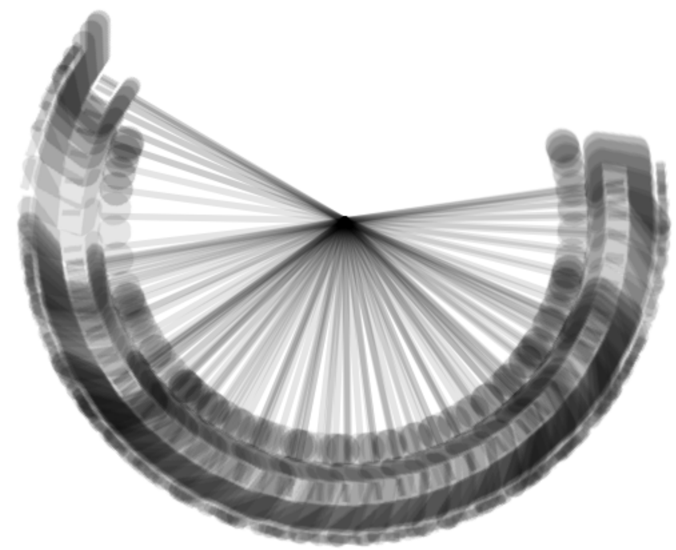
2^{-6}

step size in seconds

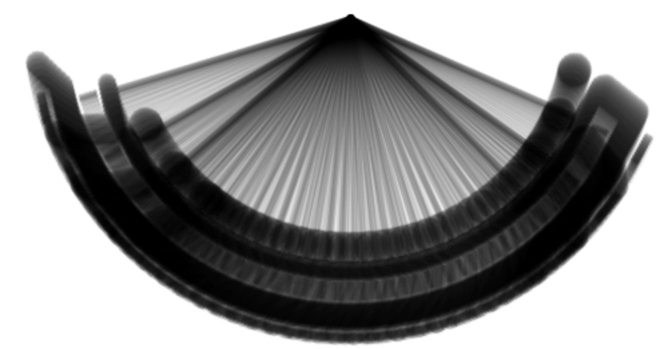
Explicit: Time Step Refinement

2^{-6}

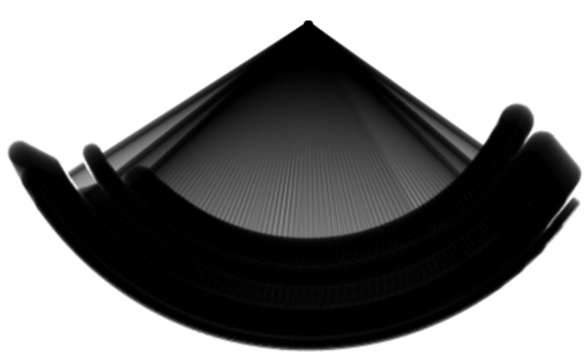
step size in seconds



2^{-7}



2^{-8}



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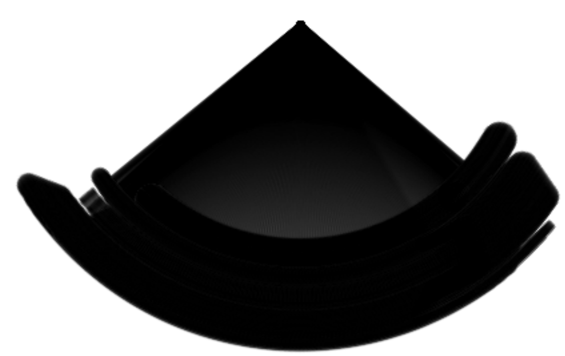
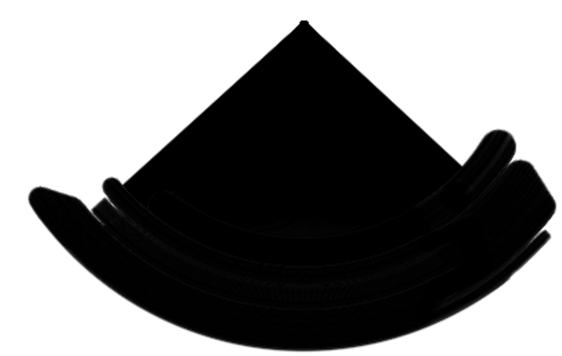


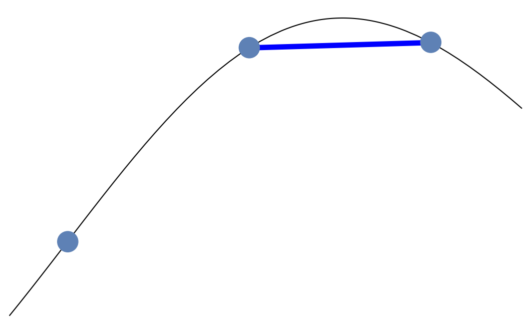
2^{-10}



2^{-11}

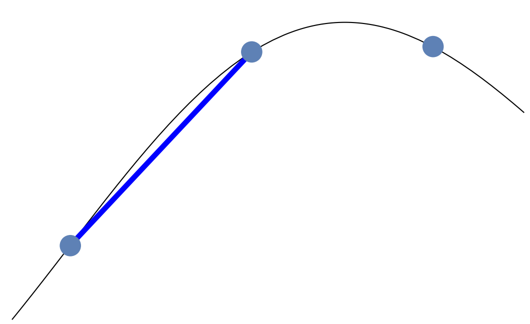
First Order Integration Schemes

Explicit (forward) Euler



$$q_{k+1} = q_k + \Delta t \, \dot{q}_k$$
$$\dot{q}_{k+1} = \dot{q}_k + \Delta t \, m^{-1}(-U'(q_k))$$

Implicit (backward) Euler



$$q_{k+1} = q_k + \Delta t \, \dot{q}_{k+1}$$
$$\dot{q}_{k+1} = \dot{q}_k + \Delta t \, m^{-1}(-U'(q_{k+1}))$$

motion “implicitly” depends on variables

First Order Integration Schemes

Implicit Euler

$$q_{k+1} = q_k + \Delta t \, \dot{q}_{k+1}$$

$$\dot{q}_{k+1} = \dot{q}_k + \Delta t \, m^{-1}(-U'(q_{k+1}))$$

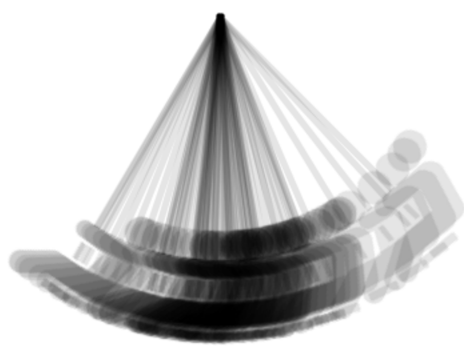
"stable" for large time steps
(stays close to true trajectories)

but

adds artificial damping

more expensive -- nonlinear solve for implicit variables

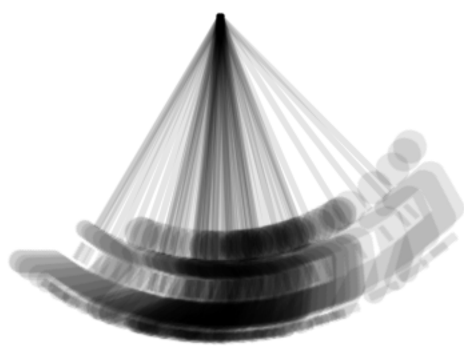
Implicit Euler



2^{-6}

step size in seconds

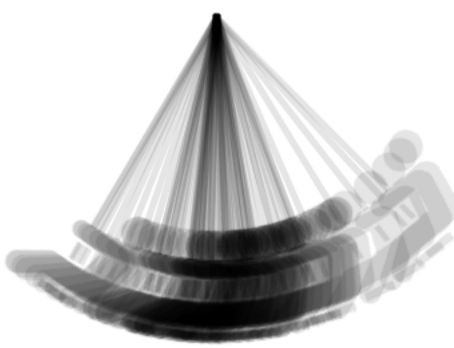
Implicit Euler



2^{-6}

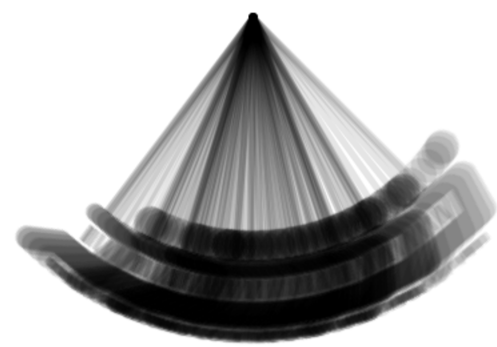
step size in seconds

Implicit: Time Step Refinement

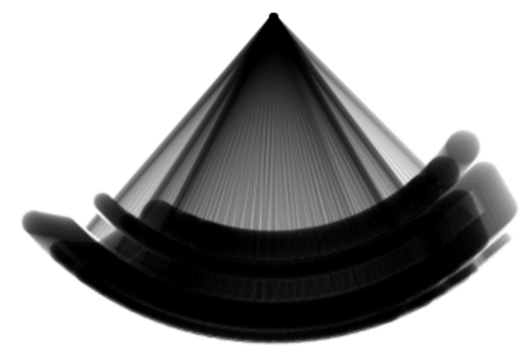


2^{-6}

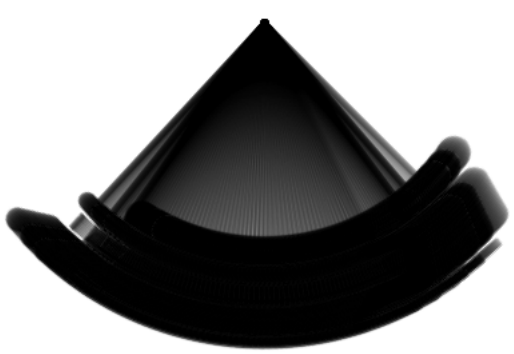
step size in seconds



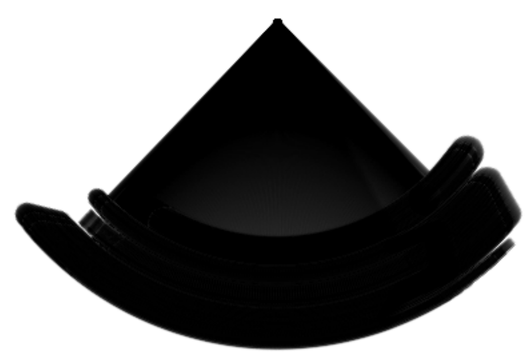
2^{-7}



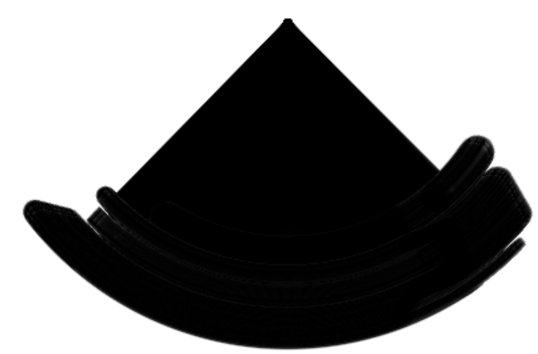
2^{-8}



2^{-9}



2^{-10}



2^{-11}

First Order Integration Schemes

Symplectic Euler Method A

$$q_{k+1} = q_k + \Delta t\, \dot{q}_k$$

$$\dot{q}_{k+1} = \dot{q}_k + \Delta t\, m^{-1}(-U'(q_{k+1}))$$

Symplectic Euler Method B

$$q_{k+1} = q_k + \Delta t\, \dot{q}_{k+1}$$

$$\dot{q}_{k+1} = \dot{q}_k + \Delta t\, m^{-1}(-U'(q_k))$$

also called “semi-implicit” Euler methods

First Order Integration Schemes

Symplectic Euler Methods, e.g.,

$$q_{k+1} = q_k + \Delta t\, \dot{q}_{k+1}$$

$$\dot{q}_{k+1} = \dot{q}_k + \Delta t\, m^{-1}(-U'(q_k))$$

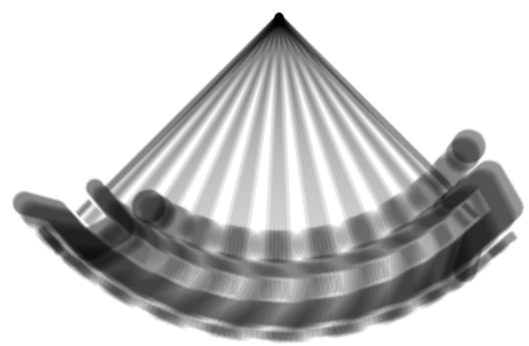
as cheap as Explicit Euler

bounded energy oscillation
(little artificial damping/driving)

conserved linear and angular momentum

also unstable for very large time steps

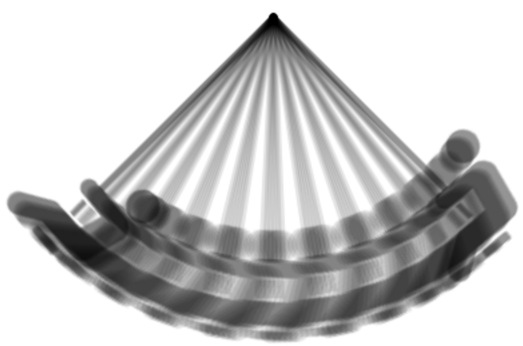
Symplectic Euler (Method B)



$$2^{-6}$$

step size in seconds

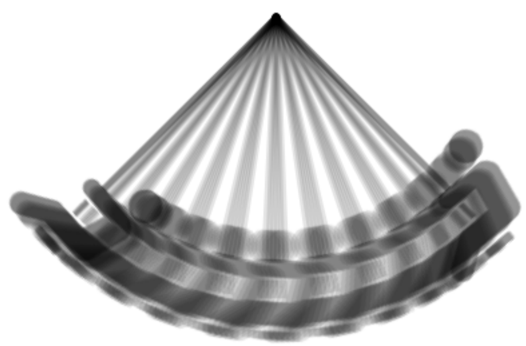
Symplectic Euler (Method B)



2^{-6}

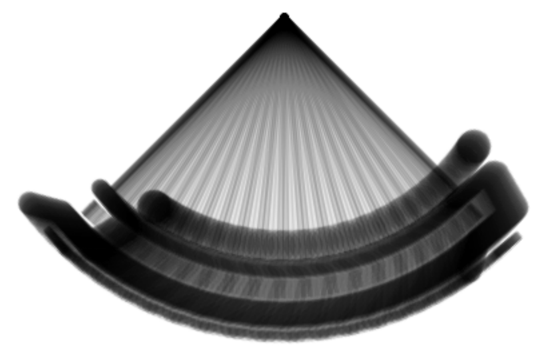
step size in seconds

Symplectic: Time Step Refinement

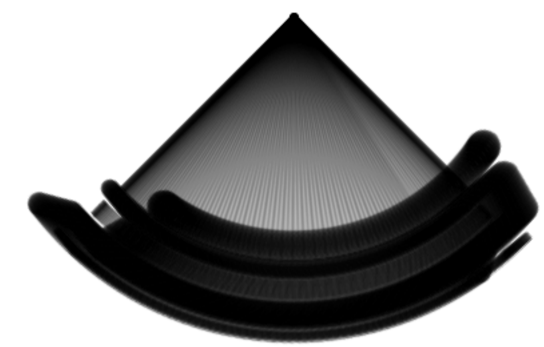


2^{-6}

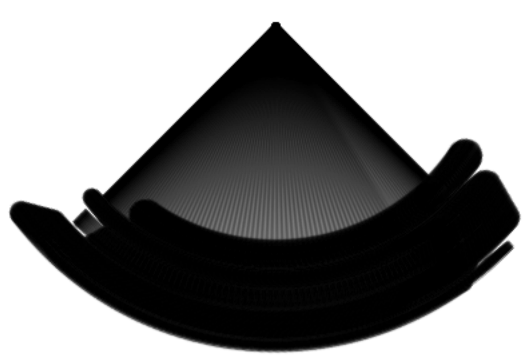
step size in seconds



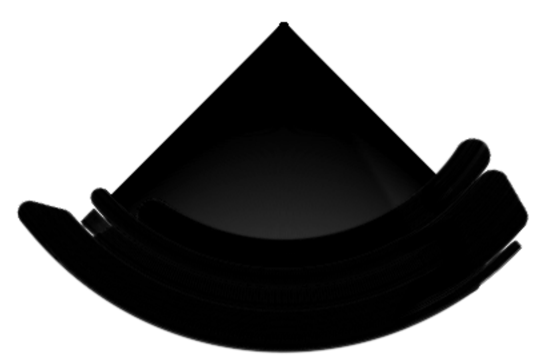
2^{-7}



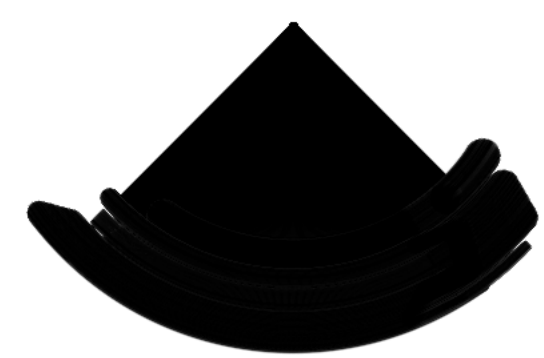
2^{-8}



2^{-9}

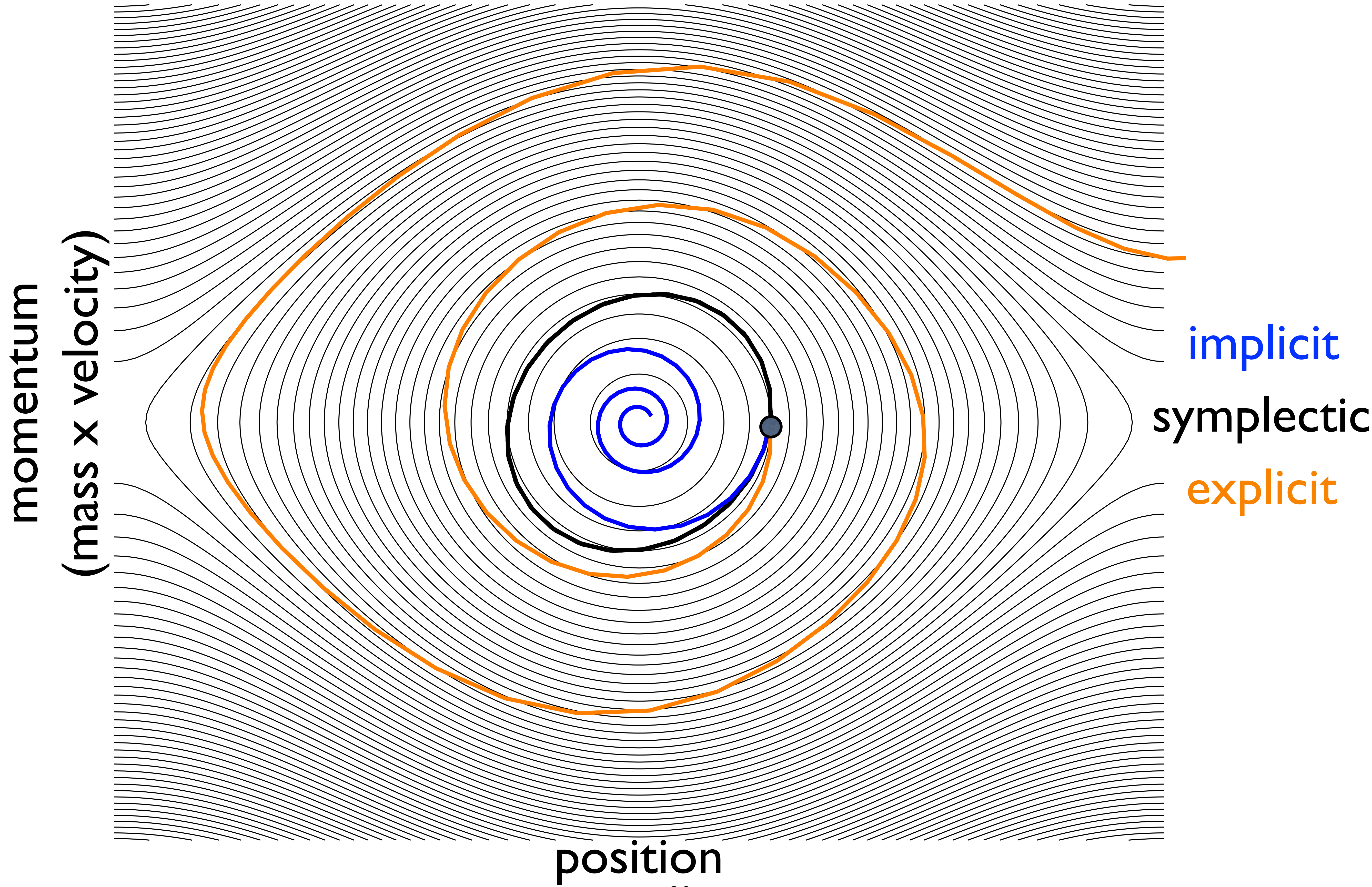


2^{-10}

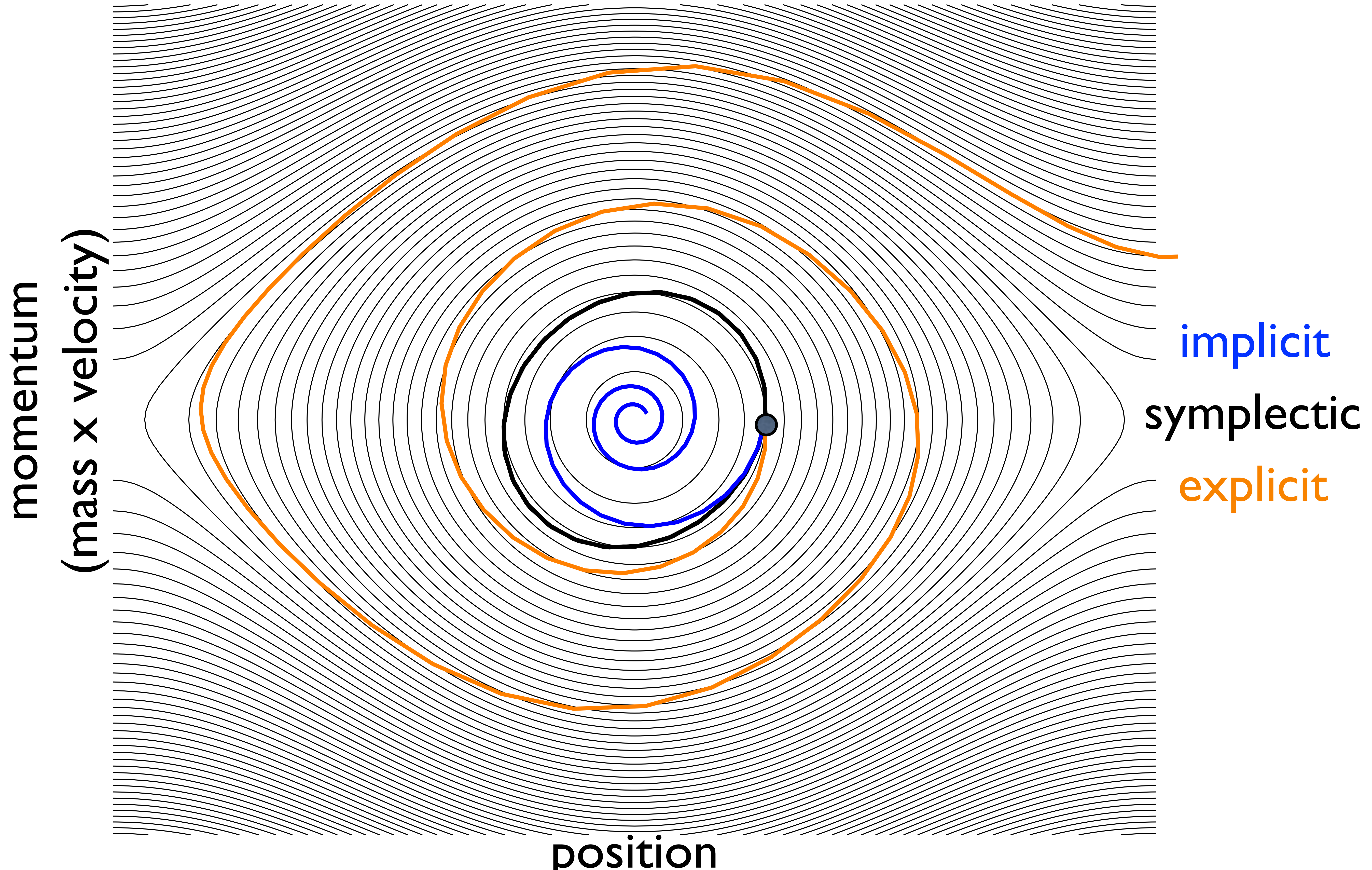


2^{-11}

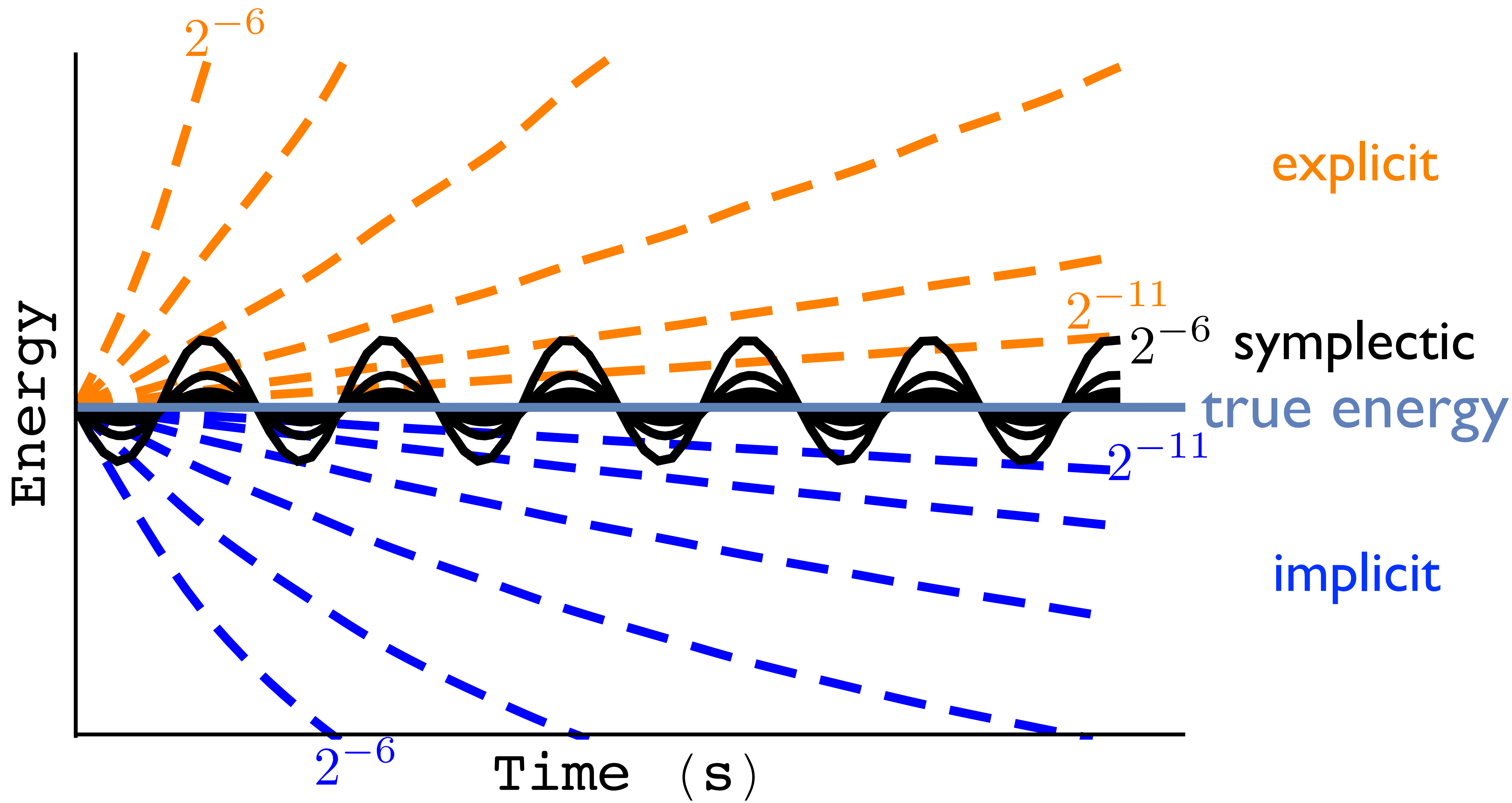
Phase Space (energy levels)



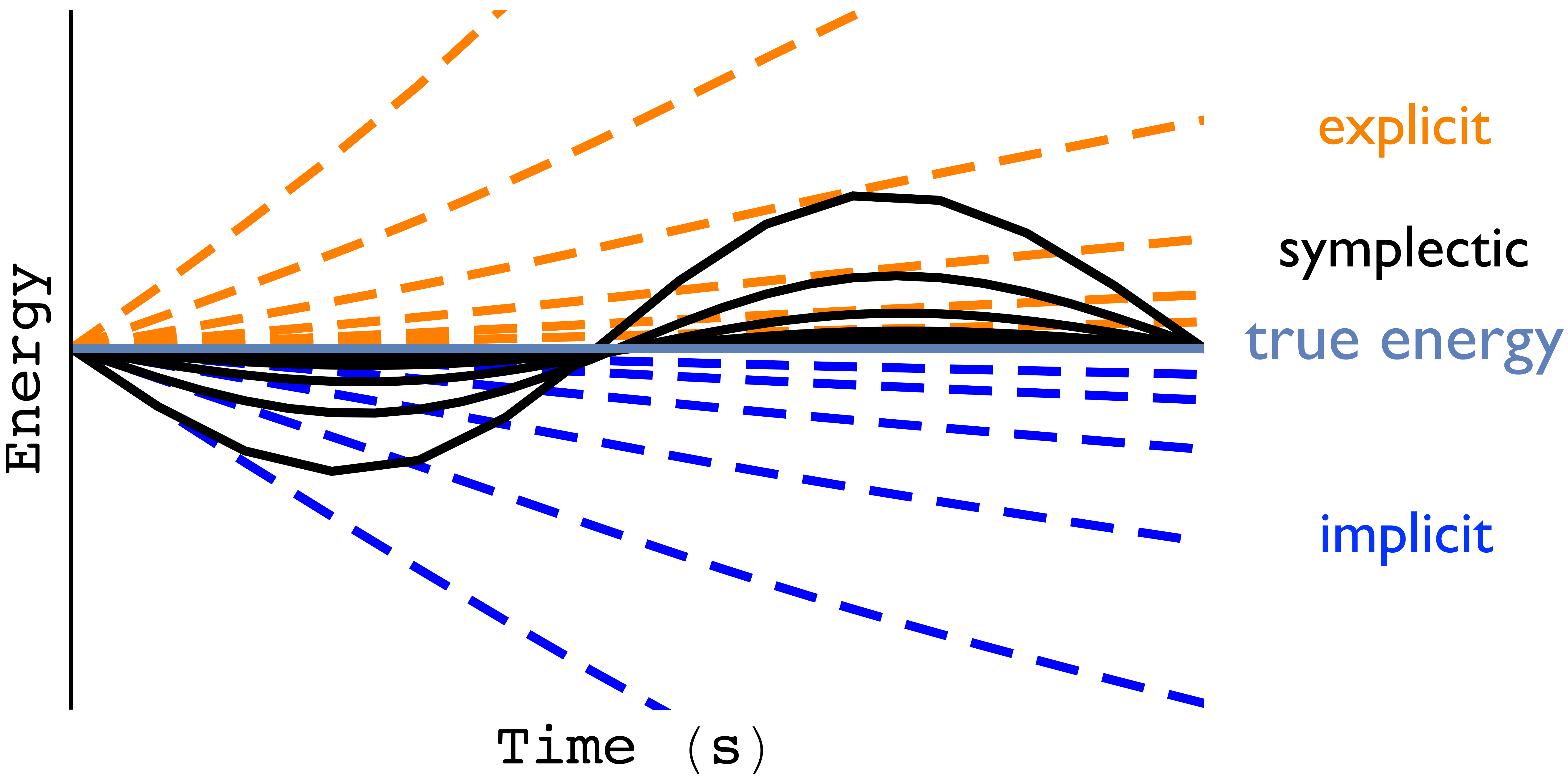
Phase Space (energy levels)



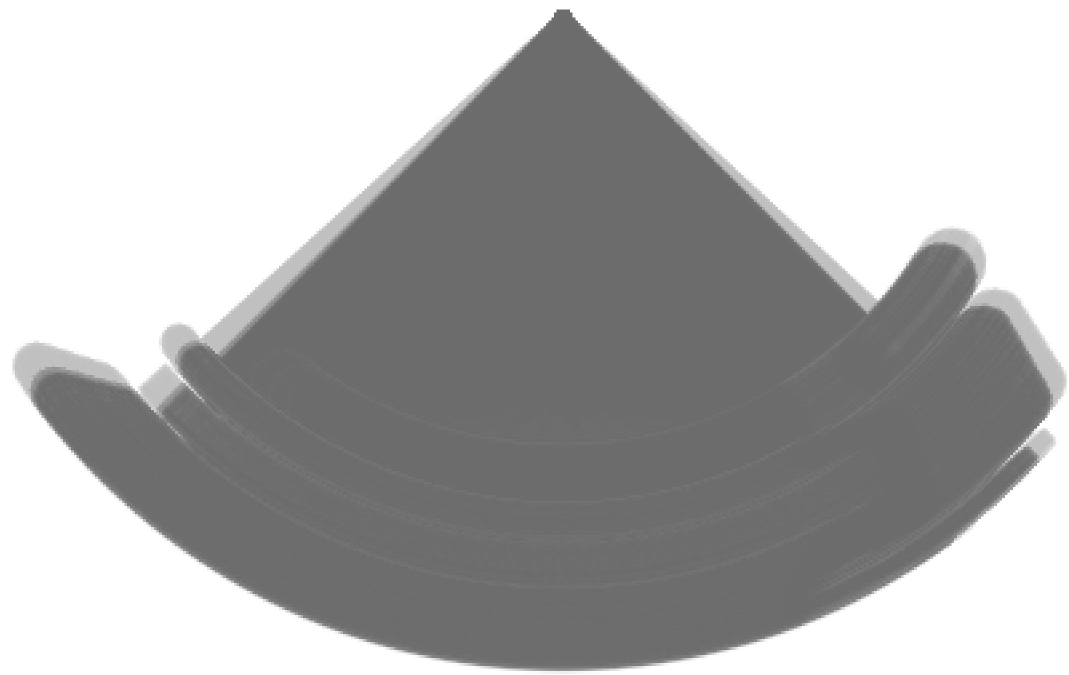
Energy Landscape Under Step Refinement

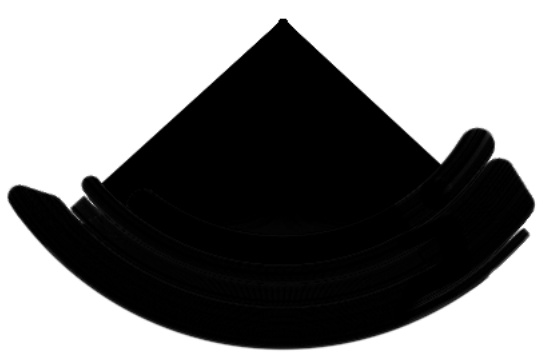


Energy Landscape Near Time Zero

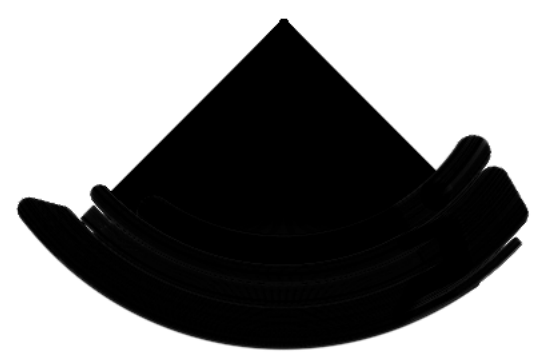


Very Small Time Step

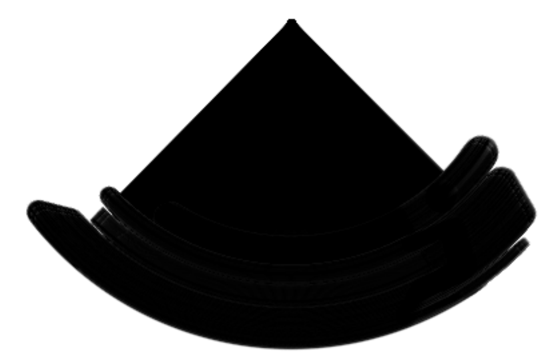




explicit

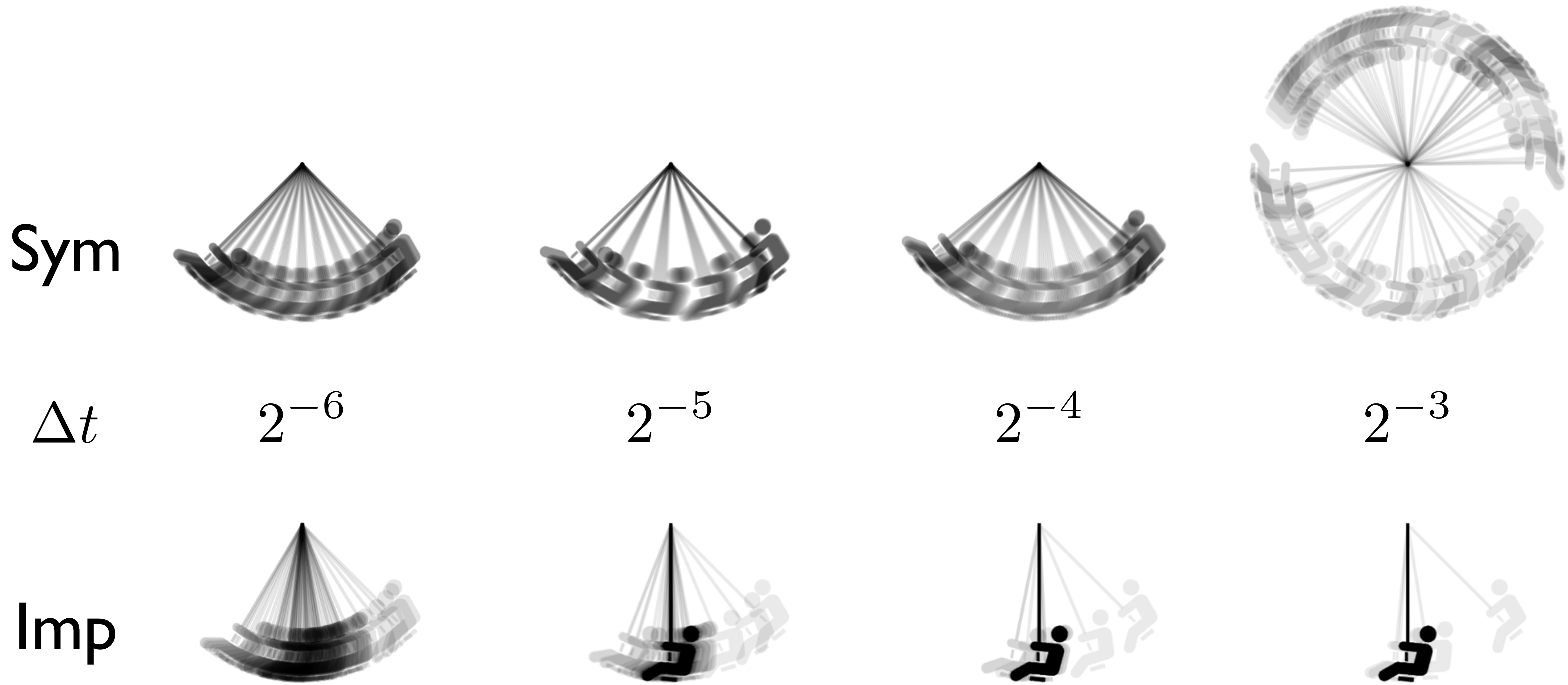


symplectic



implicit

Large Time Steps: Symplectic vs Implicit



Symplectic unstable region shown in largest time step

Implicit is stable, but damping is time step dependent

Three Integrators Summary

<u>Explicit</u>

cheap

artificial driving

unstable

<u>Variational</u>

cheap

good energy

unstable for large Δt

momenta conserved

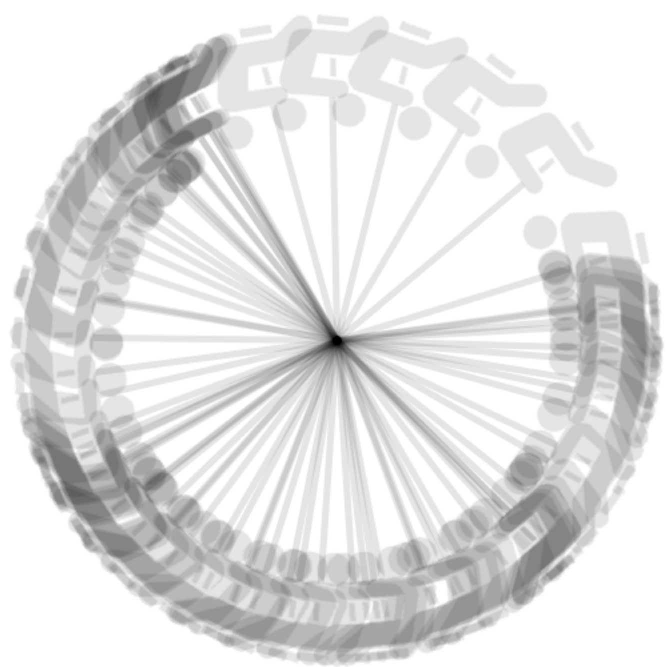
<u>Implicit</u>

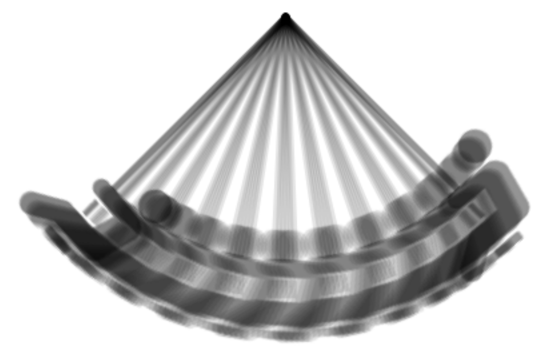
more expensive

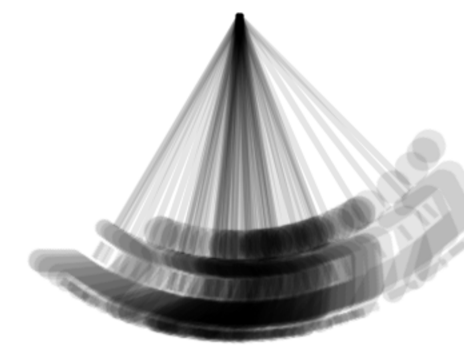
artificial damping

stable

Three Integrators Summary







Explicit	Variational	Implicit
cheap	cheap	more expensive
artificial driving	good energy	artificial damping
unstable	unstable for large Δt	stable
	momenta conserved	

Three Integrators Summary

Variational Integrators

cheap

good energy

momenta conserved

but (can't have it all!)

unstable for large Δt

Three Integrators Summary

Variational Integrators

cheap

good energy

momenta conserved

but (can't have it all!)

unstable for large Δt

Damped Systems

Want to include non-conservative forces, too

$$m\ddot{q} = -U'(q) + f(q, \dot{q})$$

Systems with non-conservative forces satisfy the

Lagrange-D'Alembert Principle

$$\delta_\eta \int_{t_1}^{t_2} \mathcal{L}(q(t), \dot{q}(t))\, dt + \int_{t_1}^{t_2} f(q(t), \dot{q}(t)) \cdot \eta\, dt = 0$$

variation of action in direction eta

integral of force in direction of variation, eta

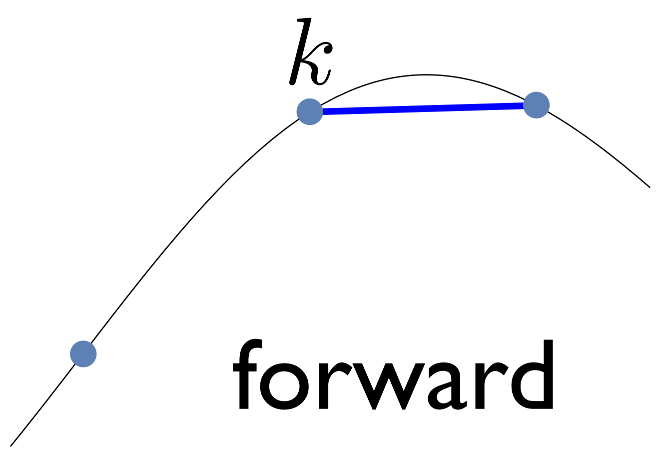
modification of Principle of Stationary Action

Damped Systems

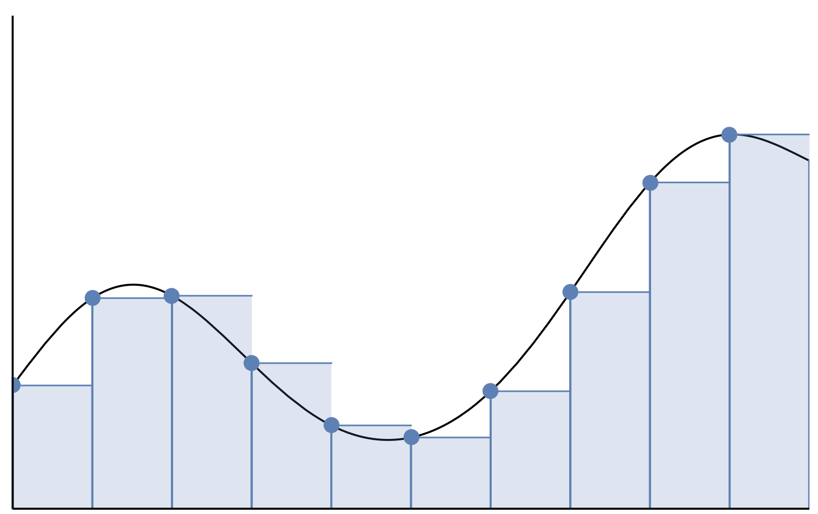
Lagrange-D'Alembert Principle

$$\delta_\eta \int_{t_1}^{t_2} \mathcal{L}(q(t), \dot{q}(t))\, dt + \int_{t_1}^{t_2} f(q(t), \dot{q}(t)) \cdot \eta \, dt = 0$$

Discretize using Variational Principle with:



forward

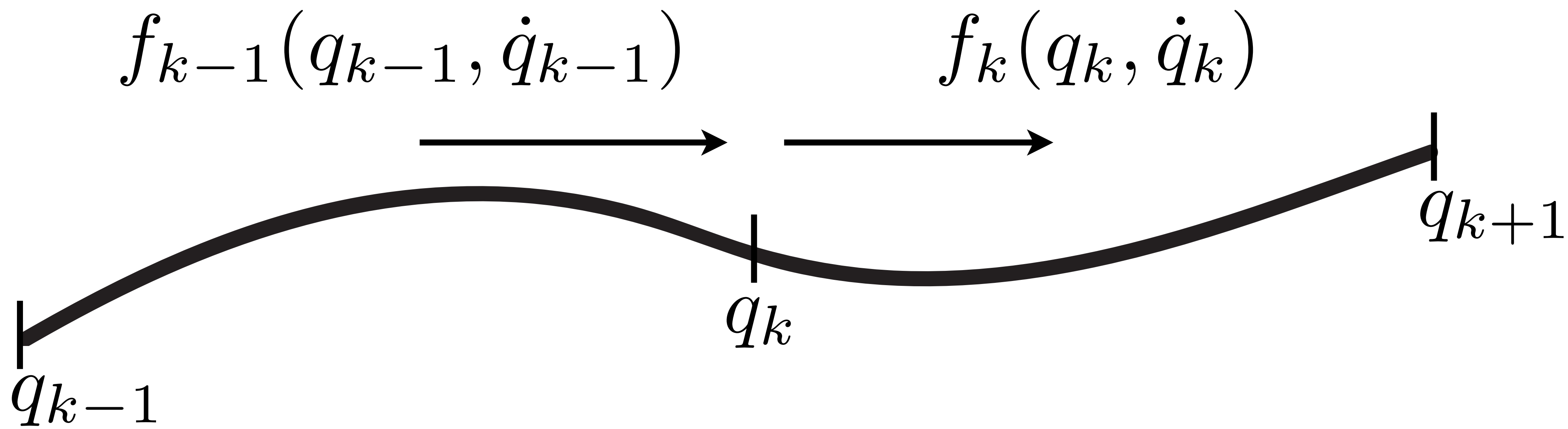


rectangular

(Forced Symplectic Euler Method)

Discrete Lagrange-D'Alembert Principle

Forced Symplectic Euler Method B

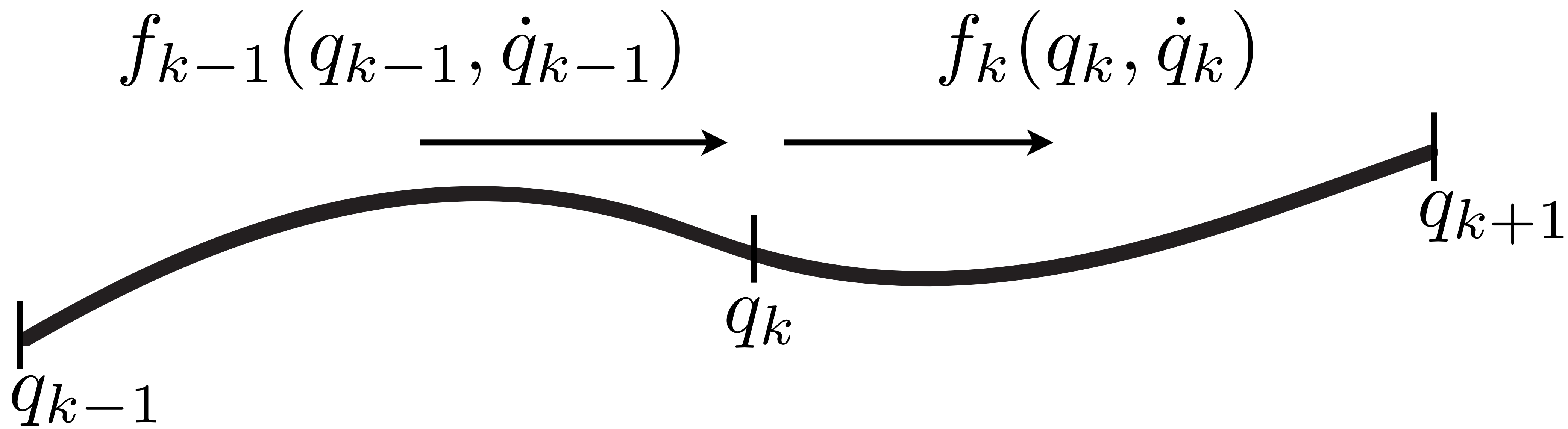


$$q_{k+1} = q_k + \Delta t\, \dot{q}_{k+1}$$

$$\dot{q}_{k+1} = \dot{q}_k + \Delta t\, m^{-1} \left(-U'(q_k) + \frac{f_{k-1} + f_k}{2} \right)$$

Discrete Lagrange-D'Alembert Principle

Forced Symplectic Euler Method B



$$q_{k+1} = q_k + \Delta t\, \dot{q}_{k+1}$$

$$\dot{q}_{k+1} = \dot{q}_k + \Delta t\, m^{-1} \left(-U'(q_k) + \frac{f_{k-1} + f_k}{2} \right)$$

e.g., air resistance

$$f_k = -c\, \dot{q}_k$$

Variational Damped Pendulum

30% damped

non-damped

Variational Damped Pendulum

30% damped

non-damped

Variational Damped Pendulum

30% damped

non-damped

behavior independent of step size
(within stable region)

Variational Damped Pendulum

non-damped

80% damped

30% damped

behavior independent of step size
(within stable region)

Variational Damped Pendulum

non-damped

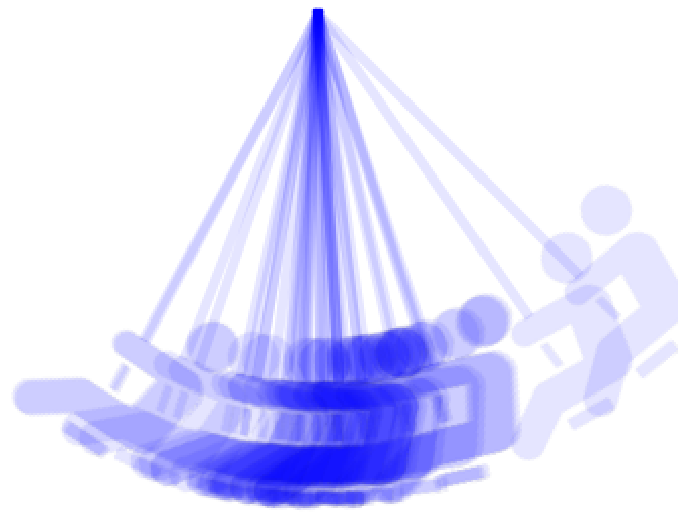
80% damped

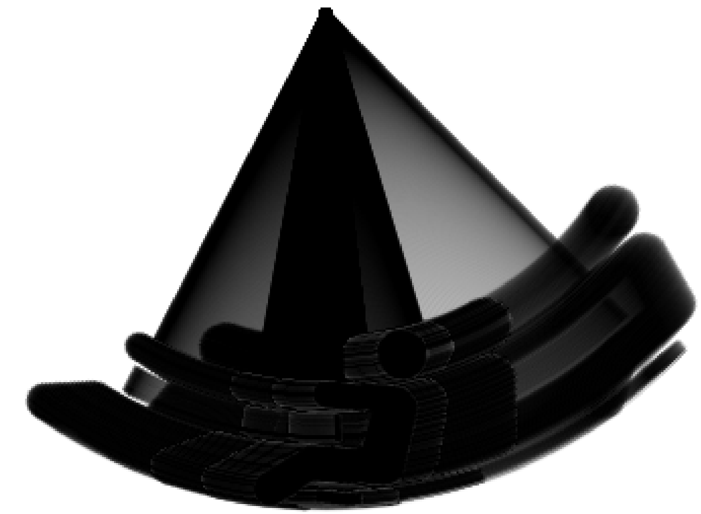
30% damped

behavior independent of step size
(within stable region)

30% Damped Pendulum

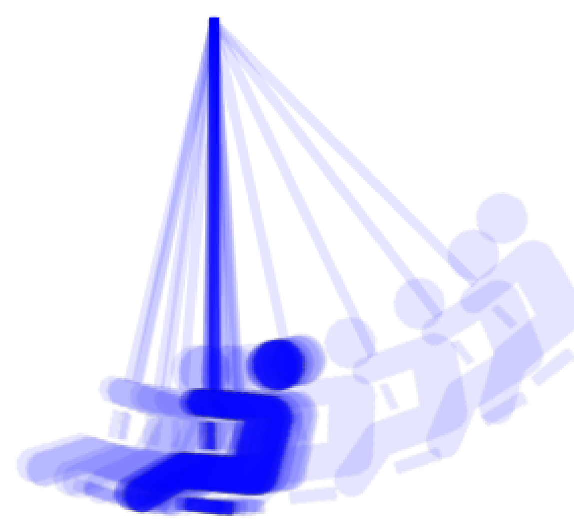
<u>Variational</u>
step size
independent

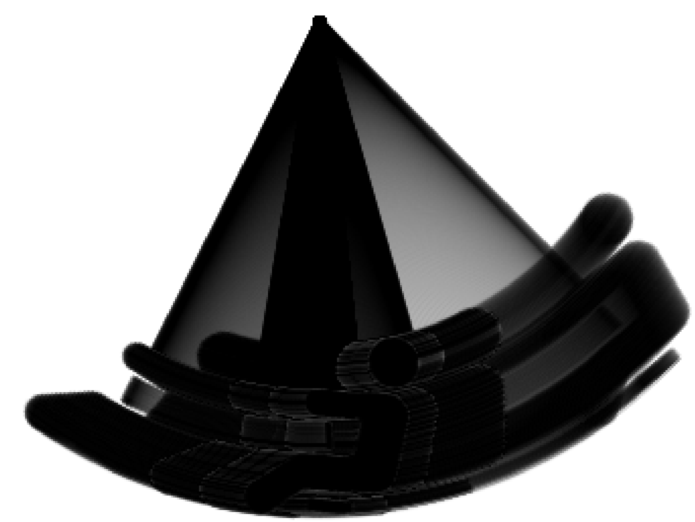




Δt 2^{-5} 2^{-10}

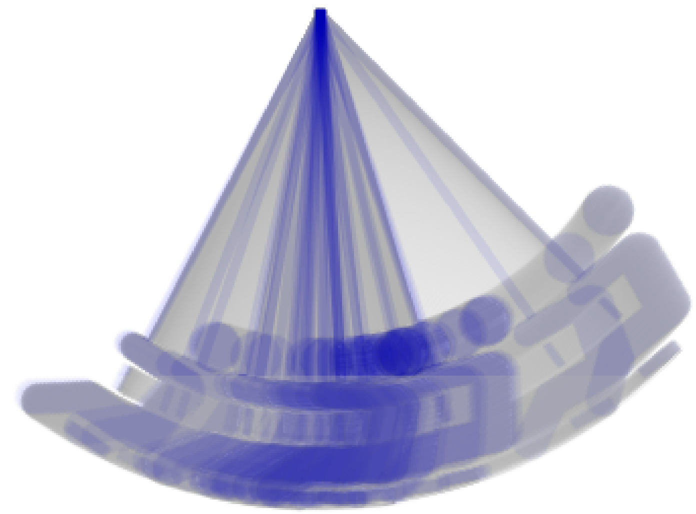
<u>Implicit</u>
step size
dependent





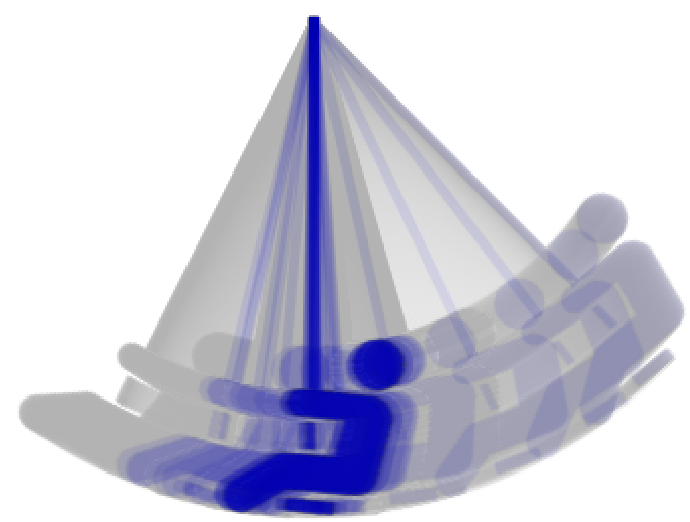
30% Damped Pendulum

<u>Variational</u>
step size
independent



Δt 2^{-5} 2^{-10}

<u>Implicit</u>
step size
dependent



30% Damped Pendulum

Variati

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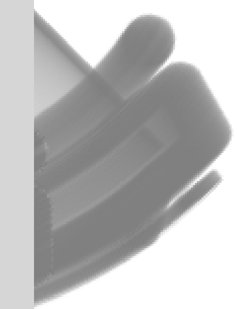
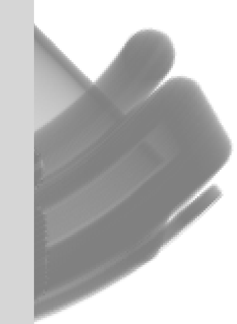




Forced Variational Integrators

cheap

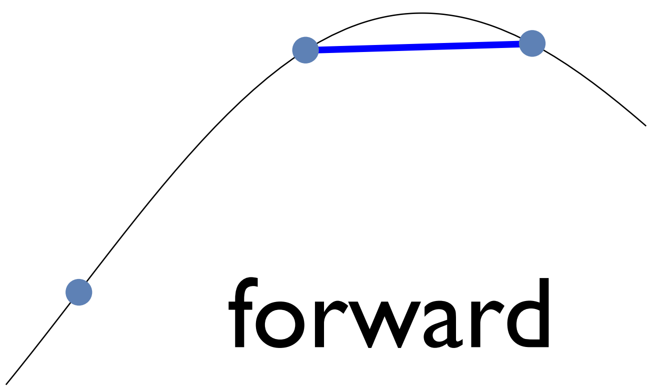
good energy behavior

behavior independent of step size (in stable region)

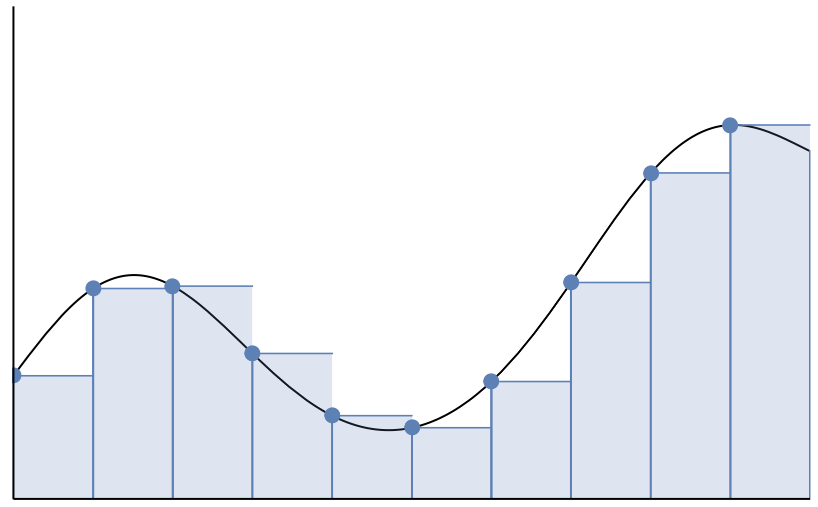
Essential for rough previews often done in Computer Graphics

Higher Order Variational Integrators

Recall:



forward



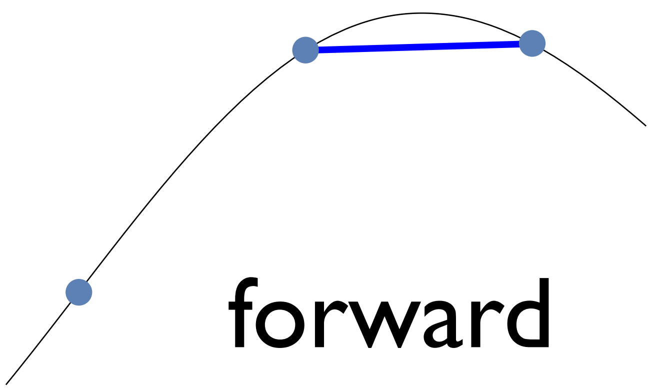
rectangular

zeroth order quadrature

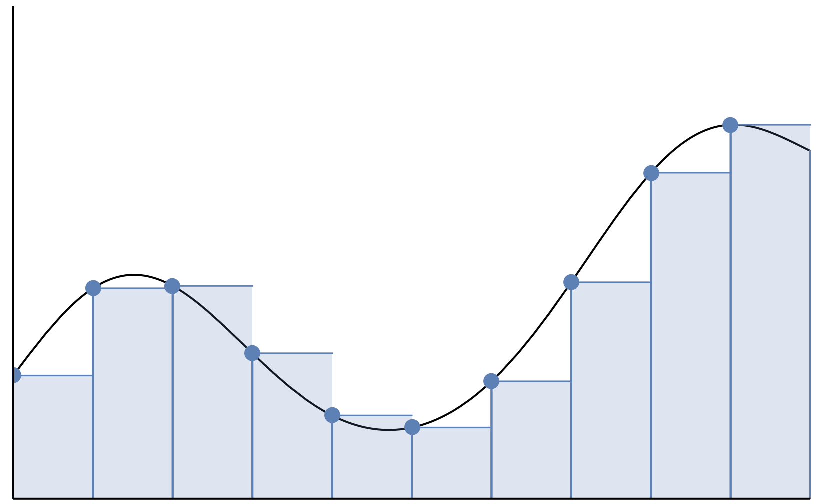
yields first order integration scheme

Higher Order Variational Integrators

Recall:



forward



rectangular

zeroth order quadrature

yields first order integration scheme

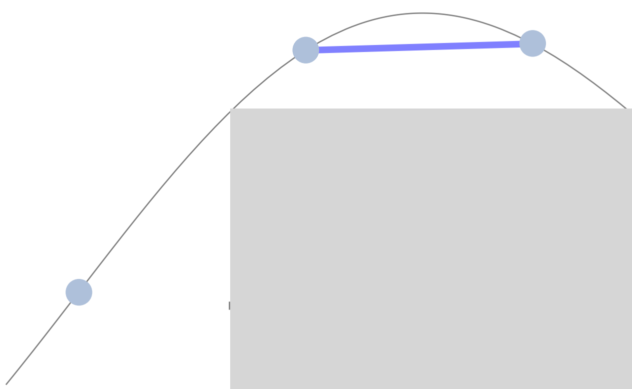
Generically:

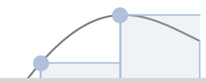
r^{th} order quadrature yields

$(r+1)^{\text{st}}$ order integrator

Higher Order Variational Integrators

Recall:





order
ture

Variational Integrators exist of all orders

r^{th} order quadrature yields

$(r+1)^{\mathrm{st}}$ order integrator

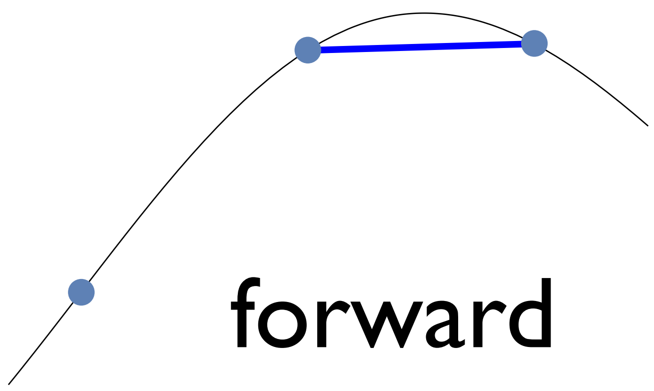
r^{th} order quadrature yields

$(r+1)^{\mathrm{st}}$ order integrator

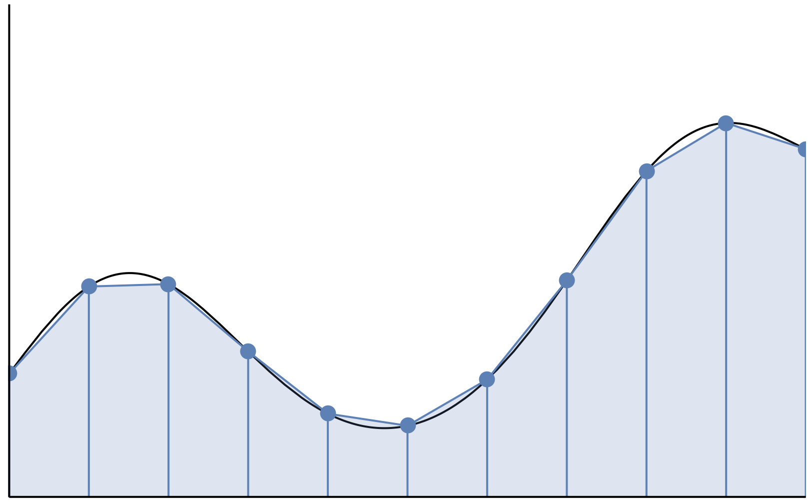
Some Well Known Variational Integrators

(of second order)

Use:



forward



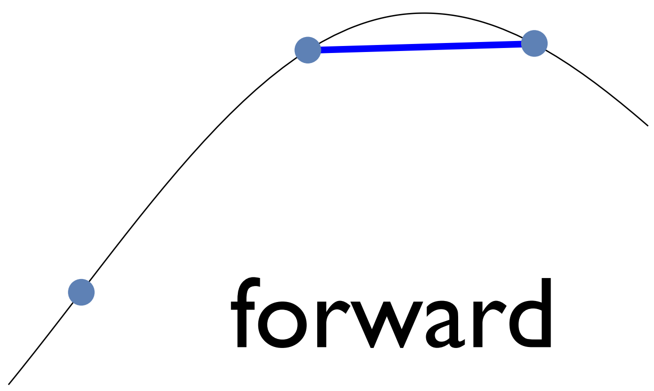
trapezoid

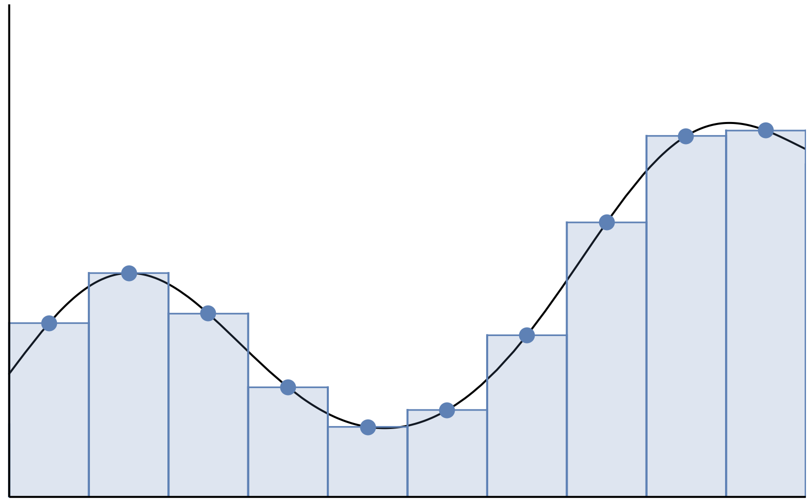
Derive: Störmer-Verlet Method

Some Well Known Variational Integrators

(of second order)

Use:





midpoint

Derive: Implicit Midpoint Method

(algebraic miracle, zeroth yields second order)

Comparison of First and Second Order Integrators

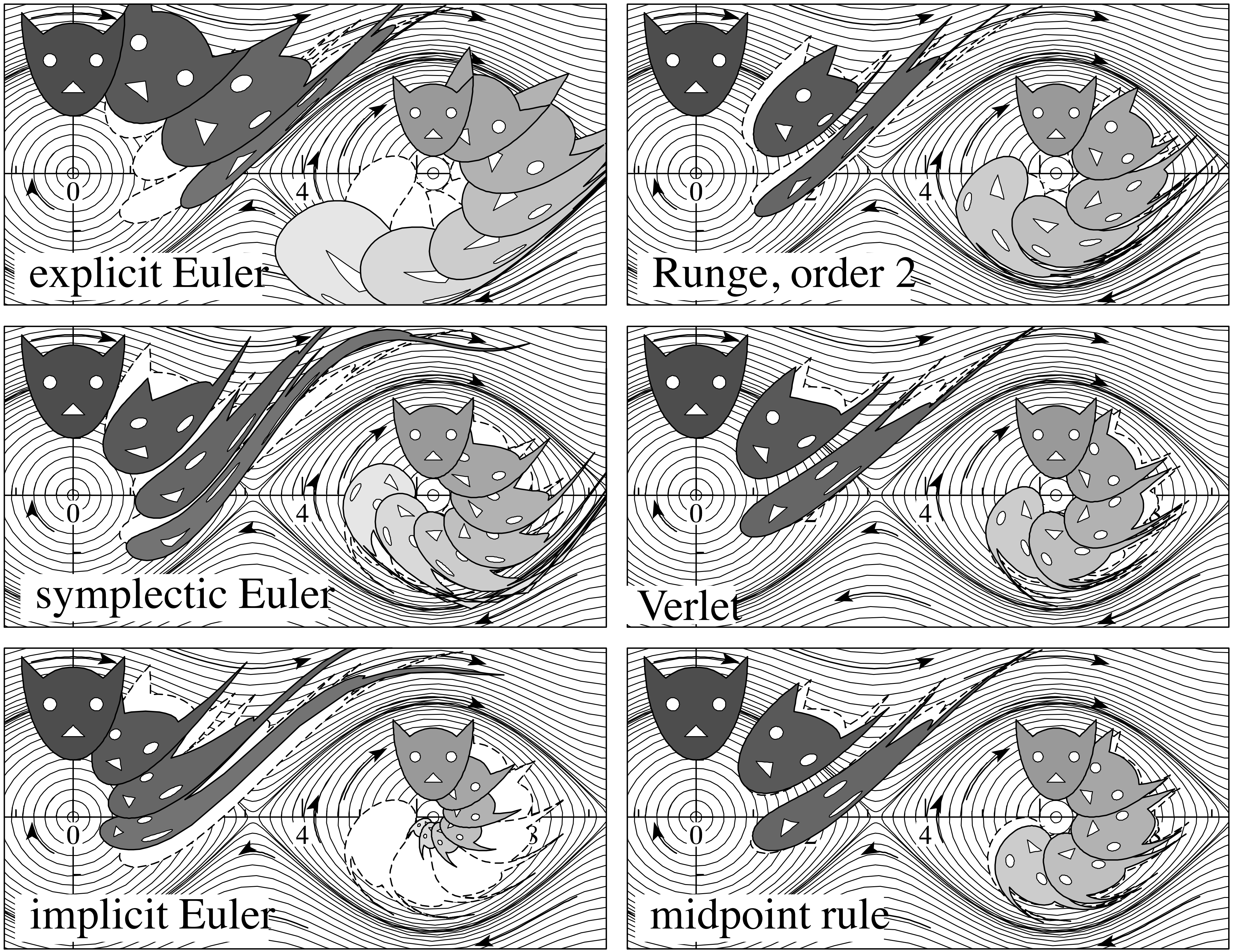


Image from Hairer, Lubich, and Wanner 2006

Summary: Variational Time Integrators

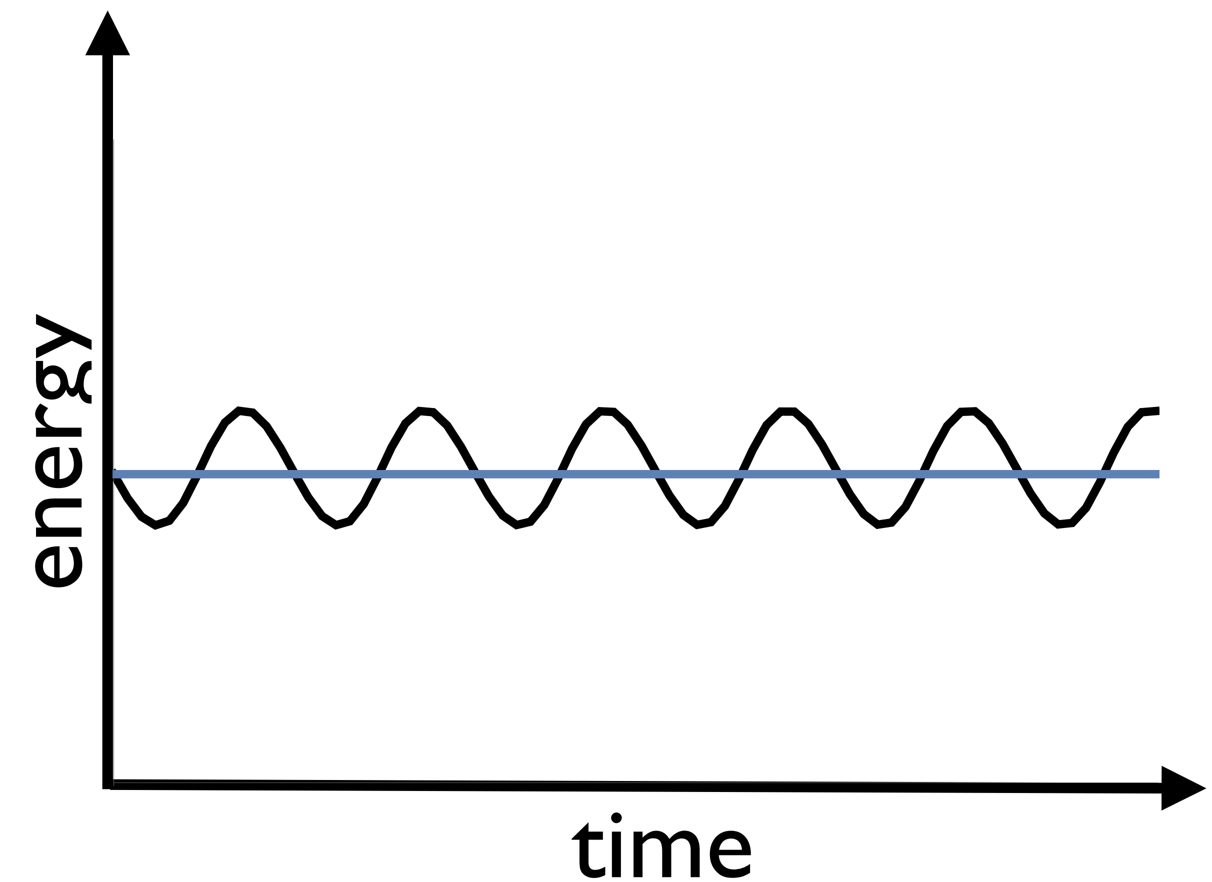
No more difficult to implement

... but have many advantages ...

Summary: Variational Time Integrators

Discrete Principle of Stationary Action

Symplectic structure guarantees good energy behavior



Noether's theorem guarantees conservation of momenta

Forced systems have behavior independent of step size (for stable time steps)

Questions?

(very incomplete list of) further reading

Principle of Least Action
Feynman Lectures on Physics II.19
http://www.feynmanlectures.caltech.edu/II_19.html

Geometric Numerical Integration: Structure-preserving Algorithms for Ordinary Differential Equations.
Hairer E, Lubich C, Wanner G. Springer; 2002.

Variational integrators.
West, Matthew (2004) Dissertation (Ph.D.), California Institute of Technology.

Geometric, variational integrators for computer animation.
L. Kharevych, Weiwei Yang, Y. Tong, E. Kanso, J. E. Marsden, P. Schröder, and M. Desbrun. 2006. In Proceedings of the 2006 ACM SIGGRAPH/Eurographics symposium on Computer animation (SCA '06).

Speculative parallel asynchronous contact mechanics.
Samantha Ainsley, Etienne Vouga, Eitan Grinspun, and Rasmus Tamstorf. 2012.
ACM Trans. Graph. 31, 6, Article 151 (November 2012), 8 pages. DOI=10.1145/2366145.2366170

Details of Movies Shown

Pendulum assumptions:

mass equals length equals one

$$-U'(q) = -\sin(q)$$

initial conditions

$$\dot{q}(0) = 0$$

$$q(0) = \pi/4$$

movies at 16 fps