Variational Integrators: Discretising the Action for Non-Hamiltonian Systems

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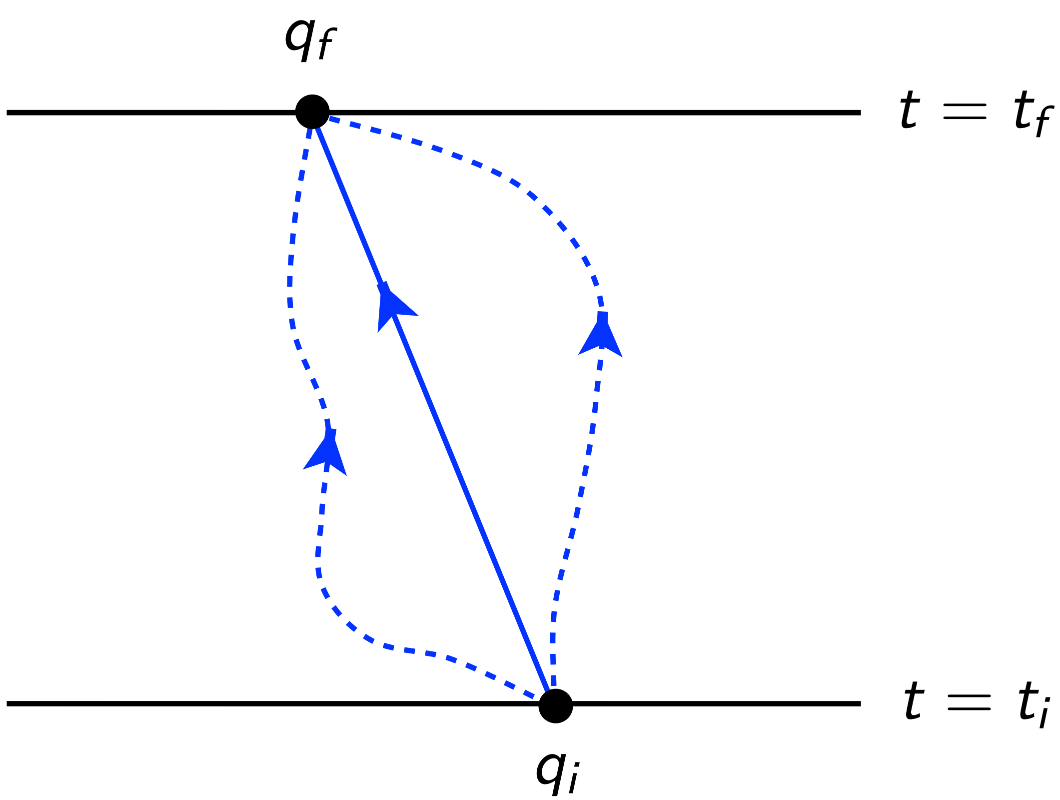
Hamilton's Principle



Hamilton's Principle states that the physical trajectories of the dynamical degrees of freedom are the solutions which extremize the action integral.

The Action: $$S[q] = \int_{t_i}^{t_f} L(q, \dot{q}, t)dt$$

Assuming appropriate boundary conditions for the variation, this implies the Euler-Lagrange equations of motion.

$$\delta S = 0 \to \frac{\partial L(q, \dot{q}, t)}{\partial q} - \frac{d}{dt}\frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}} = 0.$$

The Action As a Generating Function

Let's assume that q(t) extremizes the Action between some endpoints q_o and q_f and satisfies the E-L equation.

$$\frac{\partial S}{\partial q_o} = \underbrace{\int_{t_o}^{t_f} \left[\frac{\partial L(q,\dot{q},t)}{\partial q} - \frac{d}{dt}\frac{\partial L(q,\dot{q},t)}{\partial \dot{q}} \right] \frac{\partial q}{\partial q_o} dt}_{0} + \frac{\partial q}{\partial q_o}\frac{\partial L}{\partial \dot{q}}\bigg|_{t_o}^{t_f}$$

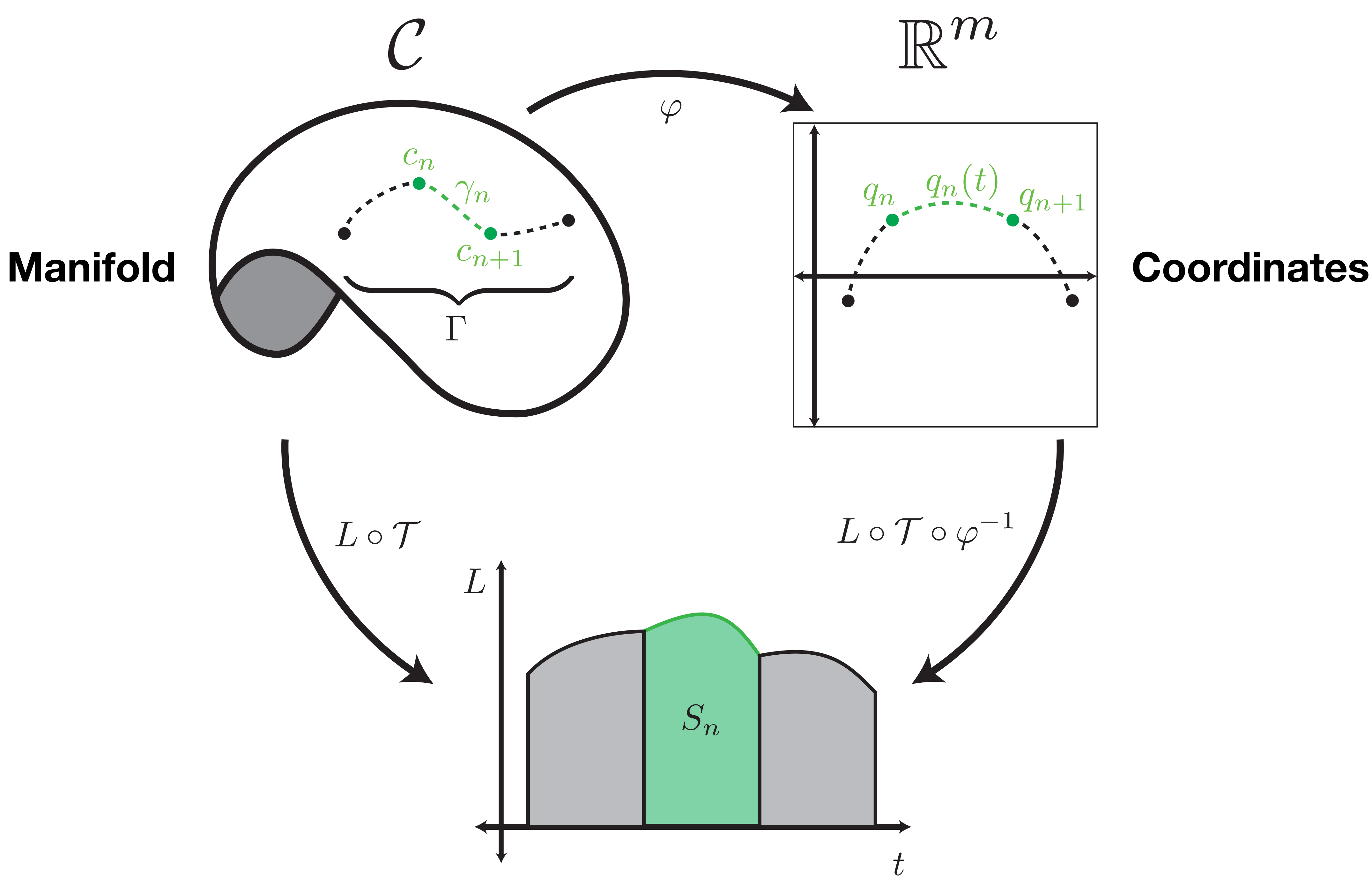
$$\frac{\partial S}{\partial q_o} = -\frac{\partial L}{\partial \dot{q}}\bigg|_{t_o} \equiv -p_o$$

Similarly, $$\frac{\partial S}{\partial q_f} = \frac{\partial L}{\partial \dot{q}}\bigg|_{t_f} \equiv p_f$$

The *extremal* action is a (Type 1) generating function for the canonical transformation that implements time evolution of the degrees of freedom (Hamilton-Jacobi theory).

Piecewise Extremal Trajectories & A "Perfect" Integrator

Let's consider a sequence of points $\{q_n\}$ that represent the positions at time $\{t_n\}$. We can connect these with a set of curves with $\{\gamma_n(t)\}$ that are piecewise connected



Piecewise Extremal Trajectories & A "Perfect" Integrator

Let's consider a sequence of points $\{q_n\}$ that represent the positions at time $\{t_n\}$.

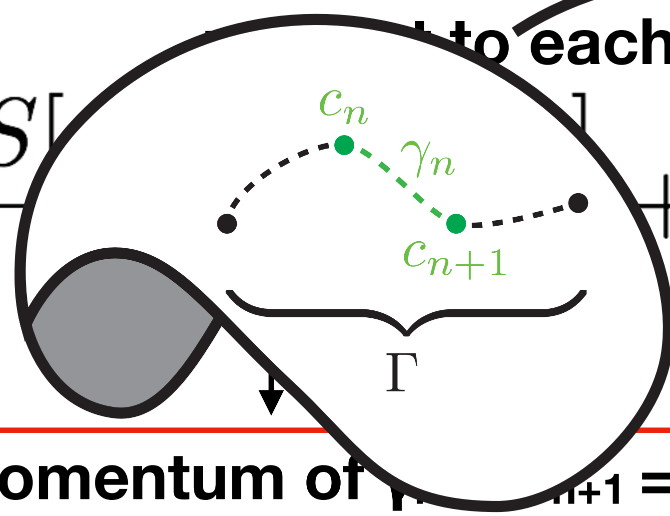
Assume each γ_n (uniquely) extremizes $S[\gamma_n]$ between points q_n and q_{n+1}.

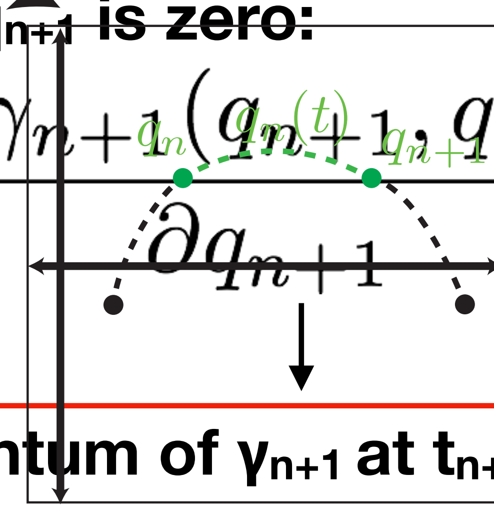
We can connect these with a set of curves with $\{\gamma_n(t)\}$ that are piecewise connected

The total action is then, $\sum_n S[\gamma_n]$

Since each subpath is extremal, the total action is extremized iff the derivative with respect to each point q_{n+1} is zero:

$$\forall n, \quad \frac{\partial S[\gamma_n(q_n, q_{n+1})]}{\partial q_{n+1}} + \frac{\partial S[\gamma_{n+1}(q_{n+1}, q_{n+2})]}{\partial q_{n+1}} = 0$$





Momentum of γ_n at t_{n+1} = Momentum of γ_{n+1} at t_{n+1}

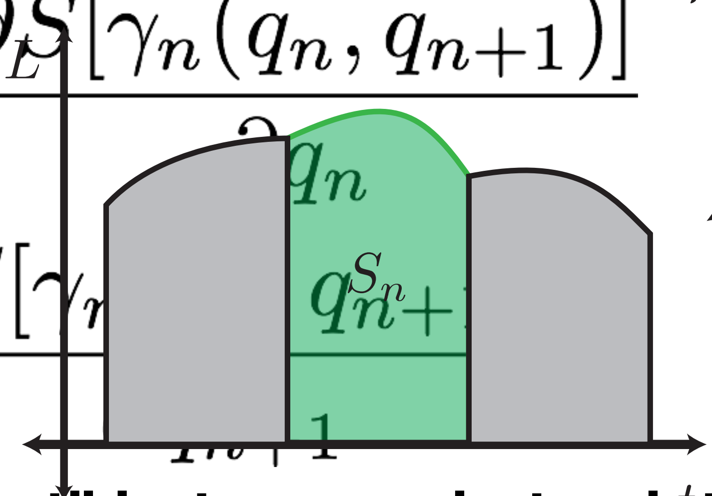
We can treat this as a mapping between $q_n, p_n \rightarrow q_{n+1}, p_{n+1}$ defined by

$$p_n \equiv -\frac{\partial S[\gamma_n(q_n, q_{n+1})]}{\partial q_n}$$

Solve for q_{n+1} in terms of q_n, p_n

$$p_{n+1} \equiv \frac{\partial S[\gamma_n(q_n, q_{n+1})]}{\partial q_{n+1}}$$

p_{n+1} from q_{n+1}, q_n



This defines a "perfect" but somewhat pointless integrator…

Variational Integrators

Consider *approximations* to the extremal action between each point in the sequence $\{q_n\}$. This *discretized action* can be constructed with 2 ingredients:

1. An approximation to the trajectory between the points

$$\gamma_n[q_n, q_{n+1}](t) \simeq \gamma_n^d[q_n, q_{n+1}](t)$$

2. An approximation to the action integral itself (numerical quadrature)

$$S[\gamma_n] \simeq S_d[\gamma_n^d].$$

These choices define different variational integrators.

Extremizing the discretized action wrt each point gives the discrete E-L equations,

$$\forall n, \quad \frac{\partial S_d[\gamma_n^d(q_n, q_{n+1})]}{\partial q_{n+1}} + \frac{\partial S_d[\gamma_{n+1}^d(q_{n+1}, q_{n+2})]}{\partial q_{n+1}} = 0$$

$$p_n^d = -\frac{\partial S_d[\gamma_n^d(q_n, q_{n+1})]}{\partial q_n}$$

Solve for q_{n+1} in terms of q_n, p_n

Or

$$p_{n+1}^d = \frac{\partial S_d[\gamma_{n+1}^d(q_n, q_{n+1})]}{\partial q_{n+1}}$$

p_{n+1} from q_{n+1}, q_n

These define mappings q_n, p_n -> q_{n+1}, p_{n+1} that are accurate to the same order as the discretized action. Symplectic with long term conservation properties.

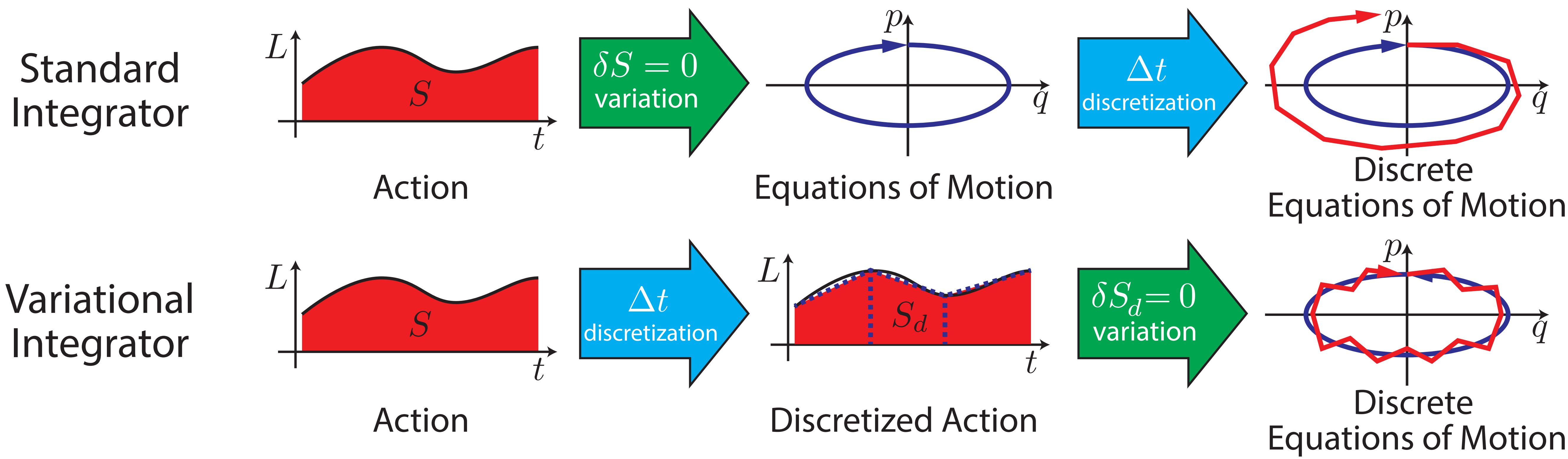
Noether's Theorem

Symmetries of the Action ⟷ **Conserved Quantities**

Time-shift sym. — Energy

Translational sym. — Momentum

Rotational sym. — Ang. Momentum



Symmetries of the Discrete Action

Conserved Quantities

Noether’s Theorem

1. An approximation to the trajectory between the points

$$\gamma_n[q_n, q_{n+1}](t) \simeq \gamma_n^d[q_n, q_{n+1}](t)$$

2. An approximation to the action integral itself (numerical quadrature)

$$S[\gamma_n] \simeq S_d[\gamma_n^d].$$

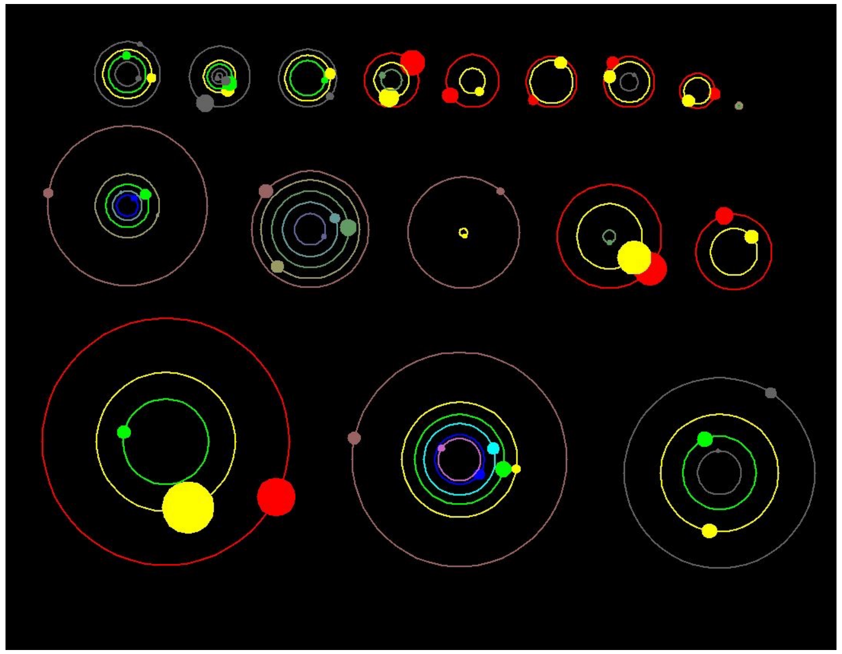
These choices define different variational integrators.

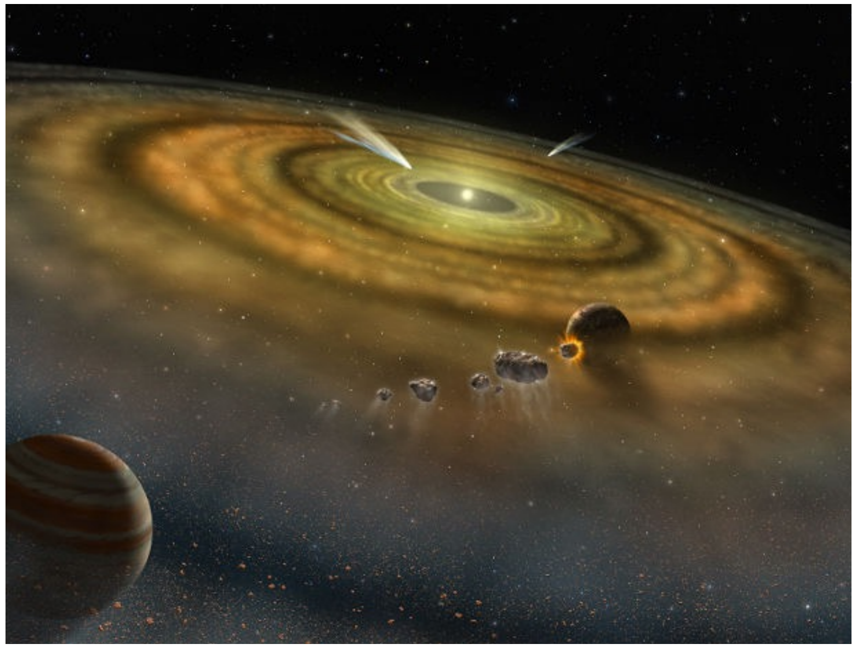
Name	Trajectory Method	Quadrature Method	Order	Notes
Galerkin-Gauss Lobatto (GGL)	Polynomial through GL pts	GL Quadrature	$\mathcal{O}(\Delta t^{2r+3})$	non-perturbative
Stormer-Verlet (2nd order GGL)	Linear through end pts	Trapezoid Rule	$\mathcal{O}(\Delta t^3)$	non-perturbative
Wisdom-Holman Gauss-Lobatto (WHGL)	Keplerian b/w end points	GL Quadrature	$\mathcal{O}(\varepsilon \Delta t^{2r+3}) + \mathcal{O}(\varepsilon^2 \Delta t^3)$	perturbative
Kick-Drift-Kick (2nd order WHGL)	Keplerian b/w end points	Trapezoid Rule	$\mathcal{O}(\varepsilon \Delta t^3) + \mathcal{O}(\varepsilon^2 \Delta t^3)$	perturbative
Wisdom-Holman Farr (WHFarr)	Keplerian b/w end points	Adaptive/Numerical Quadrature	$\mathcal{O}(\varepsilon^2 \Delta t^3)$	perturbative Effective adaptive method w/ fixed formal step size

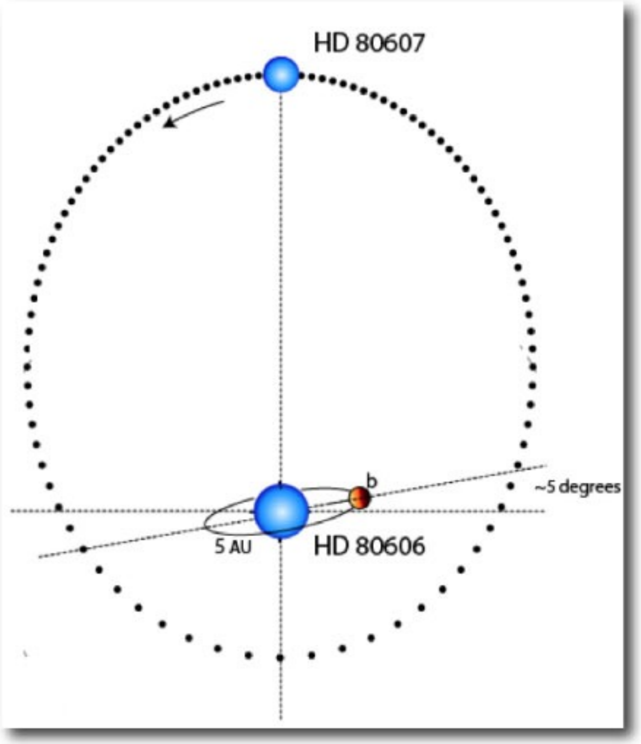
Using this ansatz it is easy to construct variational integrators that are symplectic, conserve Noether charges, and can include both position and velocity dependent forces.

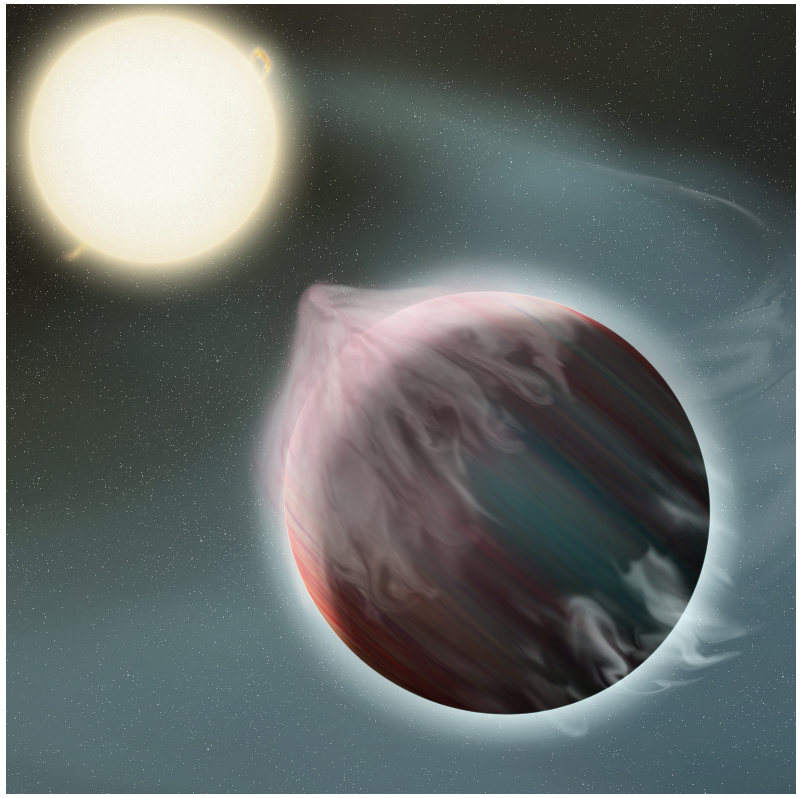
Variational Integration

… can only be applied to conservative systems?

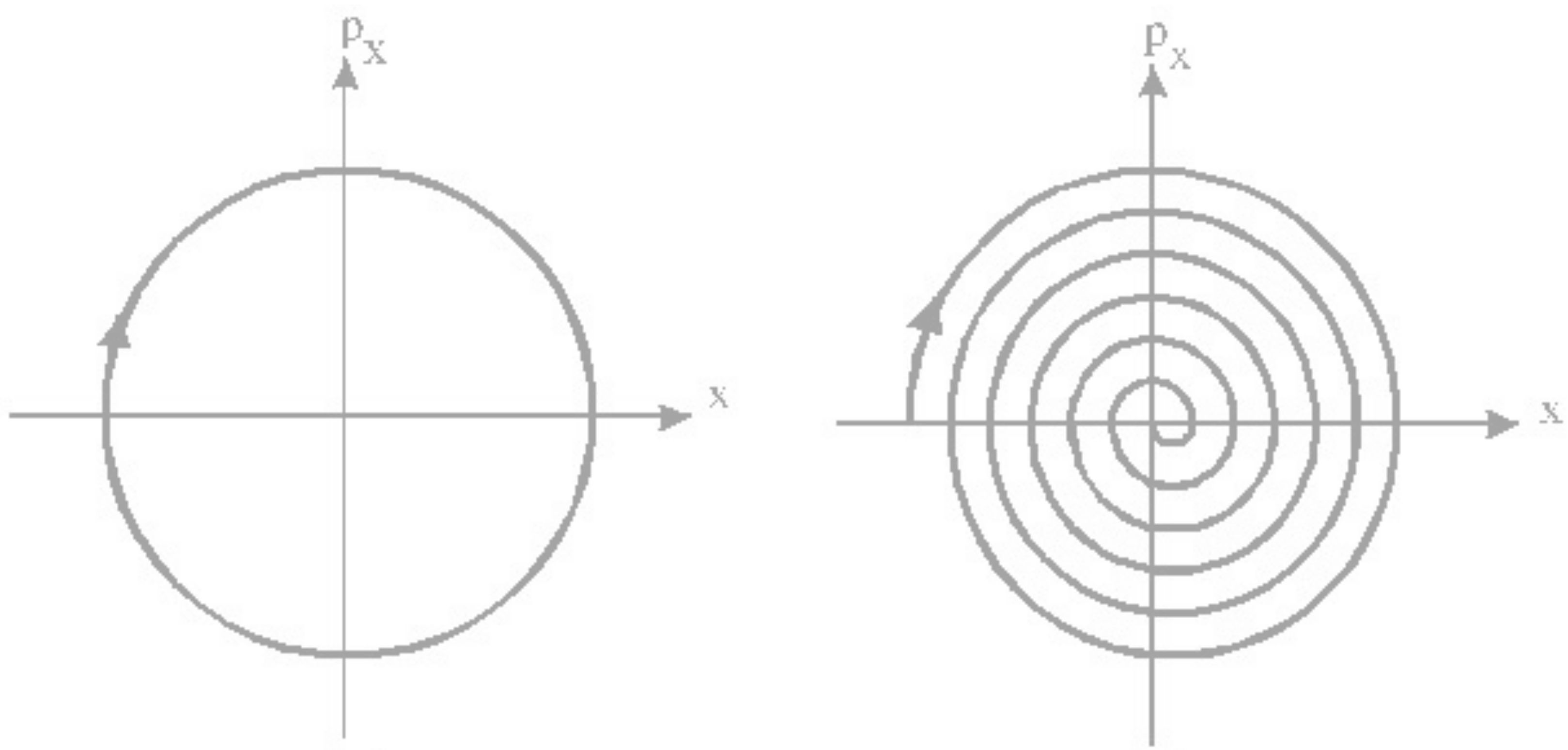






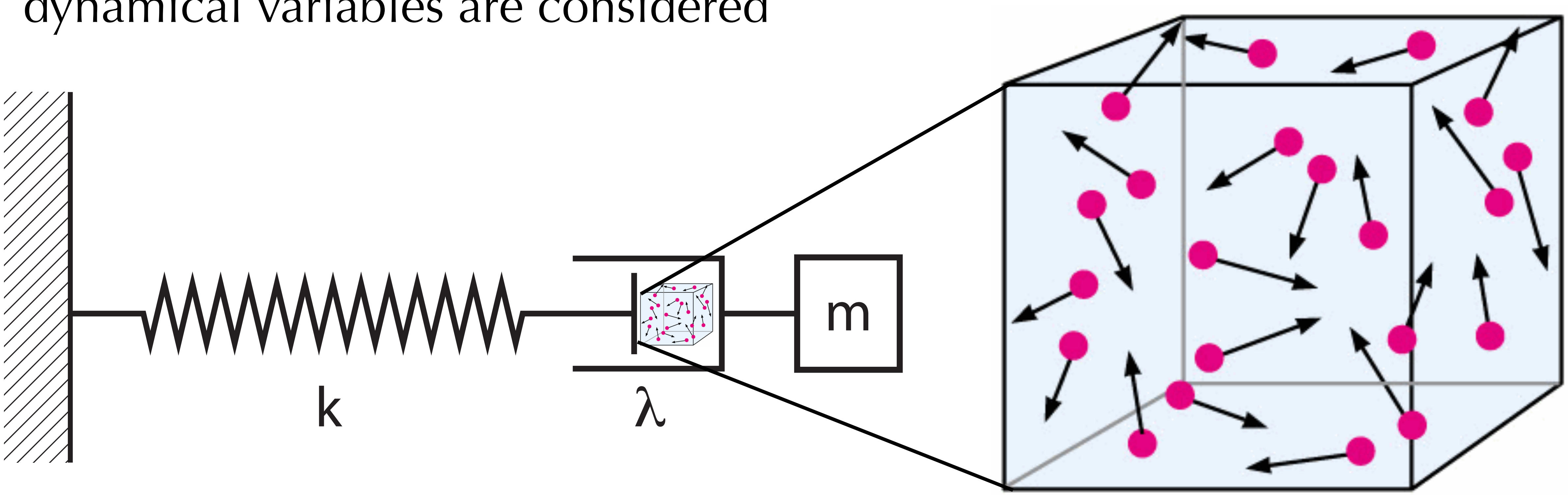


Can we build integrators for nonconservative dynamics that work as well as symplectic integrators?



How does a problem become non-conservative?

- All classical systems are micro-physically conservative
- Nonconservative effects can arise when only a subset of the dynamical variables are considered



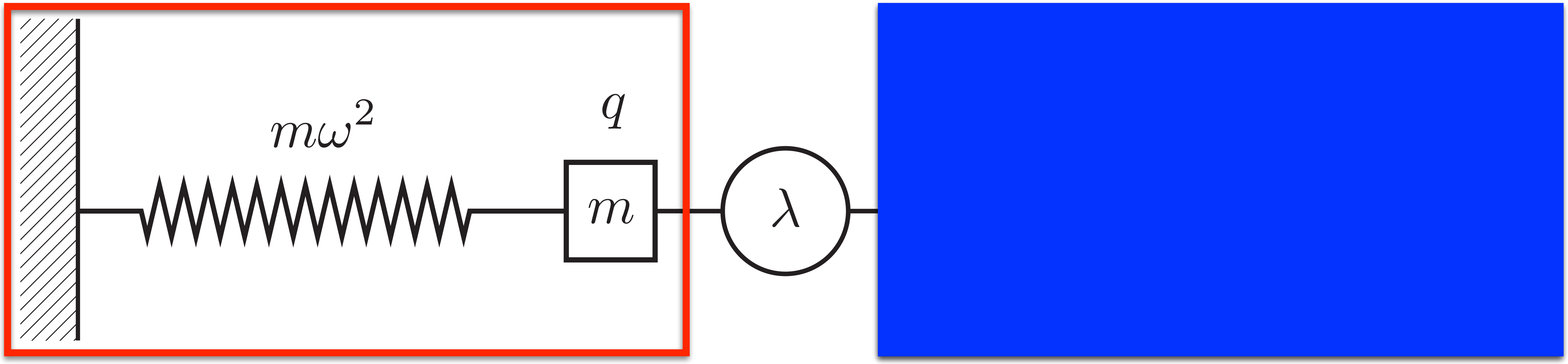
- Hierarchy of "accessible" and "inaccessible" degrees of freedom
- This hierarchy can be due to explicit choice, observational constraint, or natural separation of scales

Accessible/Inaccessible Hierarchy in Nonconservative Systems

Accessible	Inaccessible
Macroscopic or collective variables (e.g. thermodynamic)	Integrated out/coarse-grained away (e.g. individual x,v)
Explicitly tracked (e.g. particle position)	Explicitly untracked/unknown (unobserved, unmeasurable)
"Stiff" d.o.f.	"Sloppy" d.o.f.
e.g. oscillator position	e.g. thermal degrees of freedom in the damper

- Finding a way of "integrating out" degrees of freedom at the level of the Action can give us nonconservative physics, but…
- Trying this with the regular action gives non-causal solutions…

Coupled harmonic oscillators

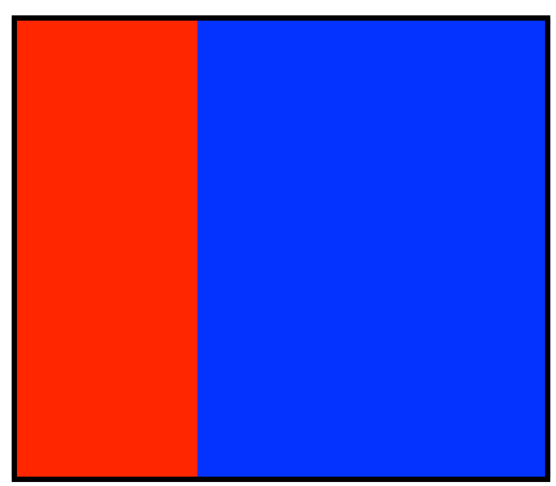


Action:

$$S[q,Q] = \int_{t_i}^{t_f} dt \left\{ \boxed{\frac{m}{2}\left(\dot{q}^2 - \omega^2 q^2\right)} + \lambda q Q + \boxed{\frac{M}{2}\left(\dot{Q}^2 - \Omega^2 Q^2\right)} \right\}$$

As a whole, the oscillators conserve energy but not individually

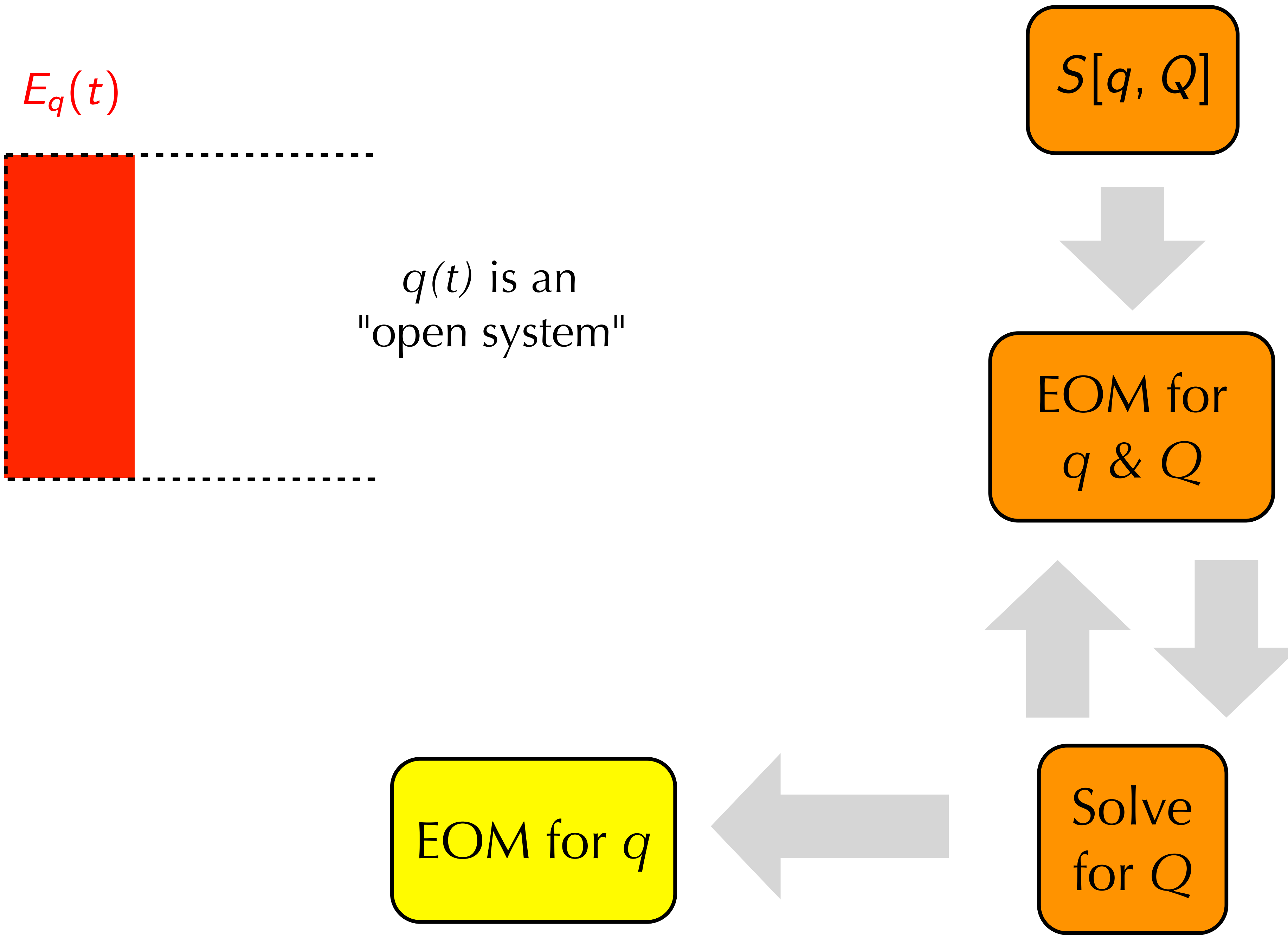
$$E = E_q(t) + E_Q(t)$$



What if we could only measure *q(t)*?

What if we could only measure $q(t)$?

What would its EOM be?



"Integrating out" or "eliminating" $Q(t)$ yields

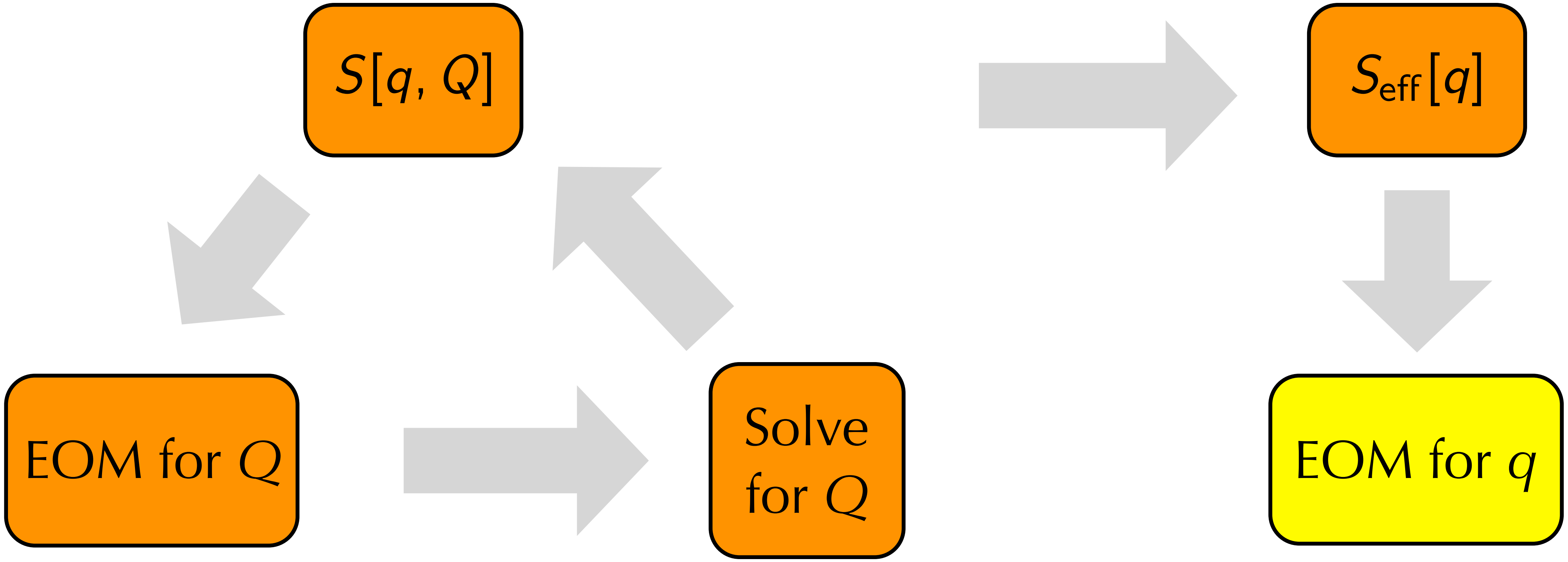
$$m\ddot{q} + m\omega^2 q = \lambda Q^{(h)}(t) + \frac{\lambda^2}{M}\int_{t_i}^{t_f} dt'\, G_{\rm ret}(t-t')\boxed{q(t')}$$

$$G_{\rm ret}(t-t') = \Theta(t-t')\frac{\sin\Omega(t-t')}{\Omega}$$

EOM for $q(t)$ are:

- Causal
- Solutions determined by initial data alone
- Dynamics at time t depends on the past history of q

What if we integrated out $Q(t)$ at the level of the action?



$$S_{\rm eff}[q] = \int_{t_i}^{t_f} dt \left\{ \frac{m}{2}\left(\dot{q}^2 - \omega^2 q^2\right) + \lambda q Q^{(h)}(t) + \frac{\lambda^2}{2M}\int_{t_i}^{t_f} dt' \, \boxed{q(t)}\, G_{\rm ret}(t-t')\, \boxed{q(t')} \right\}$$

$t \leftrightarrow t'$ symmetric

but...

$$\frac{\lambda^2}{2M}\int_{t_i}^{t_f} dt\, dt'\, q(t) \frac{G_{\rm ret}(t-t') + G_{\rm adv}(t-t')}{2} q(t')$$

$$G_{\rm adv}(t-t') = G_{\rm ret}(t'-t)$$

The EOM for $q(t)$ derived from the effective action with Hamilton's Principle is

$$m\ddot{q} + m\omega^2 q = \lambda Q^{(h)}(t) + \frac{\lambda^2}{M}\int_{t_i}^{t_f} dt' \, \frac{G_{\text{ret}}(t-t') + G_{\text{adv}}(t-t')}{2} q(t')$$

$$\frac{G_{\text{ret}}(t-t') + G_{\text{adv}}(t-t')}{2} = \frac{\sin \Omega |t-t'|}{\Omega}$$

EOM for $q(t)$ are:

- Acausal
- Solutions determined by initial and final data
- Dynamics at time t depends on the past history and future evolution of q
- Not correct...

A hint...

The problem arises because $q(t)q(t')$ is symmetric in t and t' in the two-oscillator example...

Can we "break" this symmetry somehow?

What if we use two different sets of variables?

$$\int_{t_i}^{t_f} dt\, dt'\, q(t) G_{\rm ret}(t, t') q(t') \quad \Rightarrow \quad \int_{t_i}^{t_f} dt\, dt'\, q_1(t) G_{\rm ret}(t, t') q_2(t')$$

It seems that varying with respect to $q_1(t)$ would give the correct time-asymmetric force if we set q_2=q_1 afterwards

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Classical Mechanics of Nonconservative Systems

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(Received 1 September 2012; published 22 April 2013)

Hamilton's principle of stationary action lies at the foundation of theoretical physics and is applied in many other disciplines from pure mathematics to economics. Despite its utility, Hamilton's principle has a subtle pitfall that often goes unnoticed in physics: it is formulated as a boundary value problem in time but is used to derive equations of motion that are solved with initial data. This subtlety can have undesirable effects. I present a formulation of Hamilton's principle that is compatible with initial value problems. Remarkably, this leads to a natural formulation for the Lagrangian and Hamiltonian dynamics of generic nonconservative systems, thereby filling a long-standing gap in classical mechanics. Thus, dissipative effects, for example, can be studied with new tools that may have applications in a variety of disciplines. The new formalism is demonstrated by two examples of nonconservative systems: an object moving in a fluid with viscous drag forces and a harmonic oscillator coupled to a dissipative environment.

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The principle of stationary nonconservative action for classical mechanics and field theories

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Center for Radiophysics and Space Research, Cornell University, Ithaca, NY 14853, USA

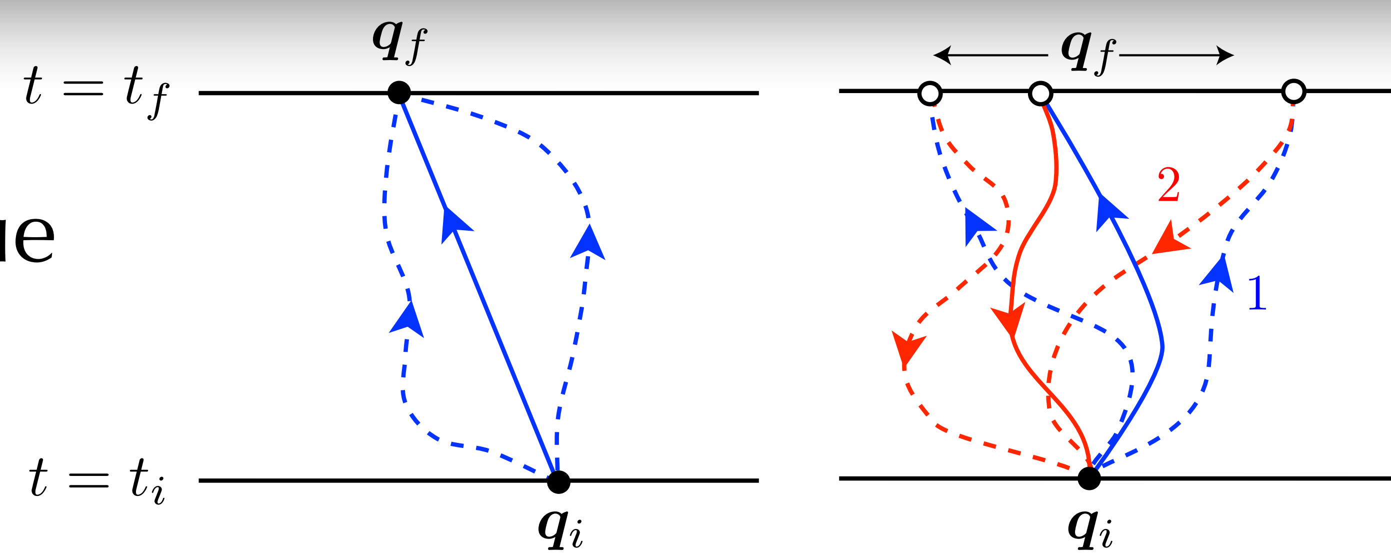
We further develop a recently introduced variational principle of stationary action for problems in nonconservative classical mechanics and extend it to classical field theories. The variational calculus used is consistent with an initial value formulation of physical problems and allows for time-irreversible processes, such as dissipation, to be included at the level of the action. In this formalism, the equations of motion are generated by extremizing a nonconservative action $\mathcal{S}$, which is a functional of a doubled set of degrees of freedom. The corresponding nonconservative Lagrangian contains a "potential" K which generates nonconservative forces and interactions. Such a nonconservative potential can arise in several ways, including from an open system interacting with inaccessible degrees of freedom or from integrating out or coarse-graining a subset of variables in closed systems. We generalize Noether's theorem to show how Noether currents are modified and no

PRL 110, 174301 (2013) PHYSICAL REVIEW LETTERS week ending 26 APRIL 2013

Classical Mechanics of Nonconservative Systems

The principle of stationary nonconservative action for classical mechanics and field theories

Boundary Value Problem



Initial Value Problem

- **allows self-consistent "integrating out" of degrees of freedom at the level of the action!**
- Physical Limit: $q_1 = q_2$
- Nonconservative (non-Hamiltonian) effects come in through nonconservative "potential" *K*, which couples the doubled paths together
- related to "closed loop" (in-in) formalism

For MUCH more info: Galley, DT, & Stein (2014) [arXiv:1412.3082]

Generalized Noether's Theorem

Symmetries of the Conservative Action

Evolution of "conserved" quantities according to the nonconservative action

Galley, DT & Stein (2014)

Nonconservative ("Slimplectic") Variational Integrators

The Astrophysical Journal Letters, 809:L9 (6pp), 2015 August 10

doi:10.1088/2041-8205/809/1/L9

"SLIMPLECTIC" INTEGRATORS: VARIATIONAL INTEGRATORS FOR GENERAL NONCONSERVATIVE SYSTEMS

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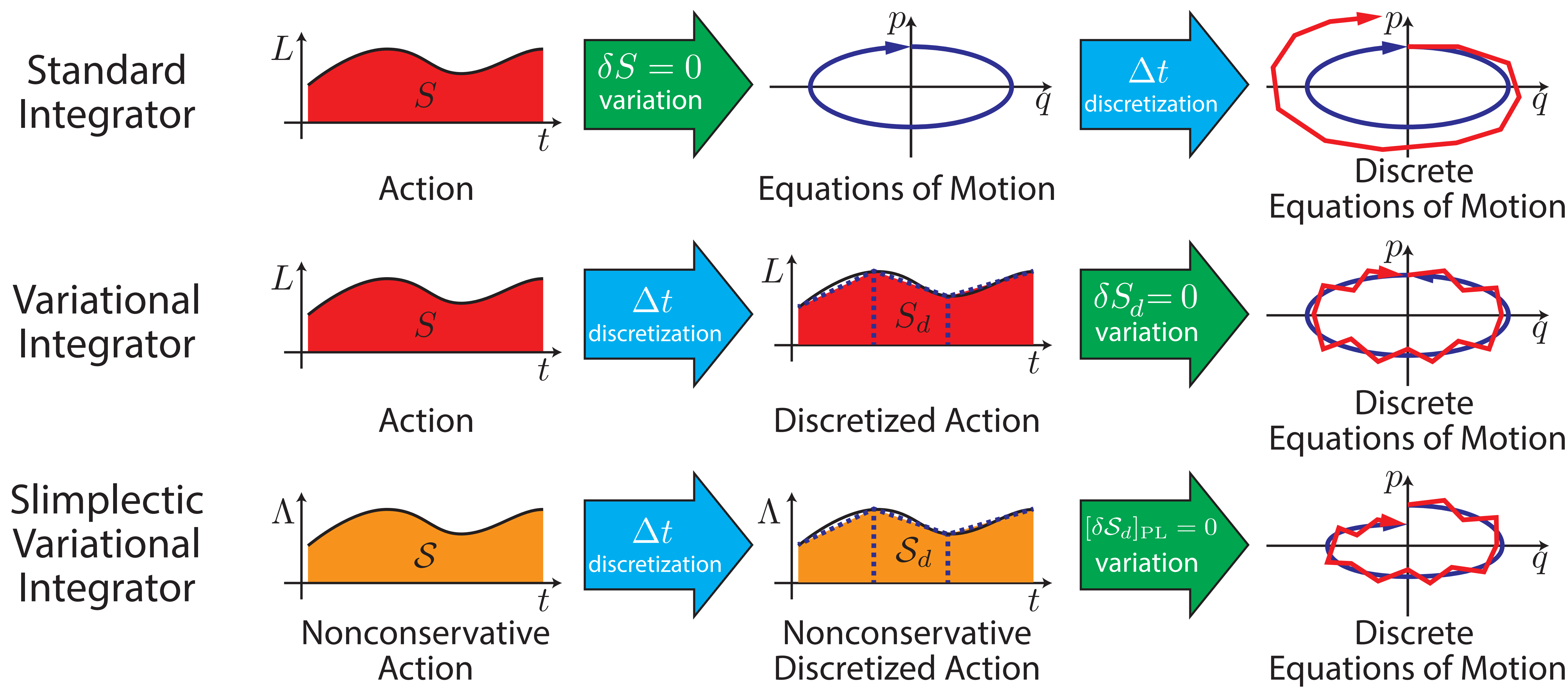
ABSTRACT

Symplectic integrators are widely used for long-term integration of conservative astrophysical problems due to their ability to preserve the constants of motion; however, they cannot in general be applied in the presence of nonconservative interactions. In this Letter, we develop the "slimplectic" integrator, a new type of numerical integrator that shares many of the benefits of traditional symplectic integrators yet is applicable to general nonconservative systems. We utilize a fixed-time-step variational integrator formalism applied to the principle of stationary nonconservative action developed in Galley et al. As a result, the generalized momenta and energy (Noether current) evolutions are well-tracked. We discuss several example systems, including damped harmonic oscillators, Poynting–Robertson drag, and gravitational radiation reaction, by utilizing our new publicly available code to demonstrate the slimplectic integrator algorithm. Slimplectic integrators are well-suited for integrations of systems where nonconservative effects play an important role in the *long-term* dynamical evolution. As such they are particularly appropriate for cosmological or celestial *N*-body dynamics problems where nonconservative interactions, e.g., gas interactions or dissipative tides, can play an important role.

Key words: celestial mechanics – methods: numerical – planets and satellites: dynamical evolution and stability

Nonconservative ("Slimplectic") Variational Integrators

Nonconservative Variational Integrators (Slimplectic Integrators) can be built by discretizing the *nonconservative* action

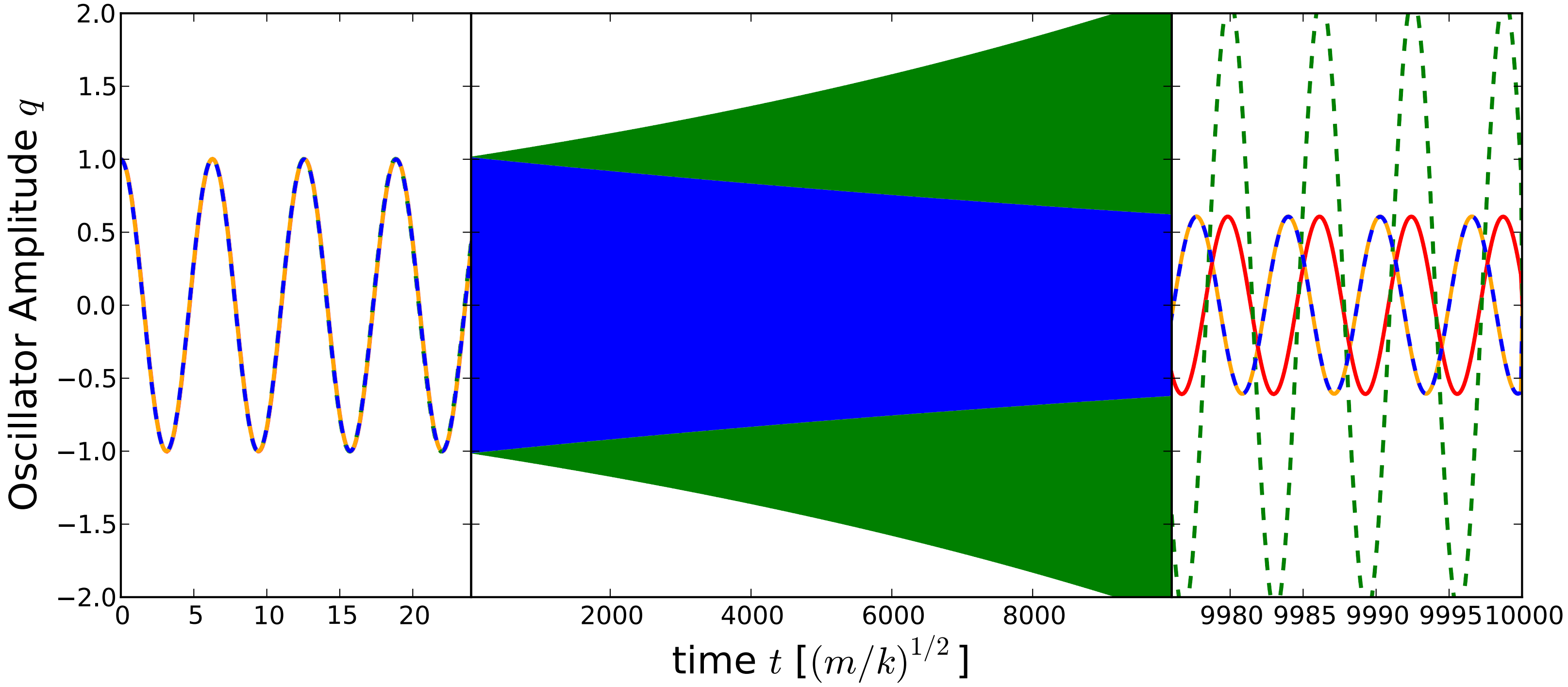


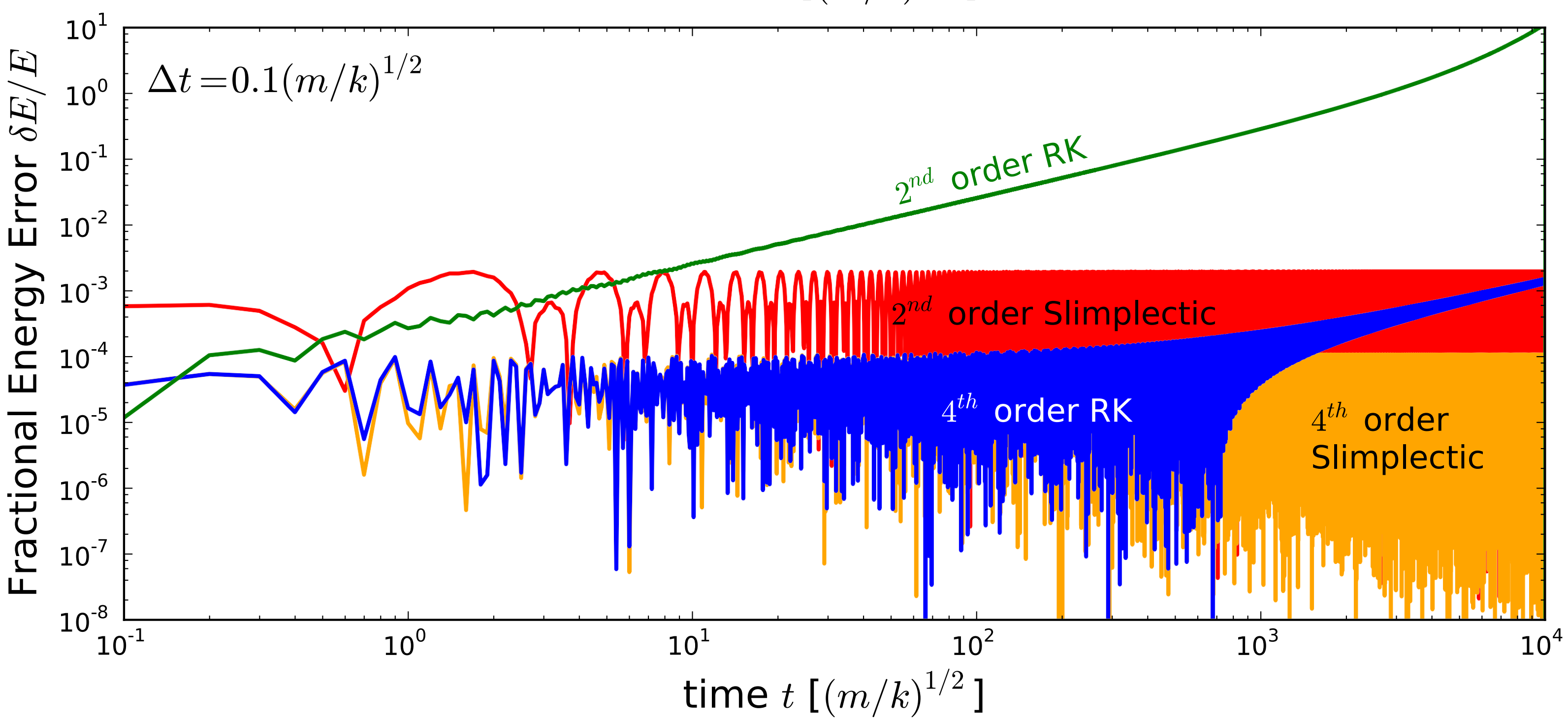
Generalized Noether's Theorem force Noether "charges" to evolve according to discretized nonconservative potential

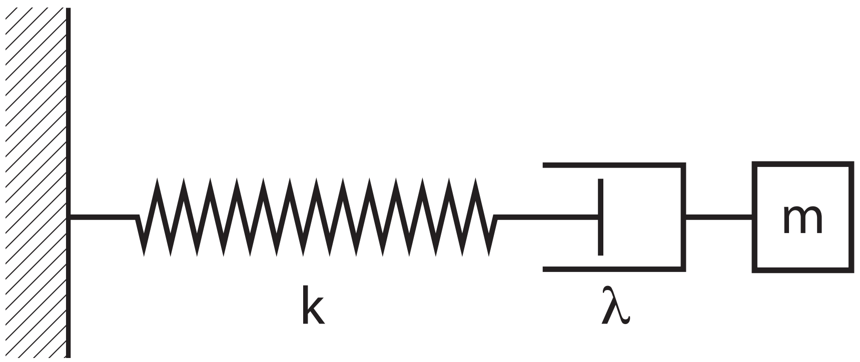
DT, Galley, & Stein (in prep)

Slimplectic Integrators

Example: Simple Damped Harmonic Oscillator







$$L = \frac{1}{2} m \dot{q}^2 - \frac{1}{2} k q^2$$

$$K = -\lambda \dot{q}_+ q_-$$

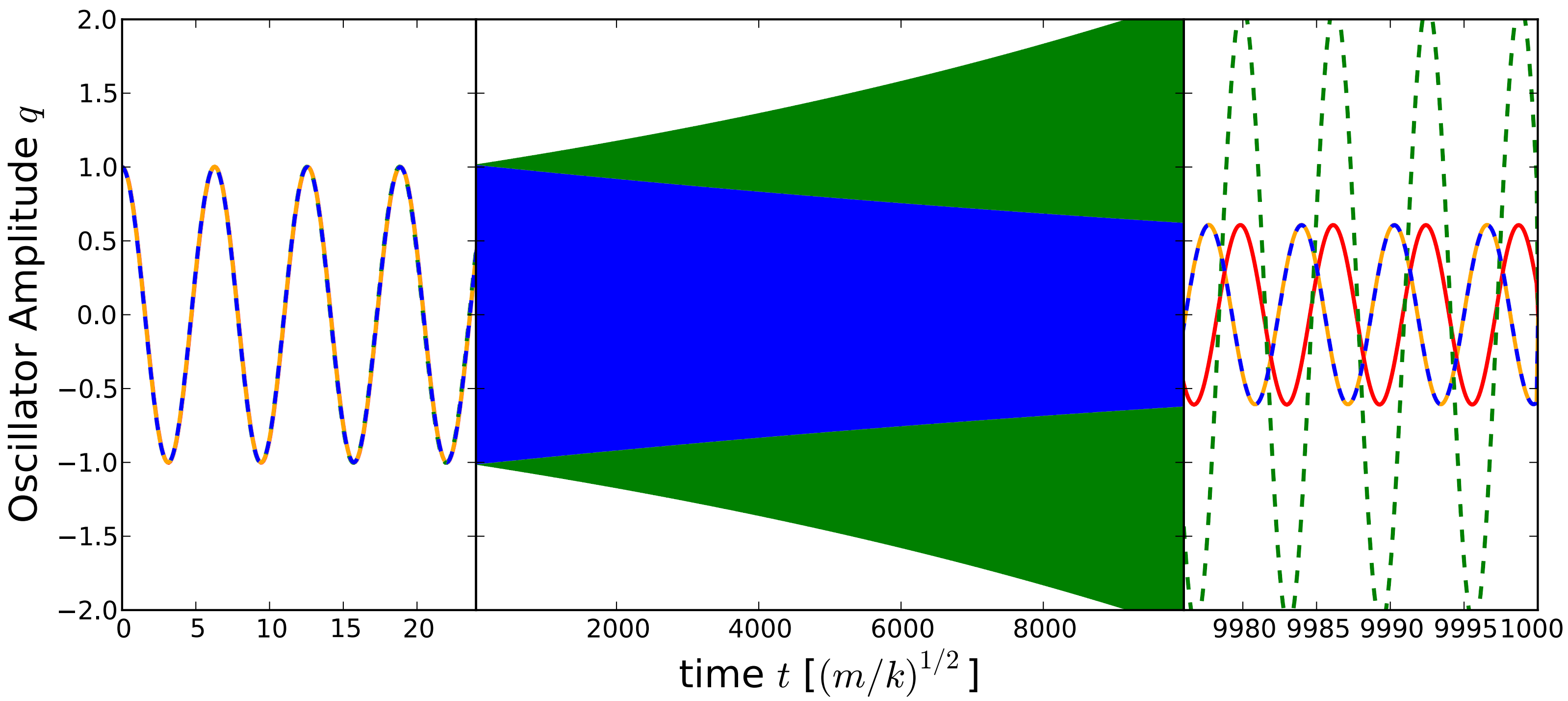
$$\lambda = 10^{-4} (mk)^{1/2}$$

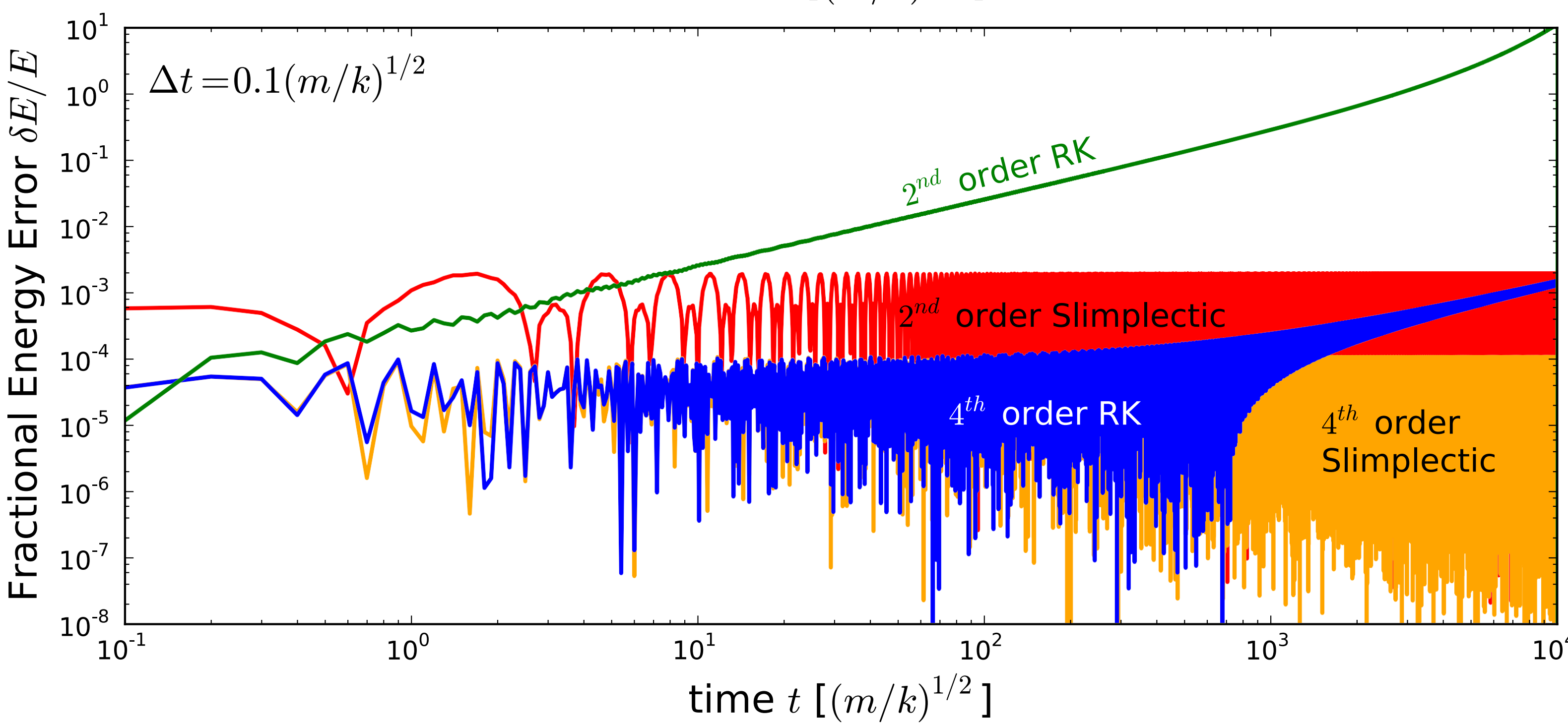
DT, Galley, Stein, & Turner (2015)

2nd order RK, 4th order RK, 2nd order “Slimplectic”, 4th order “Slimplectic”, Analytic

Slimplectic Integrators

Example: Simple Damped Harmonic Oscillator

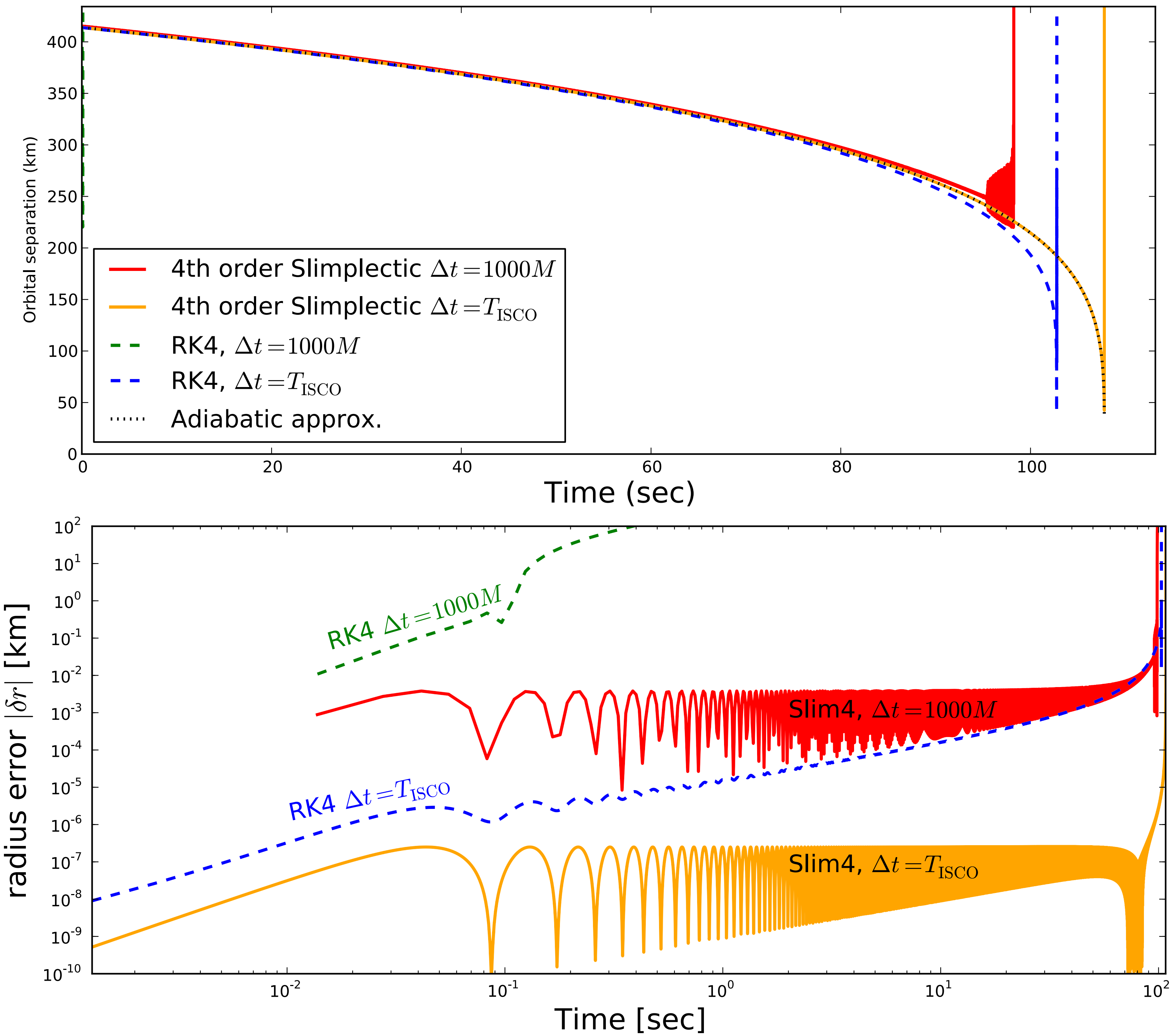


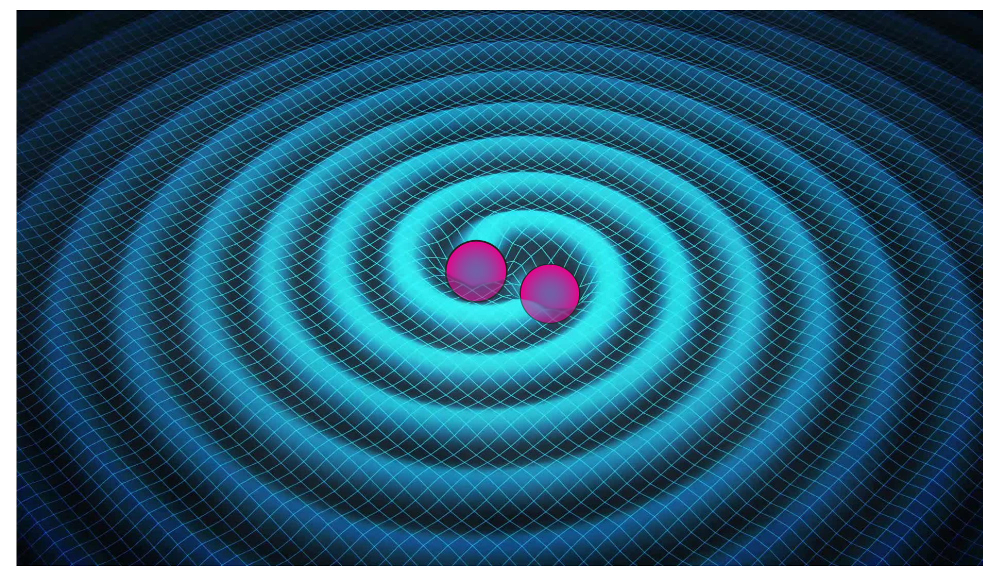


2nd order RK, 4th order RK, 2nd order “Slimplectic”, 4th order “Slimplectic”, Analytic

Slimplectic Integrators

Example: Post-Newtonian gravitational radiation reaction
(PN RR terms only, NS-NS quasi-circular inspiral)





DT, Galley, Stein, & Turner (2015)

Slimplectic Integrators

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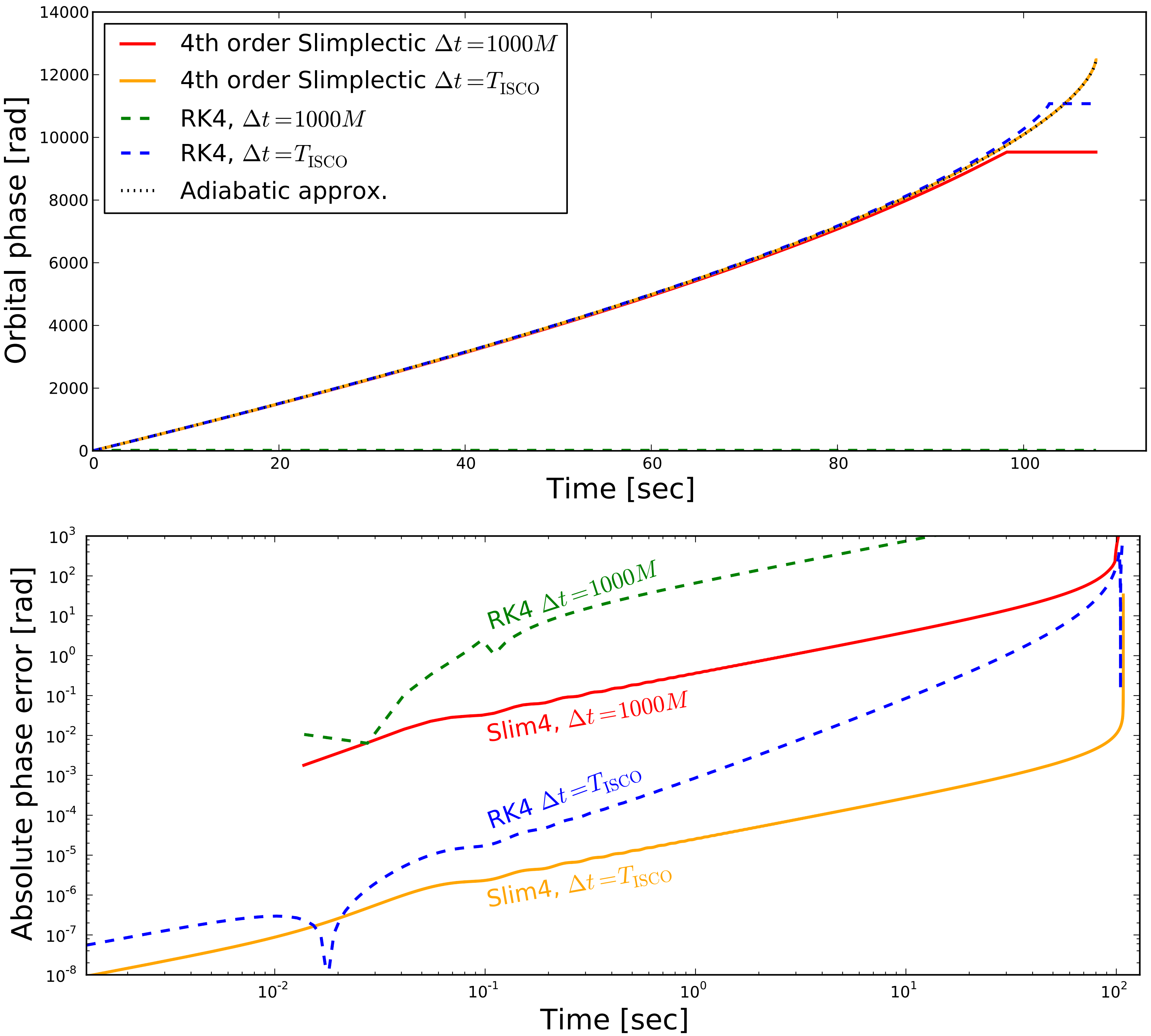
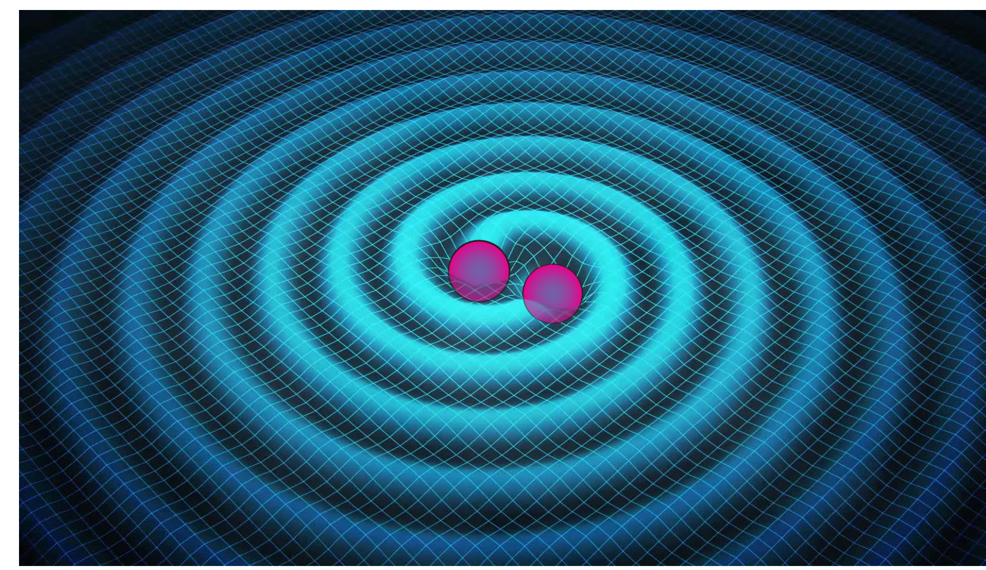
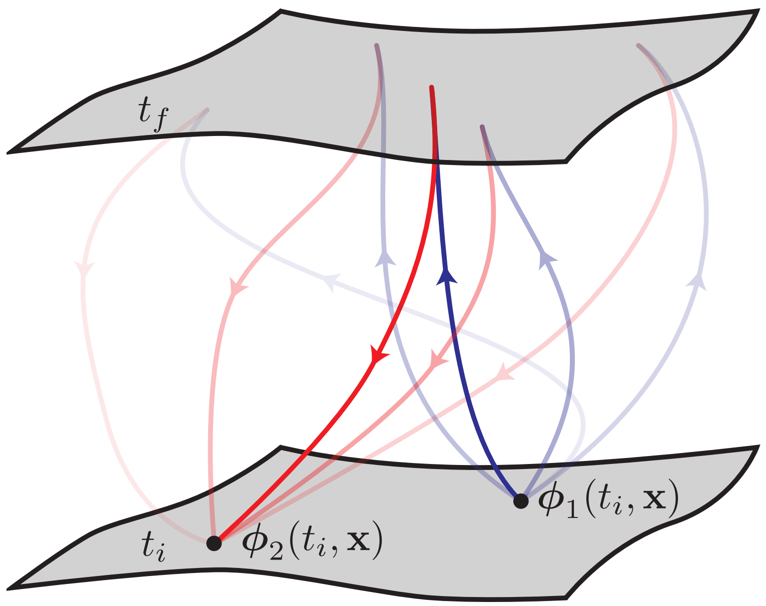
(PN RR terms only, NS-NS quasi-circular inspiral)





DT, Galley, Stein, & Turner (2015)

Nonconservative actions for classical field theories



Consider a set of fields ϕ^I. Action is total space-time integral of Lagrangian density along both paths

$$\mathcal{S}[\phi_1^I, \phi_2^I] = \int_{t_i}^{t_f} dt \int_V d^3x \, \Omega[\phi_1^I, \phi_2^I] = \int_{\mathcal{V}} d^4x \, \Omega[\phi_1^I, \phi_2^I]$$

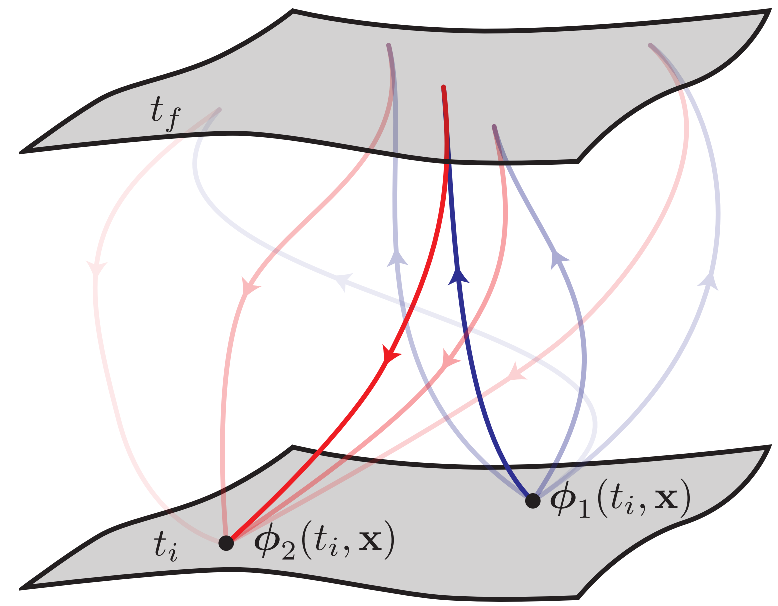
$$\Omega[\phi_1^I, \phi_2^I] = \mathcal{L}(\phi_1^I, \partial_\mu \phi_1^I, x^\mu) - \mathcal{L}(\phi_2^I, \partial_\mu \phi_2^I, x^\mu) + \mathcal{K}(\phi_1^I, \phi_2^I, \partial_\mu \phi_1^I, \partial_\mu \phi_2^I, x^\mu).$$

Being careful about the boundary conditions, we can get the E-L eqn:

$$\left[\partial_\mu \frac{\partial \Omega}{\partial(\partial_\mu \phi_-^I)} - \frac{\partial \Omega}{\partial \phi_-^I} \right]_{\mathrm{PL}} = 0,$$

$$\boxed{\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi^I)} - \frac{\partial \mathcal{L}}{\partial \phi^I} = \left[\frac{\partial \mathcal{K}}{\partial \phi_-^I} - \partial_\mu \frac{\partial \mathcal{K}}{\partial(\partial_\mu \phi_-^I)} \right]_{\mathrm{PL}} =: \mathcal{Q}_I}$$

Nonconservative actions for classical field theories



Consider a set of fields ϕ^I. Action is total space-time integral of Lagrangian density along both paths

$$S[\phi_1^I,\phi_2^I] = \int_{t_i}^{t_f} dt \int_V d^3x\, \Omega[\phi_1^I,\phi_2^I] = \int_{\mathcal{V}} d^4x\, \Omega[\phi_1^I,\phi_2^I]$$

$$\Omega[\phi_1^I,\phi_2^I] = \mathcal{L}(\phi_1^I,\partial_\mu\phi_1^I,x^\mu) - \mathcal{L}(\phi_2^I,\partial_\mu\phi_2^I,x^\mu) + \mathcal{K}(\phi_1^I,\phi_2^I,\partial_\mu\phi_1^I,\partial_\mu\phi_2^I,x^\mu).$$

Being careful about the boundary conditions, we can get the E-L eqn:

$$\left[\partial_\mu \frac{\partial\Omega}{\partial(\partial_\mu\phi_-^I)} - \frac{\partial\Omega}{\partial\phi_-^I}\right]_{\text{PL}} = 0,$$

$$\boxed{\partial_\mu \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^I)} - \frac{\partial\mathcal{L}}{\partial\phi^I} = \left[\frac{\partial\mathcal{K}}{\partial\phi_-^I} - \partial_\mu \frac{\partial\mathcal{K}}{\partial(\partial_\mu\phi_-^I)}\right]_{\text{PL}} =: \mathcal{Q}_I}$$

Noether's theorem procedure is similar:

1) Determine the continuous symmetries of the conservative action;

2) Find how the Noether currents are changed due to nonconservative potential density *K* and RHS above.

Again we have a generalized Noether's Theorem:

If the conservative action S is invariant under a continuous symmetry then there exists a shifted Noether current that changes in time according to K.

Example: The Canonical Stress-Energy Tensor

$$S = \int_{\mathcal{V}} d^4x \, \mathcal{L}\left(\phi^I(x^\alpha), \partial_\mu \phi^I(x^\alpha), x^\mu\right)$$

Consider a system where the conservative action S is symmetric under space-time translations $x^\mu \to x^\mu + \delta x^\mu$,

Taking $\delta S = 0$ and manipulating the RHS, we get

$$0 = \int_{\mathcal{V}} d^4x \, \delta x^\mu \left[\partial_\nu \boxed{\left(\partial_\mu \phi^I \frac{\partial \mathcal{L}}{\partial(\partial_\nu \phi^I)} - \mathcal{L} \right)} + \frac{\partial \mathcal{L}}{\partial x^\mu} - \partial_\mu \phi^I \boxed{\left(\partial_\nu \frac{\partial \mathcal{L}}{\partial(\partial_\nu \phi^I)} - \frac{\partial \mathcal{L}}{\partial \phi^I} \right)} \right]$$

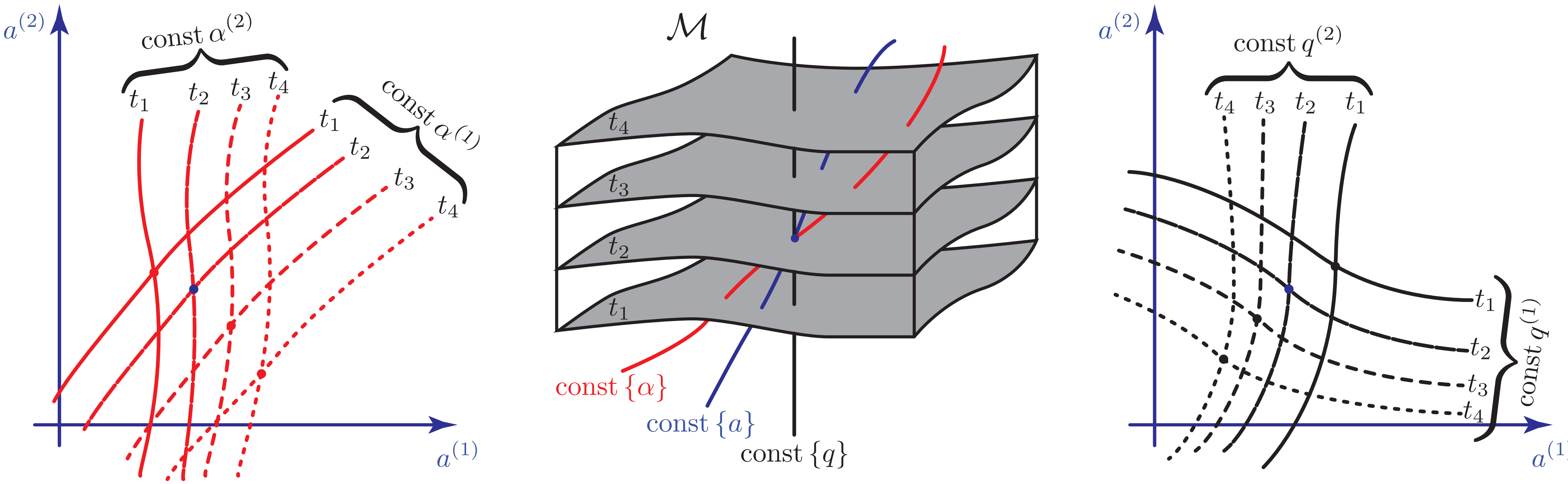
$$T_\mu{}^\nu$$

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi^I)} - \frac{\partial \mathcal{L}}{\partial \phi^I} = \left[\frac{\partial \mathcal{K}}{\partial \phi^I_-} - \partial_\mu \frac{\partial \mathcal{K}}{\partial(\partial_\mu \phi^I_-)} \right]_{\mathrm{PL}}$$

$$\Rightarrow \quad \partial_\nu \boxed{\left(T_\mu{}^\nu + \partial_\mu \phi^I \frac{\partial \mathcal{K}}{\partial_\nu \phi^I_-} \right)} = -\frac{\partial \mathcal{L}}{\partial x^\mu} + \partial_\mu \phi^I \left[\frac{\partial \mathcal{K}}{\partial \phi^I_-} \right]_{\mathrm{PL}} + \partial_\nu \partial_\mu \phi^I \frac{\partial \mathcal{K}}{\partial_\nu \phi^I_-}$$

$\mathcal{T}_\mu{}^\nu$ Total stress energy tensor (including n.c. parts)

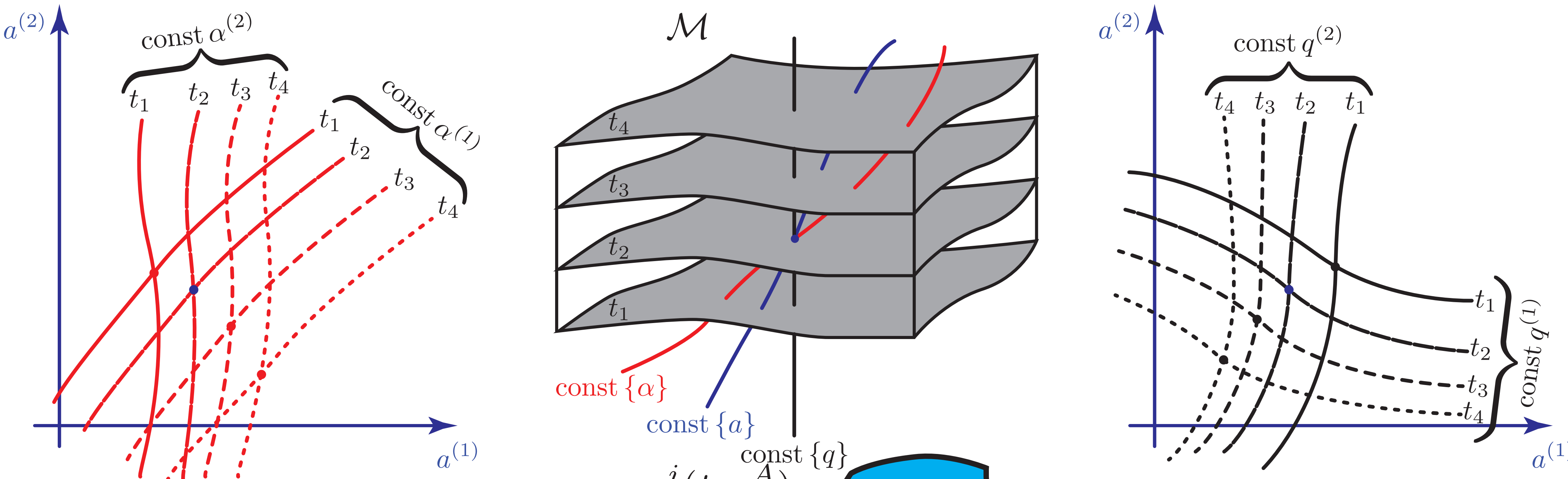
Continuum Mechanics: world lines as degrees of freedom

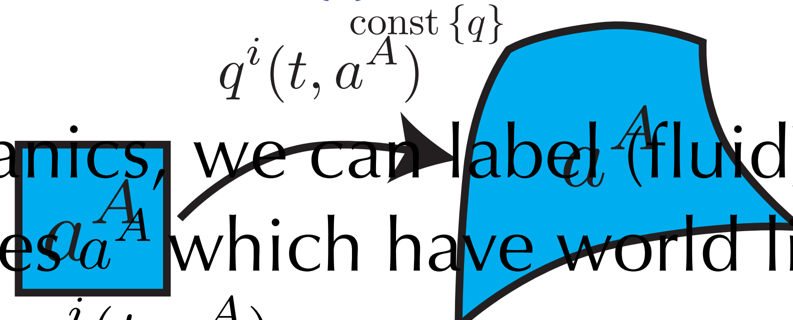


For continuum mechanics, we can label (fluid) elements with Lagrangian coordinates a^A which have world lines described by Eulerian position $q^i = q^i(t, a^A)$.

We take the Lagrangian coordinates (+ time) to be the space-time integration variables, while the world lines, q^i, are the dynamical fields.

Continuum Mechanics: world lines as degrees of freedom





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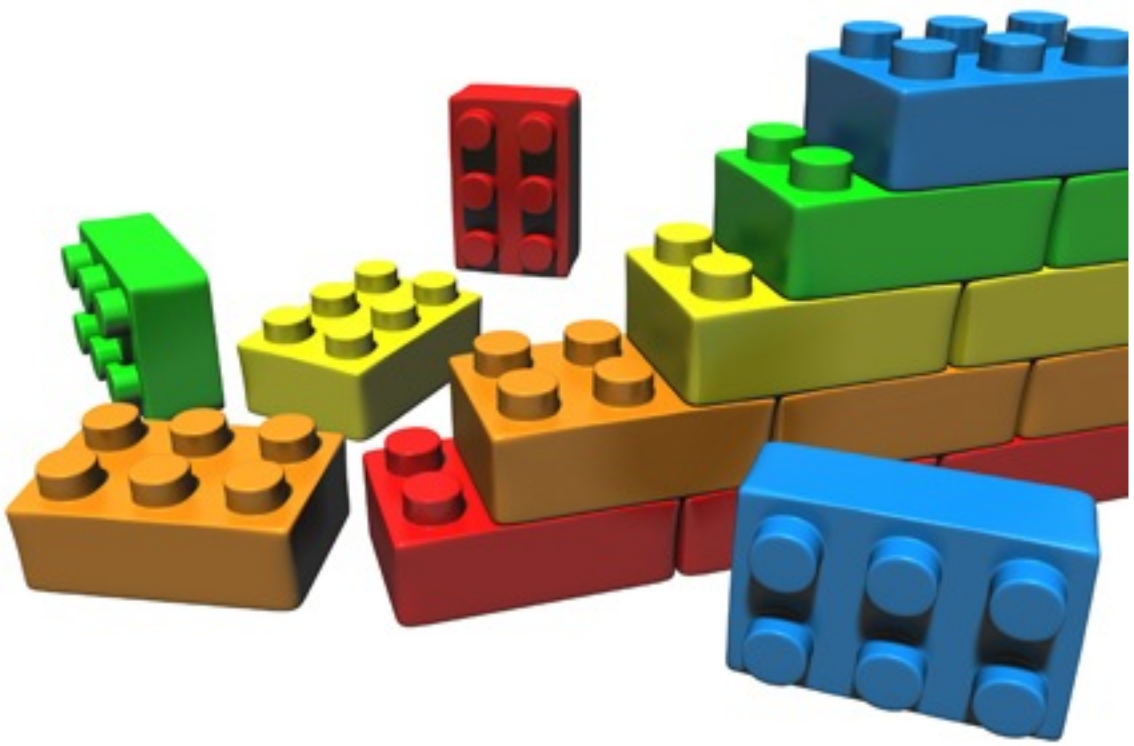
We take the Lagrangian coordinates (+ time) to be the space-time integration variables, while the world lines, q^i, are the dynamical fields.

As the material moves in the Eulerian coordinates q, the volume of an element will change. The volumes in the Lagrangian and Eulerian coordinates are related by

$$d^3a = J\, d^3q, \qquad J = \det \frac{\partial q^i}{\partial a^A}$$

Hydrodynamics: Building An Action



Hydrodynamics: The Perfect Fluid

Consider an isentropic inviscid fluid:

Assume the internal energy (Eulerian) density of the fluid to be

$$\bar{\varepsilon} = \bar{\varepsilon}(\bar{\rho}, \bar{s})$$

overbar means Eulerian density
density with no overbar means Lagrangian

such that $d\bar{\varepsilon} = \mu \, d\bar{\rho} + T \, d\bar{s}$.

The action for such a perfect fluid is given by (e.g. Morrison 98)

$$S = \int dt \, d^3a \, \mathcal{L} \qquad \text{where} \qquad \mathcal{L} = \frac{1}{2}\rho \dot{q}^2 - J\bar{\varepsilon}\left(\frac{\rho}{J}, \frac{s}{J}\right)$$

$$\frac{\delta S}{\delta q^i} = 0 \quad \Rightarrow \quad \bar{\rho}\,\bar{\partial}_t v_i + \bar{\rho} v^j \bar{\nabla}_j v_i + \bar{\nabla}_i \bar{P} = 0$$

$$\bar{P} \equiv \mu\bar{\rho} + T\bar{s} - \bar{\varepsilon}$$

$$\partial_t \rho(a^A) = 0 \quad \Rightarrow \quad \bar{\partial}_t \bar{\rho} + \bar{\nabla}_i (v^i \bar{\rho}) = 0$$

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Since action S is invariant under time and Lagrange-coordinate shifts the canonical stress-energy tensor is conserved

$$\frac{\delta S}{\delta q^i} = 0 \qquad \bar\rho\, \bar\partial_t v_i + \bar\rho v^j \bar\nabla_j v_i + \bar\nabla_i \bar P = 0$$

$$T_\mu{}^\nu \equiv \partial_\mu \phi^I \frac{\partial \mathcal{L}}{\partial(\partial_\nu \phi^I)} - \mathcal{L}\, \delta^\nu_\mu$$

$$\bar P \equiv \mu\bar\rho + T\bar s - \bar\varepsilon$$

$$\partial_\nu T_\mu{}^\nu = 0 \qquad \bar\partial_t\left(\frac{1}{2}\bar\rho v^2 + \bar\varepsilon(\bar\rho, \bar s)\right) + \bar\nabla_i\left[v^i\left(\frac{1}{2}\bar\rho v^2 + \bar\varepsilon + \bar P\right)\right] = 0$$

$$\partial_t \rho(a^A) = 0 \qquad \bar\partial_t \bar\rho + \bar\nabla_i (v^i \bar\rho) = 0$$

Energy Equation

Hydrodynamics:

Consider an isentropic viscous fluid: $\partial_t s(a^A) = 0$

$$\mathcal{S} = \int dt\, d^3a\, (\mathcal{L}_1 - \mathcal{L}_2 + \mathcal{K}) \quad \text{where} \quad \mathcal{L} = \frac{1}{2}\rho\dot{q}^2 - J\varepsilon\left(\frac{\rho}{J}, \frac{s}{J}\right)$$

$$\mathcal{K} = -[u_-]_{AB}\, \sigma_+^{AB}$$

u^{AB} is the strain tensor

$$\sigma^{AB} = \left(\eta_s P^{ABCD} + \eta_b C^{AB} C^{CD}\right) \gamma_{CD}$$ is the viscous stress tensor

γ^{AB} is the rate of strain tensor

$$\frac{\delta S}{\delta q^i} = 0 \quad \Rightarrow \quad \bar{\rho}\, \bar{\partial}_t v_i + \bar{\rho} v^j \bar{\nabla}_j v_i + \bar{\nabla}_i \bar{P} = \bar{\nabla}_j \bar{\sigma}^j{}_i$$

$$\partial_\nu \mathcal{T}_\mu{}^\nu = \ldots \quad \Rightarrow \quad \bar{\partial}_t \left[\frac{1}{2}\bar{\rho} v^2 + \bar{\varepsilon}(\bar{\rho}, \bar{s})\right] + \bar{\nabla}_i \left\{ v^i \left(\frac{1}{2}\bar{\rho} v^2 + \bar{h}\right) \boxed{- v^j\, \bar{\sigma}^i{}_j} \right\} = \boxed{-\bar{\sigma}^{ij} \bar{\nabla}_i v_j,}$$

viscous energy flux

viscous dissipation loss

Hydrodynamics: perfectly insulating fluid

Consider perfectly insulating viscous fluid:

$$\mathcal{L} = \frac{1}{2}\rho\dot{q}^2 - J\bar{\varepsilon}\left(\frac{\rho}{J}, \frac{s}{J}\right) \qquad\qquad \mathcal{K} = -[u_-]_{AB}\,\sigma_+^{AB}$$

Replace isentropic condition with the closed system "closure" condition

$$\cancel{\partial_t s(a^A) = 0} \qquad\qquad \partial_\nu \mathcal{T}_\mu{}^\nu = 0$$

The closed system condition implies the internal energy density accounts for all the energy of the inaccessible degrees of freedom.

$$\frac{\delta S}{\delta q^i} = 0 \quad \Longrightarrow \quad \bar{\rho}\,\bar{\partial}_t v_i + \bar{\rho} v^j \bar{\nabla}_j v_i + \bar{\nabla}_i \bar{P} = \bar{\nabla}_j \bar{\sigma}^j{}_i$$

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Noether’s Thm: $\partial_\nu \mathcal{T}_\mu{}^\nu = -\frac{\partial \mathcal{L}}{\partial x^\mu} + \partial_\mu \phi^I \left[\frac{\partial \mathcal{K}}{\partial \phi_-^I}\right]_{\mathrm{PL}} + \partial_\nu \partial_\mu \phi^I \mathcal{K}_I{}^\nu$

“closure” cond’n: $\partial_\nu \mathcal{T}_\mu{}^\nu = 0$

$$\frac{\delta S}{\delta q^i} = 0 \qquad \bar{\rho}\,\bar{\partial}_t v_i + \bar{\rho} v^j \bar{\nabla}_j v_i + \bar{\nabla}_i \bar{P} = \bar{\nabla}_j \bar{\sigma}^j{}_i$$

$$\bar{\partial}_t\left[\frac{1}{2}\bar{\rho}v^2 + \bar{\varepsilon}(\bar{\rho}, \bar{s})\right] + \bar{\nabla}_i\left\{v^i\left(\frac{1}{2}\bar{\rho}v^2 + \bar{h}\right) - v^j \bar{\sigma}^i{}_j\right\} = 0$$

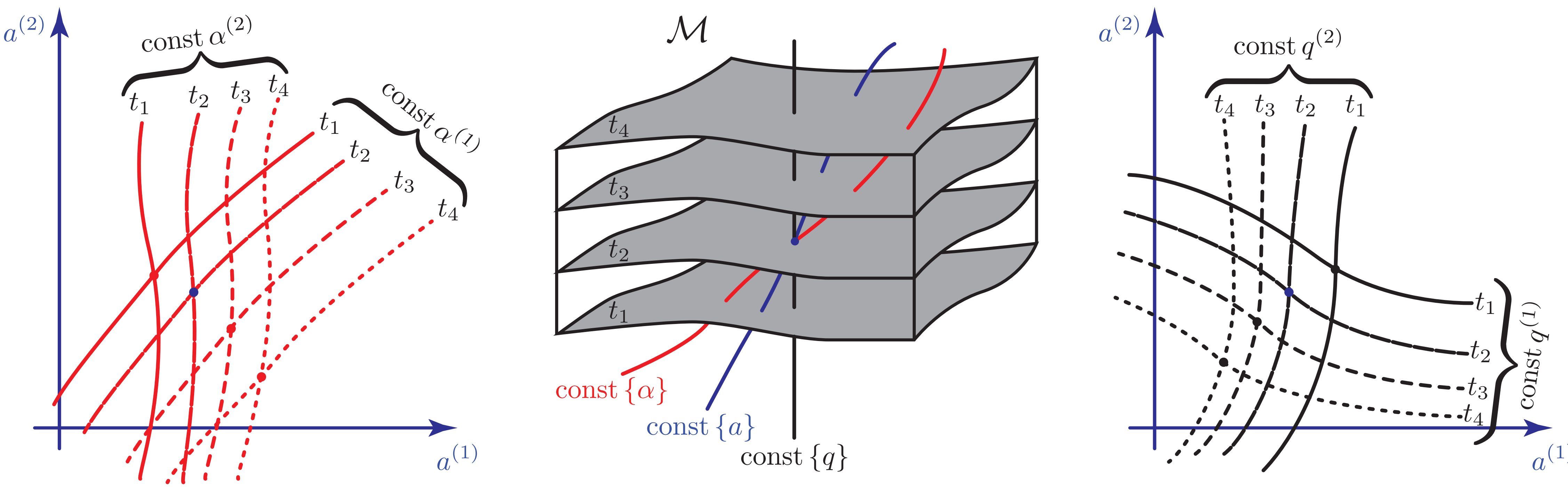
Energy Eq.

$$\bar{\partial}_t \bar{s} + \bar{\nabla}_i(v^i \bar{s}) = \frac{1}{T}\bar{\sigma}^{ij}\bar{\nabla}_i v_j.$$

Entropy Eq.

But what about heat flow?

Hydrodynamics: inviscid fluid w/ heat diffusion

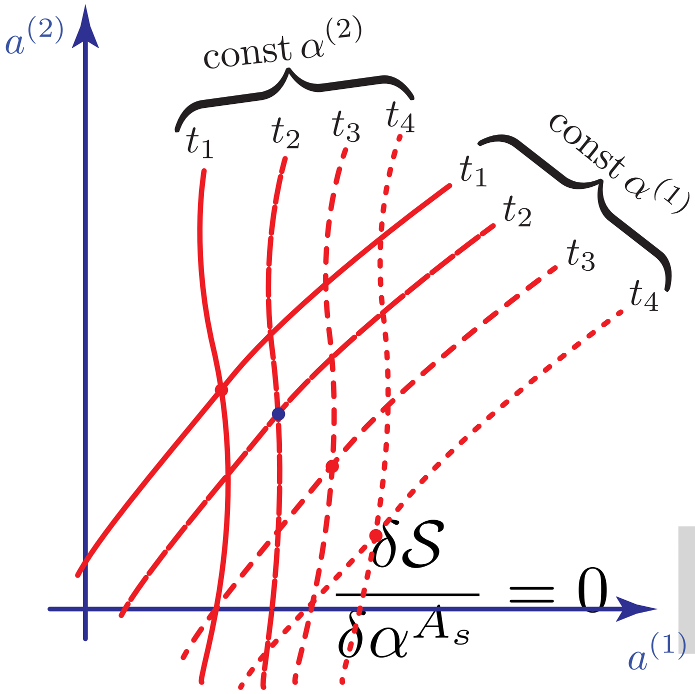


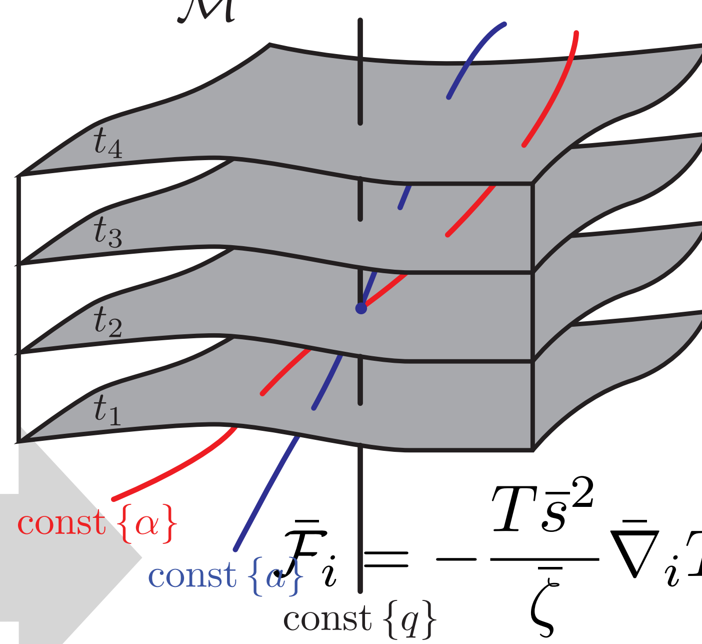
We allow the entropy "fluid" to flow.
The entropy fluid labels α^{A_s} are now degrees of freedom.

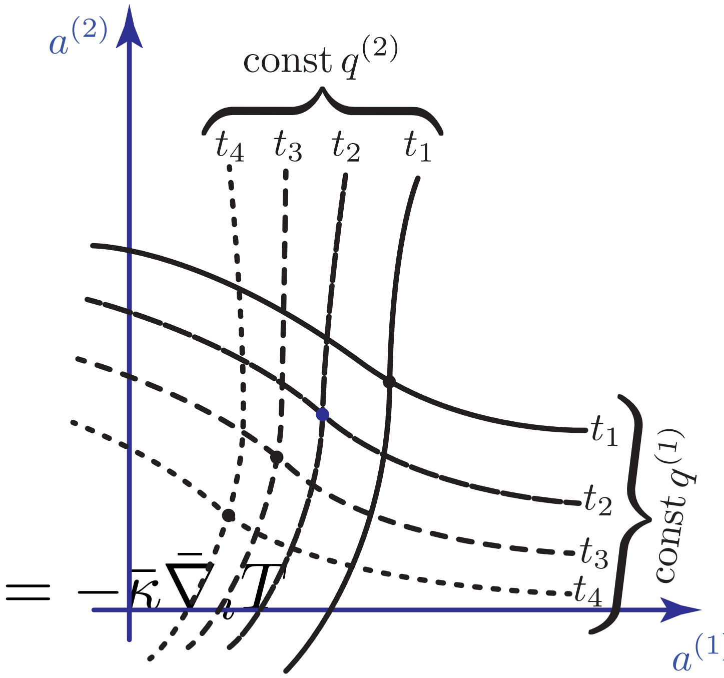
$$\mathcal{L} = \frac{1}{2}\rho\dot{q}^2 - J\bar{\varepsilon}\left(\frac{\rho}{J}, \frac{s}{J}\right) \qquad \mathcal{K} = -\zeta_+ \left[\partial_t \alpha_+\right]_{A_s} \alpha_-^{A_s}$$

$$\frac{\delta \mathcal{S}}{\delta q^i} = 0 \qquad \bar{\rho}\,\bar{\partial}_t v_i + \bar{\rho} v^j \bar{\nabla}_j v_i + \bar{\nabla}_i \bar{P} = 0$$

Hydrodynamics: inviscid fluid w/ heat diffusion







$$\frac{\delta \mathcal{S}}{\delta \alpha^{A_s}} = 0$$

$$\bar{\mathcal{F}}_i = -\frac{T\bar{s}^2}{\bar{\zeta}} \bar{\nabla}_i T = -\bar{\kappa} \bar{\nabla}_i T$$

$\bar{\mathcal{F}}^i = T\bar{s}\Delta^i$ Fourier's Law

We allow the entropy "fluid" to flow.

The entropy fluid labels α^{A_s} are now degrees of freedom.

Noether's Thm: $\partial_\nu \mathcal{T}_\mu{}^\nu = -\frac{\partial \mathcal{L}}{\partial x^\mu} + \partial_\mu \phi^I \left[\frac{\partial \mathcal{K}}{\partial \phi^I_-}\right]_{\text{PL}} + \partial_\nu \partial_\mu \phi^I \kappa^\nu_I$

$$\mathcal{L} = \frac{1}{2}\rho \dot{q}^2 - J\varepsilon\left(\frac{\rho}{J}, \frac{s}{J}\right) \qquad \mathcal{K} = -\zeta_+ \left[\partial_t \alpha_+\right]_{A_s} \alpha^{A_s}_-$$

"closure" cond'n: $\partial_\nu \mathcal{T}_\mu{}^\nu = 0$

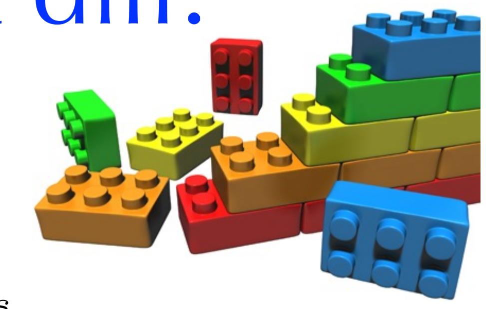
$$\frac{\delta \mathcal{S}}{\delta q^i} = 0$$

$$\bar{\rho}\,\bar{\partial}_t v_i + \bar{\rho} v^j \bar{\nabla}_j v_i + \bar{\nabla}_i \bar{P} = 0$$

$$\bar{\partial}_t\left(\frac{1}{2}\bar{\rho}v^2 + \bar{\varepsilon}\right) + \bar{\nabla}_i\left\{v^i\left(\frac{1}{2}\bar{\rho}v^2 + \bar{h}\right) - \bar{\kappa}\bar{\nabla}^i T\right\} = 0$$

$$\bar{\partial}_t \bar{s} + \bar{\nabla}_i(v^i \bar{s}) = -\frac{1}{T}\bar{\nabla}_i \bar{\mathcal{F}}^i = \frac{1}{T}\bar{\nabla}_i(\bar{\kappa}\bar{\nabla}^i T)$$

Hydrodynamics: Navier-Stokes w/ Heat diff.



Putting all the pieces together:

$$\mathcal{L} = \frac{1}{2}\rho\dot{q}^2 - J\bar{\varepsilon}\left(\frac{\rho}{J}, \frac{s}{J}\right)$$

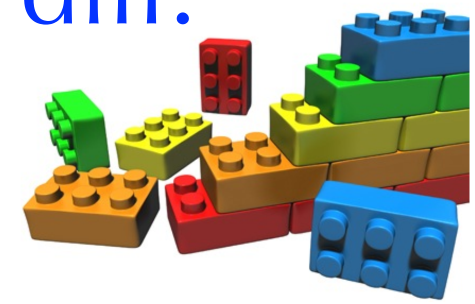
$$\mathcal{K} = -\zeta_+ \left[\partial_t \alpha_+\right]_{A_s} \alpha_-^{A_s} - [u_-]_{AB}\, \sigma_+^{AB}$$

$$\frac{\delta \mathcal{S}}{\delta q^i} = 0 \quad \Rightarrow \quad \bar{\rho}\,\bar{\partial}_t v_i + \bar{\rho} v^j \bar{\nabla}_j v_i + \bar{\nabla}_i \bar{P} = \bar{\nabla}_j \bar{\sigma}^j{}_i$$

$$\frac{\delta \mathcal{S}}{\delta \alpha^{A_s}} = 0 \quad \Rightarrow \quad \bar{\mathcal{F}}_i = -\frac{T\bar{s}^2}{\bar{\zeta}} \bar{\nabla}_i T = -\bar{\kappa} \bar{\nabla}_i T$$

$$\partial_t \rho(a^A) = 0 \quad \Rightarrow \quad \bar{\partial}_t \bar{\rho} + \bar{\nabla}_i (v^i \bar{\rho}) = 0$$

Hydrodynamics: Navier-Stokes w/ Heat diff.



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Noether's Thm

$$\partial_t \rho(a^A) = 0 \quad \Rightarrow \quad \bar{\partial}_t \bar{\rho} + \bar{\nabla}_i (v^i \bar{\rho}) = 0$$

$$\bar{\partial}_t \left(\frac{1}{2}\bar{\rho} v^2 + \bar{\varepsilon}\right) + \bar{\nabla}_i \left\{ v^i \left(\frac{1}{2}\bar{\rho} v^2 + \bar{h}\right) - v_j\, \bar{\sigma}^{ij} - \bar{\kappa} \bar{\nabla}^i T \right\} = 0$$

closure cond.

$$\bar{\partial}_t \bar{s} + \bar{\nabla}_i (v^i \bar{s}) = \frac{1}{T} \bar{\nabla}_i (\bar{\kappa} \bar{\nabla}^i T) + \frac{1}{T} \bar{\sigma}^{ij} \bar{\nabla}_i v_j$$

Name	$\mathcal{L}$	$\mathcal{K}$	DoF	System Type
Perfect Fluid §V B 1	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}(\bar{\rho},\bar{s})$	-	$\boldsymbol{q}$	conservative
Cold Stone Fluid §V B 2	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}(\bar{\rho},\bar{s})$	$-\boldsymbol{\mathcal{V}}_+::(\boldsymbol{u}_-\otimes\boldsymbol{\gamma}_+)$	$\boldsymbol{q}$	open isentropic ($\partial_t s = 0$)
Viscous Insulating Fluid §V B 3	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}(\bar{\rho},\bar{s})$	$-\boldsymbol{\mathcal{V}}_+::(\boldsymbol{u}_-\otimes\boldsymbol{\gamma}_+)$	$\boldsymbol{q}$	closed ($\partial_\nu \mathcal{T}_0{}^\nu = 0$)
Inviscid Fluid with Heat Diffusion §V B 4	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}(\bar{\rho},\bar{s})$	$-\zeta_+(\boldsymbol{\alpha}_-\cdot\partial_t\boldsymbol{\alpha}_+)$	$\boldsymbol{q},\boldsymbol{\alpha}$	closed ($\partial_\nu \mathcal{T}_0{}^\nu = 0$)
Navier-Stokes Fluid §V B 5	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}(\bar{\rho},\bar{s})$	$-\boldsymbol{\mathcal{V}}_+::(\boldsymbol{u}_-\otimes\boldsymbol{\gamma}_+) - \zeta_+(\boldsymbol{\alpha}_-\cdot\partial_t\boldsymbol{\alpha}_+)$	$\boldsymbol{q},\boldsymbol{\alpha}$	closed ($\partial_\nu \mathcal{T}_0{}^\nu = 0$)
Microhydrodynamics (Stokes Limit) §V C	$-J\bar{\varepsilon}(\bar{\rho},\bar{s})$	$-\boldsymbol{\mathcal{V}}_+::(\boldsymbol{u}_-\otimes\boldsymbol{\gamma}_+)$	$\boldsymbol{q}$	open isentropic ($\partial_t s = 0$), movable boundaries
Perfect Elastic Material	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}_o(\bar{\rho},\bar{s}) - \frac{1}{2}\boldsymbol{\mathcal{E}}::(\boldsymbol{u}\otimes\boldsymbol{u})$	-	$\boldsymbol{q}$	conservative
Cold Stone Elastic with Dissipation	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}_o(\bar{\rho},\bar{s}) - \frac{1}{2}\boldsymbol{\mathcal{E}}::(\boldsymbol{u}\otimes\boldsymbol{u})$	$-\boldsymbol{\mathcal{V}}_+::(\boldsymbol{u}_-\otimes\boldsymbol{\gamma}_+)$	$\boldsymbol{q}$	open isentropic ($\partial_t s = 0$)
Insulating Elastic with Dissipation	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}_o(\bar{\rho},\bar{s}) - \frac{1}{2}\boldsymbol{\mathcal{E}}::(\boldsymbol{u}\otimes\boldsymbol{u})$	$-\boldsymbol{\mathcal{V}}_+::(\boldsymbol{u}_-\otimes\boldsymbol{\gamma}_+)$	$\boldsymbol{q}$	closed ($\partial_\mu \mathcal{T}_0^\mu = 0$)
Elastic with Heat Diffusion	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}_o(\bar{\rho},\bar{s}) - \frac{1}{2}\boldsymbol{\mathcal{E}}::(\boldsymbol{u}\otimes\boldsymbol{u})$	$-\zeta_+(\boldsymbol{\alpha}_-\cdot\partial_t\boldsymbol{\alpha}_+)$	$\boldsymbol{q},\boldsymbol{\alpha}$	closed ($\partial_\mu \mathcal{T}_0^\mu = 0$)
Elastic with Dissipation & Heat Diffusion	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}_o(\bar{\rho},\bar{s}) - \frac{1}{2}\boldsymbol{\mathcal{E}}::(\boldsymbol{u}\otimes\boldsymbol{u})$	$-\boldsymbol{\mathcal{V}}_+::(\boldsymbol{u}_-\otimes\boldsymbol{\gamma}_+) - \zeta_+(\boldsymbol{\alpha}_-\cdot\partial_t\boldsymbol{\alpha}_+)$	$\boldsymbol{q},\boldsymbol{\alpha}$	closed ($\partial_\mu \mathcal{T}_0^\mu = 0$)
Cold Stone Maxwell Fluid	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}_o(\bar{\rho},\bar{s}) - \frac{1}{2}\boldsymbol{\mathcal{E}}::(\boldsymbol{u}_{\rm el}\otimes\boldsymbol{u}_{\rm el})$	$-\boldsymbol{\mathcal{V}}_+::(\boldsymbol{u}_{\rm pl-}\otimes\boldsymbol{\gamma}_{\rm pl+})$	$\boldsymbol{q},\boldsymbol{C}_{\rm pl}$	open isentropic ($\partial_t s = 0$)
Insulating Maxwell Fluid	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}_o(\bar{\rho},\bar{s}) - \frac{1}{2}\boldsymbol{\mathcal{E}}::(\boldsymbol{u}_{\rm el}\otimes\boldsymbol{u}_{\rm el})$	$-\boldsymbol{\mathcal{V}}_+::(\boldsymbol{u}_{\rm pl-}\otimes\boldsymbol{\gamma}_{\rm pl+})$	$\boldsymbol{q},\boldsymbol{C}_{\rm pl}$	closed ($\partial_\nu \mathcal{T}_0{}^\nu = 0$)
Viscoelastic Maxwell Fluid §V D	$\frac{1}{2}\rho\dot{\boldsymbol{q}}^2 - J\bar{\varepsilon}_o(\bar{\rho},\bar{s}) - \frac{1}{2}\boldsymbol{\mathcal{E}}::(\boldsymbol{u}_{\rm el}\otimes\boldsymbol{u}_{\rm el})$	$-\boldsymbol{\mathcal{V}}_+::(\boldsymbol{u}_{\rm pl-}\otimes\boldsymbol{\gamma}_{\rm pl+}) - \zeta_+(\boldsymbol{\alpha}_-\cdot\partial_t\boldsymbol{\alpha}_+)$	$\boldsymbol{q},\boldsymbol{C}_{\rm pl},\boldsymbol{\alpha}$	closed ($\partial_\nu \mathcal{T}_0{}^\nu = 0$)

Towards a Variational Integrator for Hydrodynamics

Discretize space (or spacetime) using simplicial meshes:

- Scalar fields degrees of freedom (Eulerian position components) become N numbers for each mesh vertex
- Action becomes a sum of discrete (N+1)-forms over (N+1)-volumes
- Use Discrete Exterior Calculus to determine (exterior) derivatives

$$\int_V d\omega = \int_{\partial V} \omega$$ **Stokes Theorem**

$$< d\omega_i, V^i >=< \omega_j, \partial V^j >$$ **Discrete Stokes Theorem**

Discrete exterior derivative $d \equiv \partial^T$ **Discrete Boundary Operator**

Towards a Variational Integrator for Hydrodynamics

2+1D Fluids

Variational Problem becomes minimisation problem for each d.o.f. on each mesh point (for each time)