

SINGULAR SOLITONS, MOMENTUM MAPS & COMPUTATIONAL ANATOMY

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“I shall speak of things . . . so singular in their oddity as in some manner to instruct, or at least entertain, without wearying.”

Lorenzo da Ponte

Collaborators & References for this talk

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Problem & Approach for Computational Anatomy

In a very large part of morphology, our essential task lies in the **comparison of related forms** rather than in the precise definition of each. . . . This process of comparison, of recognizing in one form a definite permutation or deformation of another, . . . lies within the immediate province of mathematics and finds its solution in . . . the Theory of Transformations.

– D’Arcy Thompson, “On Growth and Form” (1917)

Summary of our discussion today

- Computational Anatomy (CA) compares shapes (graphical structures) by making a *geodesic deformation* from one shape to the another.
- Among these graphical structures, landmarks and image outlines in CA are found to be singular solutions of the geodesic *EPDiff* equation.
- A *momentum map* for singular solutions of EPDiff yields their canonical Hamiltonian formulation, which provides a *complete parameterization* of the landmarks and image outlines by their *canonical positions and momenta*.

Summary of discussion (cont)

- The momentum map provides an *isomorphism* between landmarks (and outlines) for images and *singular* (weak) solutions of EPDiff. (These are solitons in 1D.)
- This isomorphism provides for CA:
 - (1) a complete and non-redundant data representation
 - (2) a dynamical paradigm in which image outlines interact by exchange of momentum
 - (3) methods for numerical simulation & data assimilation
- Euler-Poincaré theory also provides a framework for unifying and extending the various approaches in CA

The importance of momentum for CA

- Completes the representation of images (momentum of cartoons)
- Informs template matching of the possibility of soliton-like collisions and **momentum exchange in image outline interactions**
- Encodes the subsequent deformation into the **initial locus and momentum** of an image outline
- Provides numerical simulation methods using the **momentum map for right action** as a data structure.
- Accomplishes matching and data assimilation via the **adjoint linear problem** for template matching, using the **initial momentum as a control variable**.
- All these momentum properties flow from the **EPDiff** equation

Outline of the rest of the talk

- Describe the template matching variational problems of computational anatomy
- Motivate the EPDiff evolution equation.
- Describe the singular solutions for the EPDiff equation with diffeomorphism group $Diff$.
- Explain why these singular solutions exist (singular momentum map)
- Discuss the consequences of EPDiff for CA.
- Give numerical examples (by Colin J Cotter, Imperial College London)

Cost

Template matching assigns the cost for a given comparison

$$\text{Cost}(t \mapsto \varphi_t) = \int_0^1 \ell(\mathbf{u}_t) dt$$

as a functional defined on curves φ_t in a Lie group with tangents

$$\frac{d\varphi_t}{dt} = \mathbf{u}_t \circ \varphi_t, \quad \mathcal{I}_t = \varphi_t \cdot \mathcal{I}_0 \quad (1)$$

In the following, the function $\mathbf{u}_t \mapsto \ell(\mathbf{u}_t) = \|\mathbf{u}_t\|_{\mathfrak{g}}^2$ is taken as a squared functional norm on the space of velocity vectors.

The vector space of **right invariant** instantaneous velocities,

$$\mathbf{u}_t = (d\varphi_t/dt) \circ \varphi_t^{-1},$$

forms the tangent space at the identity of the considered Lie group, and is isomorphic to the group's **Lie algebra, denoted \mathfrak{g}** .

Problem statement

Given the cost of a time-dependent deformation process, defined by

$$\text{Cost}(t \mapsto \varphi_t) = \int_0^1 \|\mathbf{u}_t\|_{\mathfrak{g}}^2 dt, \quad (2)$$

most problems in CA can be formulated as:

Find the deformation path with minimal cost, under the constraint that it carries the template to the target.

Such problems have a remarkable analogy with fluid dynamics.

Mathematical analogy: template matching vs fluid dynamics

(I) The frameworks in CA and fluid dynamics both involve a **right-invariant** stationary principle with action, or cost function

$$\underbrace{A = \int_0^1 \ell(\mathbf{u}_t) dt}_{\text{Action}}, \quad \underbrace{\ell(\mathbf{u}_t) = \frac{1}{2} \|\mathbf{u}_t\|_{\mathfrak{g}}^2}_{\text{Lagrangian}}, \quad \underbrace{\mathbf{u}_t = (d\varphi_t/dt) \circ \varphi_t^{-1}}_{\text{Right invariant}}$$

The main differences are:

Template matching

Cost function is designed for the application

Optimal control problem

Fluid dynamics

Cost function is Kinetic energy

Initial value problem

Mathematical analogy: CA and fluids (cont1)

(II) The geodesic evolution for both template matching and fluid dynamics is governed by **EPDiff** [HoMaRa1998, Mumford1998, Younes1998],

$$\left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right) \mathbf{m} + (\nabla \mathbf{u})^T \cdot \mathbf{m} + \mathbf{m}(\operatorname{div} \mathbf{u}) = 0. \quad (3)$$

Here $\mathbf{u} = G * \mathbf{m}$, where $G*$ denotes convolution with the Green's kernel G for the operator \mathcal{L} , when

$$\mathbf{m} = \frac{\delta \ell}{\delta \mathbf{u}} =: \mathcal{L} \mathbf{u}$$

Here, the operator \mathcal{L} is symmetric and positive definite for the

$$\operatorname{Cost}(t \mapsto \varphi_t) = \int_0^1 \ell(\mathbf{u}_t) dt = \int_0^1 \|\mathbf{u}_t\|_{\mathfrak{g}}^2 dt = \int_0^1 \langle \mathbf{u}_t, \mathcal{L} \mathbf{u}_t \rangle dt$$

with L^2 pairing $\langle \cdot, \cdot \rangle$ whenever $\|\mathbf{u}_t\|_{\mathfrak{g}}^2$ is a norm.

Mathematical analogy: CA and fluids (cont2)

(III) The flows in CA and fluid dynamics both evolve under a left group action on a linear representation space,

$$\mathcal{I}_t = \varphi_t \cdot \mathcal{I}_0$$

They differ in the roles of their advected quantities, $a_t = a_0 \circ \varphi_t^{-1}$:

Template matching

Image properties are passive
Images are only swept along
for $\ell(\mathbf{u})$

Fluid dynamics

Advected quantities may affect fluid flows
Waves may form in fluids for $\ell(\mathbf{u}, a)$
since restoring forcing depend on a

(IV) Some features of CA are a bit more like fluid dynamics, e.g., metamorphoses have a semidirect-product structure. Can metamorphoses have waves?

How EPDiff emerges in CA

Choose the cost function for continuously morphing \mathcal{I}_0 into \mathcal{I}_1 as

$$\text{Cost}(t \mapsto \varphi_t) = \int_0^1 \ell(\mathbf{u}_t) dt = \int_0^1 \|\mathbf{u}_t\|_{\mathfrak{g}}^2 dt,$$

where u_t is the velocity of the fluid deformation at time t and

$$\|\mathbf{u}_t\|_{\mathfrak{g}}^2 = \langle \mathbf{u}_t, \mathcal{L}\mathbf{u}_t \rangle,$$

and \mathcal{L} is a positive symmetric linear operator.

Then, the momentum governing the process,

$$\mathbf{m}_t = \mathcal{L}\mathbf{u}_t, \quad \text{with Green's function } G : \mathbf{u}_t = G * \mathbf{m}_t$$

satisfies **EPDiff**. Namely,

$$\left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{m} + (\nabla \mathbf{u})^T \cdot \mathbf{m} + \mathbf{m}(\text{div } \mathbf{u}) = 0$$

This equation arises in both template matching and fluid dynamics, and it informs both fields of endeavor.

More about EPDiff

- EPDiff may be written in a **Lagrangian sense** as

$$\frac{d}{dt} \left(\mathbf{m} \cdot d\mathbf{x} \otimes d^n x \right) = 0 \quad \text{along} \quad \frac{d\mathbf{x}}{dt} = \mathbf{u} = G * \mathbf{m}$$

- That is, EPDiff **convects** the one-form density of momentum as

$$\left(\frac{\partial}{\partial t} + \mathcal{L}_{\mathbf{u}} \right) \left(\mathbf{m}_t \cdot d\mathbf{x}_t \otimes d^n x_t \right) = 0,$$

with Lie derivative $\mathcal{L}_{\mathbf{u}}$ wrt velocity \mathbf{u} .

- Consequently, the solution of EPDiff is,

$$\mathbf{m}_t \cdot d\mathbf{x}_t \otimes d^n x_t = \left(\mathbf{m}_0 \cdot d\mathbf{x}_0 \otimes d^n x_0 \right) \circ \varphi_t^{-1}$$

for velocity $\mathbf{u} = G * \mathbf{m} = \dot{\varphi}_t \circ \varphi_t^{-1}$ and $\varphi_t \in \text{Diff}$.

- Recognizing this as **coadjoint motion** will be a useful step.

Deriving EPDiff from Hamilton's principle.

Euler-Poincaré Reduction starts with a right (or left) G -invariant Lagrangian $L : TG \rightarrow \mathbb{R}$ on the tangent bundle of a Lie group G .

Right invariance of the Lagrangian may be written as

$$L(g(t), \dot{g}(t)) = L(g(t)h, \dot{g}(t)h), \text{ for all } h \in G$$

- A G -invariant Lagrangian defined on TG possesses a symmetry-reduced Hamilton's principle defined on the Lie algebra \mathfrak{g}

$$TG \mapsto TG/G \simeq \mathfrak{g}.$$

- Stationarity of the symmetry-reduced Hamilton's principle yields the **Euler-Poincaré equations** on the dual Lie algebra \mathfrak{g}^* .
- For $G = Diff$, this equation is **EPDiff**.

Theorem 0.1 (Euler-Poincaré Reduction) *Let G be a Lie group, $L : TG \rightarrow \mathbb{R}$ a right-invariant Lagrangian, and $l := L|_{\mathfrak{g}} : \mathfrak{g} \rightarrow \mathbb{R}$ be its restriction to the Lie algebra \mathfrak{g} . For a curve $g(t) \in G$, let*

$$\xi(t) = \dot{g}(t) \cdot g(t)^{-1} \in \mathfrak{g}.$$

Then the following four statements are equivalent:

(i) $g(t)$ satisfies the Euler-Lagrange equations for Lagrangian L defined on G .

(ii) The variational principle holds, for variations with fixed endpoints,

$$\delta \int_a^b L(g(t), \dot{g}(t)) dt = 0$$

(iii) The (right invariant) **Euler-Poincaré equation** holds:

$$\dot{\mu} = -\text{ad}_{\xi}^* \mu \quad \text{with} \quad \mu = \frac{\delta l}{\delta \xi} \quad \text{and} \quad l(\xi) := L(e, \dot{g}g^{-1}(t))$$

where $\xi = \dot{g}g^{-1}(t)$. **(If $G = \text{Diff}$, this is EPDiff.)**

(iv) For an arbitrary path $\eta(t)$ in \mathfrak{g} which vanishes at the endpoints, i.e., $\eta(a) = \eta(b) = 0$, the **reduced variational principle** holds on \mathfrak{g} ,

$$\delta \int_a^b l(\xi(t)) dt = 0, \quad \text{for} \quad \delta \xi = \dot{\eta} - [\xi, \eta] =: \dot{\eta} - \text{ad}_{\xi} \eta$$

Example: Outlines & momentum measures

Outline matching:

Given two collections of curves c_1, \dots, c_N and C_1, \dots, C_N in Ω , find a time-dependent diffeomorphic process ($t \mapsto \varphi_t$) of minimal action (or cost) such that $\varphi_0 = \text{id}$ and $\varphi_1(c_i) = C_i$ for $i = 1, \dots, N$.

The matching problem for the image outlines seeks *singular momentum solutions* which naturally emerge in the computation of geodesics.

Image outlines as Singular Momentum Solutions of EPDiff

For example, in the 2D plane, EPDiff has weak **singular momentum solutions** that are expressed as [CaHo1993, HoSt2003, HoMa2004]

$$\mathbf{m}(\mathbf{x}, t) = \sum_{a=1}^N \int_s \mathbf{P}_a(t, s) \delta(\mathbf{x} - \mathbf{Q}_a(t, s)) ds, \quad (4)$$

where s is a **Lagrangian coordinate** defined along a set of N curves in the plane *moving with the flow* by the equations $\mathbf{x} = \mathbf{Q}_a(t, s)$ and supported on the delta functions in the EPDiff solution (4). \Rightarrow PPT

Thus, the singular momentum solutions of EPDiff represent evolving “wavefronts” supported on delta functions defined along curves by (4).

These solutions exist in any dimension & provide CA matching for points (landmarks), curves, surfaces, in any combination.

Lagrangian representation of the singular solutions of EPDiff

Substituting the singular momentum solution formula (4) for $s \in S$ into EPDiff (3), then integrating against a smooth test function implies **canonical Hamiltonian equations for Lagrangian wavefronts**

$$\begin{aligned} \frac{\partial}{\partial t} \mathbf{Q}_a(s, t) &= \sum_{b=1}^N \int \mathbf{P}_b(s', t) G(\mathbf{Q}_a(s, t), \mathbf{Q}_b(s', t)) ds' \\ &= \mathbf{u}(\mathbf{Q}_a(s, t), t) = \frac{\delta H_N}{\delta \mathbf{P}_a}, \\ \frac{\partial}{\partial t} \mathbf{P}_a(s, t) &= - \sum_{b=1}^N \int \mathbf{P}_a(s, t) \cdot \mathbf{P}_b(s', t) \\ &\quad \frac{\partial}{\partial \mathbf{Q}_a(s, t)} G(\mathbf{Q}_a(s, t), \mathbf{Q}_b(s', t)) ds' = - \frac{\delta H_N}{\delta \mathbf{Q}_a}. \end{aligned} \tag{5}$$

The $s \in S$ are Lagrangian coordinates; $\mathbf{Q}_a(s, t)$ moves with the flow.

Canonical Hamiltonian dynamics

The singular momentum solutions (4) satisfy *geodesic* Hamiltonian phase space dynamics (5) for the canonically conjugate vector parameters $\mathbf{Q}_a(s, t)$ and $\mathbf{P}_a(s, t)$ with $a = 1, 2 \dots N$.

The Hamiltonian is

$$H_N = \frac{1}{2} \iint \sum_{a, b=1}^N (\mathbf{P}_a(s, t) \cdot \mathbf{P}_b(s', t)) G(\mathbf{Q}_a(s, t), \mathbf{Q}_b(s', t)) ds ds'$$

Here is the Geometry – Leading to the Numerics

- Basic observation that ties everything together in n –dimensions:

Theorem (Holm and Marsden, 2004):

The singular momentum solutions

$$T^*\text{Emb}(S, \mathbb{R}^n) \rightarrow \mathfrak{g}^* : (P, Q) \rightarrow \mathfrak{m}$$

define an equivariant momentum map.

- The embedded manifold S is the support set of the P 's and Q 's.
The momentum map is for left action of the diffeos on S .
The whole system is right invariant.
Its momentum map for right action is conserved.
- These constructions persist for a certain class of numerical schemes
- They apply for every choice of norm for template matching.

Wait a second, what is a momentum map? Give an example

A **momentum map** $\mathbf{J} : T^*Q \mapsto \mathfrak{g}^*$ is a Hamiltonian for canonical action of a Lie group G on phase space T^*Q . It is expressed in terms of the pairing $\langle \cdot, \cdot \rangle : \mathfrak{g}^* \times \mathfrak{g} \mapsto \mathbb{R}$ as

$$\langle \mathbf{J}, \xi \rangle = \langle p, \mathcal{L}_\xi q \rangle =: \langle q \diamond p, \xi \rangle,$$

where $(q, p) \in T_q^*Q$ and $\mathcal{L}_\xi q$ is the infinitesimal generator of the action of the Lie algebra element $\xi \in \mathfrak{g}$ on q in the manifold Q .

The standard example is $\mathcal{L}_\xi q = \xi \times q$ for $\mathbb{R}^3 \times \mathbb{R}^3 \mapsto \mathbb{R}^3$, with pairing $\langle \cdot, \cdot \rangle$ given by scalar product of vectors. The momentum map is then

$$\mathbf{J} \cdot \xi = p \cdot \xi \times q = q \times p \cdot \xi \Rightarrow \mathbf{J} = q \times p$$

This is angular momentum, the Hamiltonian for phase-space rotations.

How is the singular solution ansatz a momentum map?

A momentum map $\mathbf{J} : T^*Q \rightarrow \mathfrak{g}^*$ satisfies the defining relation,

$$\underbrace{\langle \mathbf{J}(\alpha_q), \xi \rangle}_{\langle \cdot, \cdot \rangle: \mathfrak{g}^* \times \mathfrak{g} \rightarrow \mathbb{R}} = \underbrace{\langle \langle \alpha_q, \xi_Q(q) \rangle \rangle}_{\langle \langle \cdot, \cdot \rangle \rangle: T_q^*Q \times T_qQ \rightarrow \mathbb{R}}$$

On LHS, $\alpha_q \in T_q^*Q$ and $\xi \in \mathfrak{g}$.

On RHS, ξ_Q is the infinitesimal generator of the action of Lie group G on Q (associated to Lie algebra element $\xi \in \mathfrak{g}$, the Lie algebra \mathfrak{g} of G .)
 G acts on T^*Q from the left by $g \cdot \mathbf{Q} = g \circ \mathbf{Q}$ (composition of functions)
 Singular solution ansatz does satisfy the momentum map formula, by

$$\int_{\mathbb{R}^n} \int_S (P_i(s) \delta(\mathbf{x} - \mathbf{Q}(s)) d^k s) \xi^i(\mathbf{x}) d^n x = \langle (\mathbf{Q}, \mathbf{P}), \xi \circ \mathbf{Q} \rangle$$

which verifies that both sides are equal $= \int_S P_i(s) \xi^i(\mathbf{Q}(s)) d^k s$

What about the momentum map for relabeling symmetry?

Relabeling $\eta : S \rightarrow S$ is given by the **right action**

$$\text{Diff}(S) : \mathbf{Q} \cdot \eta = \mathbf{Q} \circ \eta.$$

The infinitesimal generator of this right action is the vector field

$$X_{\text{Emb}(S, \mathbb{R}^n)}(\mathbf{Q}) = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \mathbf{Q} \circ \eta_\epsilon = T\mathbf{Q} \cdot \xi$$

where $\xi \in \mathfrak{X}$ is tangent to the curve $\eta_\epsilon \in \text{Diff}$ at $\epsilon = 0$.

Thus for right action the infinitesimal generator needed in the momentum map formula is

$$\xi_{\mathbf{Q}}(s) = T\mathbf{Q} \cdot \xi(s)$$

For right action, the momentum map formula yields:

$$\begin{aligned}
 \langle \mathbf{J}_S(\mathbf{Q}, \mathbf{P}), \xi \rangle &= \langle (\mathbf{Q}, \mathbf{P}), T\mathbf{Q} \cdot \xi \rangle \\
 &= \int_S P_i(s) \frac{\partial Q^i(s)}{\partial s^m} \xi^m(s) d^k s \\
 &= \int_S \xi \left(\mathbf{P}(s) \cdot d\mathbf{Q}(s) \right) d^k s \\
 &= \int_S \left(\mathbf{P}(s) \cdot d\mathbf{Q}(s) \otimes d^k s, \xi(s) \right) \\
 &= \left\langle \mathbf{P} \cdot d\mathbf{Q}, \xi \right\rangle
 \end{aligned}$$

for the pairing of the one-form density $\mathbf{P} \cdot d\mathbf{Q}$ with the vector field ξ .

Symmetry under relabeling implies the momentum map for right action (**relabeling momentum**) is **conserved** on the embedded surface

$$\mathbf{J}_S(\mathbf{Q}, \mathbf{P}) = \mathbf{P}(s) \cdot d\mathbf{Q}(s)$$

EPDiff dynamics informs optimal control for CA

CA must compare two geometric objects, and thus it is concerned with an **optimal control problem**.

However, the **initial value problem** for EPDiff also has **important consequences for CA applications**.

- When matching two geometric structures, the *momentum at time $t=0$ contains all required information for reconstructing the target from the template*. This is done via **Hamiltonian geodesic flow**.
- Being canonically conjugate, the momentum has exactly the same dimension as the matched structures, so there is **no redundancy**.
- Right invariance mods out the relabeling motions from the optimal solution. This symmetry also yields a **conserved momentum map**.

- Besides being one-to-one, the momentum representation is defined on a **linear space**, being dual to the velocity vectors.

This means one may, for example,:

- study linear instability of CA processes,
- take averages and
- apply statistics to the space of image contours.

The *advantage* is the ease of building, sampling and estimating statistical models on a *linear space*.

Conclusions so far

We have:

- (1) identified **momentum as a key concept** in the representation of image data for CA and
- (2) discussed analogies with fluid dynamics.

The **fundamental idea** transferring from fluid dynamics to CA is the idea of **momentum maps** corresponding to group actions.

- Relabeling by **right action** $\text{Emb}(S, \mathbb{R}^n) \times G \mapsto \text{Emb}(S, \mathbb{R}^n)$ is a symmetry of the template Hamiltonian, so its momentum map is conserved. (Right action also generates the steady EPDiff solutions.)
- **Left action** $G \times \text{Emb}(S, \mathbb{R}^n) \mapsto \text{Emb}(S, \mathbb{R}^n)$ is **not** a symmetry. Momentum map \mathbf{J} represents the **weak solution** of EPDiff supported on $\text{Emb}(S, \mathbb{R}^n)$ whose motion is a coadjoint orbit of the left action.

Examples

- Let \mathbf{Q}_0 and \mathbf{Q}_1 be two embeddings of S^1 in \mathbb{R}^2 which represent two shapes, each a closed planar curve.
- We seek a 1-parameter family of embeddings $\mathbf{Q}(t) : S^1 \times [0, 1] \rightarrow \mathbb{R}^2$ so that $\mathbf{Q}(0) = \mathbf{Q}_0$ and $\mathbf{Q}(1)$ matches \mathbf{Q}_1 (up to relabeling).

- $\mathbf{Q}(t)$ is found by minimizing the constrained norm of its velocity.
- To find the equation for \mathbf{Q} we require extremal values of the action

$$A = \int_0^1 \frac{1}{2} \|\mathbf{u}(t)\|_{\mathfrak{g}}^2 dt + \int_0^1 \int_{S^1} \mathbf{P}(s, t) \cdot (\dot{\mathbf{Q}}(s, t) - \mathbf{u}(\mathbf{Q}(s, t))) ds dt,$$

i.e. we seek time-series of vector fields $\mathbf{u}(t)$ which are minimized in some norm subject to the constraint that \mathbf{Q} is advected by the flow using the Lagrange multipliers \mathbf{P} (which we call momentum).

- The minimizing solutions are

$$\frac{\delta L}{\delta \mathbf{u}} = \int_{S^1} \mathbf{P}(s, t) \delta(\mathbf{x} - \mathbf{Q}(s, t)) \, ds,$$

$$\dot{\mathbf{P}}(s, t) = -\mathbf{P}(s, t) \cdot \nabla \mathbf{u}(\mathbf{Q}(s, t), t),$$

$$\dot{\mathbf{Q}}(s, t) = \mathbf{u}(\mathbf{Q}(s, t), t),$$

subject to $\mathbf{Q}(s, 0) = \mathbf{Q}_0(s)$.

- Now one must seek initial momentum $\mathbf{P}(s, 0)$ which takes shape $\mathbf{Q}_0(s)$ to shape $\mathbf{Q}_1(s)$.
- This last problem can be solved by using a gradient algorithm, where the gradient of the residual error with respect to $\mathbf{P}(s, 0)$ is calculated using the adjoint.

Refrain from discussing the adjoint dynamics on Tg^* and Tg

In the **movie examples** we use the Variational Particle-Mesh (VPM) method (Cotter, 2005) to discretize the equations, as follows:

- Discretize the velocity on an Eulerian grid and approximate $\|\mathbf{u}\|$ there.
- Replace S^1 by representing the shape by a finite set of Lagrangian particles $\{\mathbf{Q}_\beta\}_{\beta=1}^{n_p}$.
- Interpolate from the grid to the particles using basis functions

$$\mathbf{u}(\mathbf{Q}_\beta) = \sum_{k=1}^{n_g} \mathbf{u}_k \psi_k(\mathbf{Q}_\beta), \quad \text{with} \quad \sum_{k=1}^{n_g} \psi_k(\mathbf{x}) = 1, \quad \forall \mathbf{x}$$

The action for the continuous time motion on the grid then becomes

$$A = \int_0^1 \frac{1}{2} \|\mathbf{u}(t)\|_{grid}^2 + \sum_{\beta} \mathbf{P}_\beta \cdot \left(\dot{\mathbf{Q}}_\beta - \sum_k \mathbf{u}_k \psi_k(\mathbf{Q}_\beta) \right) dt,$$

and one can obtain a fully discrete method by discretizing the action in time. The discrete adjoint is then applied in computing the inversion.

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Relation to Metamorphosis

Consider the action for Metamorphosis,

$$A = \int_0^1 l dt = \frac{1}{2} \int_0^1 \|\mathbf{u}(t)\|_{\mathfrak{g}}^2 + \frac{1}{\sigma_X^2} \|\partial_t X + \mathcal{L}_{\mathbf{u}} X\|^2 dt$$

where X is an element of any vector representation space of G , $\mathcal{L}_{\mathbf{u}}$ denotes Lie derivative wrt velocity \mathbf{u} and we shall take the norms $\|(\cdot)\|^2$ to define appropriate pairings, $\|(\cdot)\|^2 = \langle (\cdot), (\cdot) \rangle$. Stationarity with respect to variations of the velocity \mathbf{u} yields

$$\delta \mathbf{u} : \mathcal{L} \mathbf{u} = Z_X \diamond X \in \mathfrak{g}^*$$

where

$$Z_X = \frac{1}{\sigma_X^2} \left(\partial_t X + \mathcal{L}_{\mathbf{u}} X \right) = \frac{\delta l}{\delta(\partial_t X)}$$

and the operation \diamond is defined with any chosen pairing by

$$\langle Z_X \diamond X, \eta \rangle := - \langle Z_X, \mathcal{L}_{\eta} X \rangle =: - \langle Z_X, X \eta \rangle$$

Relation to Metamorphosis (cont)

The diamond operation is skew symmetric

$$\langle X \diamond Z_X, \eta \rangle = -\langle Z_X \diamond X, \eta \rangle$$

and it satisfies the chain rule under Lie derivative,

$$\langle \mathcal{L}_\xi(Z_X \diamond X), \eta \rangle = \langle (\mathcal{L}_\xi Z_X) \diamond X, \eta \rangle + \langle Z_X \diamond \mathcal{L}_\xi X, \eta \rangle$$

Consequently, one finds

$$(\partial_t + \text{ad}_\mathbf{u}^*)\mathcal{L}\mathbf{u} = (\partial_t + \mathcal{L}_\mathbf{u})\mathcal{L}\mathbf{u} = (\partial_t + \mathcal{L}_\mathbf{u})(Z_X \diamond X) = 0$$

Euler–Poincaré equation via Clebsch relations

Stationary variations of the constrained Eulerian action,

$$\mathcal{S} = \int l(\xi, a) + \left\langle v, \frac{\partial a}{\partial t} + \mathcal{L}_\xi a \right\rangle dt$$

yield the following **Clebsch relations**,

$$\begin{aligned} \delta\xi : \frac{\delta l}{\delta \xi} - v \diamond a &= 0 \quad (\text{momentum map}) \\ \delta a : \frac{\delta l}{\delta a} - \frac{\partial v}{\partial t} - \mathcal{L}_\xi v &= 0 \\ \delta v : \frac{\partial a}{\partial t} + \mathcal{L}_\xi a &= 0 \quad (\text{advection relation}) \end{aligned} \tag{6}$$

The Clebsch relations will recover the Euler–Poincaré equations,

$$\left(\frac{\partial}{\partial t} + \text{ad}_\xi^* \right) \frac{\delta l}{\delta \xi} = \frac{\delta l}{\delta a} \diamond a \quad \text{and} \quad \frac{\partial a}{\partial t} + \mathcal{L}_\xi a = 0.$$

by using the properties of the **diamond operation** \diamond .

The **diamond operation** \diamond is defined by

$$\langle v \diamond a, \eta \rangle \equiv - \langle v, \mathcal{L}_\eta a \rangle = - \langle v, a \eta \rangle .$$

This operation is **antisymmetric**,

$$\langle v \diamond a, \eta \rangle = - \langle a \diamond v, \eta \rangle ,$$

and satisfies the **chain rule under the Lie derivative**,

$$\langle \mathcal{L}_\xi (v \diamond a), \eta \rangle = \langle (\mathcal{L}_\xi v) \diamond a, \eta \rangle + \langle v \diamond (\mathcal{L}_\xi a), \eta \rangle .$$

These two properties of the \diamond operation and the Clebsch relations (6) together imply

$$\left(\frac{\partial}{\partial t} + \mathcal{L}_\xi \right) (v \diamond a) = \frac{\delta l}{\delta a} \diamond a$$

This manipulation recovers the EP **motion equation**, since

$$\mathcal{L}_\xi \frac{\delta l}{\delta \xi} = \text{ad}_\xi^* \frac{\delta l}{\delta \xi} ,$$

for one-form densities such as $\delta l / \delta \xi = v \diamond a$.