Geometric and Computational Dynamics

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Von Neumann Lecture
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For papers, movies, etc., visit:
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Lagrangian Coherent Structures (LCS)

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Let's first have a look at an example of what the LCS tool can reveal in a particular fluid system.

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LCS for a GLAS-II Airfoil

How this is computed:

1. Get hold of the velocity field
2. Compute the LCS (below)
3. Place particles on either side of the computed LCS
4. Let things flow

Take Home: LCS divides particles with different dynamical behavior—like a separatrix

Not so easy to do “by hand” for unsteady flows

\[a\] In this case a CFD computation that was provided by Jeff Eldredge, UCLA
\[b\] The computation was done by Shawn Shadden
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$$\dot{x} = v(x, t)$$
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**Deformation Gradient**: $F = \text{derivative of the solution } x \text{ wrt initial conditions (start time } t_0, \text{ end time } t = t_0 + T); F \text{ is an } n \times n \text{ matrix.}$
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**Cauchy Green tensor**: the matrix $C = F^T F$; measures how the flow deforms the inner product.
FTLE Field

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- **Cauchy Green tensor**: the matrix $C = F^TF$; measures how the flow deforms the inner product.

- **FTLE (Finite Time Liapunov Exponent)** is
  \[ \sigma = \frac{1}{|T|} \log \sqrt{\lambda_{\text{max}}(C)} \].
An **LCS** (*Lagrangian Coherent Structure*) is a *ridge* in the FTLE field. LCS are time dependent *curves in 2d flows* and *surfaces in 3d flows*.
Definition of LCS

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- An LCS depends on the variable starting time; choose the **run time** $T$ long enough so the computations resolve.

- For $T > 0$ one gets a **repelling LCS** (like a stable manifold), while for $T < 0$, one gets an **attracting LCS** (like an unstable manifold).
LCS in Monterey Bay

Hard to tell what the LCS is from the velocity field alone

1. Get hold of the velocity field
2. Compute the LCS
3. Place particles on either side of the computed LCS
4. Let things flow

Take Home: LCS divides the particles with different dynamical behaviors, like a separatrix

LCS still works for rather complex multiscale flows

\[^{a}\text{Data obtained from radar (Jeff Paduan) or from HOPS (Harvard Ocean Prediction System)}\]
Can compare the movement of real drifters placed in the Bay with the evolution of the LCS

LCS also help to navigate efficiently—such as invariant manifolds in the solar systems (later)

LCS also correlate with interesting ocean features, such as biological fronts
Step 1: seed the domain with a grid of tracers
Step 2: advect groups of particles on the grid
LCS Computation

- **Step 2**: advect groups of particles on the grid

- **Step 3**: Compute $F$ approximately using, for example, central differences.
LCS Computation

- **Step 2**: advect groups of particles on the grid

- **Step 3**: Compute $F$ approximately using, for example, central differences.

- **Step 4**: Plug into the definition of the FTLE field, color code the values of the FTLE field, and compute the ridges to get the LCS.
Software

□ Software—**Mangen** (MANIFOLD GENERATOR) that is able to compute, reasonably automatically, LCS structures as well as other things of interest, such as transport rates.²

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- One must be able to compute lots of particle trajectories, and *systematically* analyze them (compute FTLE fields and then ridges in these fields).

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LCS as Lagrangian Barriers

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- The main result says that if the FTLE ridge is reasonably sharp and if the run time $T$ is reasonably large, then the LCS is indeed a Lagrangian barrier.

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The main result says that if the FTLE ridge is reasonably sharp and if the run time $T$ is reasonably large, then the LCS is indeed a Lagrangian barrier.

Numerical tests show that in practice, the flux is indeed small.

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LCS can be used for studying pollution release

1. Get hold of the velocity field
2. Compute the LCS
3. Release pollutants on either side of the LCS
4. Let things flow

*Take Home:* LCS can give insight into what happens to the release of pollutants.

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Vortex rings are ubiquitous

- Naturally occur in biology; eg, jellyfish, squid\textsuperscript{a}
- Useful for certain highly manoeuvrable underwater vehicles (Helmholtz cavities)
- Create vortex rings in the lab\textsuperscript{b}

\textsuperscript{a}John Dabiri et al., \textit{J. of Experimental Biology}, \textbf{209} (2005)

LCS and Vortex Boundaries

LCS can detect the boundaries of vortex rings.\textsuperscript{4}

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LCS and Vortex Boundaries

- LCS can detect the boundaries of vortex rings.  
- Computation uses experimental data (PIV).
- Can you guess what the boundary is?

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LCS and Vortex Boundaries

☐ How correct were you?

☐ How do we know that LCS really is the boundary?
Vortex Ring Entraining

LCS gives detail about how entraining occurs

- First movie shows that LCS really is a good boundary

- Second shows what looks like “heteroclinic lobes” and how they are responsible for entraining and detraining
Progress on extending these types of calculations to 3D using *GAIO—Global Analysis of (Almost) Invariant Objects*\(^5\)

\(^5\)More on GAIO shortly; this calculation was done by Kathrin Padberg, Paderborn.
Future LCS Computations

- Cardiovascular studies (Charley Taylor, Mory Gharib, John Dabiri)
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Future LCS Computations

- Cardiovascular studies (Charley Taylor, Mory Gharib, John Dabiri)
- Atmospheric studies such as the polar vortex and the South Pole ozone hole break up (following Jones and Winkler, Paul Newton, Shane Ross, Tapio Schneider)
- Microfluidics (Igor Mezic, Sandra Trojan)
Context: Dynamics and transport problems in fluid mechanics, astrodynamics, celestial mechanics, mission design, chemical reaction rates.
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Example Transport in the solar system and application to Mars crossers

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Many applications to molecular and other systems\(^7\)

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Almost invariant sets and planetary crosser lines in the three-body system: *Sun-Jupiter-third body*.

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Invariant manifold tubes play an important role in mission design, from the Genesis Discovery Mission, to cheap missions to the moon, to the Lunar gateway, to multi-moon orbiters,...  

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Molecular Tubes

- Tubes mediate transport between realms & are present in molecular systems—connecting, e.g., *reactants* and *products*.
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○ CDS tools enable reaction rate computation for 3+ dof systems.9

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Galactic Sized Tubes

- From *Shane Ross*. Tubes are known to govern structure and motion even over galactic scales. The huge tails emanating out of some star clusters in orbit about our galaxy are due to stars slipping into tubes connecting the star cluster with the space outside.
The figure shows a *million body simulation* by Combes, Leon, and Meylan [1999]. It is believed that this process can eventually lead to the ‘evaporation’ of some star clusters over tens of billions of years. The estimation of this evaporation time scale is possible using a very simple model, in principle similar to the three-body model.
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Also shown schematically is the star cluster is modelled as a smooth potential (due to the cluster stars) plus the steady tidal field of the galaxy. Stars which are above the energy of the Lagrange points escape via tubes. From the tubes themselves, the half-life, or evaporation time scale can be determined semi-analytically.
Galactic Sized Tubes

Tadpole Galaxy and its 280 thousand light-year long tail. Presumably a passing smaller galaxy pulled off the stars in the tail.

Photo credit: NASA ACS Science & Engineering Team.
Monterey Bay studies done in the context of a big AOSN-II experiment done in summer 03 (MBARI) and continuing as ASAP in 06 (Naomi Leonard at Princeton, Steve Ramp at NPS).
Optimal strategies for gliders—to optimally gather data or to optimize trajectories. Done with NTG.\textsuperscript{10}

More Optimization: ESA Darwin study

- Group of spacecraft in a halo orbit about $L_2$ for the Earth-Sun-spacecraft 3-body system.
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- **Goal:** Optimally reconfigure the group to achieve a hexagonal configuration, including collision avoidance, e.g., pointing to an interesting distant solar system.\textsuperscript{11}

\textsuperscript{11}Provided courtesy of Sina Ober-Blöbaum and Oliver Junge.
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- **DMOC:** $N = 10$ time intervals, SQP-method: **E04UEF** (NAG).

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More Optimization: ESA Darwin study

Darwin Movie
Use discrete mechanics to discretize the equations.
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Optimize a given cost function (such as the control effort) using this with standard SQP methods using the discrete equations of mechanics as constraints.
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Similar examples using, e.g., orbit transfer of Earth-bound satellites using low thrust.
Discrete Mechanics: Example

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\[^{12}\text{Kane, C., J.E. Marsden, M. Ortiz, M. West [2000], \textit{Variational integrators \& the Newmark alg. for conserv. and dissip. mech. systems}, Int. J. Num. Meth. Eng. 49, 1295–1325.}\]
Discrete Mechanics: Example

- Particle in $\mathbb{R}^2$ moving in the field of a radially symmetric polynomial potential (left); with small dissipation (right).\(^{12}\)

- Good energy behavior in both the conservative and dissipative/controlled cases; the integrator, in the absence of dissipation is symplectic and angular momentum preserving.

Discrete Mechanics: Example

- Gets key coarse variables right: statistical computations.\textsuperscript{13}

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Excellent performance in the computation of the "temperature" (time average of the kinetic energy) of a system of interacting particles.

Why Variational?

- The flexibility of the variational view allows for a natural extension to PDEs, asynchronous computations, etc.

- The framework is not symplectic maps or geometry, but *multi-symplectic geometry*\(^a\)

Theory Highlights

• **Basis:** discrete mechanics & Hamilton’s Principle
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- **Flexible and Broad:** includes explicit or implicit algorithms, extends naturally to include multisymplectic schemes for PDE.
- **Structure Preserving:** symplectic and momentum conserving (for the non-forced case).
- **Discrete Reduction:** Discrete analogs of symplectic and Poisson reduction theory.
Key Idea: Approximate the action integral with a quadrature rule—gives a discrete Lagrangian:

\[ L_d(q_0, q_1, h) \approx \int_0^h L(q(t), \dot{q}(t)) \, dt \]

where \( q(t) \) is the exact solution of the Euler–Lagrange equations for \( L \) joining \( q_0 \) to \( q_1 \) over the time step interval \( 0 \leq t \leq h \).

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\(^{14}\)See Marsden, J.E. and M. West [2001], *Discrete variational mechanics and variational integrators*, Acta Numerica 10, 357–514 for a survey of the theory.
Key Idea: Approximate the action integral with a quadrature rule—gives a *discrete Lagrangian*:

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Using the exact value and not an approximation would lead to a solution to the *Hamilton-Jacobi equation* (Jacobi, 1840)

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Given a discrete Lagrangian, form the action sum:

\[ S_d = \sum_{k=0}^{N-1} L_d (q_k, q_{k+1}, h_k) \]
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Discrete variational (Hamilton) principle: Extremize \( S_d \) with fixed end points, \( q_0 \) and \( q_N \)
vary the point $q_i$; the only terms in the sum that are affected are $L_d(q_{i-1}, q_i, h_{i-1}) + L_d(q_i, q_{i+1}, h_i)$; this gives the **DEL**, that is, the **Discrete Euler–Lagrange** equations:

$$D_2L_d(q_{i-1}, q_i, h_{i-1}) + D_1L_d(q_i, q_{i+1}, h_i) = 0$$
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This defines the DEL \textit{algorithm}:

$$(q_{i-1}, q_i) \mapsto (q_i, q_{i+1})$$
Let $M$ be a positive definite symmetric $n \times n$ matrix and $V : \mathbb{R}^n \to \mathbb{R}$ be a given potential. Lagrangian: $L(q, \dot{q}) = \frac{1}{2} \dot{q}^T M \dot{q} - V(q)$. 
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Choose the discrete Lagrangian to be

$$L_d(q_0, q_1, h) = h \left[ \frac{1}{2} \left( \frac{q_1 - q_0}{h} \right)^T M \left( \frac{q_1 - q_0}{h} \right) - V(q_0) \right]$$
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Use the “rectangle rule” on the action integral and the approximation $\dot{q} \approx (q_1 - q_0)/h$. 
Simple Example

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○ Use the “rectangle rule” on the action integral and the approximation $\dot{q} \approx (q_1 - q_0)/h$.

○ DEL equations are a discretization of Newton’s equations:

$$M \left( \frac{q_{k+1} - 2q_k + q_{k-1}}{h^2} \right) = -\nabla V(q_k)$$
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Many Other Examples: Midpoint rule, Newmark algorithms, symplectic partitioned Runge-Kutta algorithms, Verlet, etc etc.
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Forced or Controlled Case

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□ For this (and the dissipative case) one discretizes the Lagrange-d’Alembert principle:

\[ \delta \int L(q, \dot{q}) \, dt + \int f \cdot \delta q \, dt = 0 \]
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\[
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- In addition to approximating the action with the discrete Lagrangian, we approximate the virtual work:

\[
f_k^- \cdot \delta q_k + f_k^+ \cdot \delta q_{k+1} \approx \int_{k+1}^{(k+1)h} f(t) \cdot \delta q(t) \, dt,
\]

where \( f_k^-, f_k^+ \in T^*Q \) are the left and right discrete forces.
**Optimization**

- **Idea:** merge discrete mechanics and optimal control
Optimization

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DMOC respects the energy budget well and needs remarkably few division points. That is, can take large time steps, \(\Delta t\).

Minimize a cost function

\[ J(x, u) = \int_{t_0}^{t_f} C(x(t), u(t)) \, dt \]

subject to dynamical (plus other) constraints:

\[ \dot{x}(t) = f(x(t), u(t)) \]

subject to initial conditions \( x(t_0) = x^0 \) and final conditions \( x(t_f) = x^f \).
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- **Theory.** Centered on Pontryagin maximum principle, receding horizon control,...
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□ Theory. Centered on Pontryagin maximum principle, receding horizon control,....

□ Practice. Brute force optimization software.
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Most current software packages use \textit{SQP (sequential quadratic programing)} to do the basic optimization.

For the Lagrange problem, one has to also deal with the constraints of the equations of motion. How these are handled is one of the key differences between software packages.
□ **Mechanical Case:** Equations are of Euler–Lagrange type with control forces, which are determined from the “variational” principle of *Lagrange-d’Alembert type.*

\[
\delta \int_{t_0}^{t_f} L(q(t), \dot{q}(t)) \, dt + \int_{t_0}^{t_f} u(t) \delta q(t) \, dt = 0
\]

for a given Lagrangian \( L : TQ \rightarrow \mathbb{R} \).
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for a given Lagrangian \( L : TQ \to \mathbb{R} \).

**Our strategy\(^1\):** make use of direct SQP methods for dealing with optimization—but *replace the equations of motion by their discrete variational counterpart.*

\(^1\)Junge, O., J. E. Marsden, and S. Ober-Blöbaum [2005], *Discrete mechanics and optimal control*, 2005 IFAC Proceedings.
Procedure.

- Choose a discrete $L_d$ using a chosen quadrature method
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- Result: *purely algebraic constraints*

\[ D_1 L_d(q_k, q_{k+1}) + D_2(q_{k-1}, q_k) + u^-(u_k, u_{k+1}) + u^+(u_{k-1}, u_k) = 0 \]
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- Discretize the cost functional

$$J_d(q_d, u_d) = \sum_{k=0}^{N-1} C_d(q_k, q_{k+1}, u_k, u_{k+1})$$
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- Hand this off to standard and powerful SQP packages, enforcing the initial and final conditions and any other constraints.
A group of hovercraft are asked to move from a given starting position to a hexagonal final formation shown in an optimal way. (The hovercraft themselves need to decide who goes where).
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Model: mechanical systems with 3 degrees of freedom (position \((x, y)\), heading angle \(\theta\)), so \(Q = \mathbb{R}^2 \times S^1\)
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**Model:** mechanical systems with 3 degrees of freedom (position $(x, y)$, heading angle $\theta$), so $Q = \mathbb{R}^2 \times S^1$

**Two actuation forces**—one along the axis of the hovercraft (forward acceleration), and a perpendicular force towards the rear of the hovercraft, not through the center of mass of the hovercraft (sideways slip and steering).
The system is \textit{underactuated}. The Lagrangian for the system is the standard kinetic energy of the hovercraft and the equations of motion are the standard Euler–Lagrange equations with forcing.
System is *underactuated*, but is *configuration controllable*—each point in $Q$ can be reached by applying suitably chosen forces $f_1(t)$ and $f_2(t)$. 
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The Lagrangian $= \text{kinetic energy}$:

$$L(q, \dot{q}) = \frac{1}{2}(m\dot{x}^2 + m\dot{y}^2 + J\dot{\theta}^2),$$

where $q = (x, y, \theta)$, $m$ is the mass of the hovercraft and $J$ its moment of inertia. The forces acting in $x$-, $y$- and $\theta$- direction resulting from $f_1$ and $f_2$ are

$$f(t) = \begin{pmatrix} \cos \theta(t)f_1(t) - \sin \theta(t)f_2(t) \\ \sin \theta(t)f_1(t) + \cos \theta(t)f_2(t) \\ -rf_2(t) \end{pmatrix}. $$
Forced discrete Euler-Lagrange equations

\[
\frac{1}{h} M (-q_{k-1} + 2q_k - q_{k+1}) + \frac{h}{2} \left( \frac{f_{k-1} + f_k}{2} + \frac{f_k + f_{k+1}}{2} \right) = 0,
\]

\[k = 1, \ldots, N - 1, \text{ where } M = \begin{pmatrix} m & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & J \end{pmatrix}.
\]

Let \( q_i = (x_i, y_i, \theta_i) \) the configuration of the \( i \)-th hovercraft and by \( f_i = (f_{i1}, f_{i2}) \) the corresponding forces.
Goal: minimize the control effort needed to attain the final formation.
◮ **Goal**: minimize the control effort needed to attain the final formation.

◮ **Sample Cost Function**: Add the costs for each hovercraft

\[
J(q_i, f_i) = \int_0^1 f_{i1}^2(t) + f_{i2}^2(t) \, dt,
\]
Left: Optimal rearrangement of a group of three hovercraft from an initial configuration along a line into a triangle

Right: Optimal rearrangement of a group of six hovercraft from a random initial configuration into a hexagon.
Hovercraft Example

Hovercraft
Articulated bodies in fluids\textsuperscript{17}

\textsuperscript{17}Kanso, E., J. E. Marsden, C. W. Rowley, and J. Melli-Huber [2004], \textit{Locomotion of articulated bodies in a perfect fluid}, \textit{J. Nonlinear Science (to appear)}. We owe a lot to Scott Kelly and Jim Radford!
Articulated bodies in fluids

Coupled rigid bodies (simulating and elastic swimming fish) interacting dynamically with potential flow.

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Locomotion Optimization

- Articulated bodies in fluids

- Coupled rigid bodies (simulating and elastic swimming fish) interacting dynamically with potential flow.

- Symplectic reduction theory from geometric mechanics (cotangent bundle reduction theorem) proves useful; one uses this to get rid of the fluid particle relabeling symmetry (which gives Kelvin’s theorem).

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Locomotion Optimization

- Attractive feature of DMOC: not hard to implement
- This problem: find optimal controls that achieve a given forward movement with the least amount of expended energy. (The underlying theory is related to the falling cat theorem).\(^a\)

\(^a\)Kanso, E. and J. E. Marsden [2005], *Optimal motion of an articulated body in a perfect fluid*, Proc. CDC (submitted). The optimal flapper is due to Shane Ross.
Use GAIO, Perron Frobenius eigenfunctions, and coarse-fine techniques to separate local from global minima.
More Future Directions

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- Extend DMOC to the AVI context and use hierarchical and network optimization (primal-dual ideas).
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□ Further work on optimization and collision avoidance using collision potentials, gyroscopic controls, and self organized patterns.18

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- Extend DMOC to the AVI context and use hierarchical and network optimization (primal-dual ideas).
- Further work on optimization and collision avoidance using collision potentials, gyroscopic controls, and self organized patterns.\(^{18}\)
- Discrete geometry (Whitney forms) for fluids and solid mechanics

\(^{18}\)Chang, D., S. Shadden, J. E. Marsden, and R. Olfati-Saber [2003], *Collision avoidance for multiple agent systems*, *Proc. CDC* 42, 539–543.
The End

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