Lagrangian Coherent Structures: applications to living systems

Bradly Alicea

http://www.msu.edu/~aliceab
Introduction: basic scientific problem

Q: How can we quantify emergent structures? Use Lagrangian Coherent Structures (LCS) approach.

* hard to capture higher-level relationships using simple pairwise comparisons or aggregate measurements (curse of dimensionality).

* swarms, herds, colonies, and flocks: all share a common set of principles – self-organized behaviors (weak, strong emergence).

* behaviors, formation of structure occurs in a medium (air, liquid, etc) and so are analogous to or explicitly involve flows (mechanical representation).

* interactions are also dynamic – need a dynamical systems approach.
Introduction: key people and papers

Key people/hot papers in this area:


Lagrangian introduction

Lagrangian: function that summarizes system dynamics (special case of classical mechanics).

\[ L = T - V \]

If Lagrangian known, equations of motion used instead, becomes PDE.

\[ T = \text{kinetic energy}, \; V = \text{potential energy.} \]

* combines conservation of momentum with conservation of energy.

First-order Lagrangian: constraints (motion\(\mid\)energy) explicit in form of equations (Lagrangian multipliers).

**Second-order Lagrangian:** constraints (motion\(\mid\)energy) explicit in form of a generalized coordinate system (LCS method).

Stationary action: assume well-defined trajectory bounded in space and time.

\[ S = \int L \, dt \quad S (\text{Joules} \cdot \text{sec}) \]
Finite Lyapunov exponents

**Key tool for LCS:** finite-time and finite-size Lyapunov exponents (FTLE or FSLE):

* FTLE = evolution of collective particle trajectories over time (find distance for given time interval).

* FSLE = evolution of collective particle trajectories across space (find time for given set of distances).

LCS is a flexible dynamical system:

* Lagrangian representation of mechanics (special case of classical mechanics). Use where Eulerian representations are incomplete….

Points in a flow have an initial position. The relationship between these points deformed (flow travels apart) over time:

* distance between points quantified using Lyapunov exponent.

* ridges form in flow map over time/space = coherent structures.
Finite Lyapunov exponents (con’t)

Finite Lyapunov exponent (related to $\gamma$, key parameter in dynamical systems) defined by:

Lyapunov exponent (scalar value)  Movement of particles (advection)  Coordinate system (interpolation)

A matter of diffusion….
* particles diffuse across a coordinate system at rate $r$.
* if there is underlying order, particles will aggregate into larger-scale structures.
* stochastic component (diffusion speed),
deterministic component (interface between regimes).

Flow maps and transport dynamics

Flow maps: visualizations of how particles diffuse, travel, and aggregate over time.

Major structures visible in flow map: vortex rings, streaks, tracks, streams, etc.

Characterized indirectly using LCS method (indicator of, influential in natural processes).

Flow map examples:
Flow maps and transport dynamics (con’t)

Coherent structures = distinguished set of fluid particles.

Stability properties = impact on fluid mixing.

In time-periodic laminar flow ~ complex tangles predicted for chaotic advection.

* velocity measurements for small # of tracer particles (e.g. dye) can provide a highly resolved velocity field.

  * particles yield more information about velocity field as time progresses.

  * high degree of noise, spatial complexity work against this.

Re (Reynolds #): \[ \text{Re} = \frac{\rho (V \cdot V)}{\mu V} = \frac{L}{\mu V (L \cdot L)} \]

Re >> 0, turbulent (inertial).
Re ~ 0, laminar (viscous).

Ro (Rossby #):

\[ \text{Ro} = \frac{U}{L (2 \Omega \varphi)} \]

Ro >> 0, centrifugal, inertial.
Ro ~ 0, coriolis.
Flow maps and transport dynamics (con’t)

\( \text{Ro} \) = ratio of inertial to Coriolis forces.

\( \text{Re} \) = ratio of inertial to viscous forces.

FTLE (time):

Actual trajectory unknown, inferred by repeated measurements of \( \lambda \) over interval

FSLE (size):

Courtesy:
http://www.cds.caltech.edu/~marsden/lcs/fluid-transport
Flow maps and transport dynamics (con’t)

Experiment: 50x40 cm tank, 0.4 Hz rotation.

2D flow laminar flow regime at top of tank.

* Re = 1000, Ro = 0.3

* velocity field = 1500x1500 grid.

* Δt = .004 sec.

* Lt(xo) along particle paths is large only in small regions of flow.

Integrated Lagrangian divergence:

\[ L_t(x_0) = \int_t^{t+1} (\nabla - \nu) |F_t^s(x_0)| ds \]

Direct Lyapunov exponent (DLE):

\[ \delta_{t_0} (x) = \frac{ln \lambda_{max}(t,x_0,x_0)}{2t-t_0} \]

Dabiri’s Pinch-off (Chaos, 2010) approach:

Flow map (maps fluid particles from initial position t_o over interval T):

\[ \Phi_{t_0}^{t_0+T} : x(t_0) \rightarrow x(t_0 + T) \]

FTLE:

Linearized divergence of trajectories over interval T

\[ \sigma_{t_0}^{T} = \frac{1}{|T|} \ln \left| \frac{dx(t_0 + T)}{dx(t_0)} \right| \]

Deformation tensor
Flow maps and transport dynamics (con’t)

Features of flow:
* long-lived vortices and jets in laminar regime with diversity of sizes.

* coherent structures are columnar (vertical across 2D, quasi-2D and 3D turbulence regimes).

Visualizations of LCS:
* \( t >> t_0 \) = repelling LCS at \( t_0 \) are locally maximizing curves (ridges).

* \( t << t_0 \) = attracting LCS at \( t_0 \) are locally maximizing curves (ridges).

Results invariant for \( T \) values (integration) for 1-16.

Integration = ratio of deformed area at \( t + T \): original area around \( x_0 \) at \( t \).

Flow maps and transport dynamics (con’t)

Perform time-integration in two ways, derive two distinct structural modes:

Attracting LCS, backwards in time: Maximum values of FSLE = lines that approximate unstable manifolds. Neighboring fluid trajectory attracted, escapes hyperbolic points.

Example: fluid funneling down a drain (towards attractor point, away from slopes).

Repelling LCS, forwards in time: Maximum values of FSLE form "ridges" that delineate fluids with distinct origins. Neighboring trajectories repelled and form lines that strongly modulate fluid flow, act as transport barriers.

Example: advancing front of soap scum or ripple of water.

Again, a matter of diffusion:
For example: uniform diffusion from a glob of particles (initial condition) can create a repelling LCS that forms a continuous ridge (ring).
**Dabiri Paper (Chaos, 2010)**

**Vortex Rings:** Wide variety of biological flows, fluid column of length (L) pushed through aperture of distance (D). \( L/D = \) formation 

* boundary layers form with movement (piston up and down in column), rolls up into a vortex ring.

* vorticity flux fuels growth. \( L/D > 4 \), wake formation begins to trail ring.

* disconnection of velocity and vorticity fields = pinch-off.

**Challenges:** previous approaches to understanding pinch off.

* pinch-off was not directly observed during vortex ring evolution.

* trouble controlling, disentangling interactions in the dynamics.

* in low Re flows, vortex ring evolution confused with viscous diffusion.

Proposed criterion to ID vortex ring pinch-off in axisymmetric jet flow:

* starting jet of L/D ~ 12.

* termination of previous LCS precedes appearance of new LCS (independent). Marks initiation of pinch-off.

* LCS can either form a spiral (persistent vortices) or merge with existing LCS (merger of vortices in shear layer).

LCS = finite-time invariant manifolds in time-dependent, aperiodic system:

Repelling: diverge forward in time.

Attracting: diverge backward in time.
Streamlines (left) and pathlines (right) for three different times.

Streaklines (left) and timelines (right) for three different times.
Dabiri Paper (Chaos, 2010 - con’t)

LCS are most effective as a quantitative indicator of relative Lagrangian trajectories over time, not pinch-off *per se*.

* regions of high particle separation between regions of qualitatively different flows.

* suited to ID separation different regions of vorticity-carrying flows that occurs during pinch-off.

* robust ID of vortex structure in unsteady flows.

* frame-independent FTLE allows for time-history of motion.

LCS may be useful to understand optimal vortex formation, implications for a number of biological systems:

* flow of blood/particulates through circulatory system.

* swimming and flying motions.

Courtesy: Sinauer & Associates.
Tew Kai Paper (PNAS, 2009)

Problem: ocean eddies (turbulence) influence primary production, community structure, and predation.

* predators use boundary between 2 eddies, generates strong dynamic interface.
* occurs at multiple temporal and spatial scales, but especially at spatial scales (<10km), not directly observable using satellite altimetry.

How do predators locate these structures?
* map observations to horizontal velocity field. Apply to FSLE.
* compute from marine surface velocity data, mixing activity, and coherent structures.

1) FSLE: measures how fast fluid particles separate to a specified distance.
2) LCS: ID as ridges (location with maximum value of Lyapunov exponent fields).

* dispersion rates of tracer particles - integrate trajectories towards the future (forward) or towards past (backward).
Quantifiers:
1) $\text{FSLE}_f$: repel neighboring trajectories (positive value).
2) $\text{FSLE}_b$: attract neighboring trajectories (negative value).

* dispersion rates of tracer particles allow us to integrate trajectories towards the future ($\text{FSLE}_f$) or towards past ($\text{FSLE}_b$).

LCS by FSLE: stretching and contractile properties of transport.

* compute time $\tau$ it takes 2 tracer particles initially separated by distance $\delta_o$ to reach final separation distance $\delta_f$ in velocity field.

**FSLE at position x and time t:**

$$\lambda(x,t,\delta_o,\delta_f) = \frac{1}{\tau} \log \left( \frac{\delta_f}{\delta_o} \right)$$

* depend on choice of 2 length scales $= \delta_o$ and $\delta_f$. Here, $\delta_o = .025^\circ$ and $\delta_f = 1^\circ$.

* other studies: FSLE adequate to characterize horizontal mixing and transport structures, correlate with tracer fields like temperature and chlorophyll.
Top: flow maps for geographical region of interest. Show structure of FSLEs.

Lower left: histograms for relative frequency of FSLEs.

Lower right: migration of birds during observed trips (follow FSLEs).

* as predicted by dissipative structures (Prigogine) and constructal theory (Bejan).

* higher energy density structures in active flows.
Applications of LCS methodology

**Drug delivery and diagnosis:**
* characterize flow patterns in bloodstream as indicative of arterial clogging.
* where in circulatory system are laminar, other flow conditions maximized?

**Morphogenesis:**
* so-called morphogen gradients may be characterized as ridges from different sources.
* especially interesting in tissue engineering contexts (using complex forces to differentiate stem cells).

Applications of LCS methodology (con’t)

Analysis of Biological Complexity:
LCS “ridges” as basis for rugged energy, fitness landscapes.

* Stu Kauffman’s NK-boolean networks, ruggedness = complexity.

* characterizing patterns of local (and even global) minima/maxima may allow for higher-order interpretation.

Soft Active Material Dynamics:
How do we describe higher-level order in complex monolayers, bilayers?

* nematic (left) to smectic (right) transitions in self-assembly.

* complex patterns in materials, surfaces.

Reaction-Diffusion Computing:

* computers that use B-Z reactions, other physical models.

* how do we characterize outputs (binary and non-binary)?