Geometric and probabilistic descriptions of chaotic phase space transport

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MultiSTEPS: MultiScale Transport in Environmental & Physiological Systems, www.multisteps.esm.vt.edu
Motivation: application to real data

- Many systems defined from data or large-scale simulations — experimental measurements, observations
- e.g., from fluid dynamics, biology, social sciences
- Aperiodic, finite-time, finite resolution — in general, no fixed points, periodic orbits, or other invariant sets (or their stable and unstable manifolds) to organize phase space
Motivation: application to real data

- Perhaps can find appropriate analogs to the objects; adapt previous results to this setting
- Try some numerical explorations; see what merit furthers study
Chaotic phase space transport via lobe dynamics

□ As our dynamical system, we consider a discrete map\(^1\)

\[ f : \mathcal{M} \rightarrow \mathcal{M}, \]

e.g., \( f = \phi_t^{t+T} \), where \( \mathcal{M} \) is a differentiable, orientable, two-dimensional manifold e.g., \( \mathbb{R}^2, S^2 \)

□ To understand the transport of points under the map \( f \), we consider the invariant manifolds of unstable fixed points

□ Let \( p_i, i = 1, \ldots, N_p \), denote a collection of saddle-type hyperbolic fixed points for \( f \).

\(^1\)Following Rom-Kedar and Wiggins [1990]
Partition phase space into regions

- Natural way to partition phase space
  - Pieces of $W^u(p_i)$ and $W^s(p_i)$ partition $\mathcal{M}$.

Unstable and stable manifolds in red and green, resp.
Partition phase space into regions

- Intersection of unstable and stable manifolds define boundaries.
Partition phase space into regions

- These boundaries divide the phase space into regions.
Label mobile subregions: ‘atoms’ of transport

- Can label mobile subregions based on their past and future whereabouts under one iterate of the map, e.g., \((\ldots, R_3, R_3, [R_1], R_1, R_2, \ldots)\)
Primary intersection points (pips) and boundaries

$q$ is a primary intersection point (pip), $\bar{q}$ is not a pip.
Suppose $W^u(p_i)$ and $W^s(p_j)$ intersect in the pip $q$. Define $B \equiv U[p_i, q] \cup S[p_j, q]$ as a **boundary** between “two sides,” $R_1$ and $R_2$. 

\[ B = U[p_i, q] \cup S[p_j, q] \]
Let $q_0, q_1 \in W^u(p_i) \cap W^s(p_j)$ be two adjacent pips, i.e., there are no other pips on $U[q_0, q_1]$ and $S[q_0, q_1]$. The region interior to $U[q_0, q_1] \cup S[q_0, q_1]$ is a lobe.
Lobe dynamics: transport across a boundary $B$

$f^{-1}(q)$ is a pip. $f$ is orientation-preserving $\Rightarrow$ there’s at least one pip on $U[f^{-1}(q), q]$ where the $W^u(p_i), W^s(p_j)$ intersection is topologically transverse.
Lobe dynamics: transport across a boundary $B$

$U[f^{-1}(q), q] \cup S[f^{-1}(q), q]$ forms boundary of two lobes; one in $R_1$, labeled $L_{1,2}(1)$, or equivalently $([R_1], R_2)$, where $f(([R_1], R_2)) = (R_1, [R_2])$, etc. for $L_{2,1}(1)$
Lobe dynamics: transport across a boundary $B$

- Under one iteration of $f$, only points in $L_{1,2}(1)$ can move from $R_1$ into $R_2$ by crossing $B$, etc.
- The two lobes $L_{1,2}(1)$ and $L_{2,1}(1)$ are called a turnstile.
Lobe dynamics: transport across a boundary $B$

- Essence of lobe dynamics: the dynamics associated with crossing $B$ is reduced to the dynamics of the turnstile lobes associated with $B$.
Identifying atoms of transport by itinerary

- In a complicated system, can still identify manifolds ...

Unstable and stable manifolds in red and green, resp.
Identifying atoms of transport by itinerary

... and lobes

Significant amount of fine, filamentary structure.
Identifying atoms of transport by itinerary

- e.g., with three regions \( \{R_1, R_2, R_3\} \), label lobe intersections accordingly.
  - Denote the intersection \((R_3, [R_2]) \cap ([R_2], R_1)\) by \((R_3, [R_2], R_1)\)
Identifying atoms of transport by itinerary

$(R_3, [R_2], R_1)$

Longer itineraries...
Identifying atoms of transport by itinerary

... correspond to smaller pieces of phase space; horseshoe dynamics, etc
Lobe Dynamics: example

- rest. 3-body problem: chaotic sea contains unstable fixed points.
Compute a boundary
Transport btwn Two Regions

• The evolution of a lobe of species $S_1$ into $R_2$

Transport between Two Regions

Phase Space Volume

Species Distribution: Species $S_1$ in Region $R_2$

$F_{1,2} =$ flux of species $S_1$ into region $R_2$ on the $n$th iterate

$T_{1,2} =$ total amount of $S_1$ contained in $R_2$ immediately after the $n$th iterate

$n =$ Iterate of Poincare Map

$1 \leq n \leq 10$
Lobe dynamics: fluid example

Fluid example: time-periodic Stokes flow

Model for microfluidic mixer

System has parameter $\tau_f$, which we treat as a bifurcation parameter — critical point $\tau_f^* = 1$; above and next few slides show $\tau_f > 1$

Computations by Mohsen Gheisarieh and Mark Stremler (Virginia Tech)
Lobe dynamics: fluid example

Fluid example: Poincaré map

some invariant manifolds of saddles
Lobe dynamics: fluid example

Fluid example: Poincaré map

regions and lobes labeled
Stable/unstable manifolds and lobes in fluids

Fluid example: Poincaré map

material blob at $t = 0$
Stable/unstable manifolds and lobes in fluids

Fluid example: Poincaré map

material blob at $t = 5$
Stable/unstable manifolds and lobes in fluids

Fluid example: Poincaré map

some invariant manifolds of saddles
Stable/unstable manifolds and lobes in fluids

Fluid example: Poincaré map

material blob at $t = 10$
Stable/unstable manifolds and lobes in fluids

Fluid example: Poincaré map

material blob at $t = 15$
Stable/unstable manifolds and lobes in fluids

Fluid example: Poincaré map

material blob and manifolds
Stable/unstable manifolds and lobes in fluids

Fluid example: Poincaré map

material blob at $t = 20$
Stable/unstable manifolds and lobes in fluids

Fluid example: Poincaré map

material blob at $t = 25$
Stable/unstable manifolds and lobes in fluids

Fluid example: Poincaré map

- Saddle manifolds and lobe dynamics provide template for motion
Stable/unstable manifolds and lobes in fluids

• Concentration variance; a measure of homogenization

• Homogenization has two exponential rates: slower one related to lobes
Braiding of stirrers

- Large-scale braiding provides the faster scale — and an alternative point-of-view

$R_N$: 2D fluid region with $N$ stirring ‘rods’

- stirrers move on periodic orbits
- stirrers = solid objects or fluid particles
- stirrer motions generate diffeomorphism $f: R_N \rightarrow R_N$
- stirrer trajectories generate braids in 2+1 dimensional space-time
Thurston-Nielsen classification theorem

- A stirrer motion $f$ is isotopic to a stirrer motion $g$ of one of three types (i) finite order (f.o.): the $n$th iterate of $g$ is the identity (ii) pseudo-Anosov (pA): $g$ has dense orbits, Markov partition with transition matrix $A$, topological entropy $h_{TN}(g) = \log(\lambda_{PF}(A))$, where $\lambda_{PF}(A) > 1 = $ Perron-Frobenius eigenvalue of $A$ (iii) reducible: $g$ contains both f.o. and pA regions
- $h_{TN}$ computed from ‘braid word’, e.g., $\sigma_{-1}\sigma_{2}$
- $\log(\lambda_{PF}(A))$ provides a lower bound on the true topological entropy
- i.e., non-trivial material lines grow like $\ell \sim \ell_{0}\lambda^n$, where $\lambda \geq \lambda_{TN}$
Identifying ‘ghost rods’: periodic points

- For $\tau_f > 1$, groups of elliptic and saddle periodic points of period 3 — streamlines around groups resemble fluid motion around a solid rod
- At $\tau_f = 1$, points merge into parabolic points
- Below $\tau_f < 1$, periodic points vanish
Identifying ‘ghost rods’: periodic points

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Identifying ‘ghost rods’: periodic points

- Periodic points of period 3 ⇒ act as ‘ghost rods’
- Their braid ⇒ $h_{TN} = 0.96242$ from TNCT
- Actual $h_{\text{flow}} \approx 0.964$
- ⇒ $h_{TN}$ is an excellent lower bound
Identifying ‘ghost rods’: periodic points

- Homogenization has two exponential rates: slower one related to lobes
- Fast rate due to braiding of ‘ghost rods’!
Topological entropy continuity across critical point

topological entropy as a function of $\tau_f$
Identifying ‘ghost rods’?

Poincaré section for $\tau_f < 1 \Rightarrow$ no obvious structure!

- Note the absence of any elliptical islands
- No periodic orbits of low period were found
- Is the phase space featureless?
Almost-invariant set (AIS) approach

- Take probabilistic point of view (recall, e.g., Oliver Junge’s talk)
- Partition phase space into loosely coupled regions

AISs \approx \text{“Leaky” regions with a long residence time}^2

3-body problem phase space is divided into several invariant and almost-invariant sets.

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Almost-invariant set (AIS) approach

- Create box partition of phase space $\mathcal{B} = \{ B_1, \ldots B_q \}$, with $q$ large
- Consider a $q$-by-$q$ transition (Ulam) matrix, $P$, for our dynamical system, where

$$ P_{ij} = \frac{m(B_i \cap f^{-1}(B_j))}{m(B_i)} , $$

the transition probability from $B_i$ to $B_j$ using, e.g., $f = \phi_{t+T}^t$

- $P$ approximates our dynamical system via a finite state Markov chain.
Almost-invariant set (AIS) approach

- A set $B$ is called almost invariant over the interval $[t, t + T]$ if
  \[ \rho(B) = \frac{m(B \cap \phi^{-1}(B))}{m(B)} \approx 1. \]

- Can maximize value of $\rho$ over all possible combinations of sets $B \in \mathcal{B}$.

- In practice, AIS or relatedly, almost-cyclic sets (ACS), identified via eigenvectors (of eigenvalues with $|\lambda| \approx 1$) of $P$ or graph-partitioning.

- Appropriate for non-autonomous, aperiodic, finite-time settings.
Identifying ‘ghost rods’: almost-cyclic sets

- Return to $\tau_f > 1$ case, where periodic points and manifolds exist
- Agreement between AIS boundaries and manifolds of periodic points
- Known previously\(^3\) and applies to more general objects than periodic points, i.e. normally hyperbolic invariant manifolds (NHIMs)

Identifying ‘ghost rods’: almost-cyclic sets

Poincaré section for $\tau_f < 1 \Rightarrow$ no obvious structure!

- Return to $\tau_f < 1$ case, where no periodic orbits of low period known
- Is the phase space featureless?

- Consider transition matrix $P_{t+\tau_f}^t$ induced by Poincaré map $\phi_{t+\tau_f}^t$
Identifying ‘ghost rods’: almost-cyclic sets

Top six eigenvalues for $\tau_f = 0.99 < \tau_f^*$
Identifying ‘ghost rods’: almost-cyclic sets

The zero contour (black) is the boundary between the two almost-invariant sets.

- Three-component AIS made of 3 almost-cyclic sets (ACSs) of period 3
- ACS effectively replace compact region bounded by saddle manifolds
- Also a remnant of the global ‘stable and unstable manifolds’ of the saddle points, even there are no more saddle points
Identifying ‘ghost rods’: almost-cyclic sets

Almost-cyclic sets stirring the surrounding fluid like ‘ghost rods’ — works even when periodic orbits are absent!

Movie shown is second eigenvector for $P_t^{t+\tau_f}$ for $t \in [0, \tau_f)$
Identifying ‘ghost rods’: almost-cyclic sets

Braid of ACSs gives lower bound of entropy via Thurston-Nielsen
— One only needs approximately cyclic blobs of fluid
— Even though the theorems require exactly periodic points!
Topological entropy vs. bifurcation parameter

$h$ vs. $\tau_f$

$h_{TN}$ shown for ACS braid on 3 strands
Movie shows change in eigenvector branch, marked with ‘− □ −’ above, as parameter decreases from a to f ⇒
Bifurcation of ACSs

For example, braid on 13 strands for $\tau_f = 0.92$

Movie shown is second eigenvector for $P_t^{t+\tau_f}$ for $t \in [0, \tau_f)$

Thurson-Nielsen for this braid provides lower bound on topological entropy
Bifurcation of ACSs

(a) Initial state

(b) First half-period

(c) Second half-period

(d) State after 1 period
Bifurcation of ACSs

representation of braid
Sequence of ACS braids bounds entropy

For various braids of ACSs, the calculated entropy is given, bounding from below the true topological entropy over the range where the braid exists.
Aperiodic, finite-time setting

- Data-driven, finite-time, aperiodic setting
- How do we get at transport?
- Recall the flow, \( x \mapsto \phi_{t+T}^t(x) \)
Identify regions of high sensitivity of initial conditions

- Small initial perturbations $\delta x(t)$ grow like

$$
\delta x(t + T) = \phi^{t+T}(x + \delta x(t)) - \phi^{t+T}(x)
= \frac{d\phi^{t+T}(x)}{dx} \delta x(t) + O(\|\delta x(t)\|^2)
$$
Identify regions of high sensitivity of initial conditions

- Small initial perturbations \( \delta x(t) \) grow like

\[
\delta x(t + T) = \phi_{t+T}^t(x + \delta x(t)) - \phi_{t+T}^t(x) = \frac{d\phi_{t+T}^t(x)}{dx} \delta x(t) + O(\|\delta x(t)\|^2)
\]
Invariant manifold analogs: FTLE-LCS approach

- The finite-time Lyapunov exponent (FTLE),
  \[
  \sigma^T_t(x) = \frac{1}{|T|} \log \left\| \frac{d\phi^t+T(x)}{dx} \right\|
  \]
  measures the maximum stretching rate over the interval \( T \) of trajectories starting near the point \( x \) at time \( t \)

- Ridges of \( \sigma^T_t \) are candidate hyperbolic codim-1 surfaces; finite-time analogs of stable/unstable manifolds; Lagrangian coherent structures\(^4\)

\(^4\)cf. Bowman, 1999; Haller & Yuan, 2000; Haller, 2001; Shadden, Lekien, Marsden, 2005
Invariant manifold analogs: FTLE-LCS approach
Invariant manifold analogs: FTLE-LCS approach
Invariant manifold analogs: FTLE-LCS approach

- We can define the FTLE for Riemannian manifolds\(^3\)

\[
\sigma^T_t(x) = \frac{1}{|T|} \ln \left\| D\phi^{t+T} \right\| = \frac{1}{|T|} \log \left( \max_{y \neq 0} \frac{\left\| D\phi^t(y) \right\|}{\|y\|} \right)
\]

with \(y\) a small perturbation in the tangent space at \(x\).

\(^3\)Lekien & Ross [2010] Chaos
Transport barriers: LCS

- Ridges correspond to dynamical barriers\(^3\) or Lagrangian coherent structures (LCS): repelling surfaces for \( T > 0 \), attracting for \( T < 0 \)

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\(^3\)Lekien & Ross [2010] Chaos
Atmospheric flows: Antarctic polar vortex

ozone data
Atmospheric flows: Antarctic polar vortex

ozone data + LCSs (red = repelling, blue = attracting)
Atmospheric flows: Antarctic polar vortex

air masses on either side of a repelling LCS
Atmospheric flows: continental U.S.

LCSs: orange = repelling, blue = attracting
Atmospheric flows and lobe dynamics

orange = repelling LCSs, blue = attracting LCSs

Hurricane Andrea, 2007

Atmospheric flows and lobe dynamics

Hurricane Andrea at one snapshot; LCS shown (orange = repelling, blue = attracting)
Atmospheric flows and lobe dynamics

orange = repelling (stable manifold), blue = attracting (unstable manifold)
Atmospheric flows and lobe dynamics

orange = repelling (stable manifold), blue = attracting (unstable manifold)
Atmospheric flows and lobe dynamics

Portions of lobes colored; magenta = outgoing, green = incoming, purple = stays out
Atmospheric flows and lobe dynamics

Portions of lobes colored; magenta = outgoing, green = incoming, purple = stays out
Atmospheric flows and lobe dynamics

Sets behave as lobe dynamics dictates
Coherent sets and set-based definition of FTLE

- Consider, e.g., a flow \( \phi^{t+T}_t \) in \( (x_1, x_2) \in \mathbb{R}^2 \).
- Treat the evolution of set \( B \subset \mathbb{R}^2 \) as evolution of two random variables \( X_1 \) and \( X_2 \) defined by probability density function \( f(x_1, x_2) \), initially uniform on \( B \), \( f = \frac{1}{\mu(B)} \chi_B \), with \( \chi_B \) the characteristic function of \( B \).
- Under the action of the flow \( \phi^{t+T}_t \), \( f \) is mapped to \( Pf \) where \( P \) is the associated Perron-Frobenius operator.
- Let \( I(f) \) be the covariance of \( f \) and \( I(Pf) \) the covariance of \( Pf \).

Deformation of a disk under the flow during \([t, t + T]\)
**Definition.** The covariance-based FTLE of $B$ is

$$\sigma_I(B, t, T) = \frac{1}{|T|} \log \left( \frac{\sqrt{\lambda_{\text{max}}(I(P f))}}{\sqrt{\lambda_{\text{max}}(I(f))}} \right).$$

• Reduces to usual definition of FTLE in the limit that the linearization approximation (i.e., line-stretching method) is valid.

Deformation of a disk under the flow during $[t, t + T]$
Coherent sets and set-based definition of FTLE

- The **coherence** of a set $B$ during $[t, t + T]$ is $\sigma_I(B, t, T)$.
- A set $B$ is **almost-coherent** during $[t, t + T]$ if $\sigma_I(B, t, T) \approx 0$.

- Captures the essential feature of a coherent set: it does not mix or spread significantly in the domain.
- This definition also can identify non-mixing **translating** sets.

- **Values of** $\sigma_I(B, t, T)$ **determine the family of sets of various degrees of coherence**.
- Need to set a heuristic threshold on the value of $\sigma_I(B, t, T)$ to determine coherent sets.

- Notice, coherent sets will be separated by ridges of high FTLE, i.e., LCS
Coherent sets in lid-driven cavity flow

FTLE from line-stretching (conventional) during $[0, \tau_f]$
Coherent sets in lid-driven cavity flow

FTLE from covariance-based approach during $[0, \tau_f]$
Sets of coherences $\sigma_I(0, \tau_f) < 1.6$
Coherent sets in lid-driven cavity flow

Compare with AIS from second eigenvector of $P$
Coherent sets in the atmosphere

- FTLE from covariance during 24 hours starting 09:00 1 May 2007
Coherent sets in the atmosphere

- Coherent sets during 24 hours starting 09:00 1 May 2007
Final words on chaotic transport

What are robust descriptions of transport which work in data-driven aperiodic, finite-time settings?

- Possibilities: finite-time lobe dynamics / symbolic dynamics may work — finite-time analogs of homoclinic and heteroclinic tangles

- Probabilistic, geometric, and topological methods — invariant sets, almost-invariant sets, almost-cyclic sets, coherent sets, stable and unstable manifolds, Thurston-Nielsen classification, FTLE, LCS

- Many links between these notions — e.g., LCS locate analogs of stable and unstable manifolds — boundaries between coherent sets are naturally LCS — periodic points $\Rightarrow$ almost-cyclic sets — their ‘stable/unstable invariant manifolds’ $\Rightarrow$ ???
Main Papers: