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

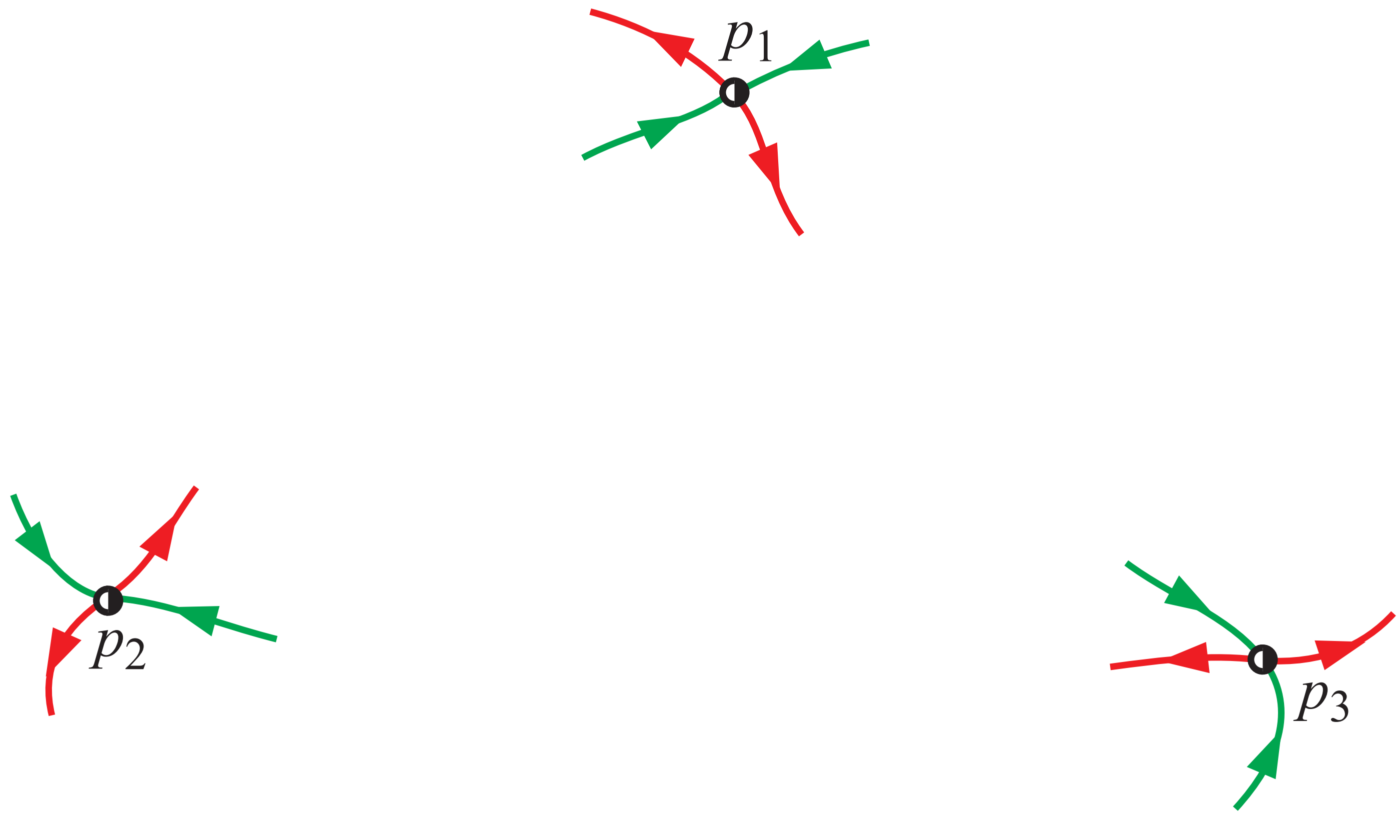
- To understand the transport of points under the map f, we consider the **invariant manifolds of unstable fixed points**

- Let $p_i, i = 1, ..., N_p$, denote a collection of saddle-type hyperbolic fixed points for f.

[1]Following Rom-Kedar and Wiggins [1990]

Partition phase space into regions

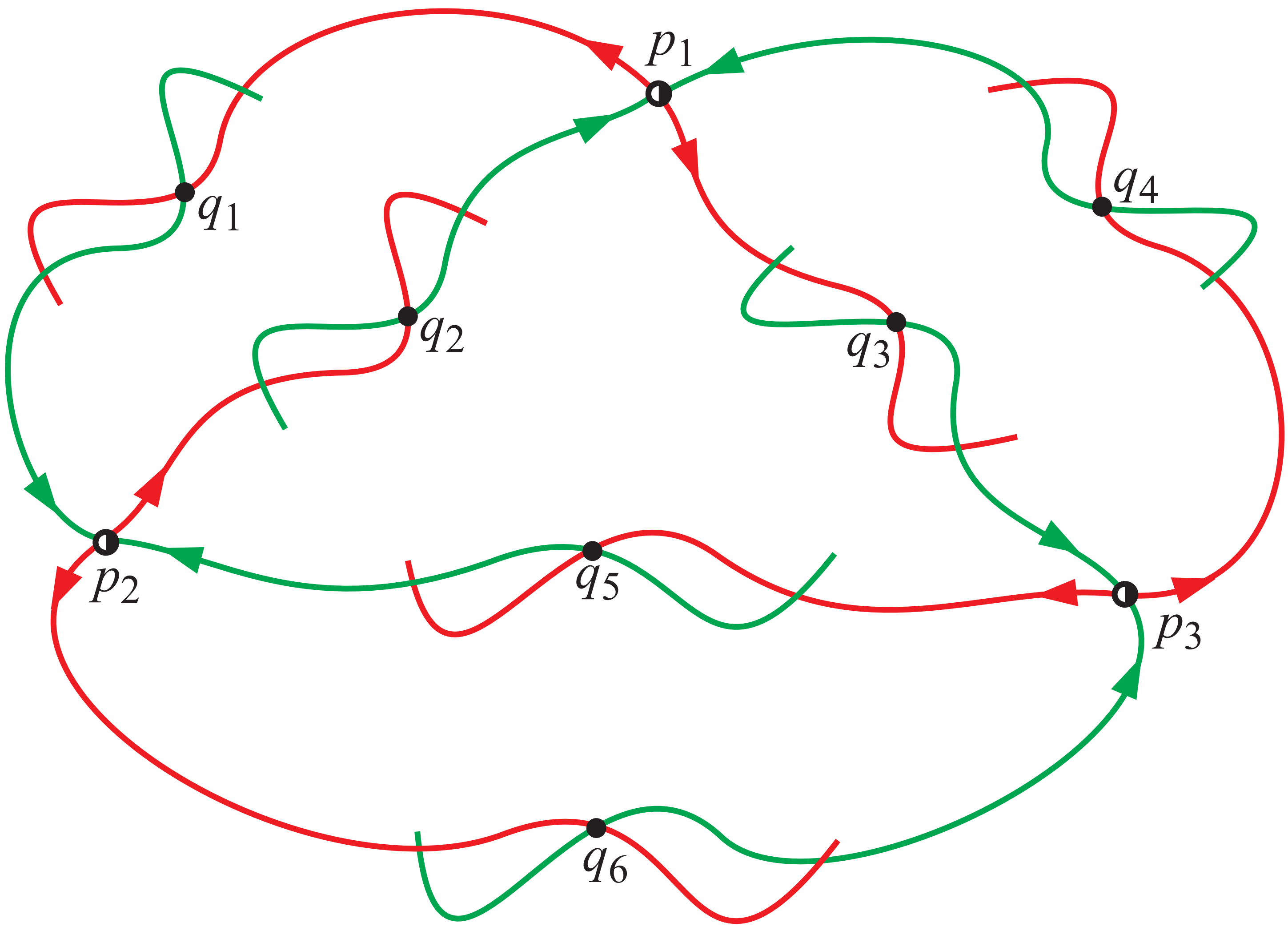
- Natural way to partition phase space
  - Pieces of $W^u(p_i)$ and $W^s(p_i)$ partition $\mathcal{M}$.



Unstable and stable manifolds in **red** and **green**, resp.

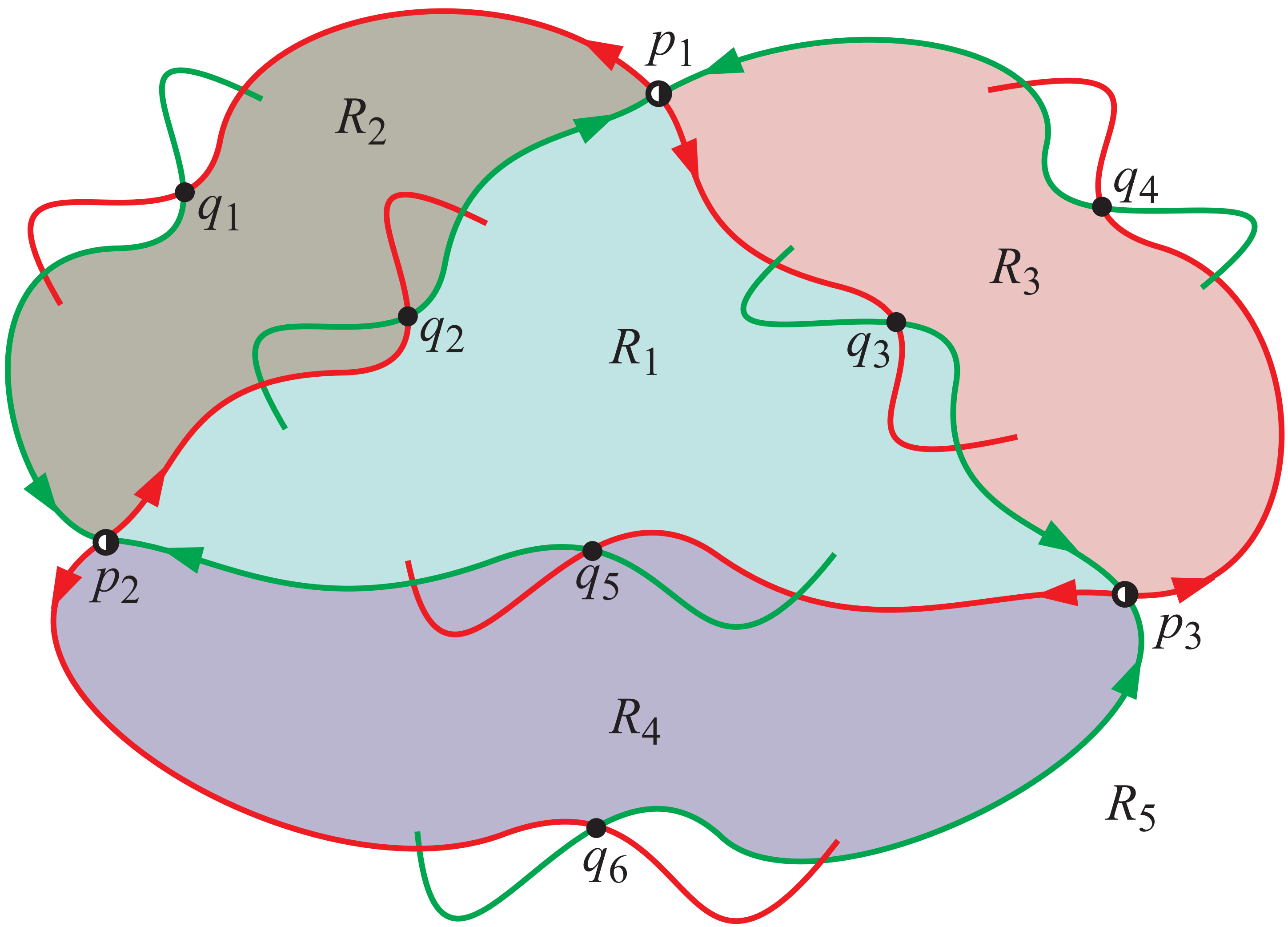
Partition phase space into regions

- Intersection of unstable and stable manifolds define **boundaries**.



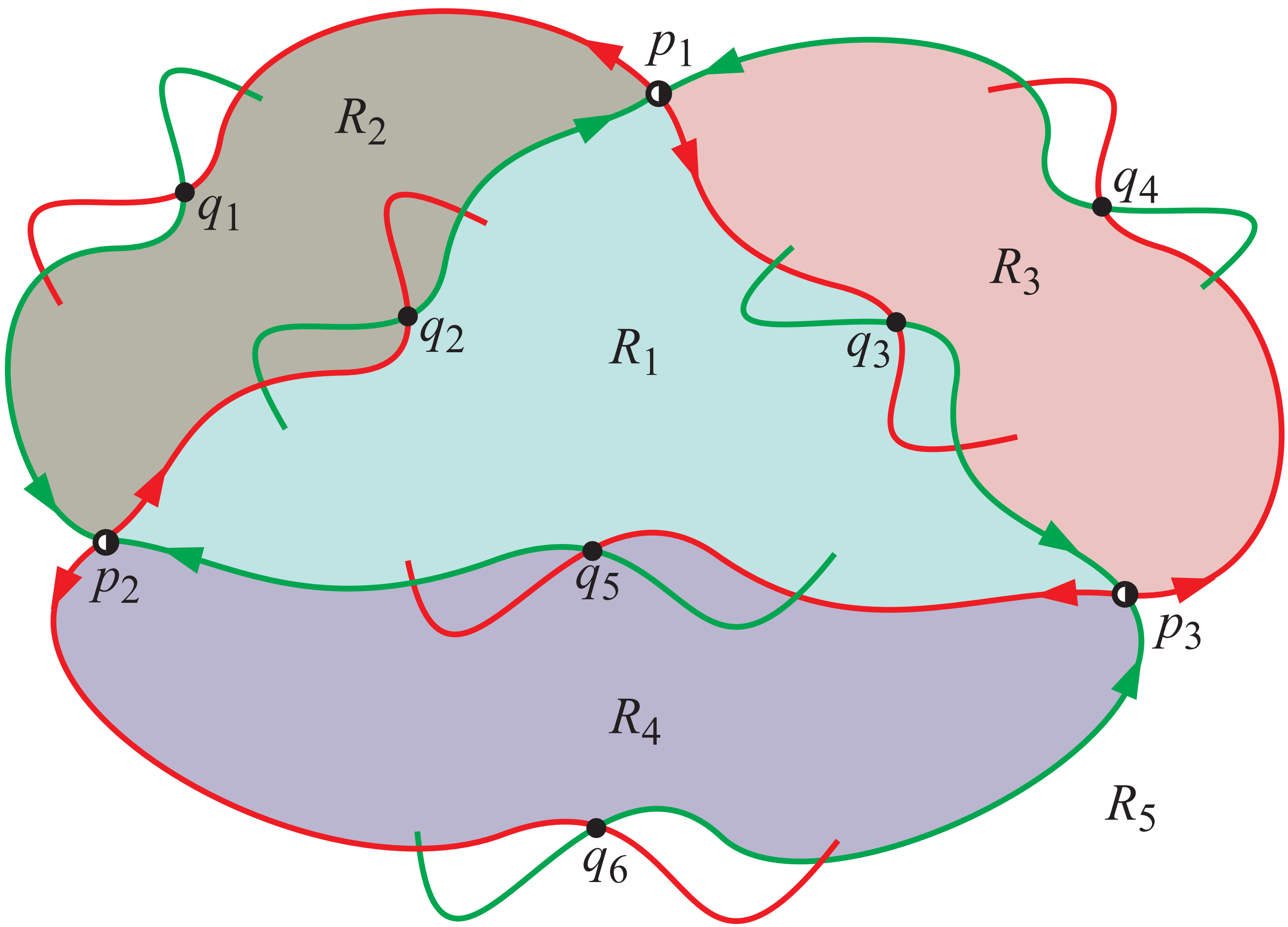
Partition phase space into regions

- These boundaries divide the phase space into **regions**.



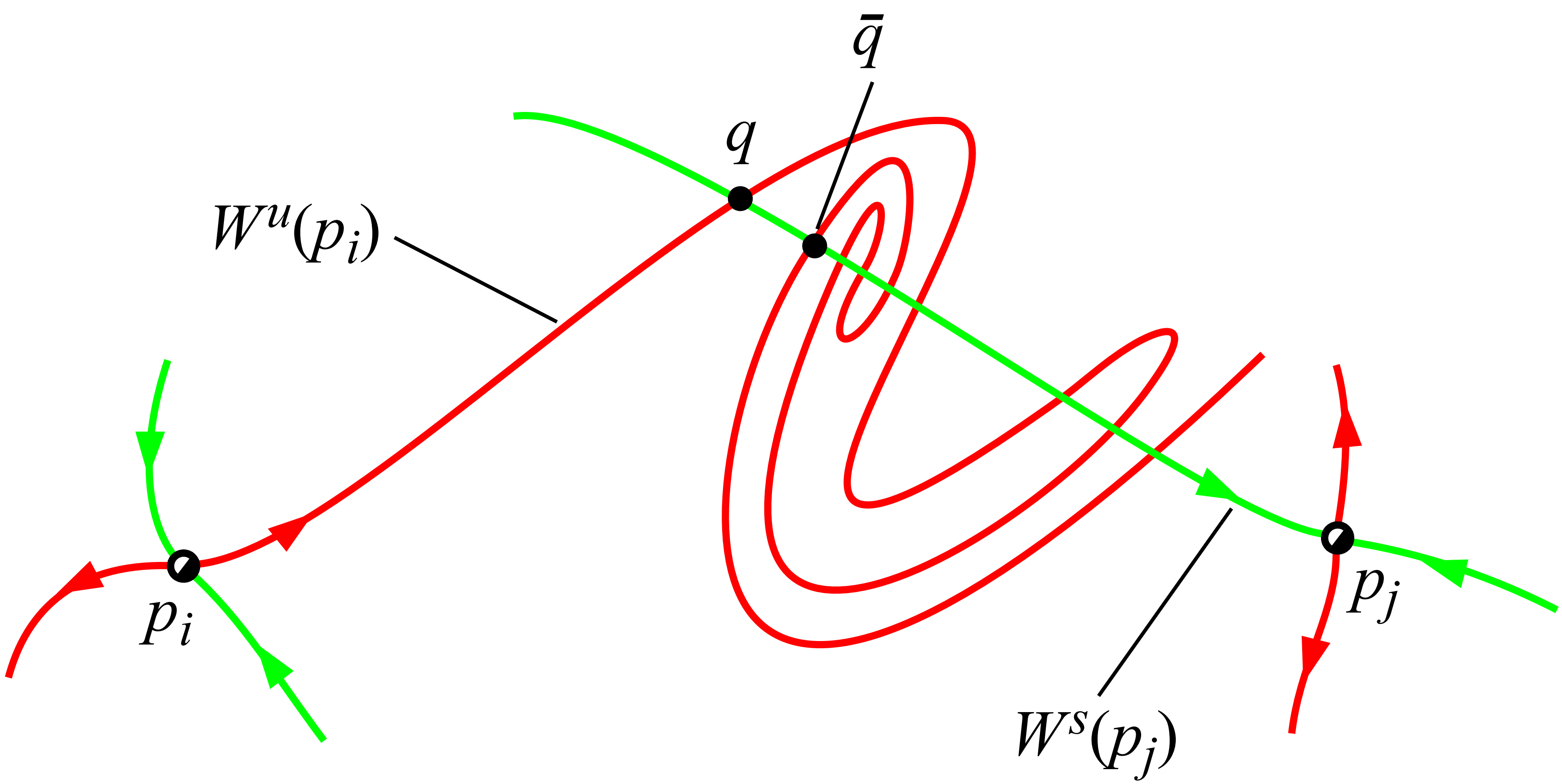
Label mobile subregions: 'atoms' of transport

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



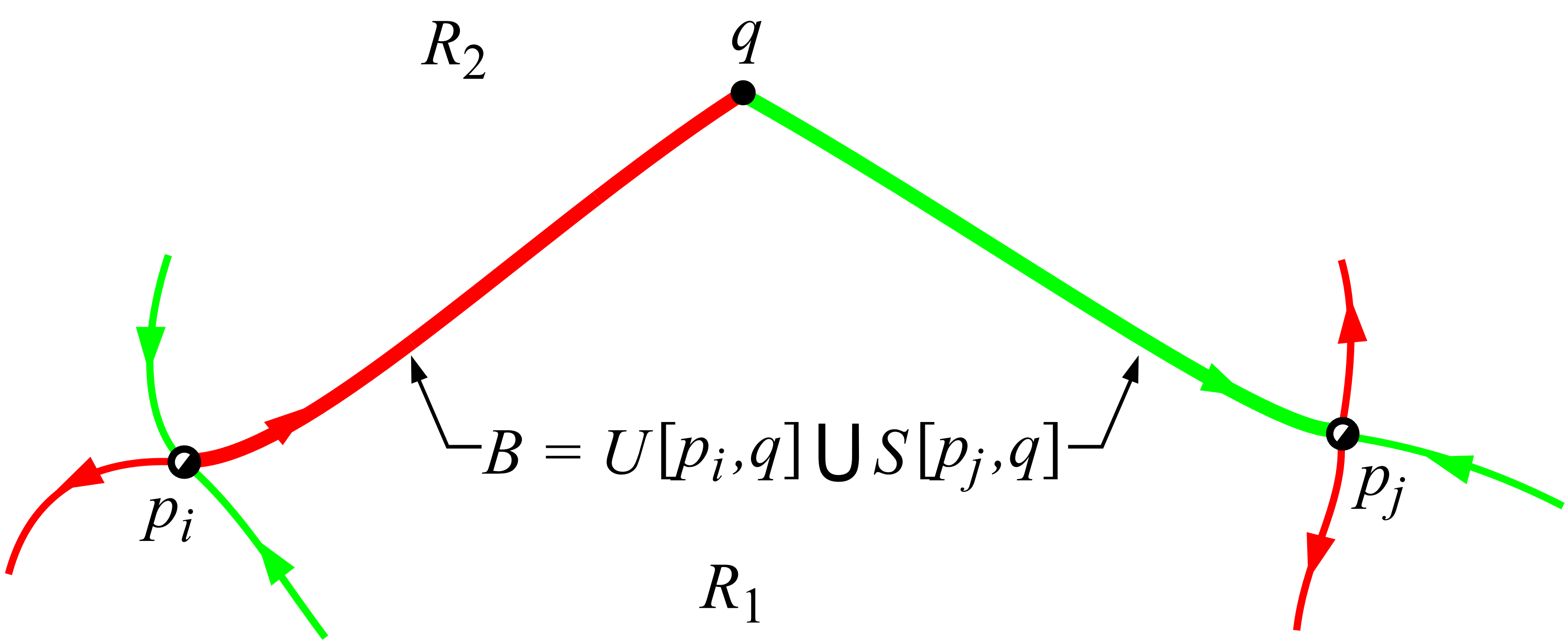
Primary intersection points (pips) and boundaries

- q is a primary intersection point (pip), $\bar{q}$ is not a pip.



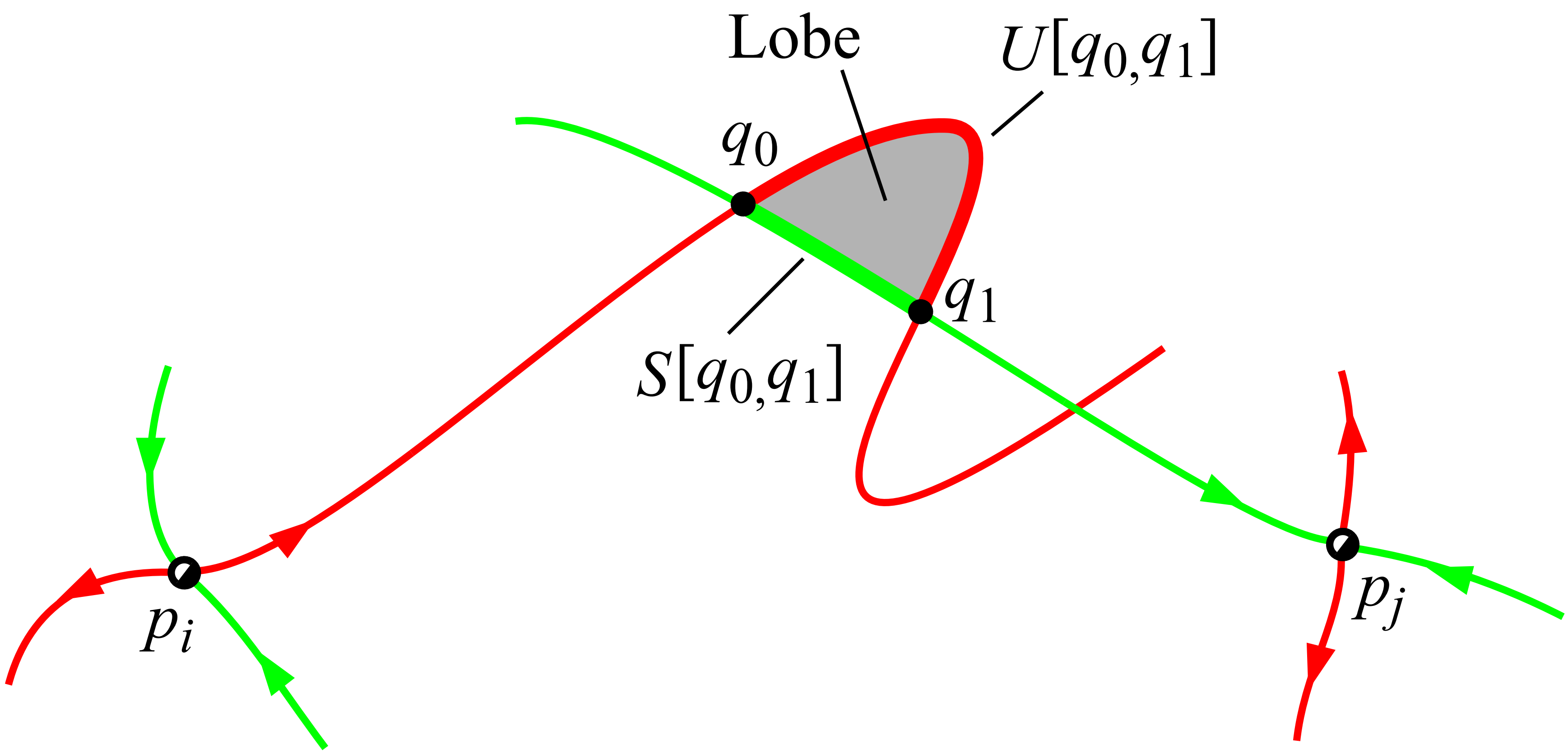
Primary intersection points (pips) and boundaries

- Suppose $W^u(p_i)$ and $W^s(p_j)$ intersect in the pip q. Define $B \equiv U[p_i, q] \bigcup S[p_j, q]$ as a **boundary** between "two sides," R_1 and R_2.



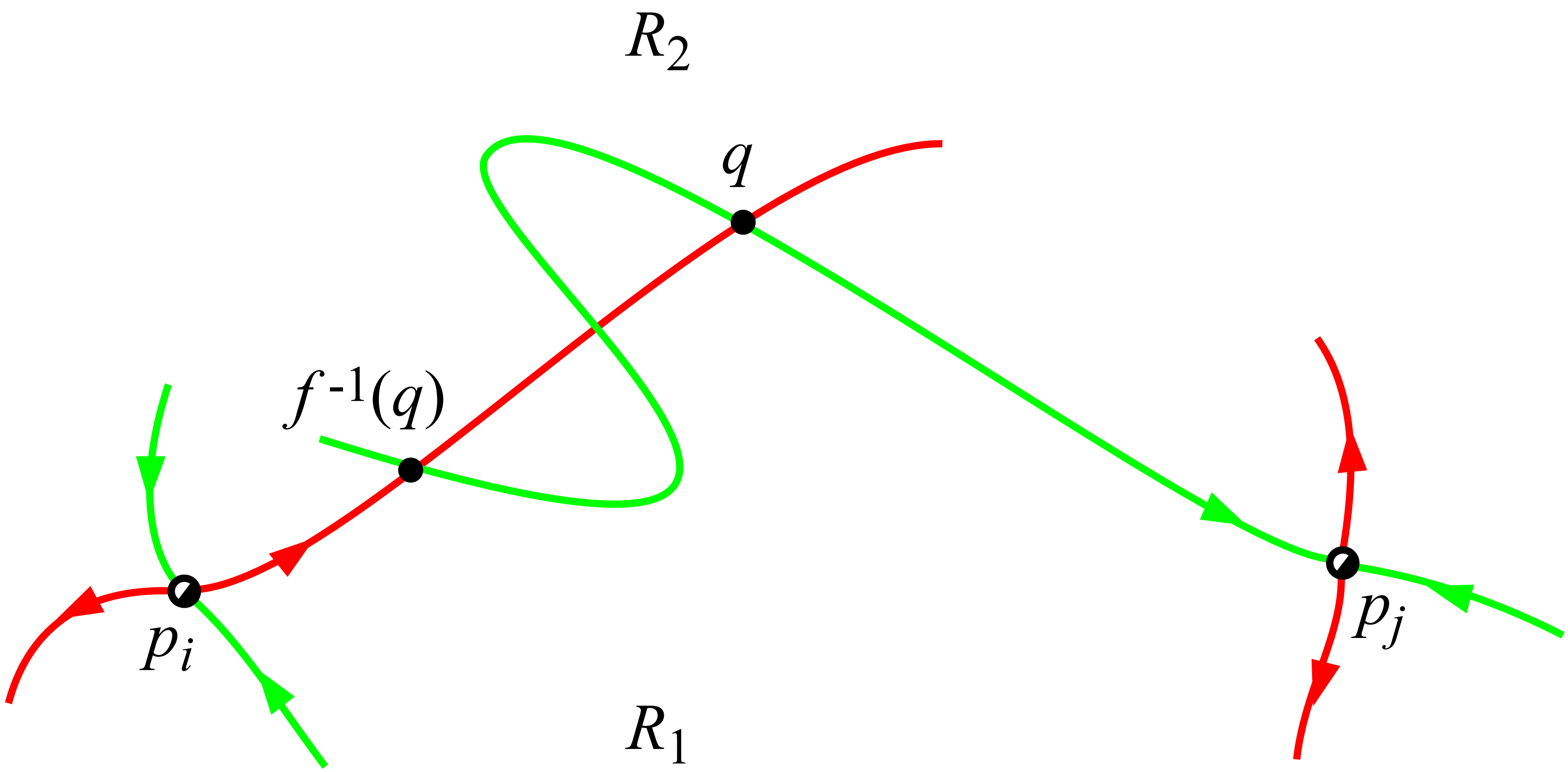
Lobes: the mobile subregions

- Let $q_0, q_1 \in W^u(p_i) \bigcap W^s(p_j)$ 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 $U[q_0, q_1] \bigcup S[q_0, q_1]$ is a **lobe**.



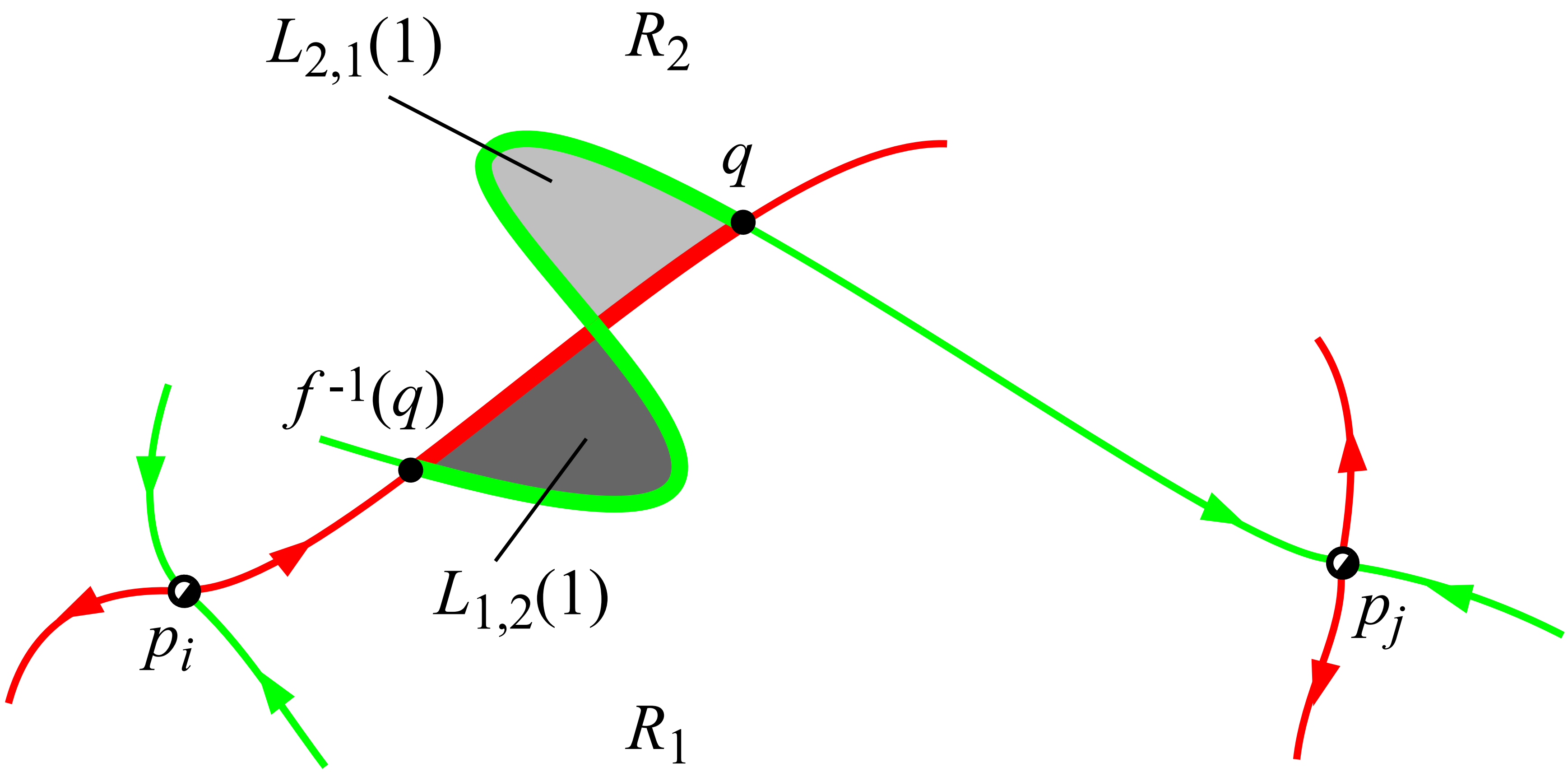
Lobe dynamics: transport across a boundary B

- $f^{-1}(q)$ 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.



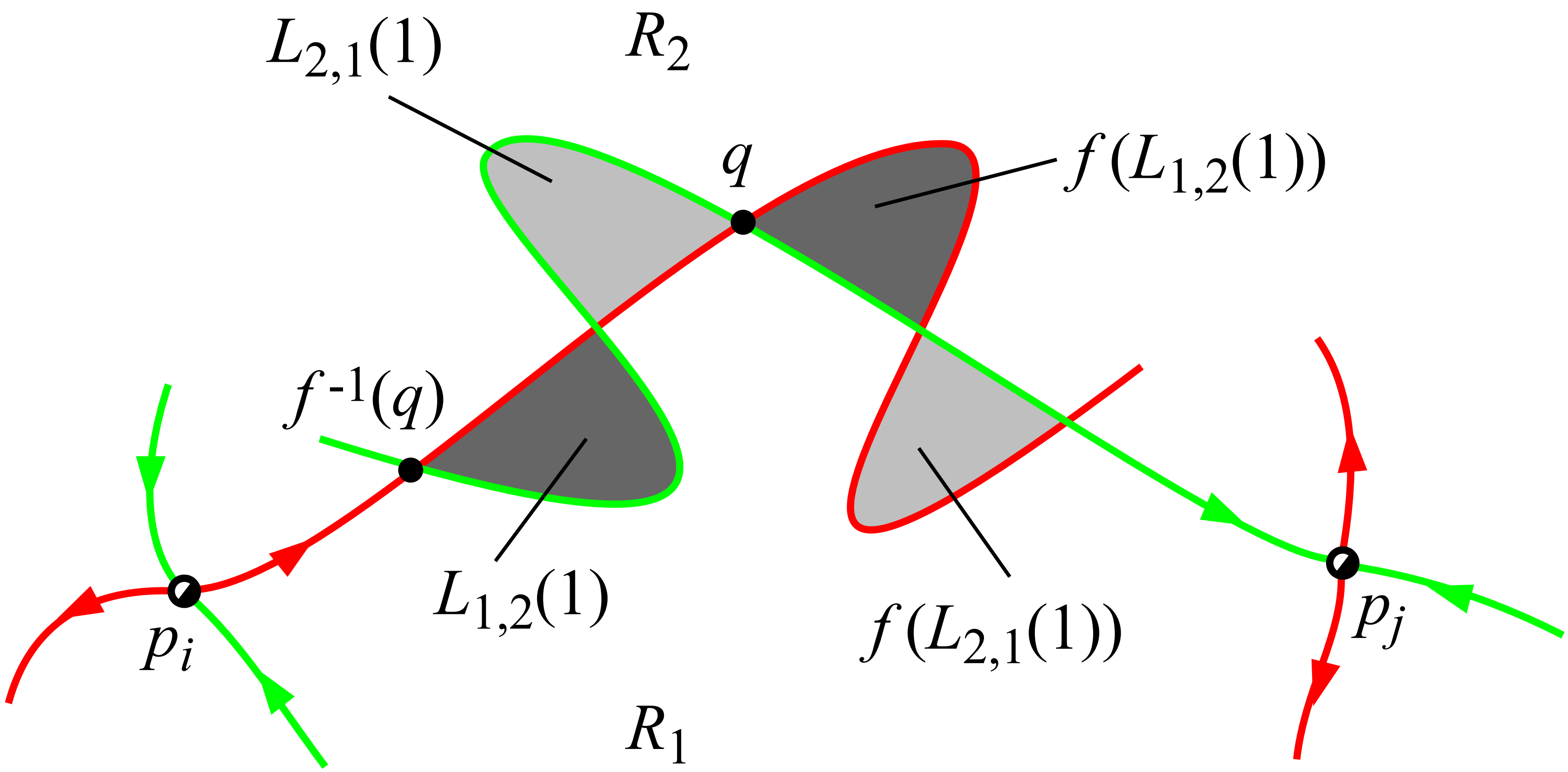
Lobe dynamics: transport across a boundary B

- $U[f^{-1}(q), q] \bigcup S[f^{-1}(q), q]$ 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 $L_{2,1}(1)$



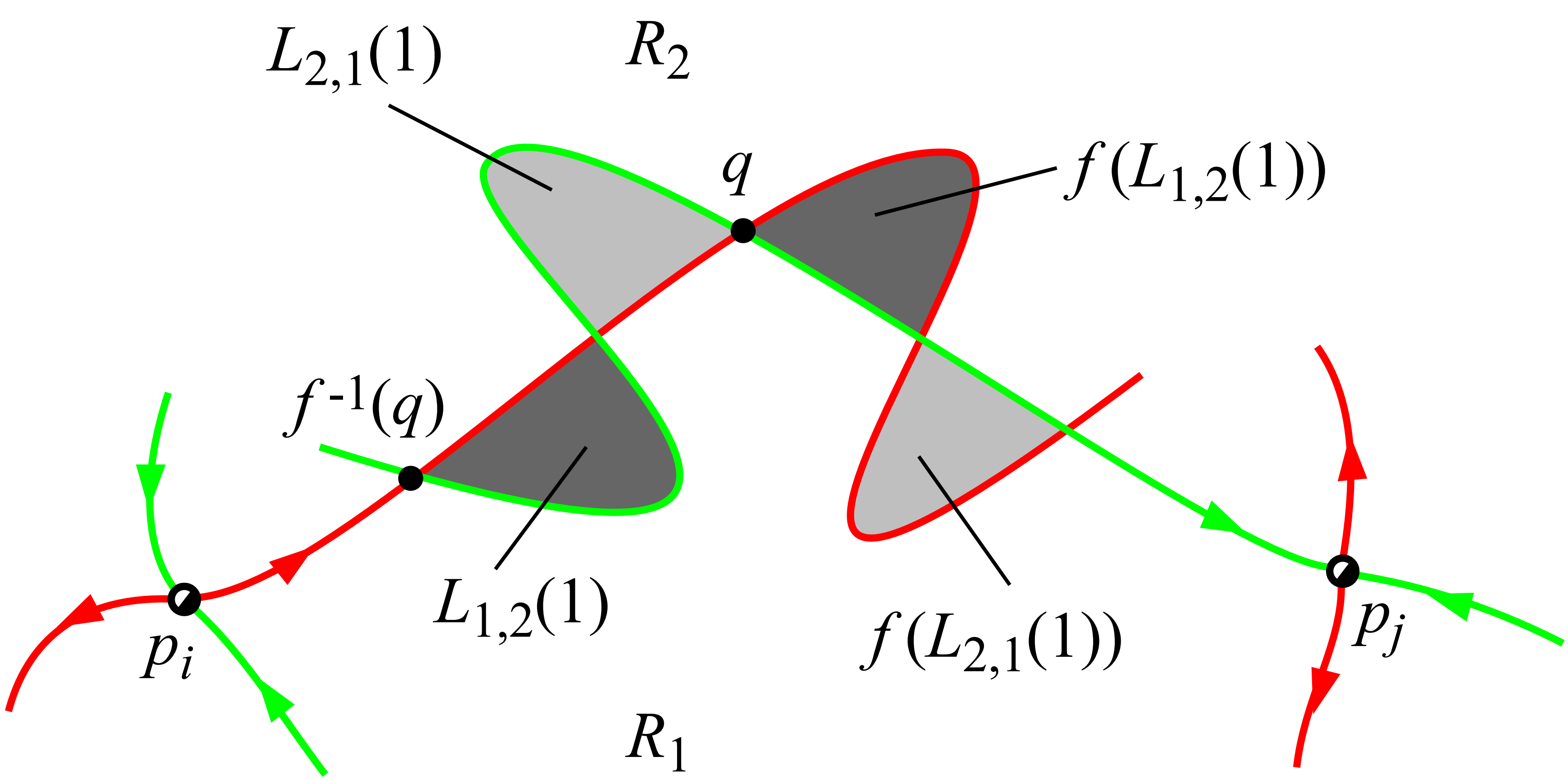
Lobe dynamics: transport across a boundary B

- 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**.



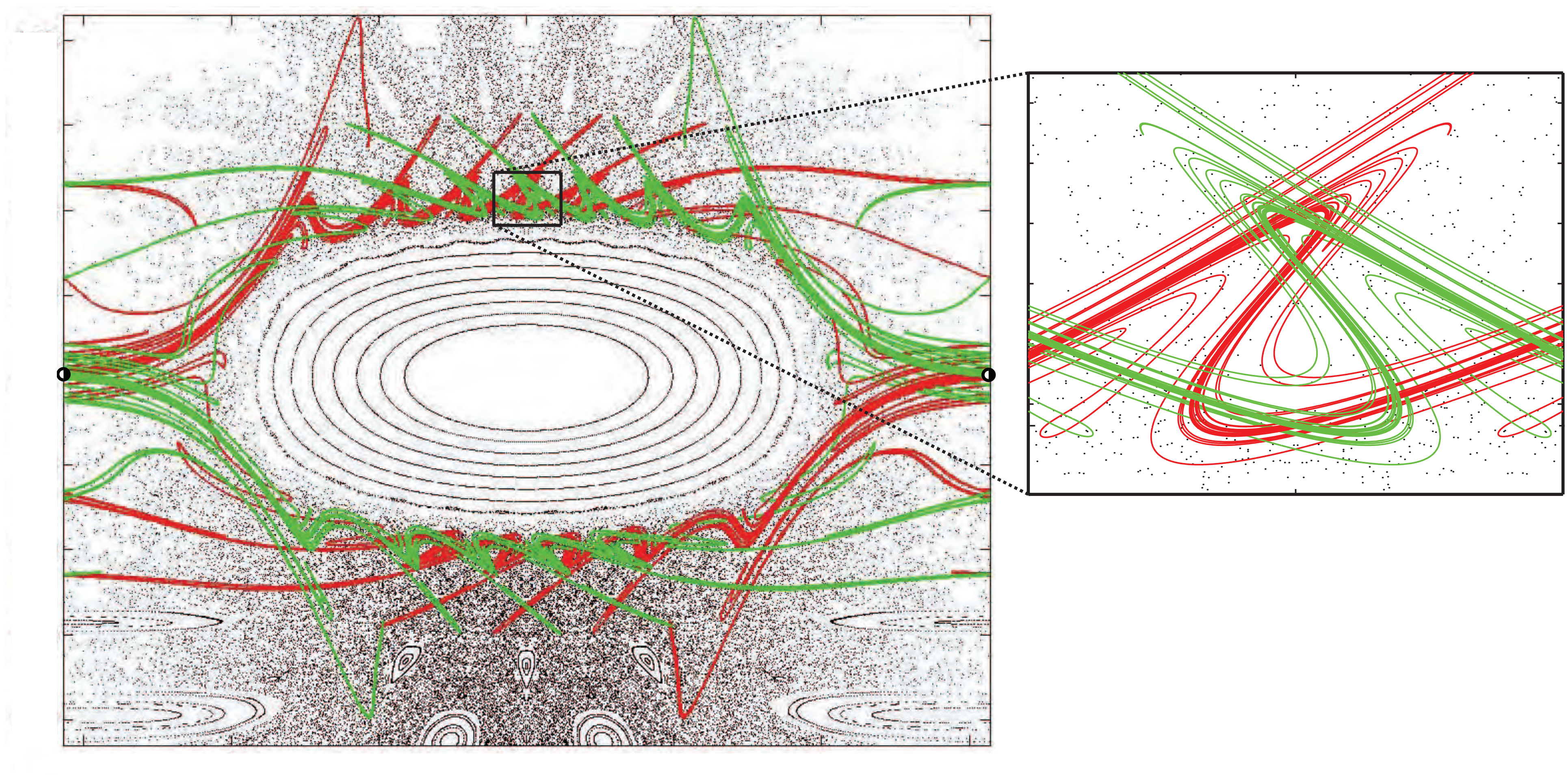
Lobe dynamics: transport across a boundary B

- 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

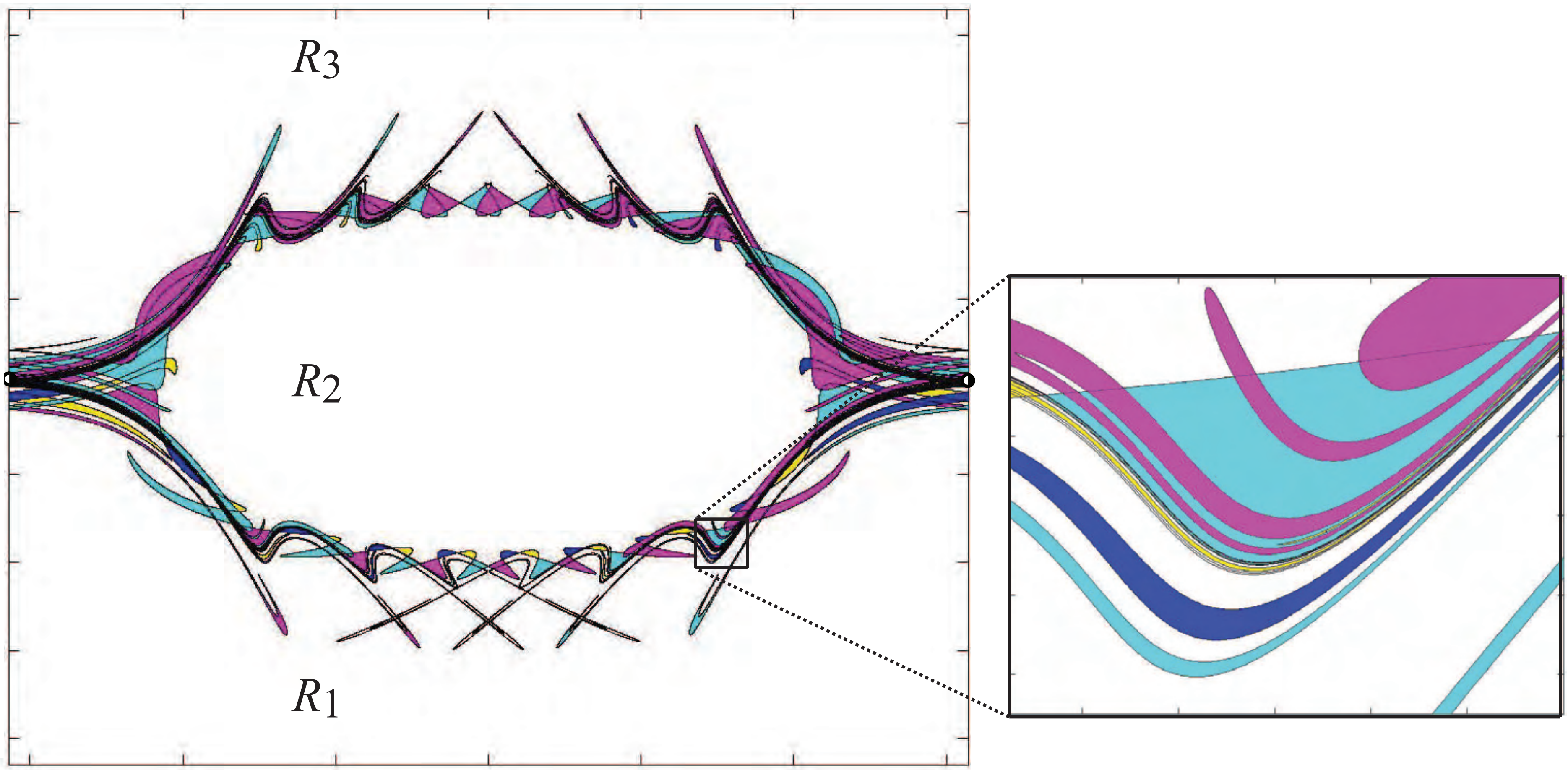
- In a complicated system, can still identify manifolds ...



Unstable and stable manifolds in **red** and **green**, resp.

Identifying atoms of transport by itinerary

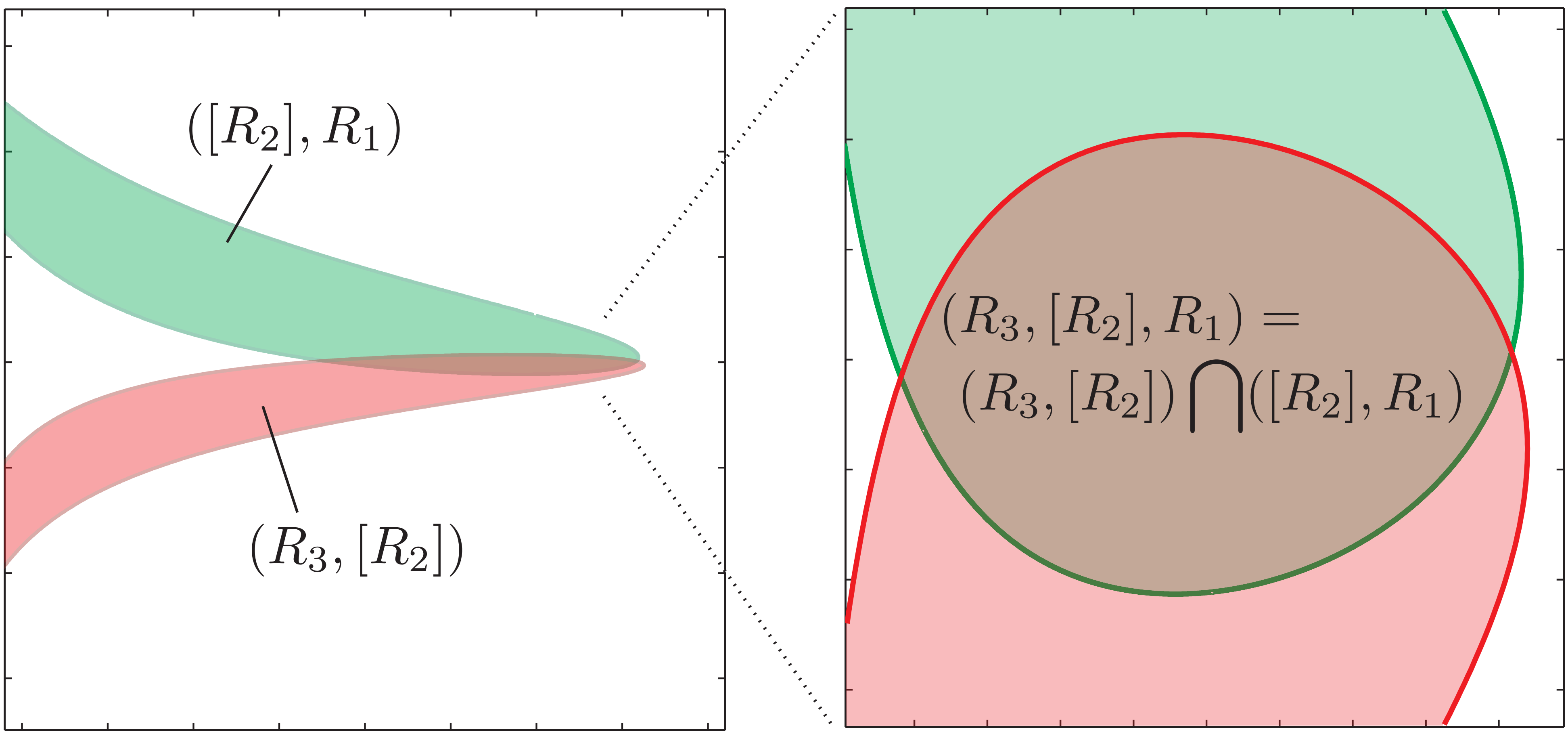
- ... and lobes



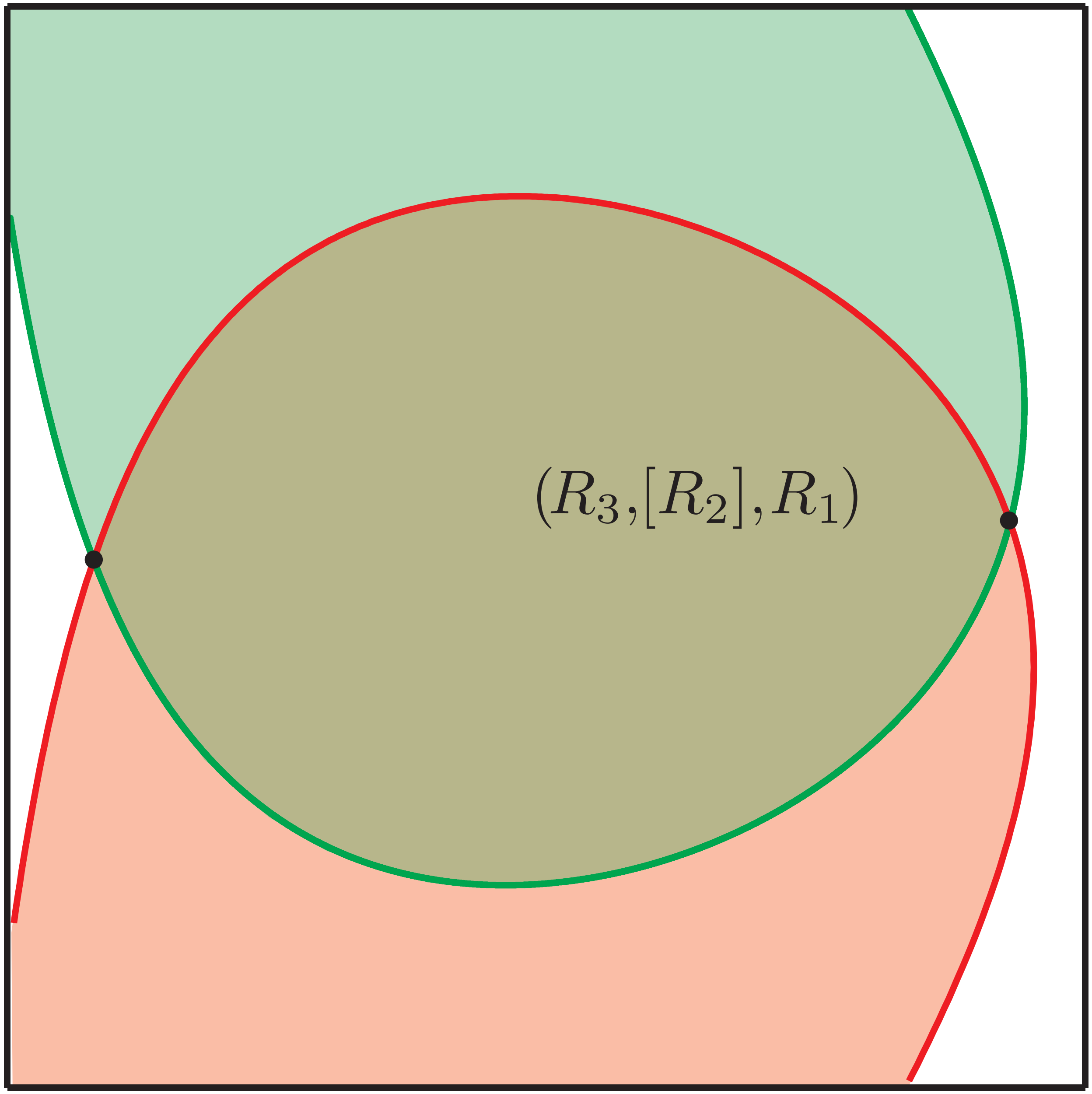
Significant amount of fine, filamentary structure.

Identifying atoms of transport by itinerary

- e.g., with three regions $\{R_1, R_2, R_3\}$, label lobe intersections accordingly.
  - Denote the intersection $(R_3, [R_2]) \bigcap ([R_2], R_1)$ by $(R_3, [R_2], R_1)$

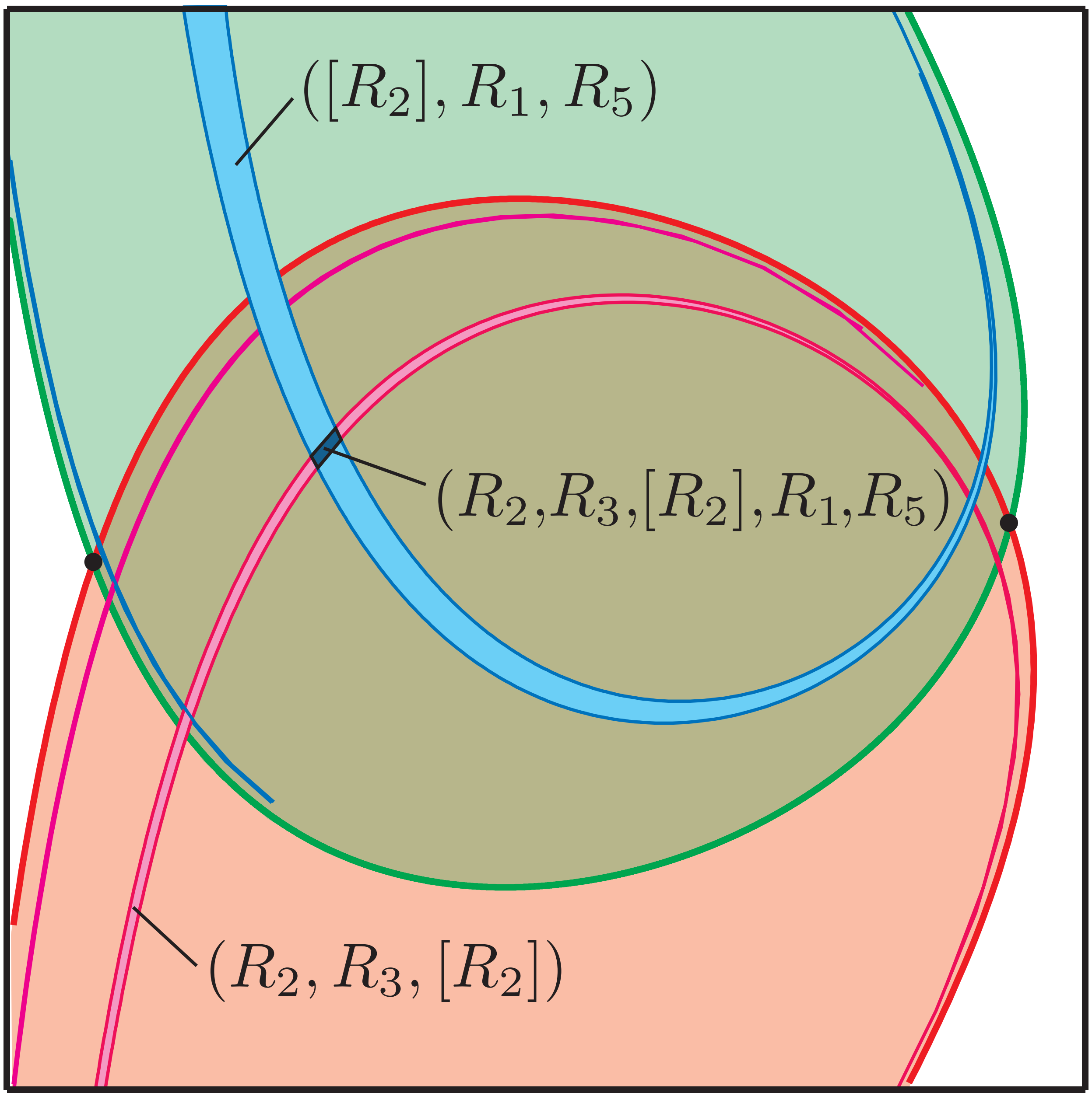


Identifying atoms of transport by itinerary



Longer itineraries...

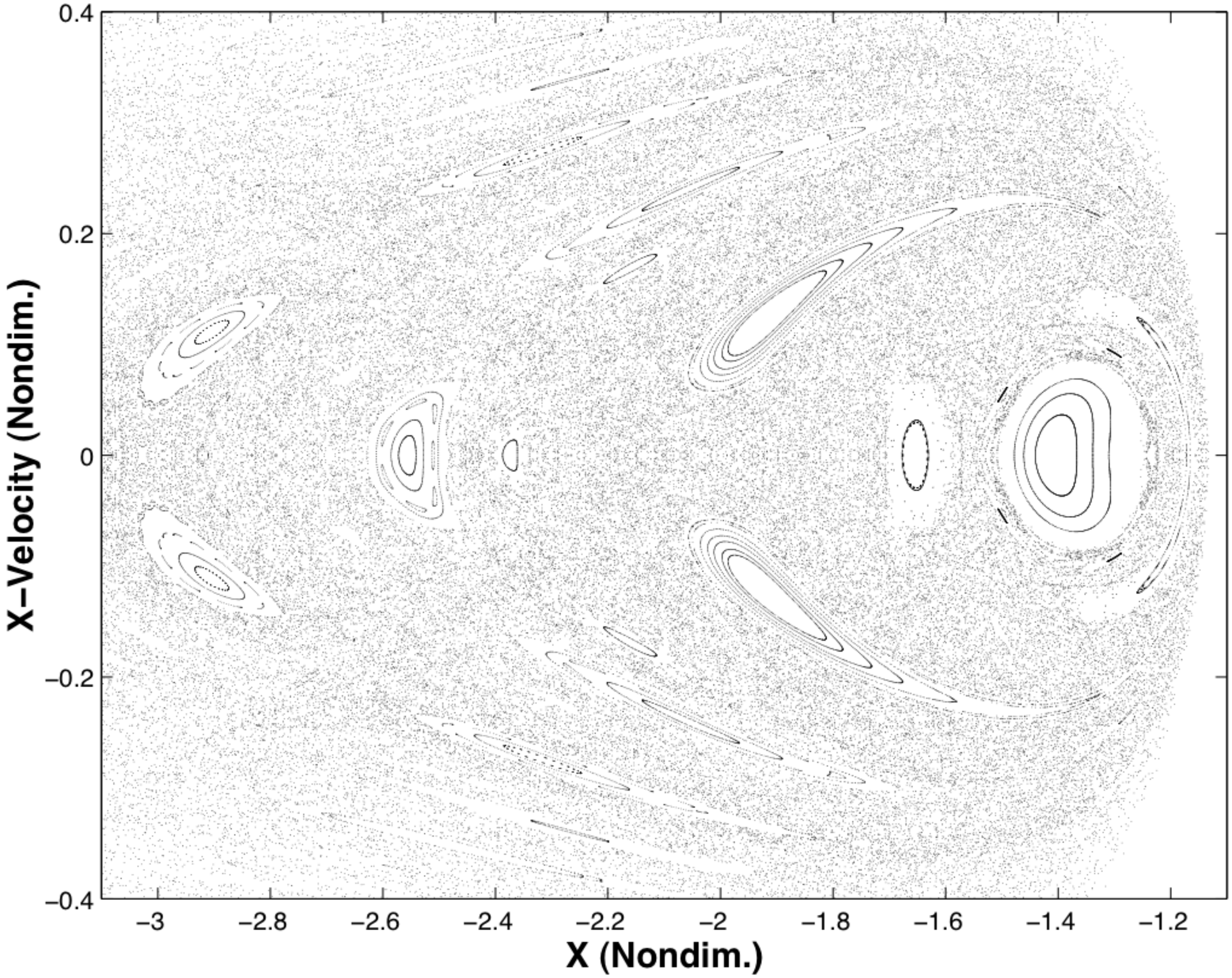
Identifying atoms of transport by itinerary



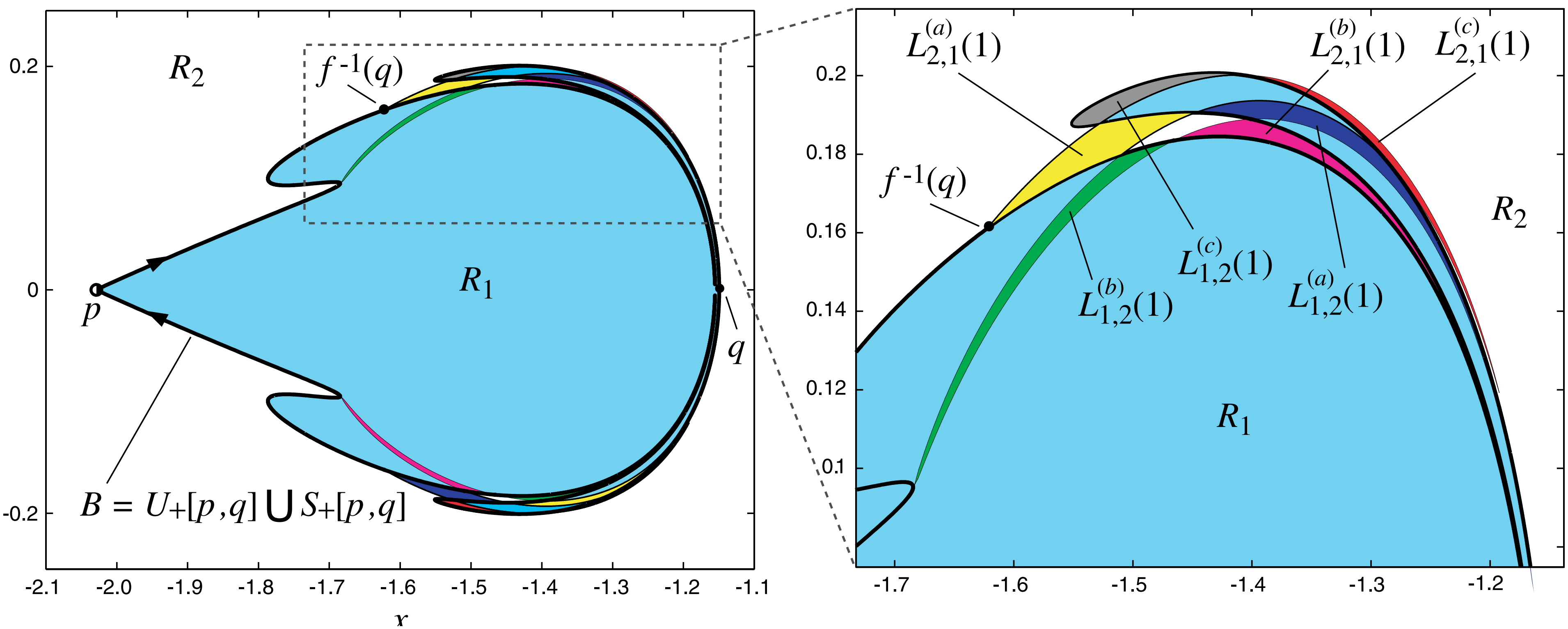
... correspond to smaller pieces of phase space; horseshoe dynamics, etc

Lobe Dynamics: example

- rest. 3-body problem: chaotic sea contains unstable fixed points.



Compute a boundary

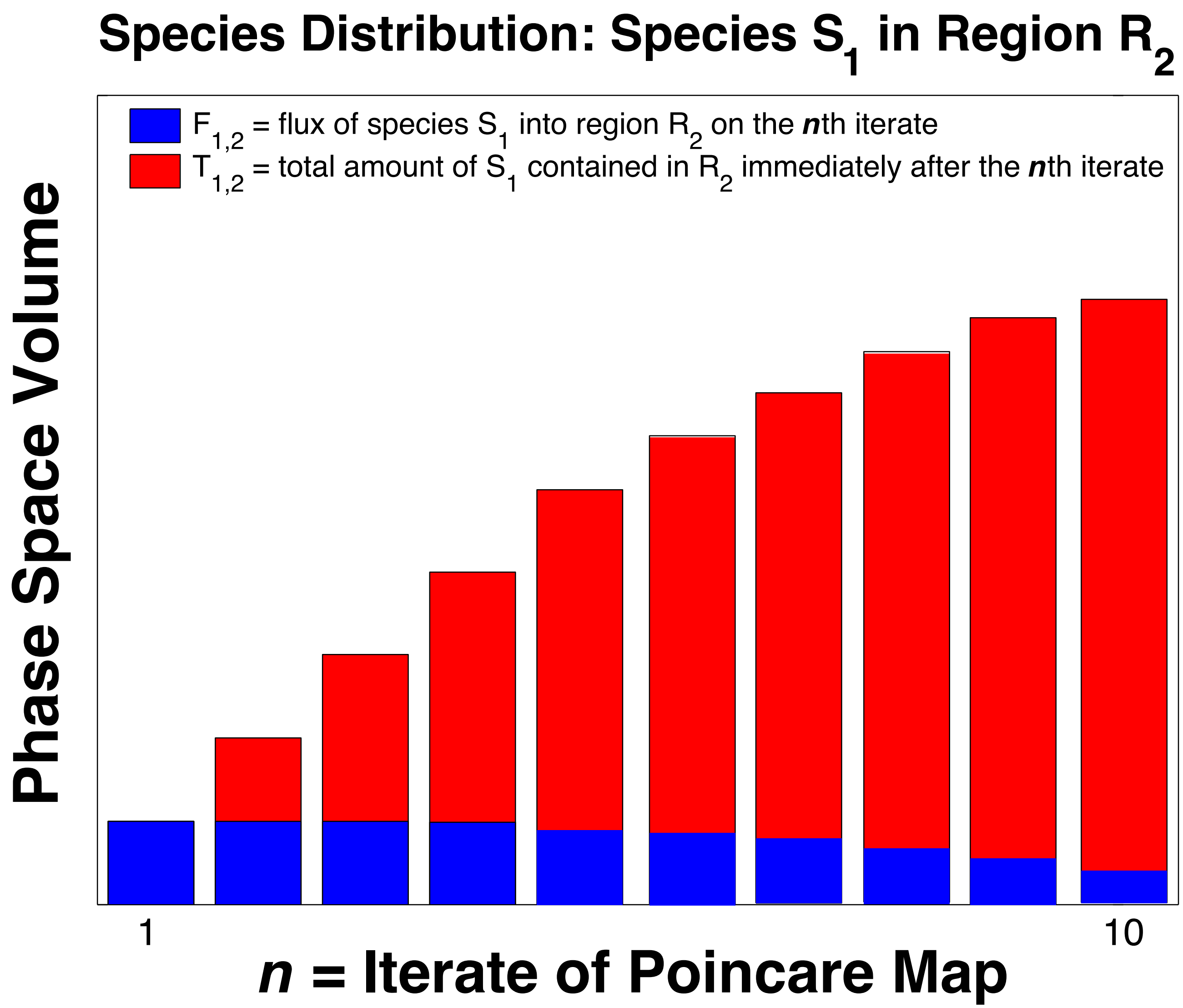


Transport btwn Two Regions

- The evolution of a lobe of species S_1 into R_2

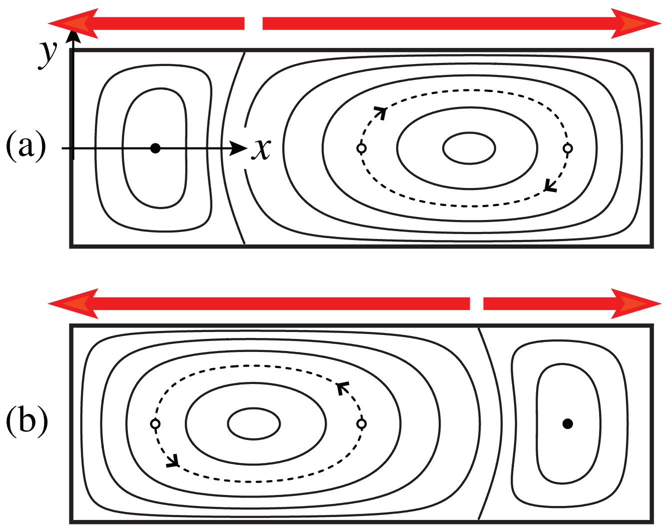
Dellnitz, Junge, Lo, Marsden, Padberg, Preis, Ross, Thiere [2005] Physical Review Letters

Transport btwn Two Regions



Lobe dynamics: fluid example

- Fluid example: time-periodic Stokes flow



streamlines

tracer blob

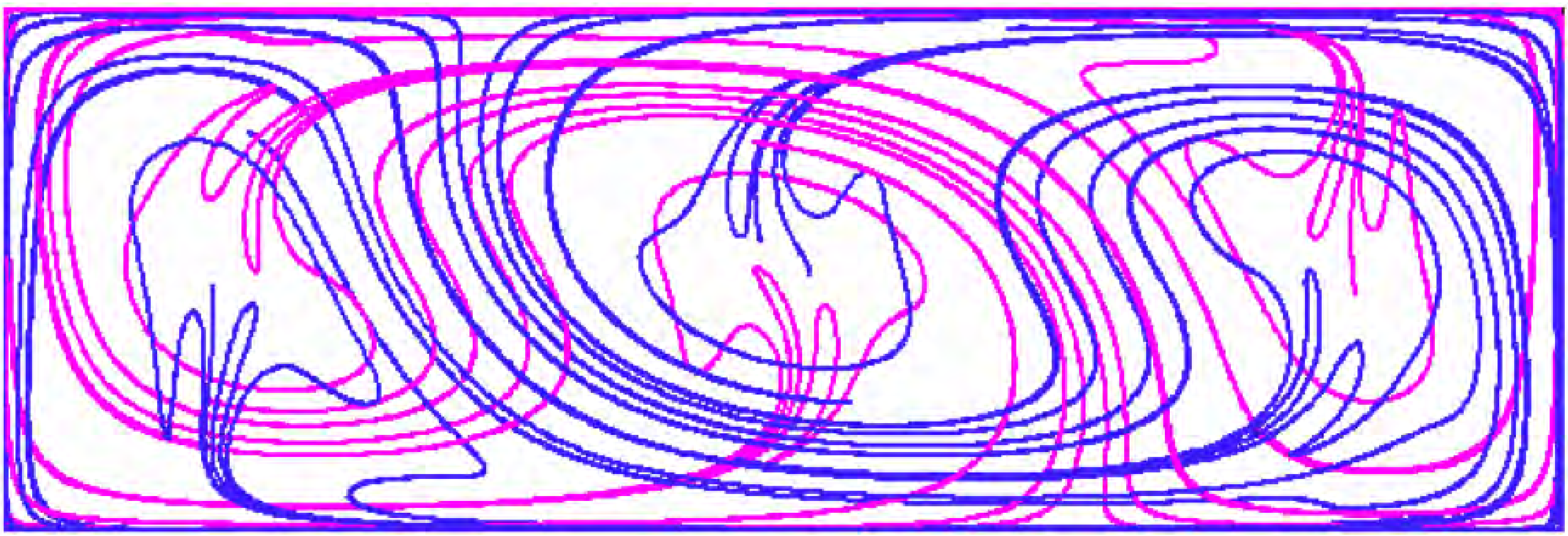
Lid-driven cavity flow

- Model for microfluidic mixer
- System has parameter τ_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 Gheisarieha and Mark Stremler (Virginia Tech)

Lobe dynamics: fluid example

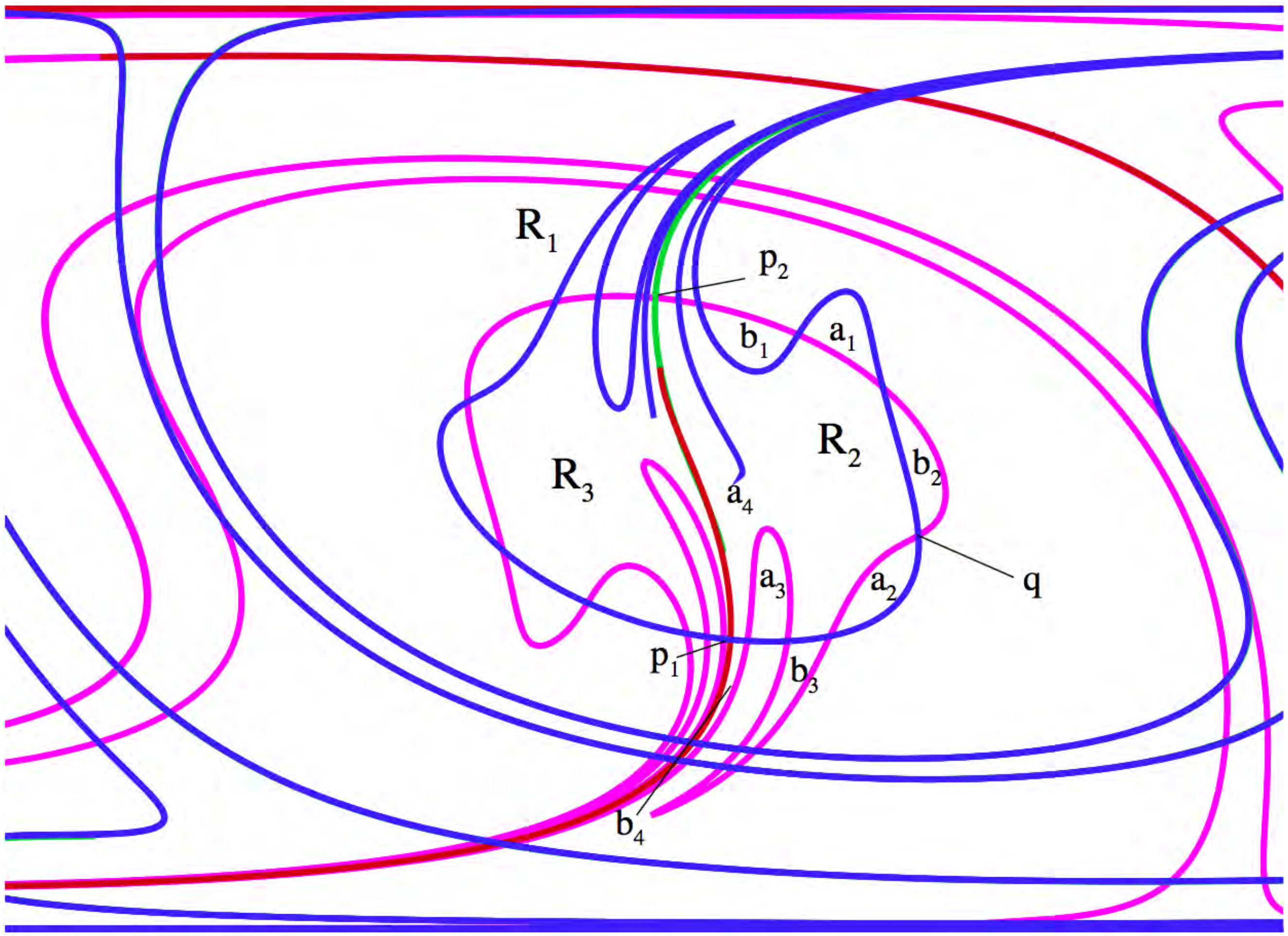
- Fluid example: Poincaré map



some invariant manifolds of saddles

Lobe dynamics: fluid example

- Fluid example: Poincaré map



regions and lobes labeled

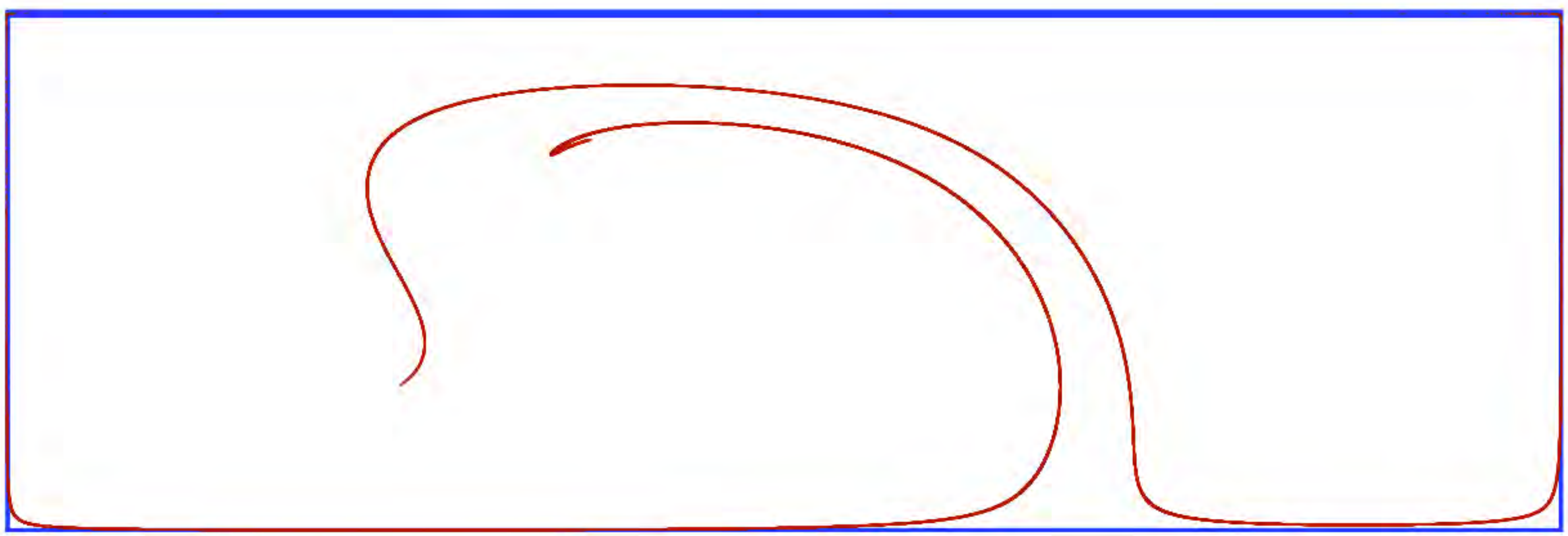
Stable/unstable manifolds and lobes in fluids

- Fluid example: Poincaré map

material blob at $t = 0$

Stable/unstable manifolds and lobes in fluids

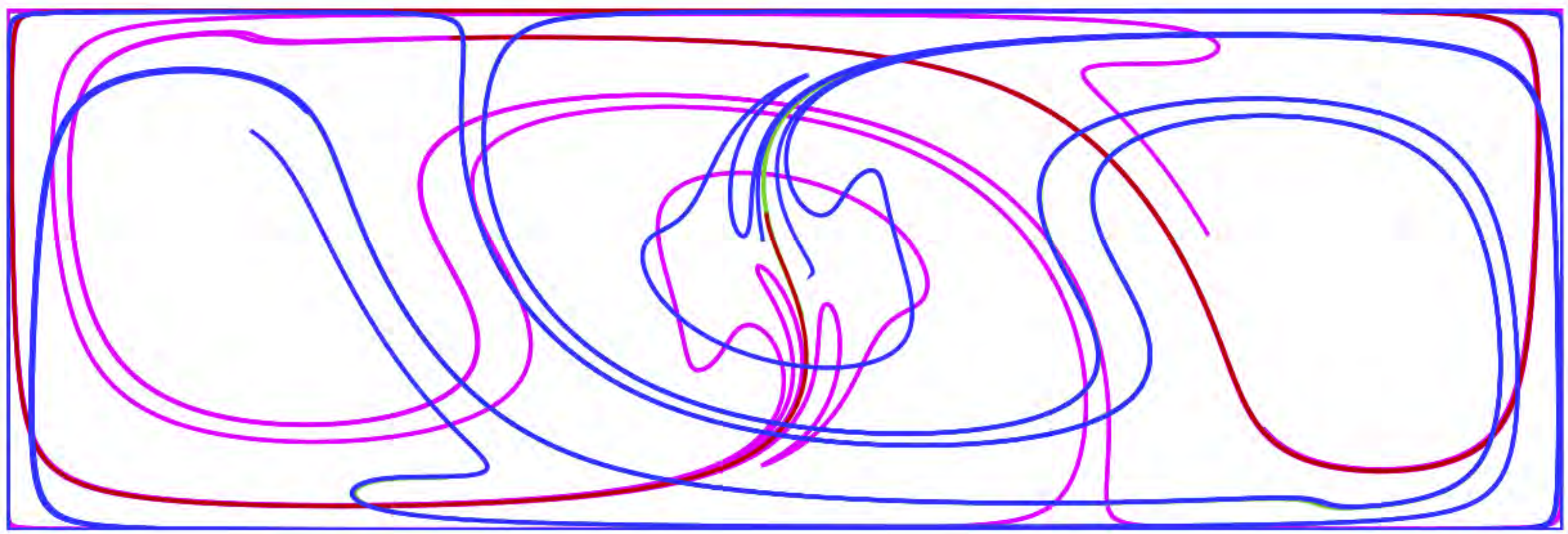
- Fluid example: Poincaré map



material blob at $t = 5$

Stable/unstable manifolds and lobes in fluids

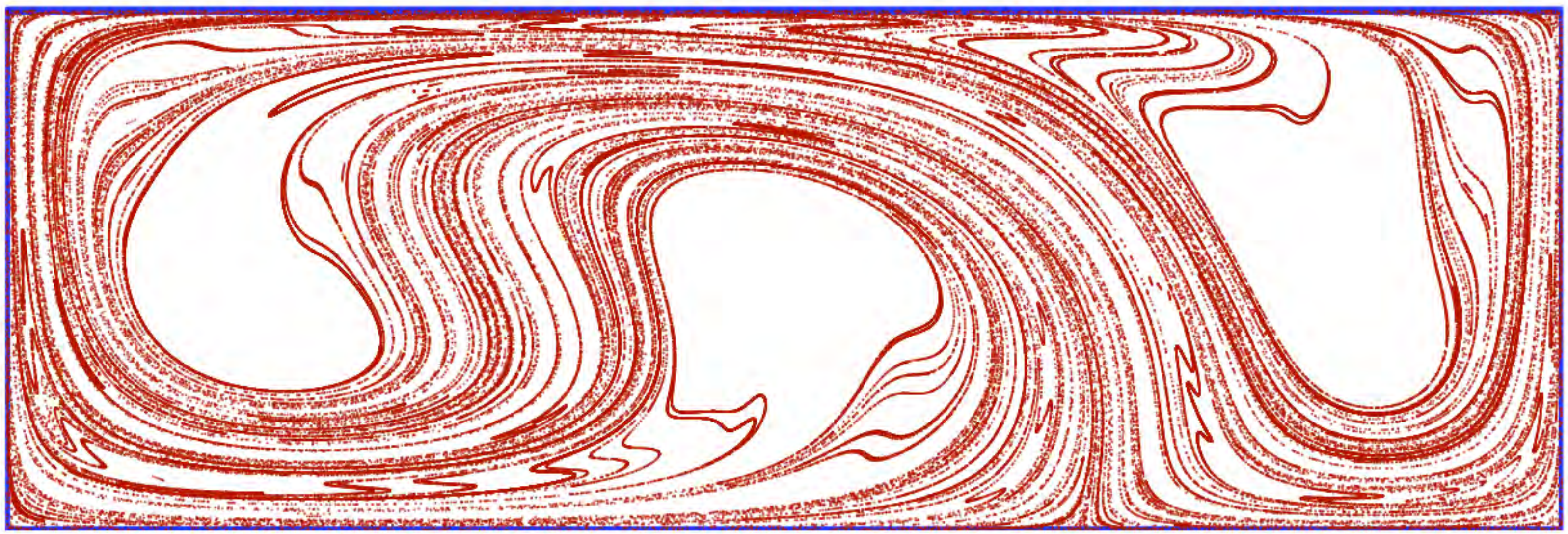
- Fluid example: Poincaré map



some invariant manifolds of saddles

Stable/unstable manifolds and lobes in fluids

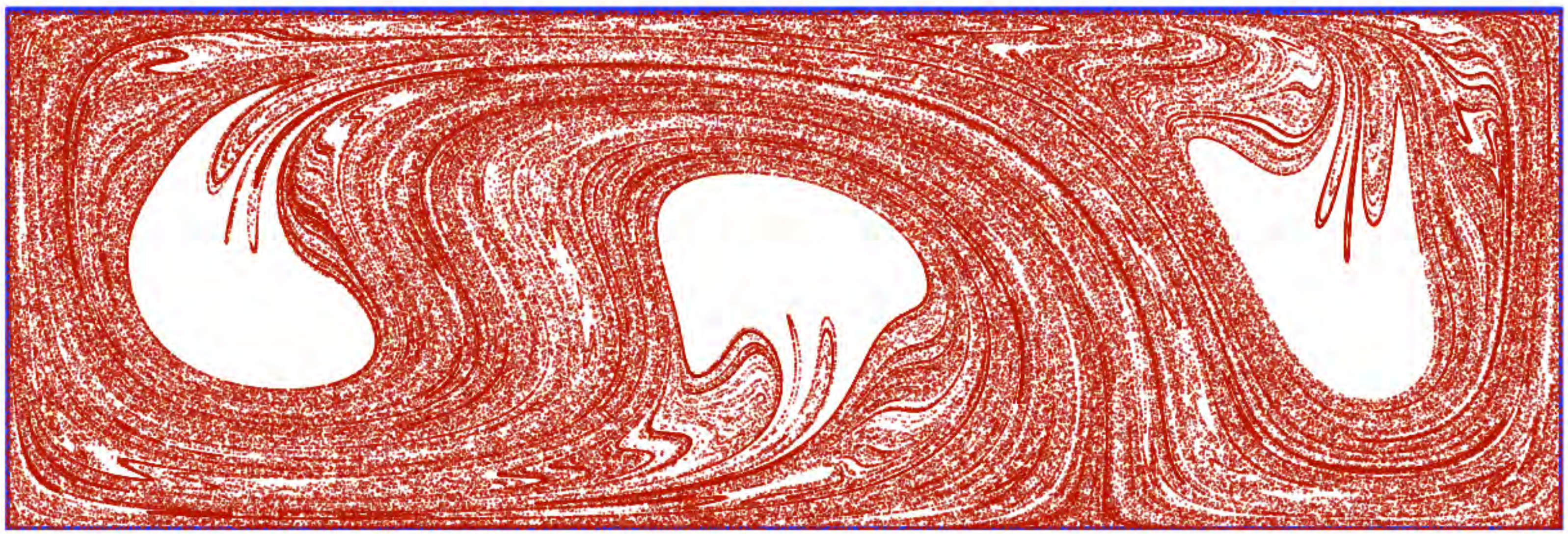
- Fluid example: Poincaré map



material blob at $t = 10$

Stable/unstable manifolds and lobes in fluids

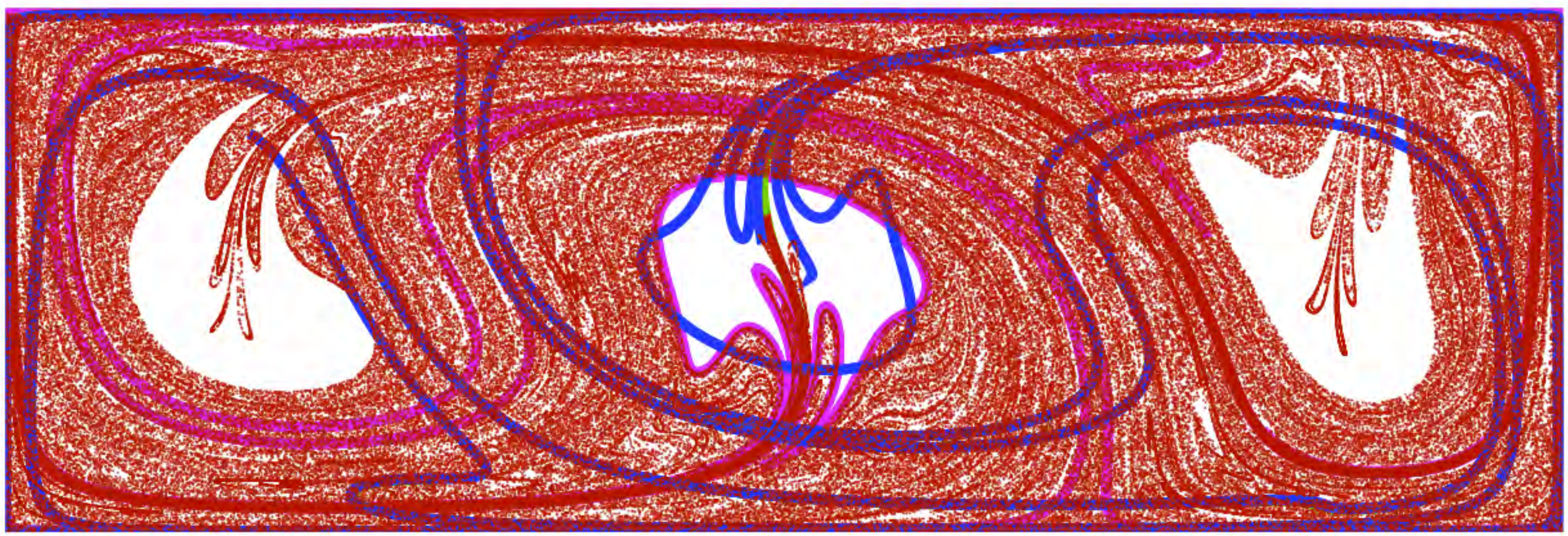
- Fluid example: Poincaré map



material blob at $t = 15$

Stable/unstable manifolds and lobes in fluids

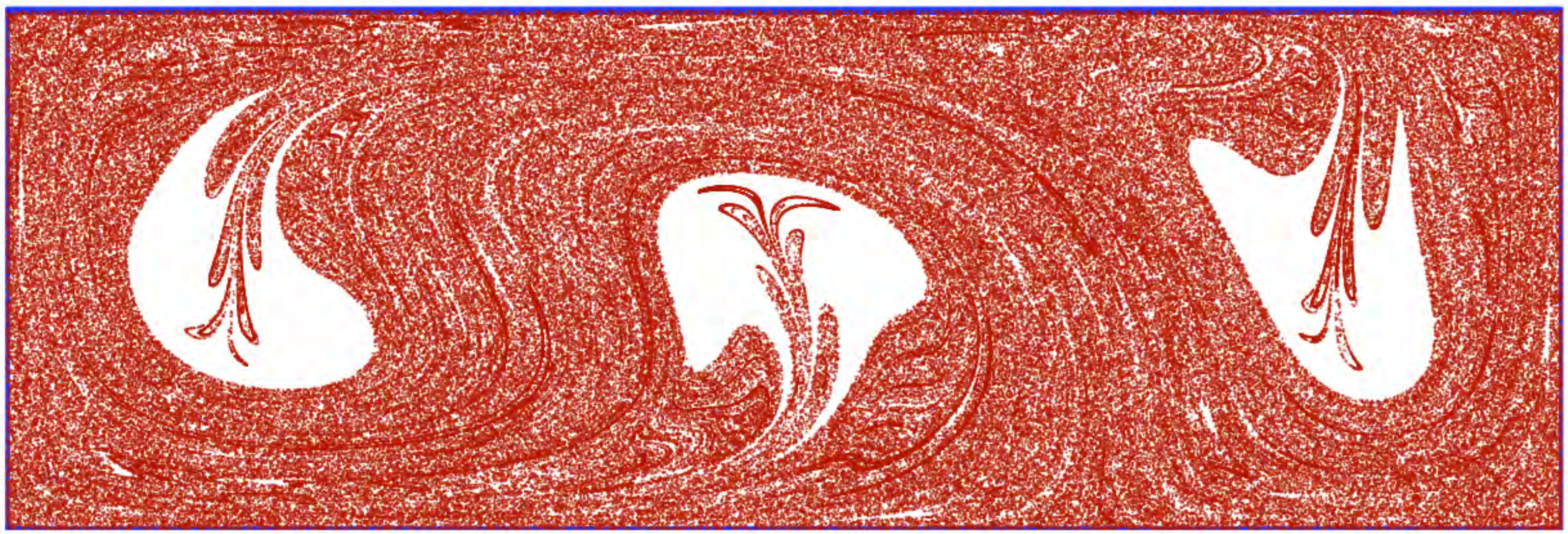
- Fluid example: Poincaré map



material blob and manifolds

Stable/unstable manifolds and lobes in fluids

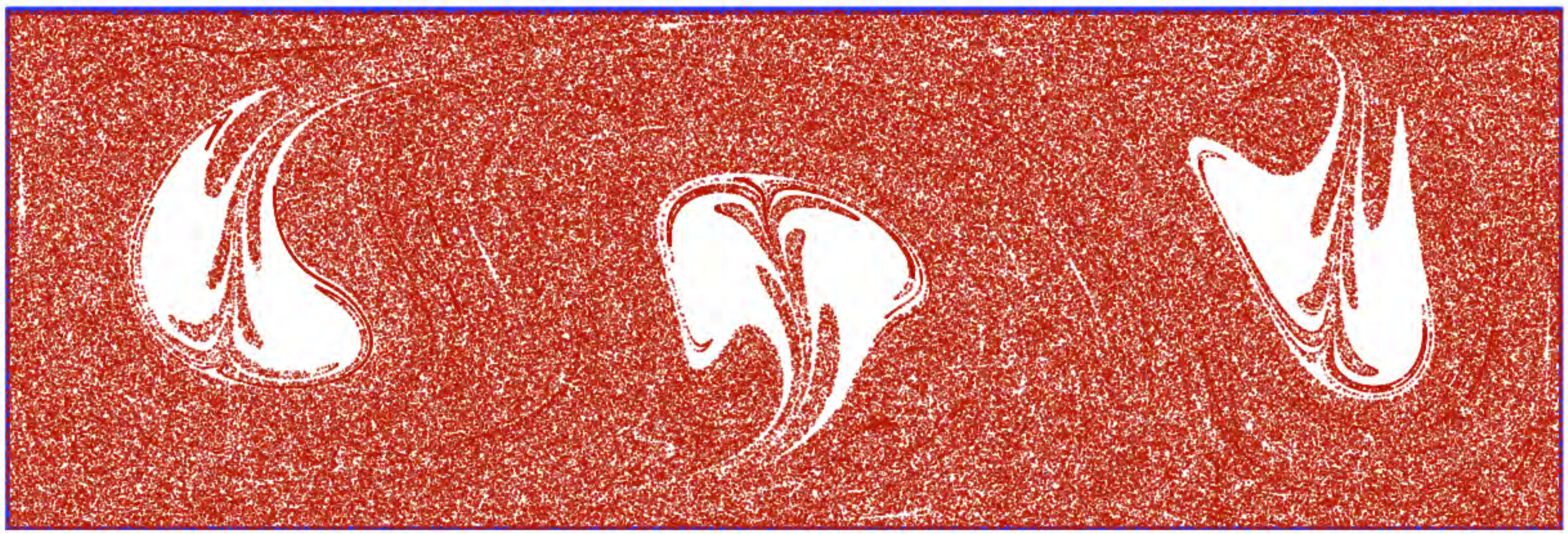
- Fluid example: Poincaré map



material blob at $t = 20$

Stable/unstable manifolds and lobes in fluids

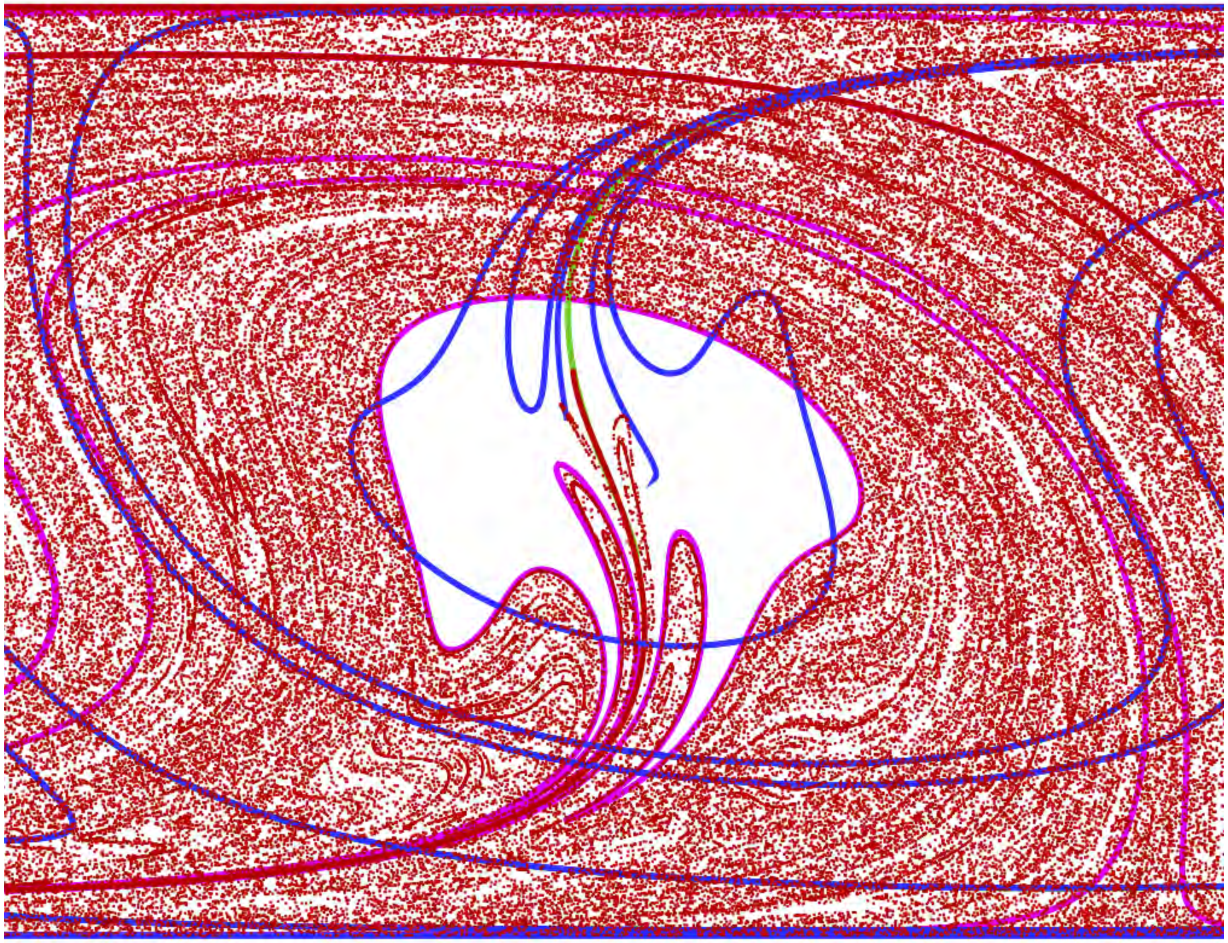
- Fluid example: Poincaré map



material blob at $t = 25$

Stable/unstable manifolds and lobes in fluids

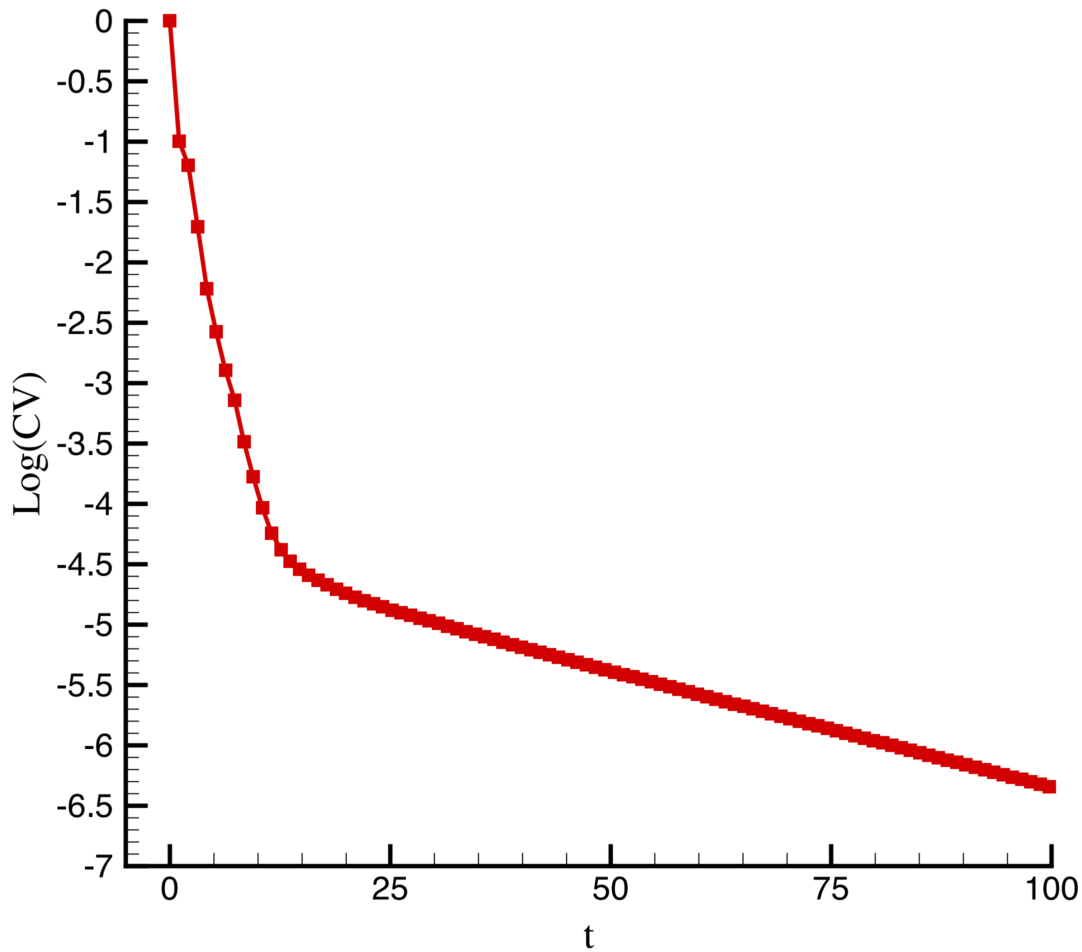
- Fluid example: Poincaré map



- Saddle manifolds and lobe dynamics provide template for motion

Stable/unstable manifolds and lobes in fluids

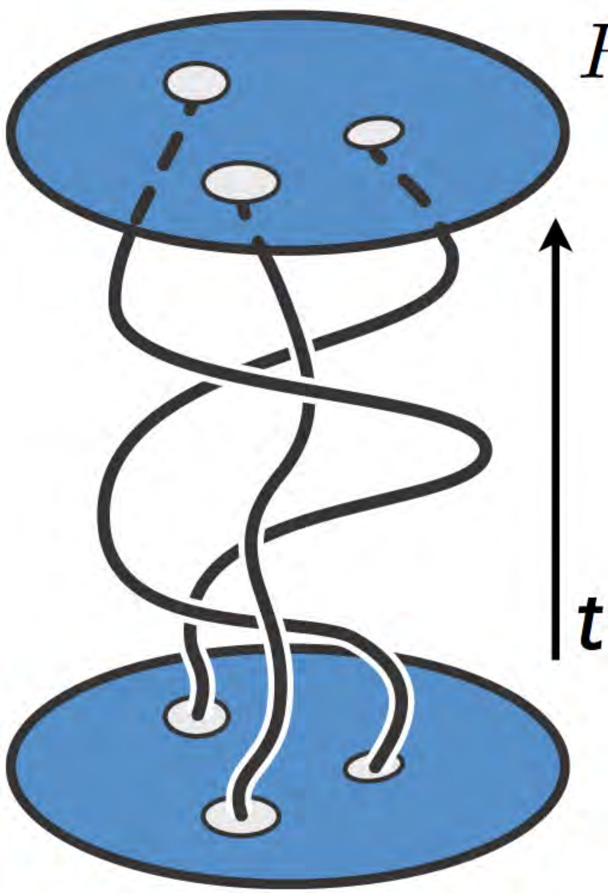
- Concentration variance; a measure of homogenization



- 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

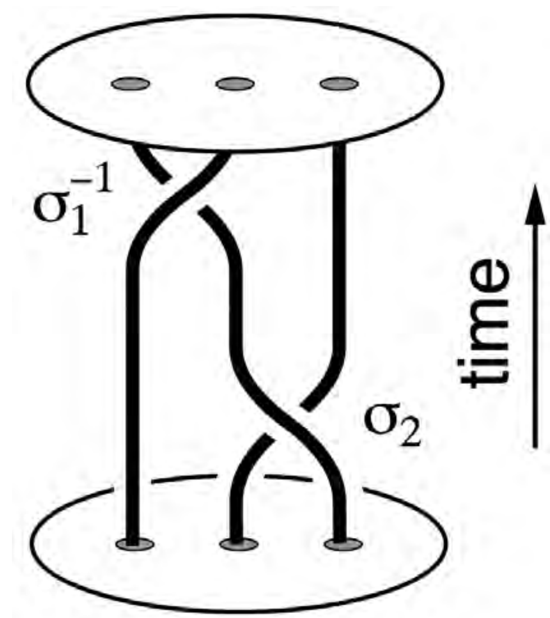


R_N : 2D fluid region with N stirring 'rods'

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

Thurston-Nielsen classification theorem

- Thurston (1988) Bull. Am. Math. Soc.
- A stirrer motion f is isotopic to a stirrer motion g of one of three types (i) finite order (f.o.): the nth iterate of g is the identity (ii) pseudo-Anosov (pA): g has dense orbits, Markov partition with transition matrix A, topological entropy $h_{\mathrm{TN}}(g) = \log(\lambda_{PF}(A))$, where $\lambda_{\mathrm{PF}}(A) > 1 =$ Perron-Frobenius eigenvalue of A (iii) reducible: g contains both f.o. and pA regions
- h_{TN} computed from 'braid word', e.g., $\sigma_{-1}\sigma_2$

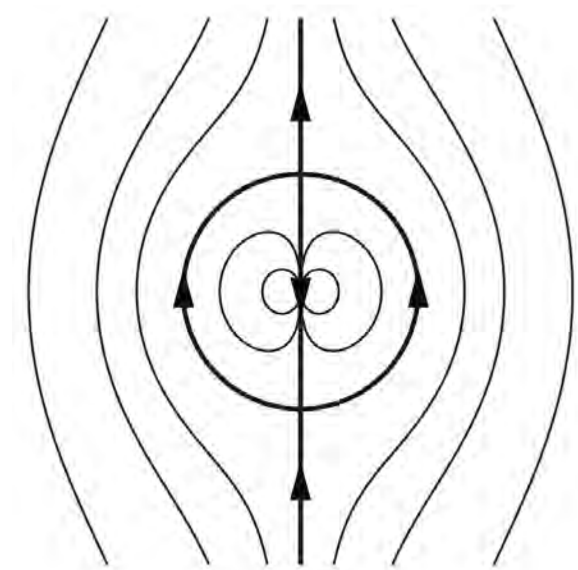


- $\log(\lambda_{PF}(A))$ provides a **lower bound** on the true topological entropy
- i.e., non-trivial material lines grow like $\ell \sim \ell_0 \lambda^n$, where $\lambda \geq \lambda_{\mathrm{TN}}$

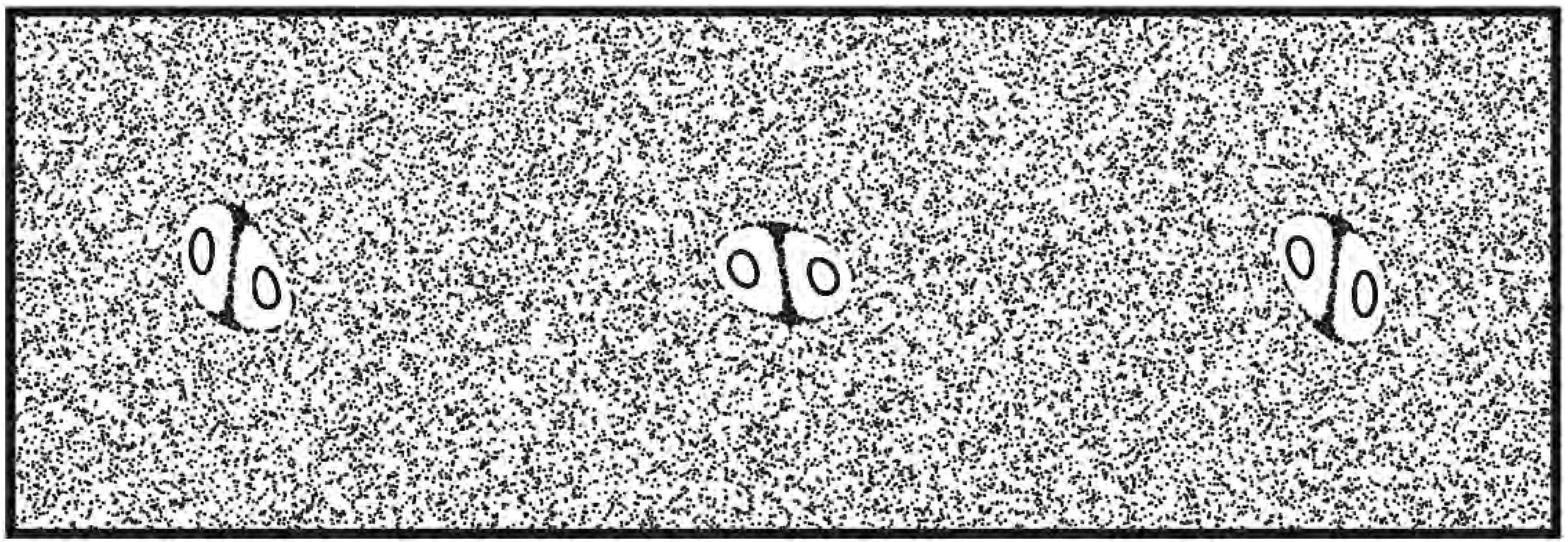
Identifying 'ghost rods': periodic points

tracer blob for $\tau_f > 1$

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



Identifying ‘ghost rods’: periodic points



Poincaré section for $\tau_f > 1$

- For $\tau_f > 1$, groups of elliptic and saddle periodic points of period 3
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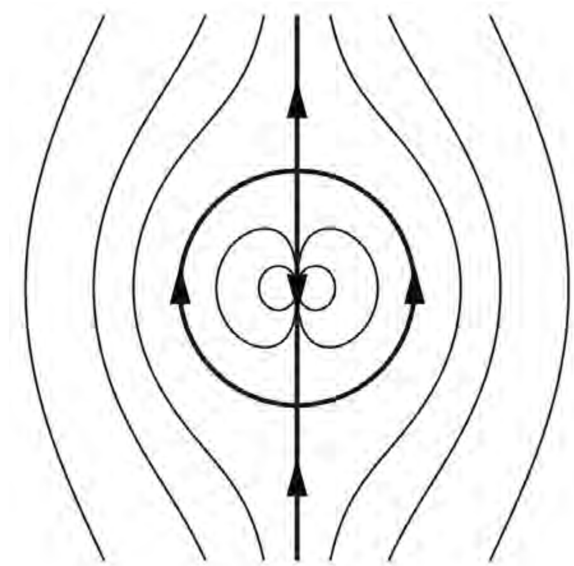
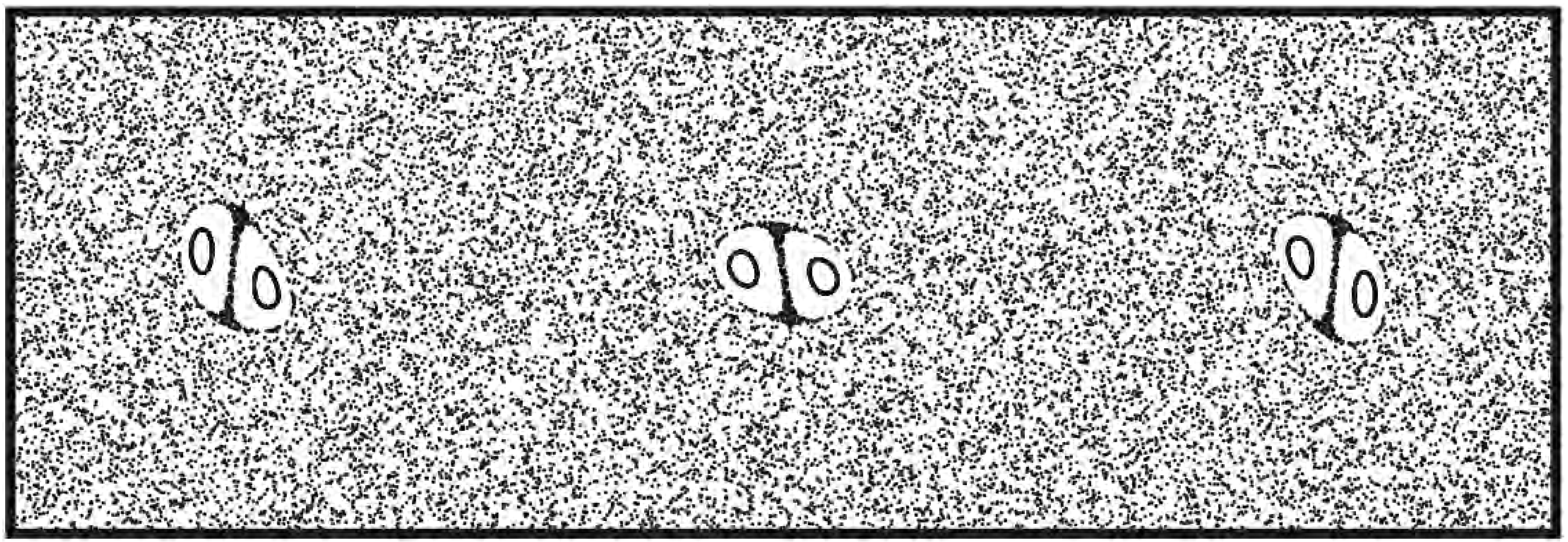
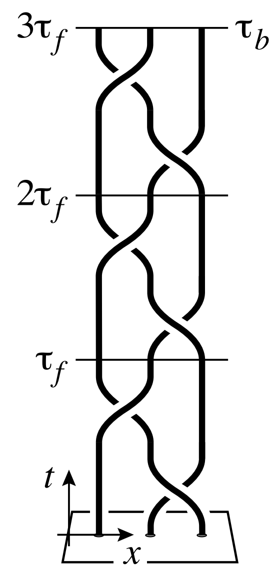


Identifying 'ghost rods': periodic points

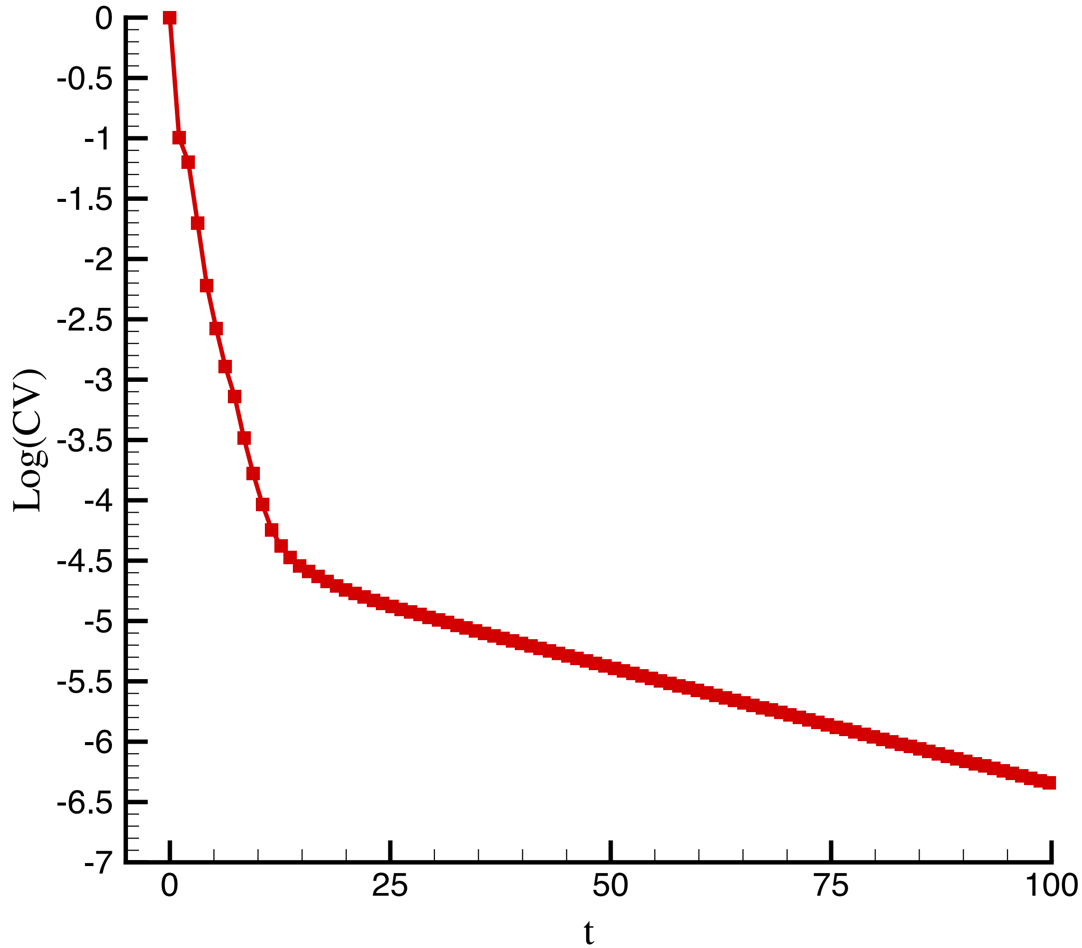


Poincaré section for $\tau_f > 1$



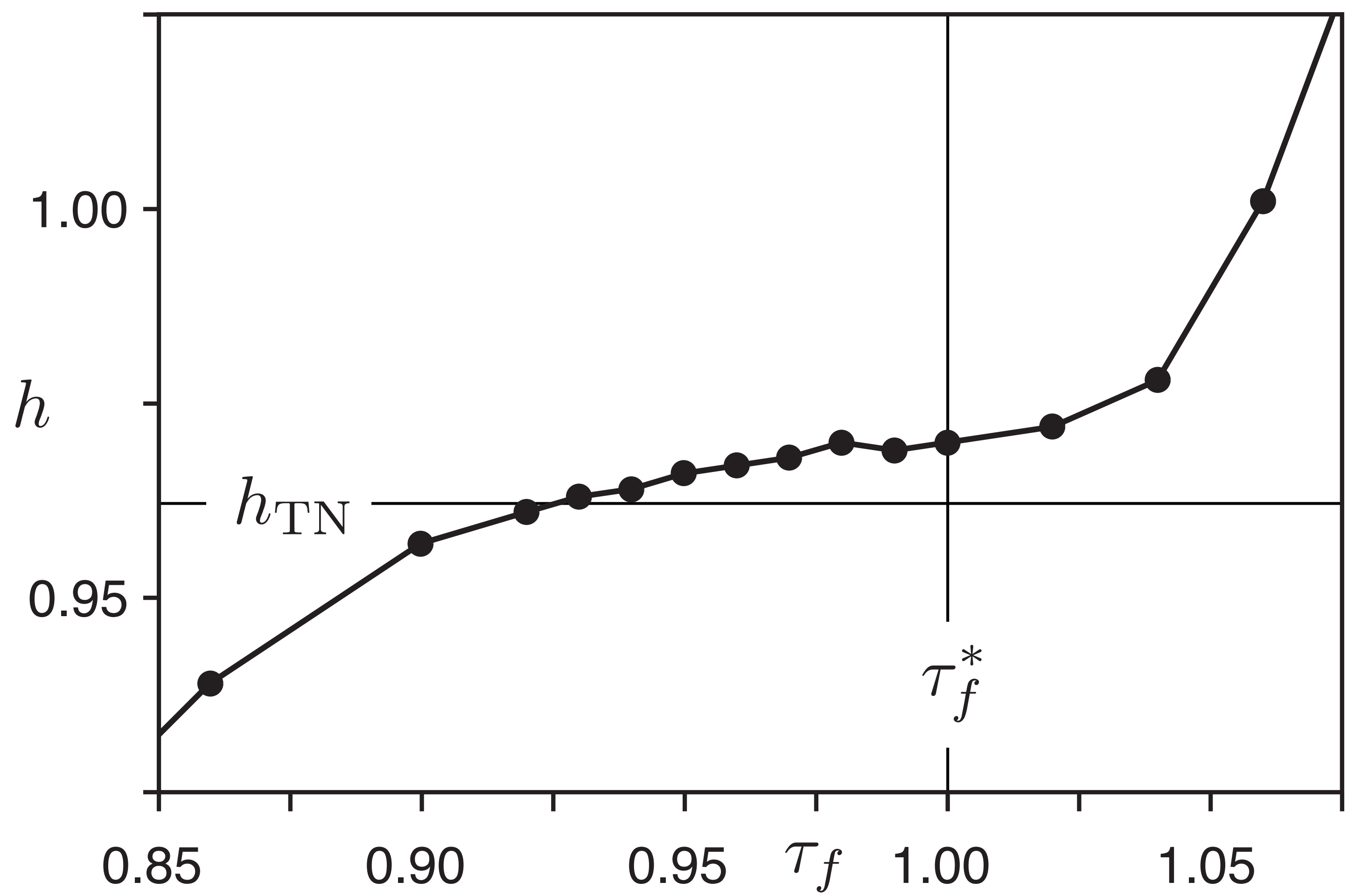
- Periodic points of period 3 $\Rightarrow$ act as 'ghost rods'
- Their braid $\Rightarrow h_{\mathrm{TN}} = 0.96242$ from TNCT
- Actual $h_{\mathrm{flow}} \approx 0.964$
- $\Rightarrow h_{\mathrm{TN}}$ is an excellent lower bound

Identifying 'ghost rods': periodic points



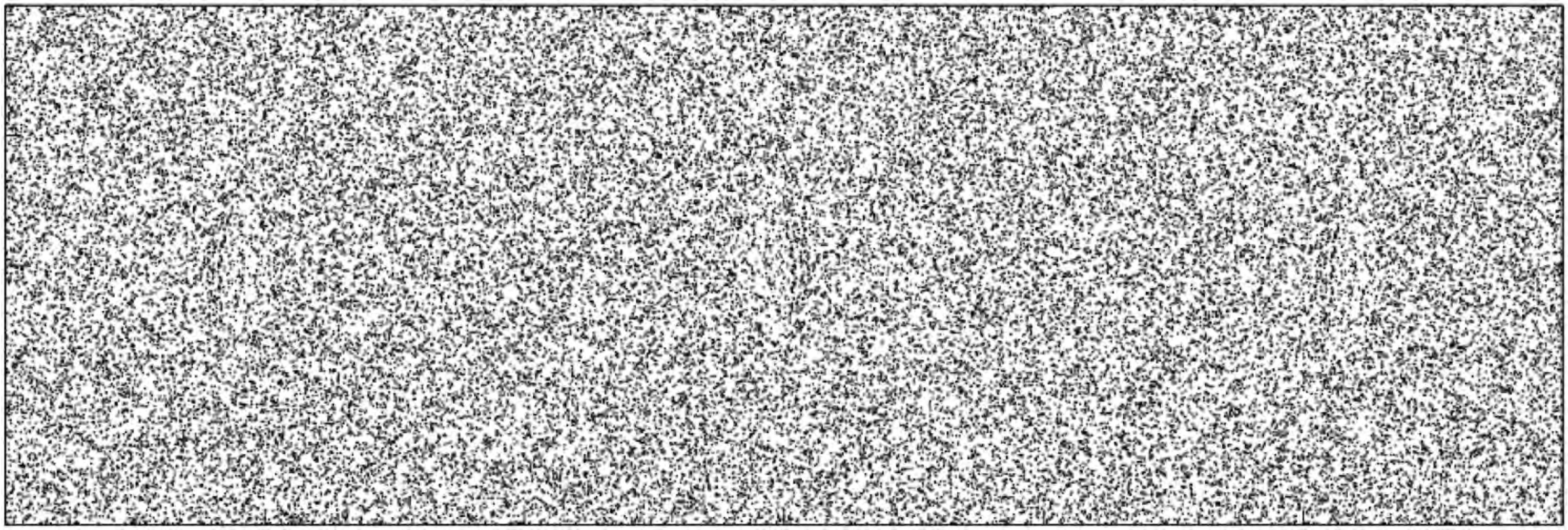
- Homogenization has two exponential rates: slower one related to lobes
- **Fast rate due to braiding of 'ghost rods'!**

Topological entropy continuity across critical point



topological entropy as a function of τ_f

Identifying 'ghost rods'?



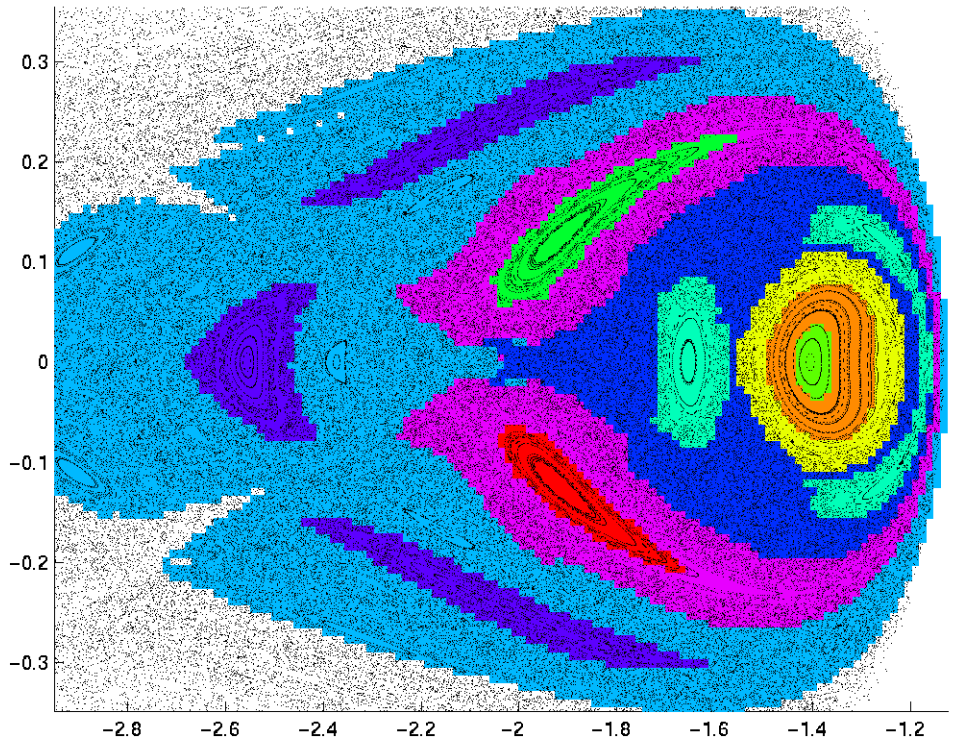
Poincaré section for $\tau_f < 1 \Rightarrow$ no obvious structure!

- 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 $\approx$ "Leaky" regions with a long residence time[2]



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

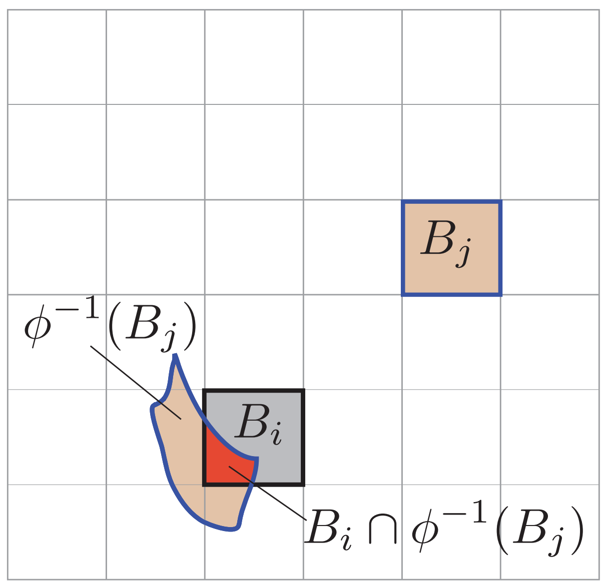
[2]Dellnitz, Junge, Koon, Lekien, Lo, Marsden, Padberg, Preis, Ross, Thiere [2005] Int. J. Bif. Chaos

Almost-invariant set (AIS) approach

- Create box partition of phase space $\mathcal{B} = \{B_1, \dots B_q\}$, 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., $f = \phi_t^{t+T}$

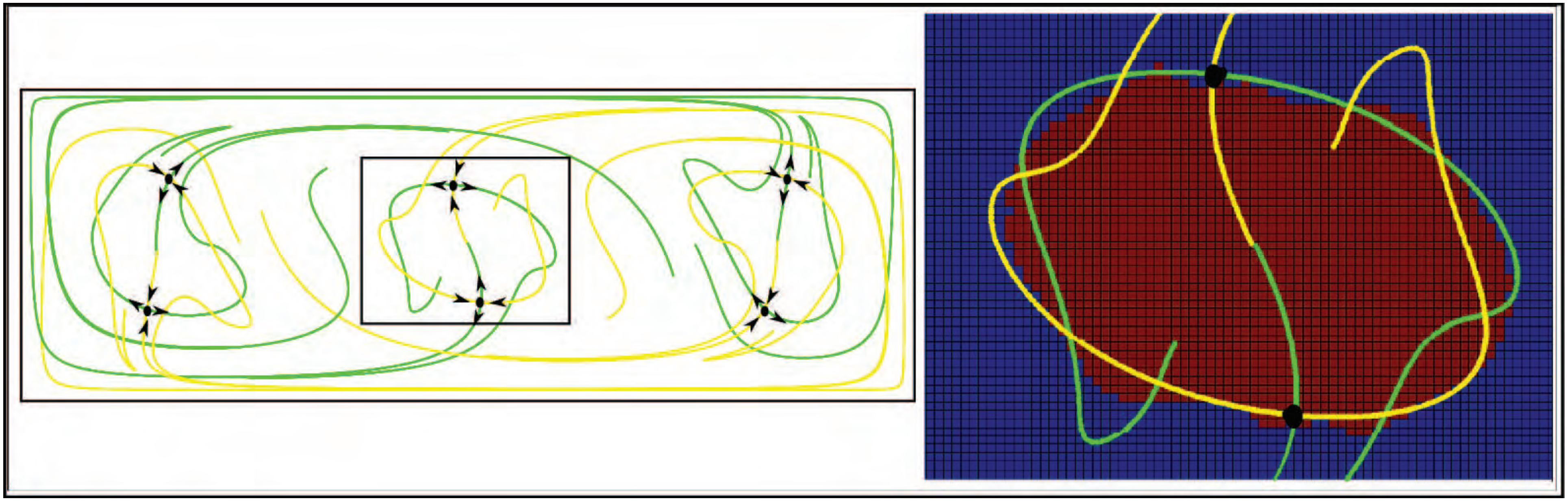


- P approximates our dynamical system via a finite state Markov chain.

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 ρ 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

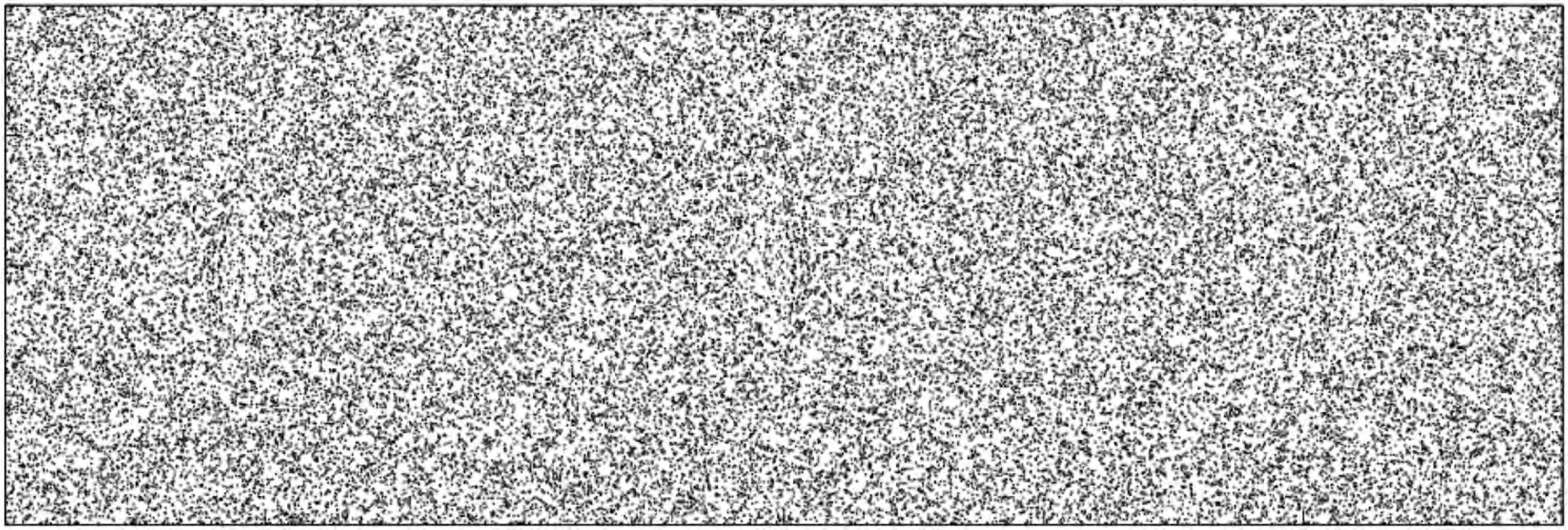
Identifying 'ghost rods': almost-cyclic sets



- 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)

[3] Dellnitz, Junge, Lo, Marsden, Padberg, Preis, Ross, Thiere [2005] Phys. Rev. Lett.; Dellnitz, Junge, Koon, Lekien, Lo, Marsden, Padberg, Preis, Ross, Thiere [2005] Int. J. Bif. Chaos

Identifying 'ghost rods': almost-cyclic sets



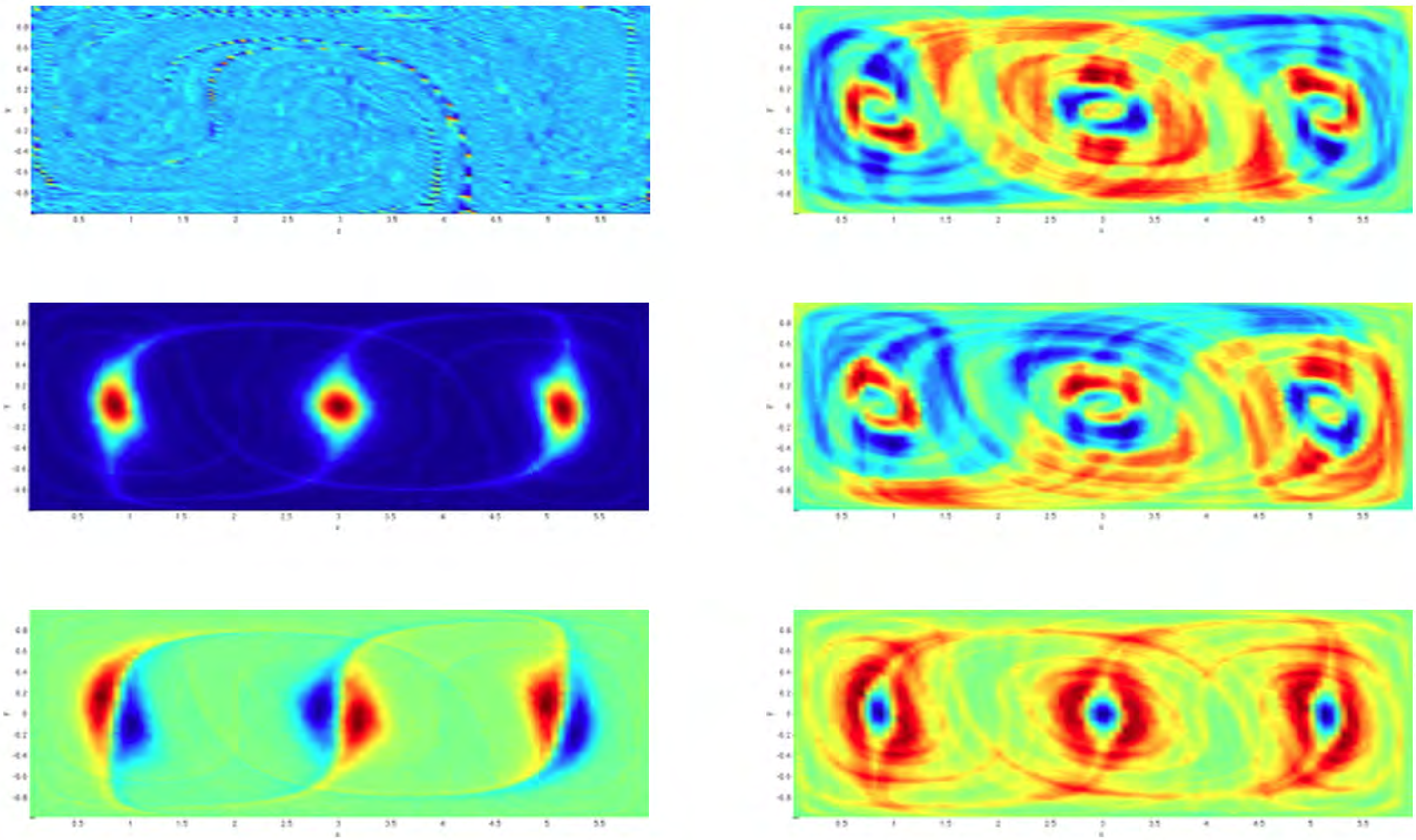
Poincaré section for $\tau_f < 1 \Rightarrow$ no obvious structure!

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

- Consider transition matrix $P_t^{t+\tau_f}$ induced by Poincaré map $\phi_t^{t+\tau_f}$

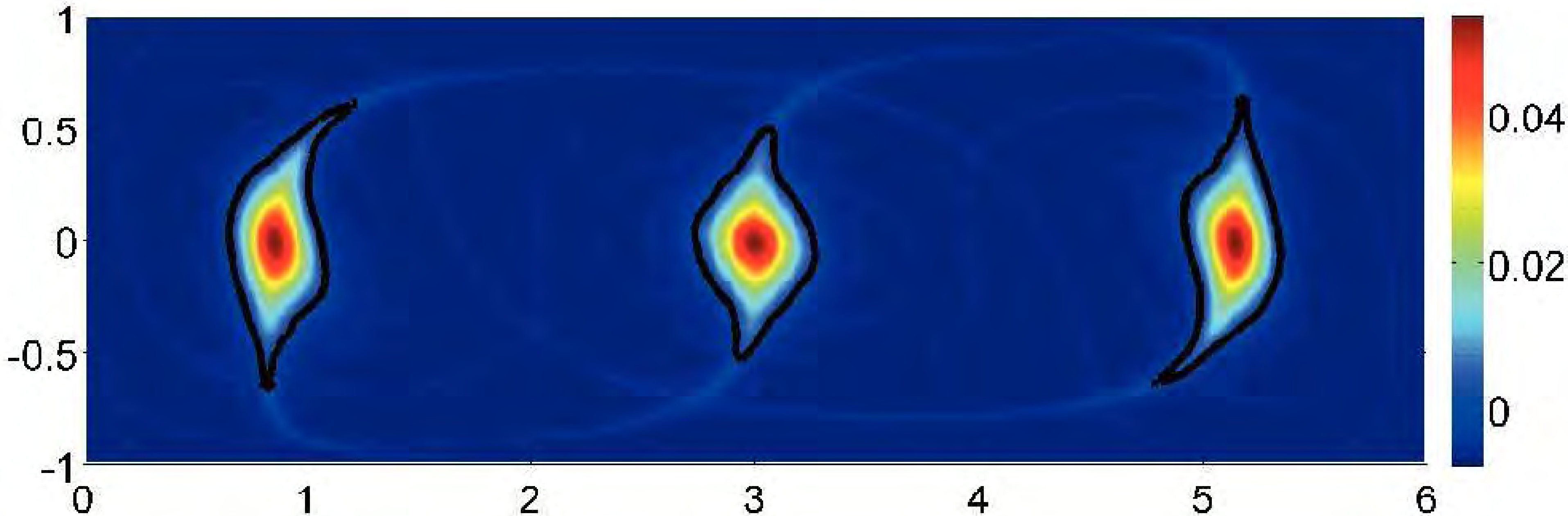
Identifying 'ghost rods': almost-cyclic sets

1 2 3 4 5 6



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.

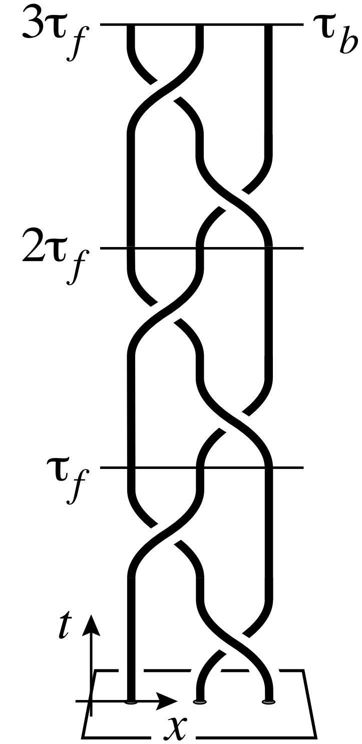
- Three-component AIS made of 3 almost-cyclic sets (ACSs) of period 3
- ACS effectively replace compact region bounded by saddle manifolds
- Also a remnant of the global 'stable and unstable manifolds' of the saddle points, even there are no more saddle points

Identifying ‘ghost rods’: almost-cyclic sets

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

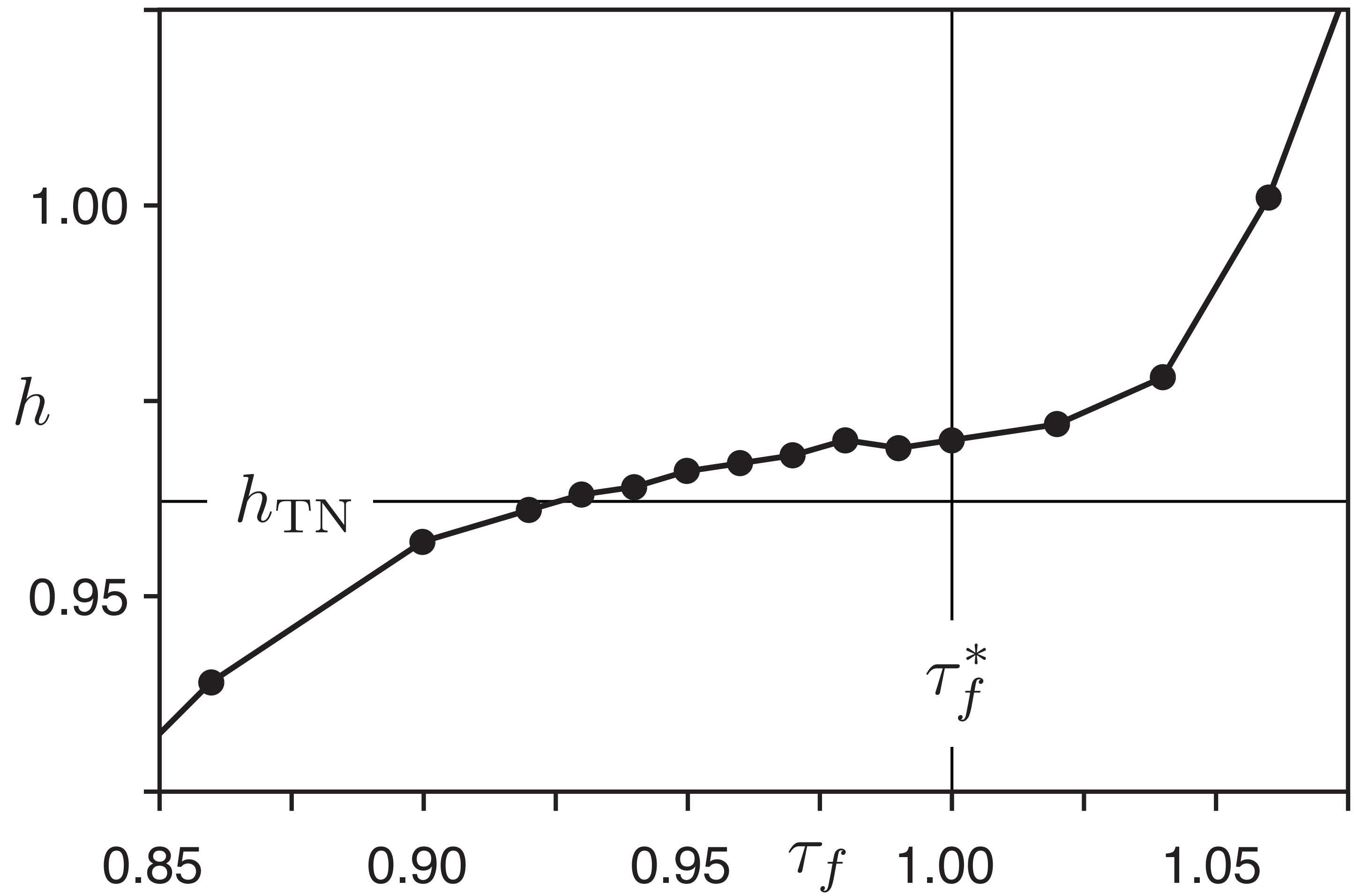
Movie shown is second eigenvector for $P_t^{t+\tau_f}$ for $t \in [0, \tau_f)$

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!
— Stremler, Ross, Grover, Kumar [2011] Phys. Rev. Lett.

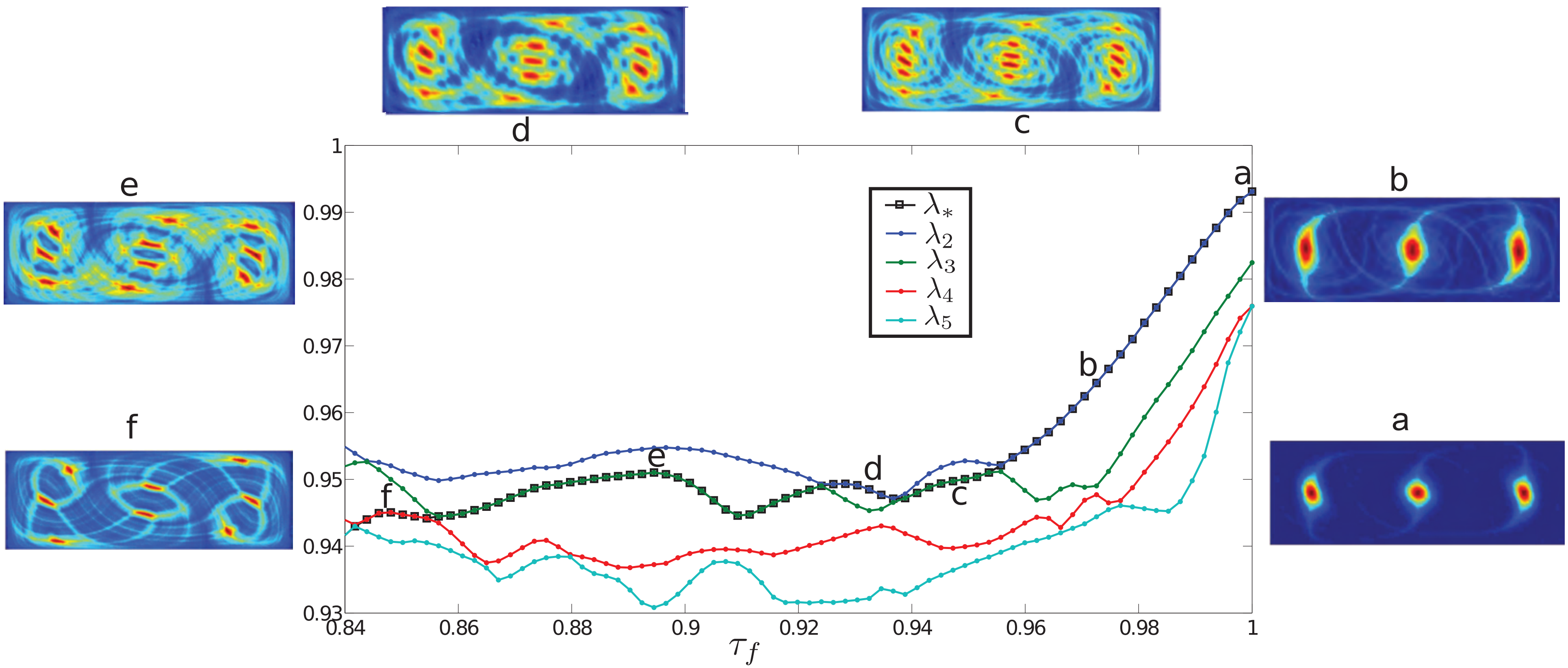
Topological entropy vs. bifurcation parameter



topological entropy as a function of τ_f

- h_{TN} shown for ACS braid on 3 strands

Eigenvalues/eigenvectors vs. bifurcation parameter



Movie shows change in eigenvector branch, marked with '$-\square-$' above, as parameter decreases from a to f $\Rightarrow$

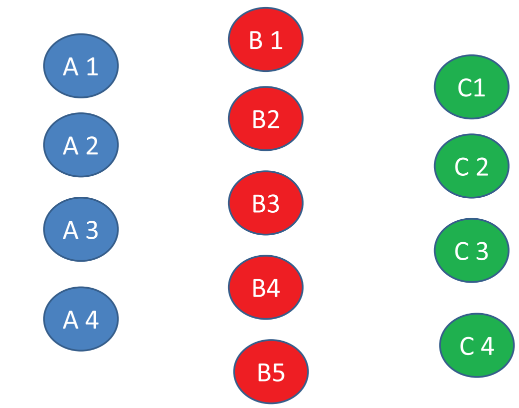
Bifurcation of ACSs

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

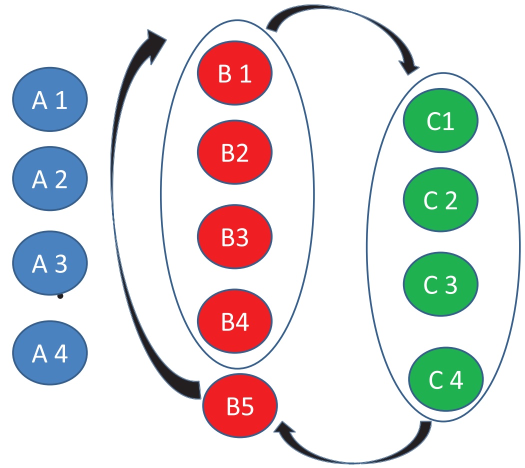
Movie shown is second eigenvector for $P_t^{t+\tau_f}$ for $t \in [0, \tau_f)$

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

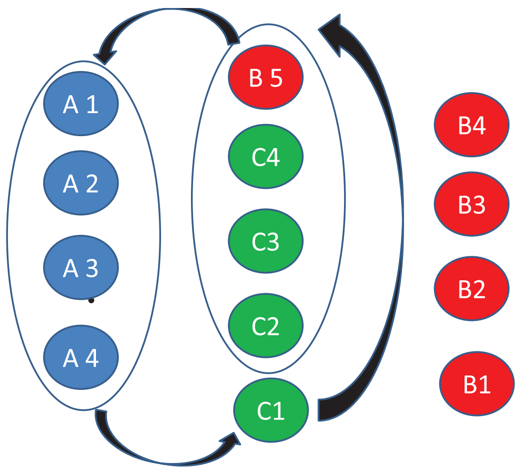
Bifurcation of ACSs



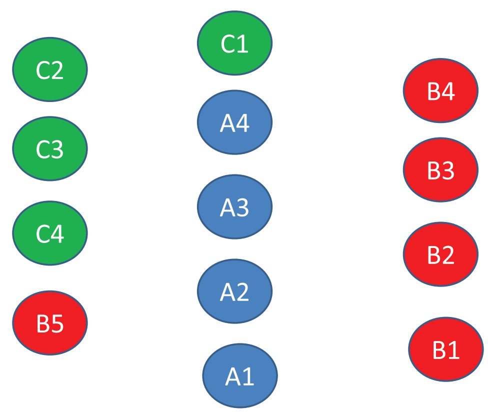
(a) Initial state



(b) First half-period

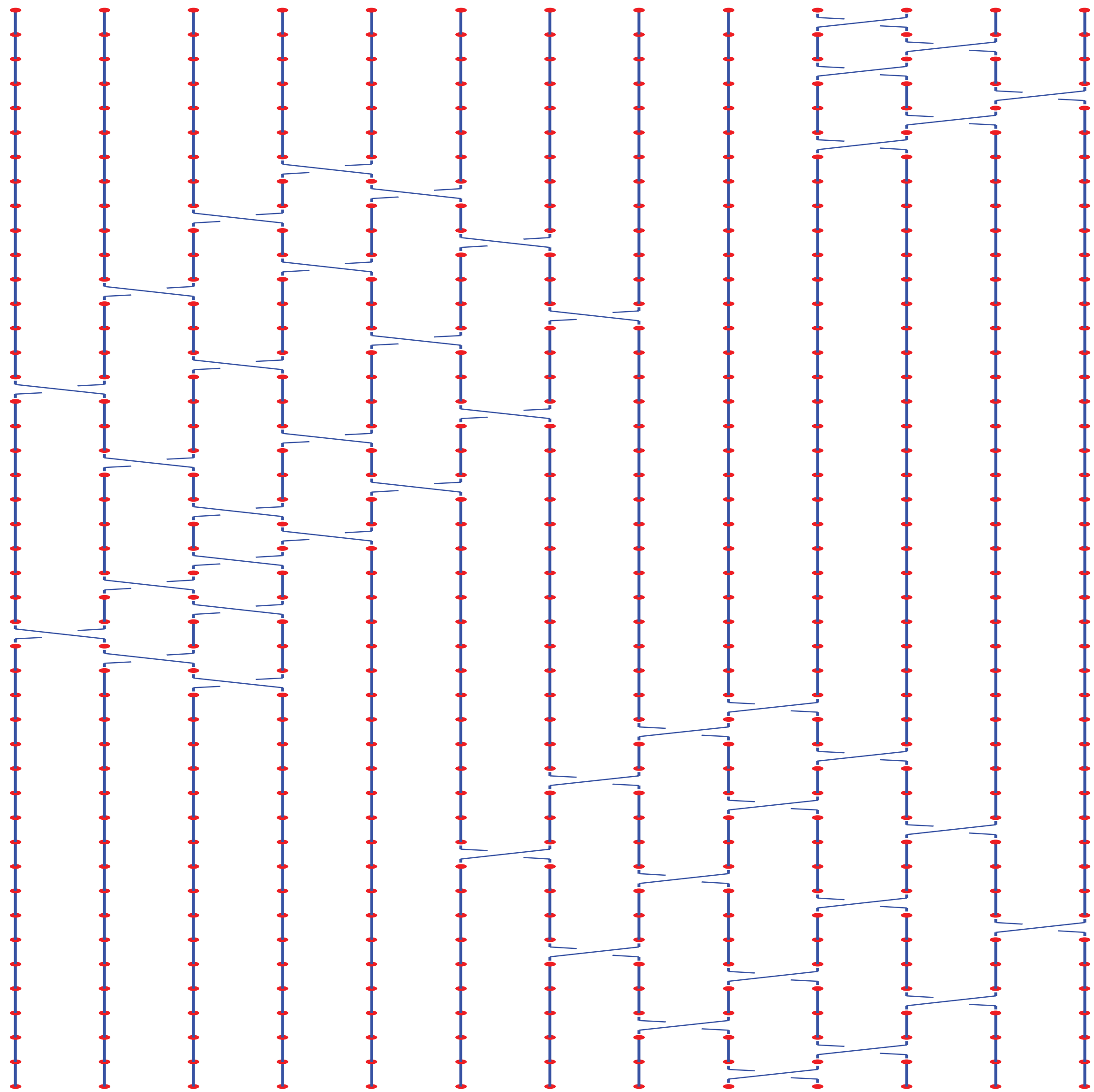


(c) Second half-period



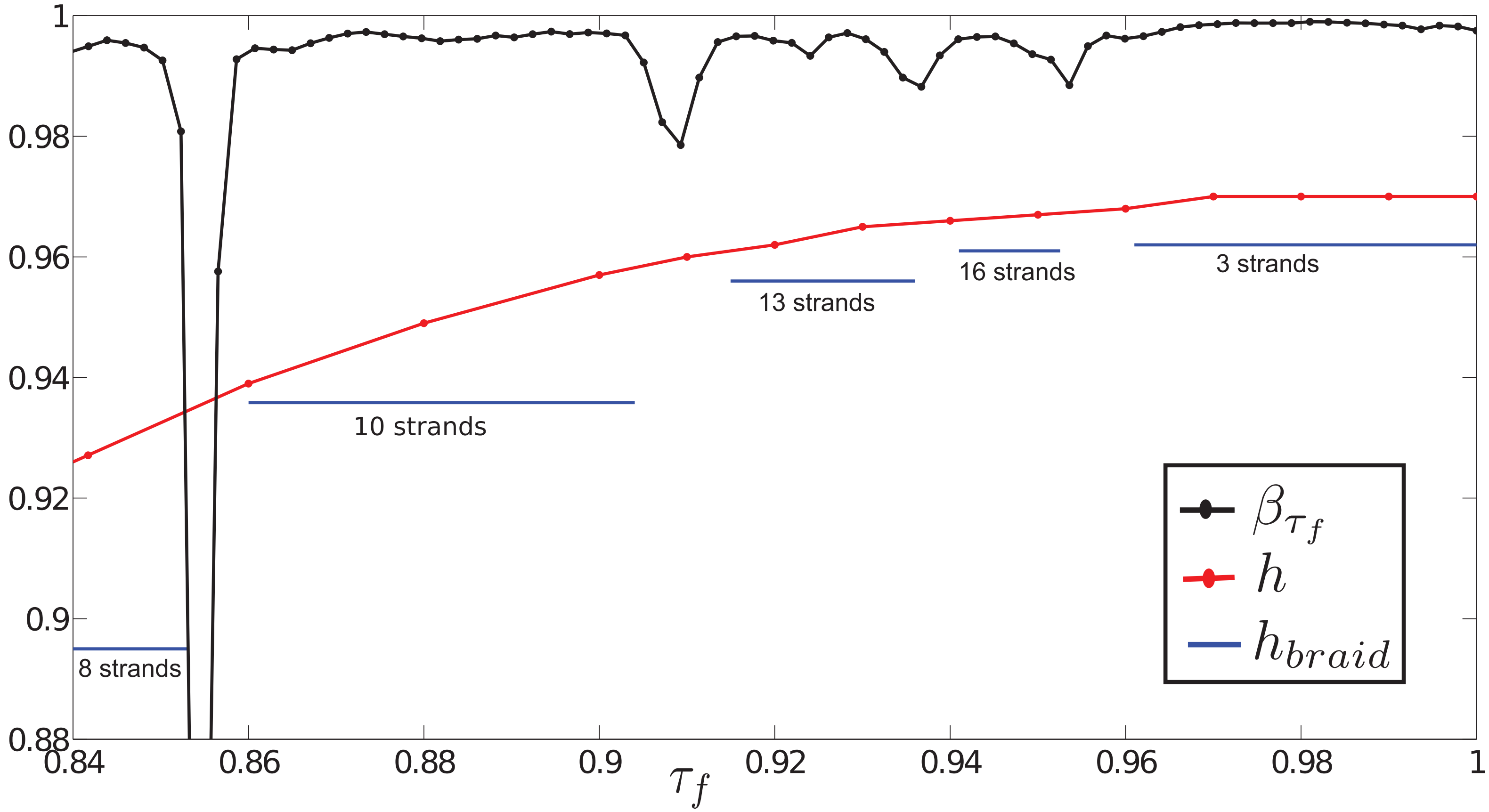
(d) State after 1 period

Bifurcation of ACSs



representation of braid

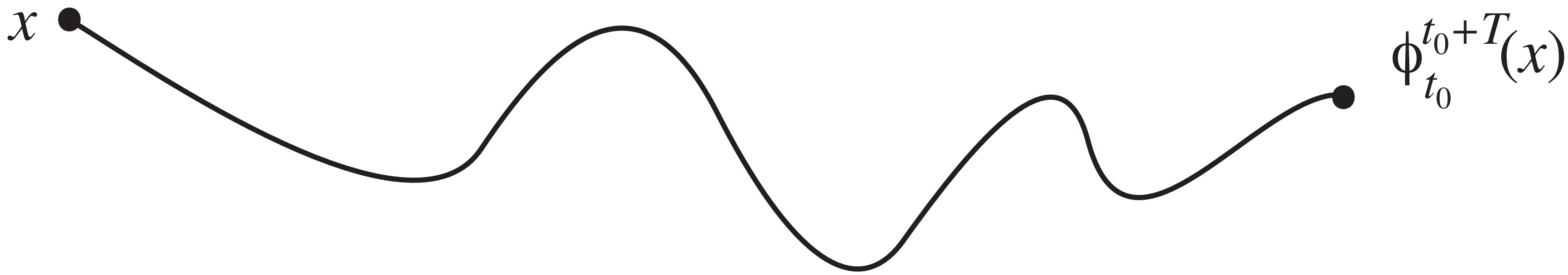
Sequence of ACS braids bounds entropy



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

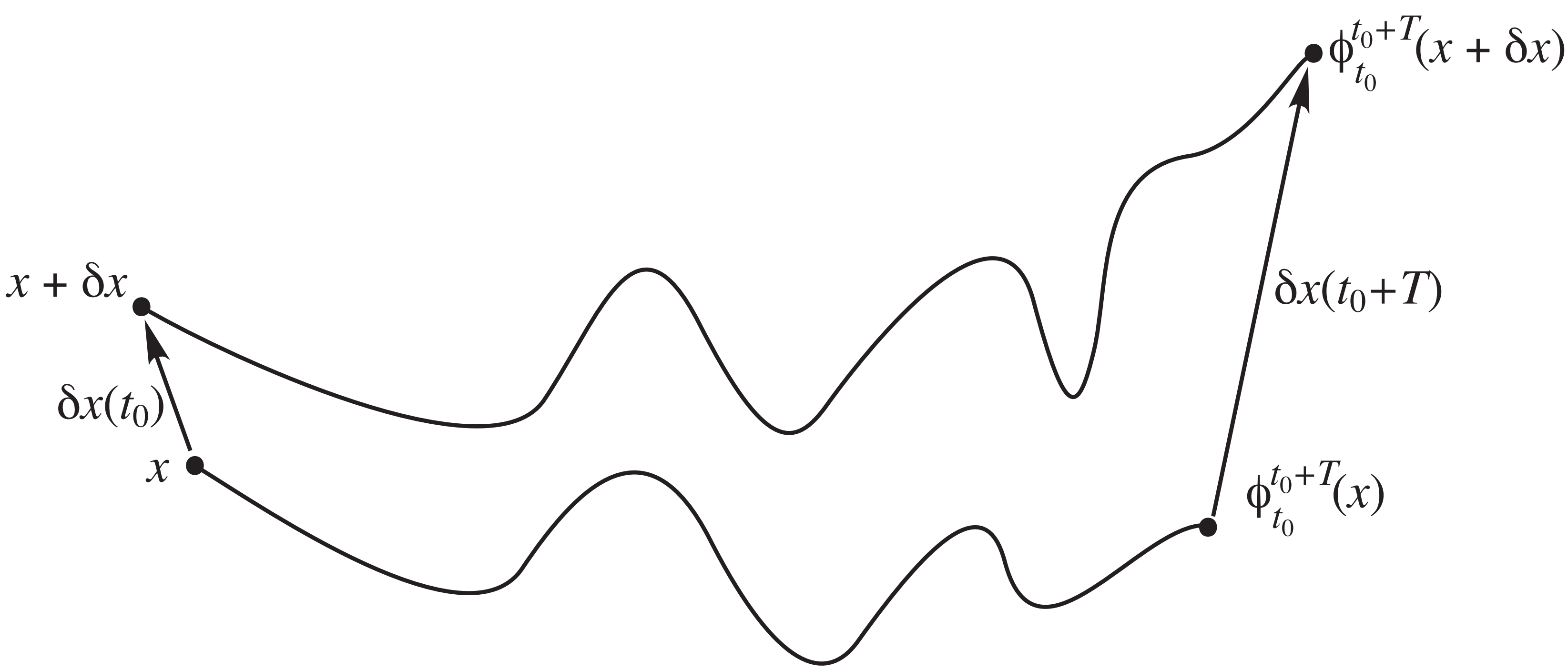
- Data-driven, finite-time, aperiodic setting
- How do we get at transport?
- Recall the flow, $x \mapsto \phi_t^{t+T}(x)$



Identify regions of high sensitivity of initial conditions

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

$$\begin{aligned}\delta x(t+T) &= \phi_t^{t+T}(x+\delta x(t)) - \phi_t^{t+T}(x) \\ &= \frac{d\phi_t^{t+T}(x)}{dx}\delta x(t) + O(||\delta x(t)||^2)\end{aligned}$$



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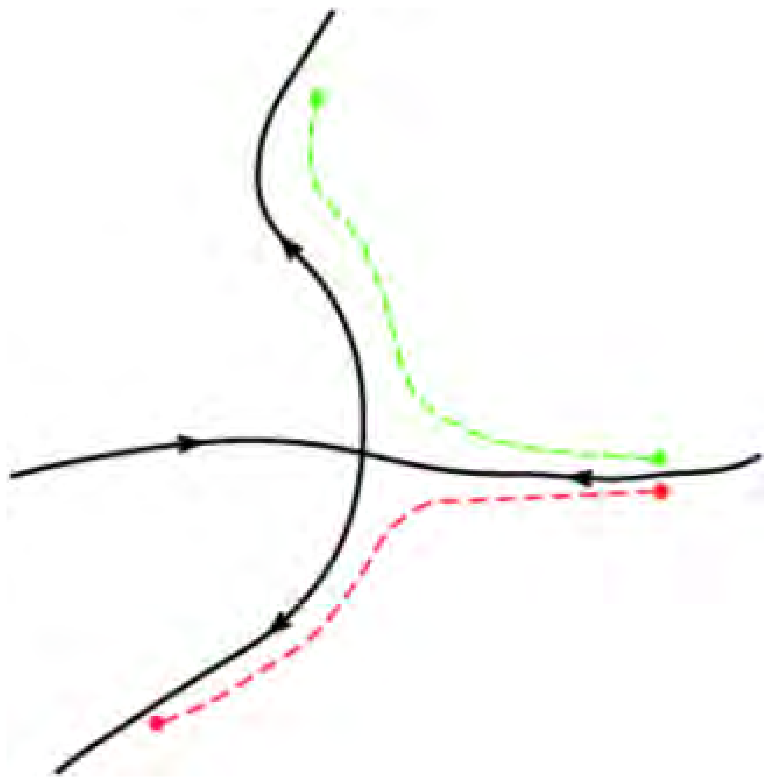
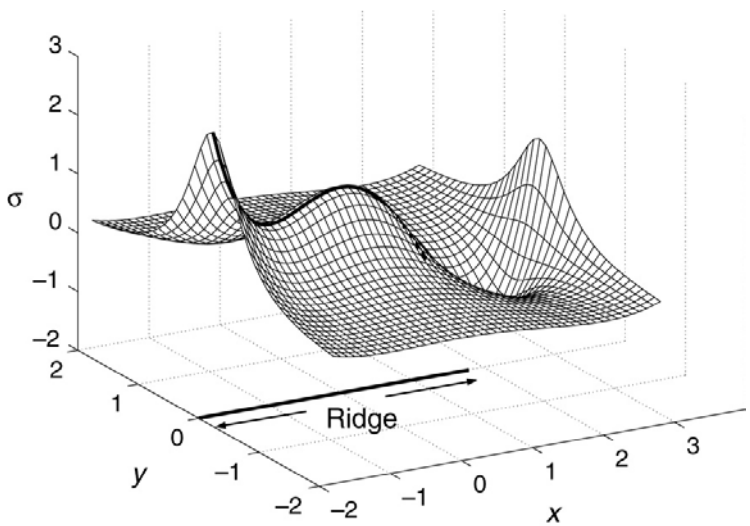


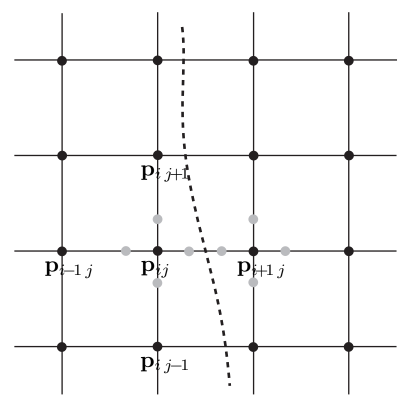
Invariant manifold analogs: FTLE-LCS approach

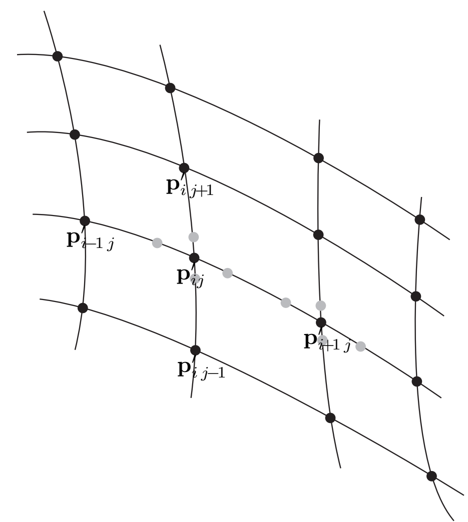
- The finite-time Lyapunov exponent (FTLE),

$$\sigma_t^T(x) = \frac{1}{|T|} \log \left\| \frac{d\phi_t^{t+T}(x)}{dx} \right\|$$

  measures the maximum stretching rate over the interval T of trajectories starting near the point x at time t
- Ridges of σ_t^T are candidate hyperbolic codim-1 surfaces; finite-time analogs of stable/unstable manifolds; Lagrangian coherent structures[4]

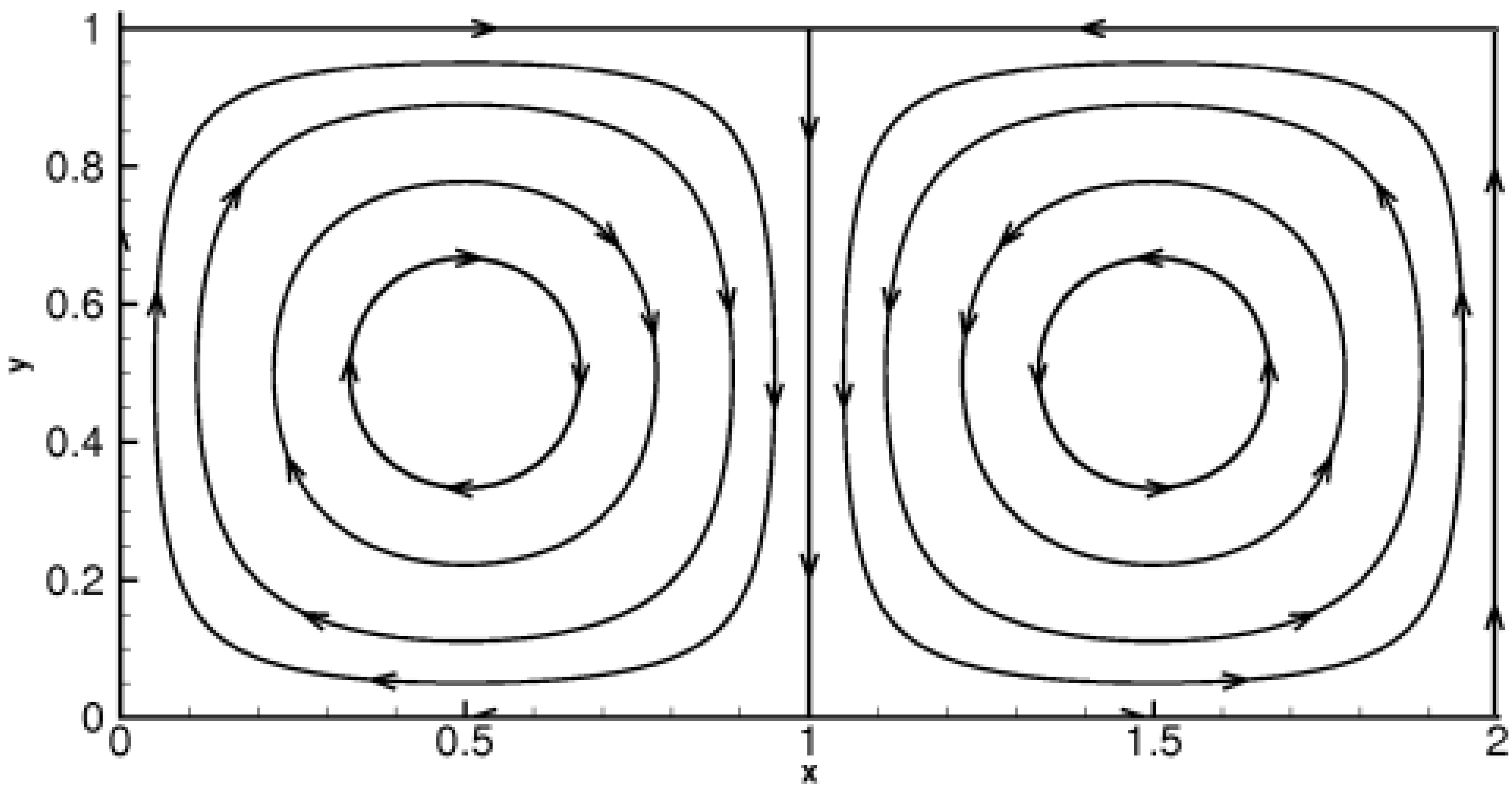




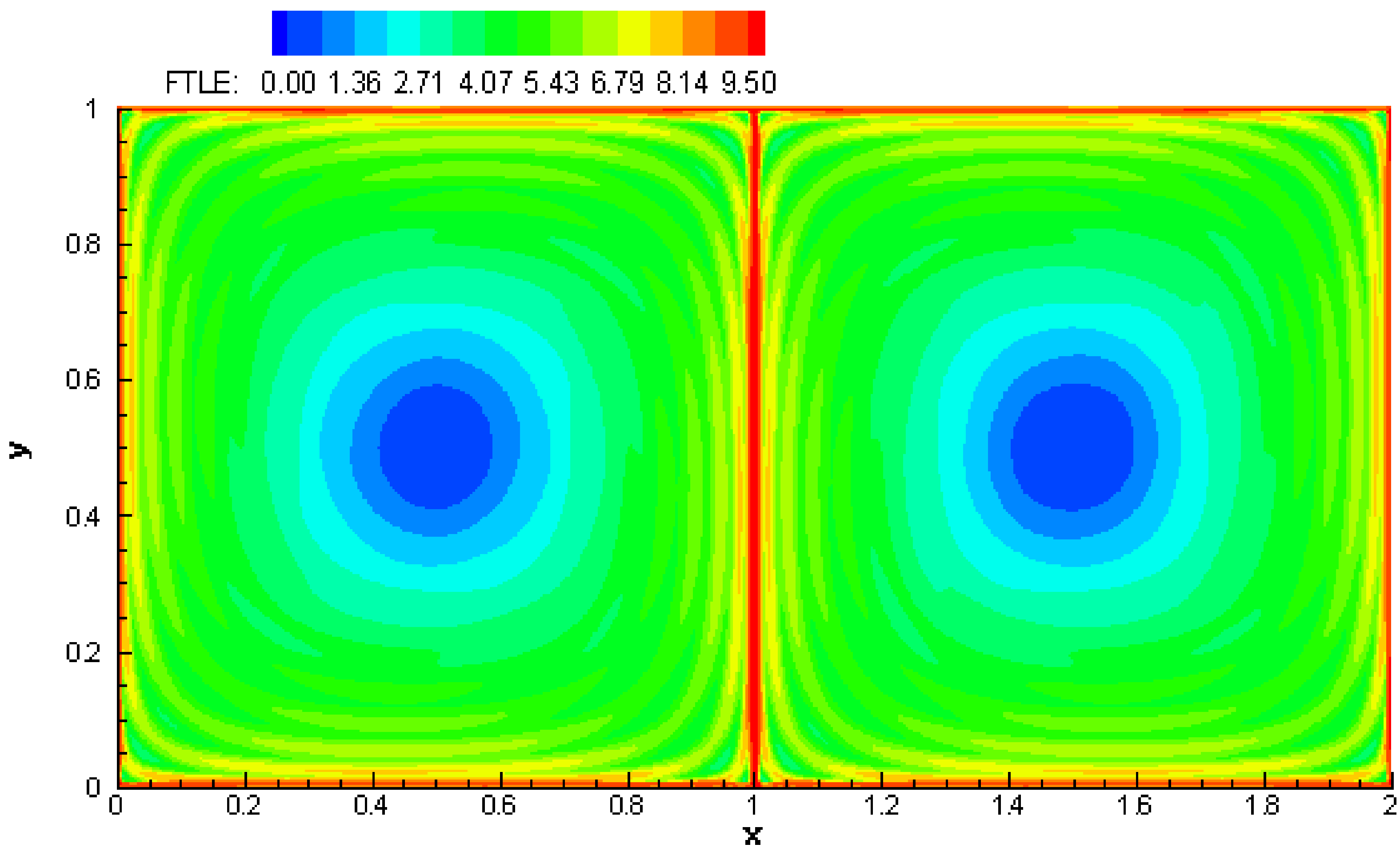


[4] cf. Bowman, 1999; Haller & Yuan, 2000; Haller, 2001; Shadden, Lekien, Marsden, 2005

Invariant manifold analogs: FTLE-LCS approach



Invariant manifold analogs: FTLE-LCS approach

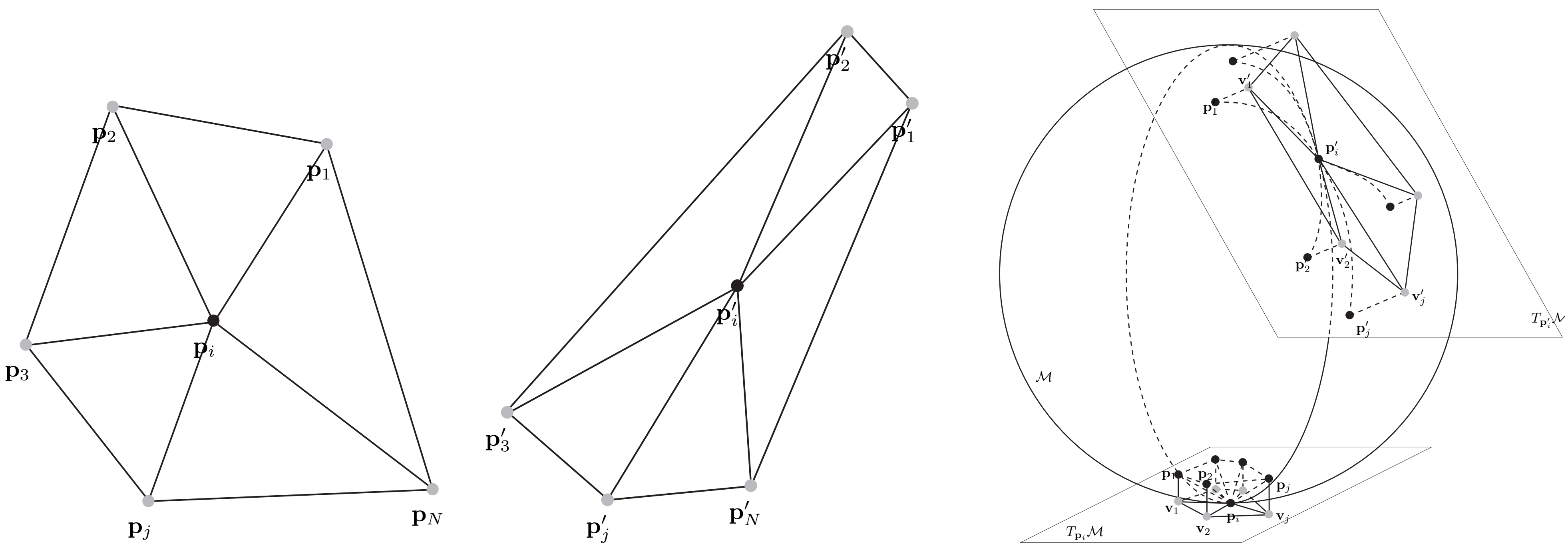


Invariant manifold analogs: FTLE-LCS approach

- We can define the FTLE for Riemannian manifolds[3]

$$\sigma_t^T(x) = \frac{1}{|T|} \ln \left\| \mathrm{D}\phi_t^{t+T} \right\| \doteq \frac{1}{|T|} \log \left(\max_{\mathrm{y} \neq 0} \frac{\left\| \mathrm{D}\phi_t^{t+T}(\mathrm{y}) \right\|}{\|\mathrm{y}\|} \right)$$

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 $T < 0$

cylinder

Moebius strip

Each frame has a different initial time t

[3] Lekien & Ross [2010] Chaos

Atmospheric flows: Antarctic polar vortex

ozone data

Atmospheric flows: Antarctic polar vortex

ozone data + LCSs (red = repelling, blue = attracting)

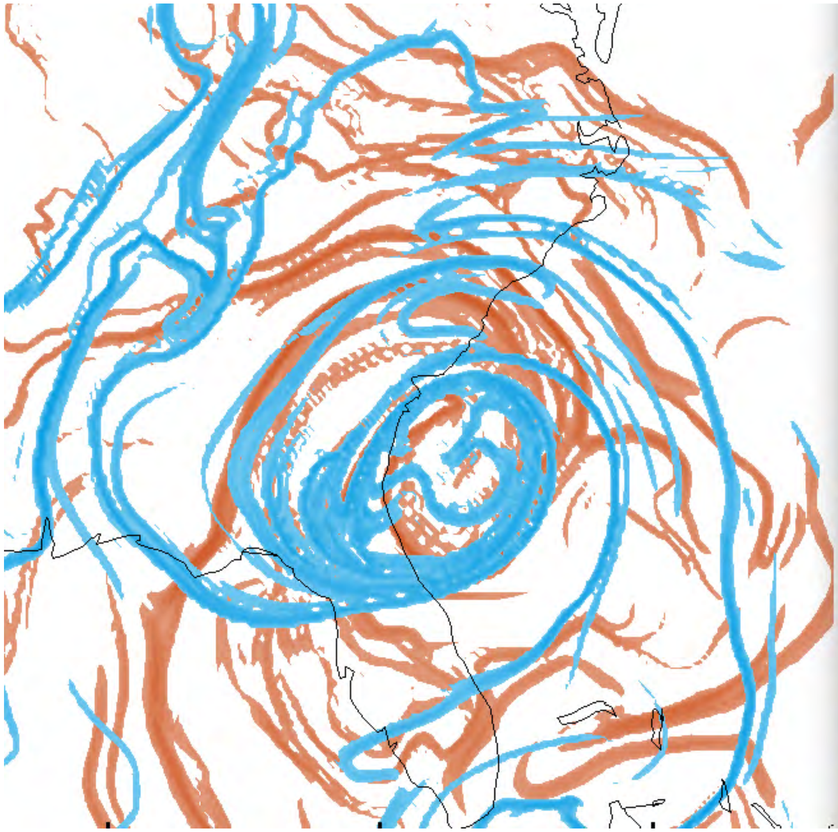
Atmospheric flows: Antarctic polar vortex

air masses on either side of a repelling LCS

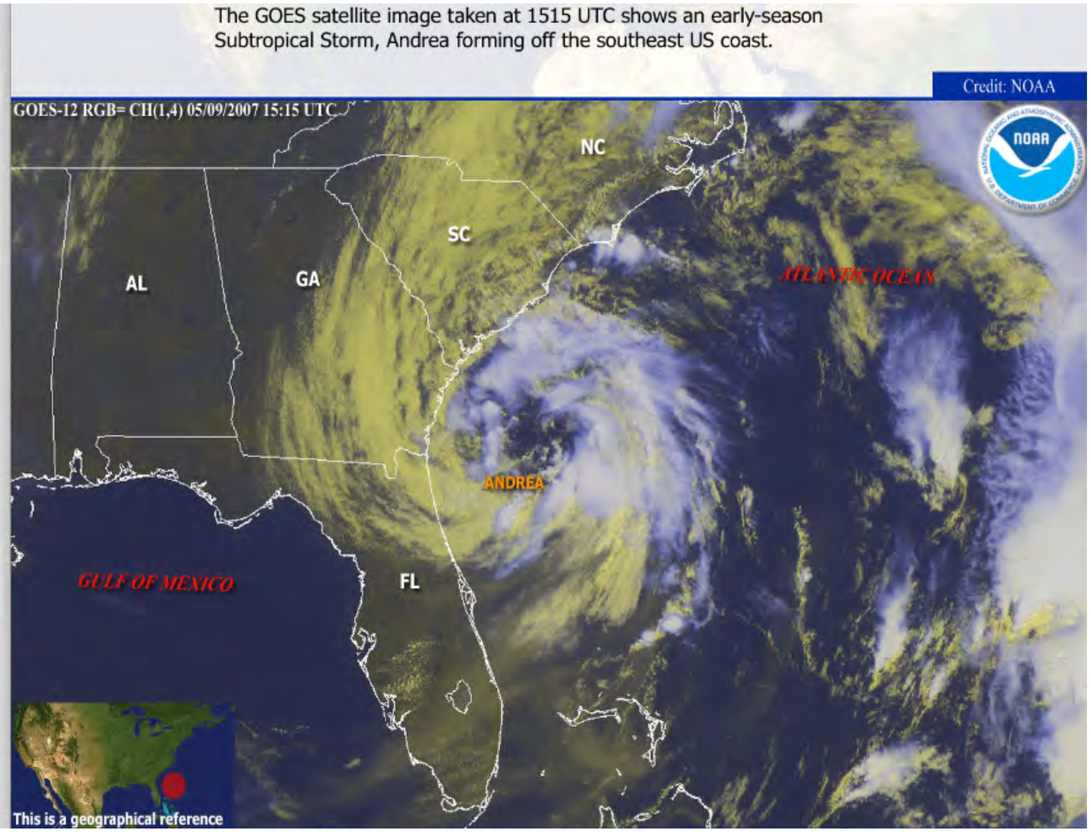
Atmospheric flows: continental U.S.

LCSs: orange = repelling, blue = attracting

Atmospheric flows and lobe dynamics



orange = repelling LCSs, blue = attracting LCSs



satellite

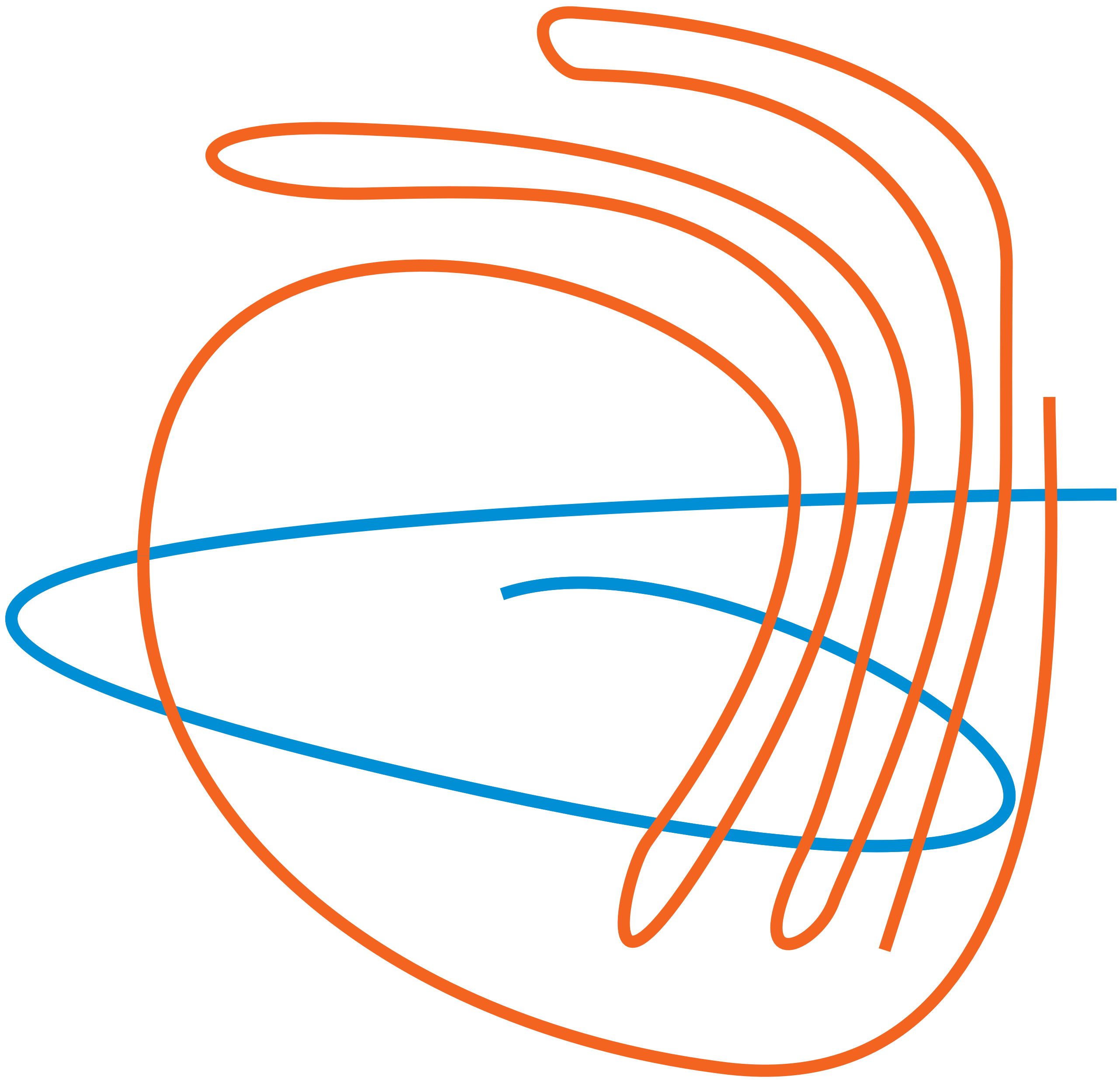
Hurricane Andrea, 2007

cf. Sapsis & Haller [2009], Du Toit & Marsden [2010], Lekien & Ross [2010], Tallapragada & Ross [2011]

Atmospheric flows and lobe dynamics

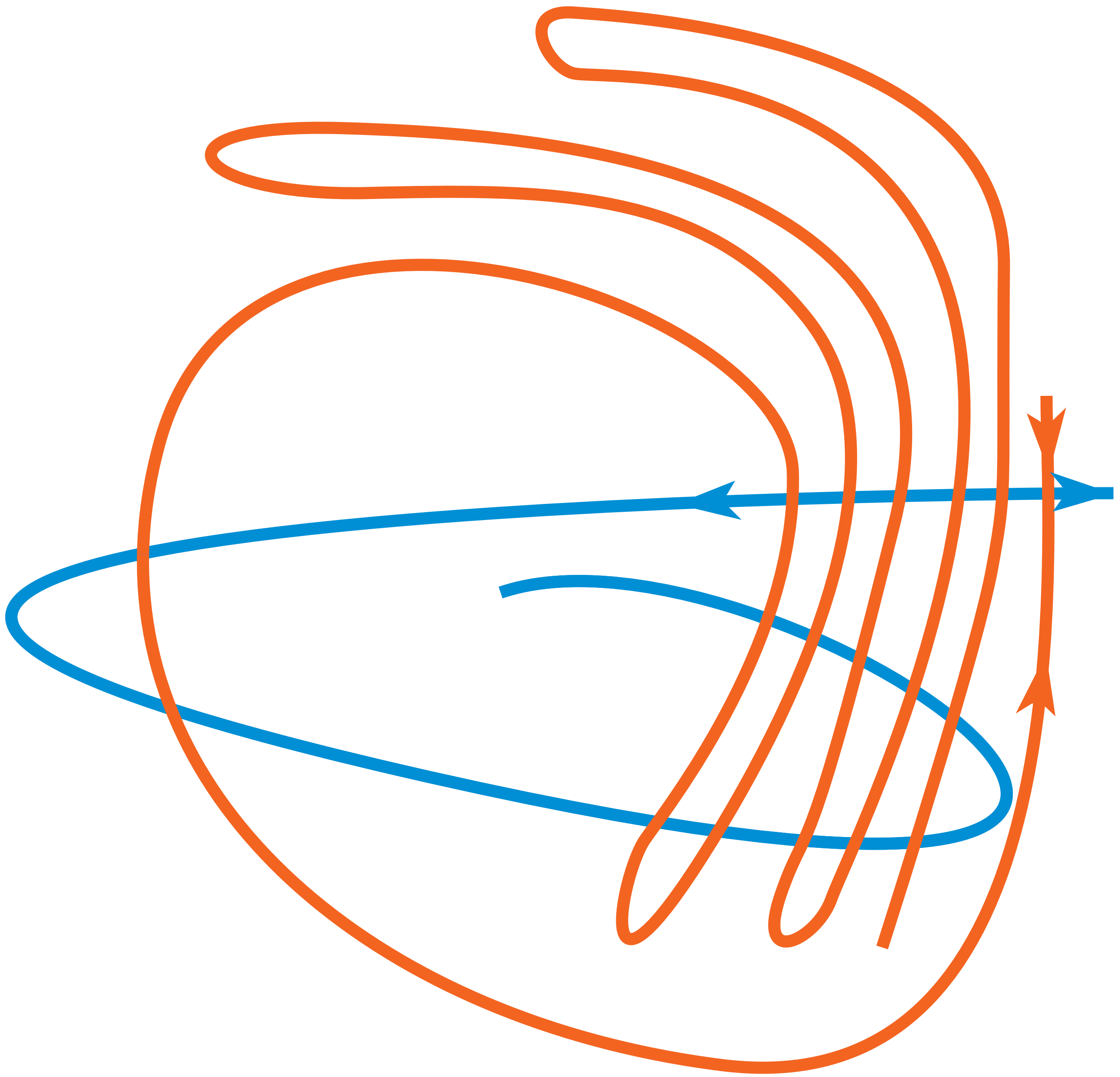
Hurricane Andrea at one snapshot; LCS shown (orange = repelling, blue = attracting)

Atmospheric flows and lobe dynamics



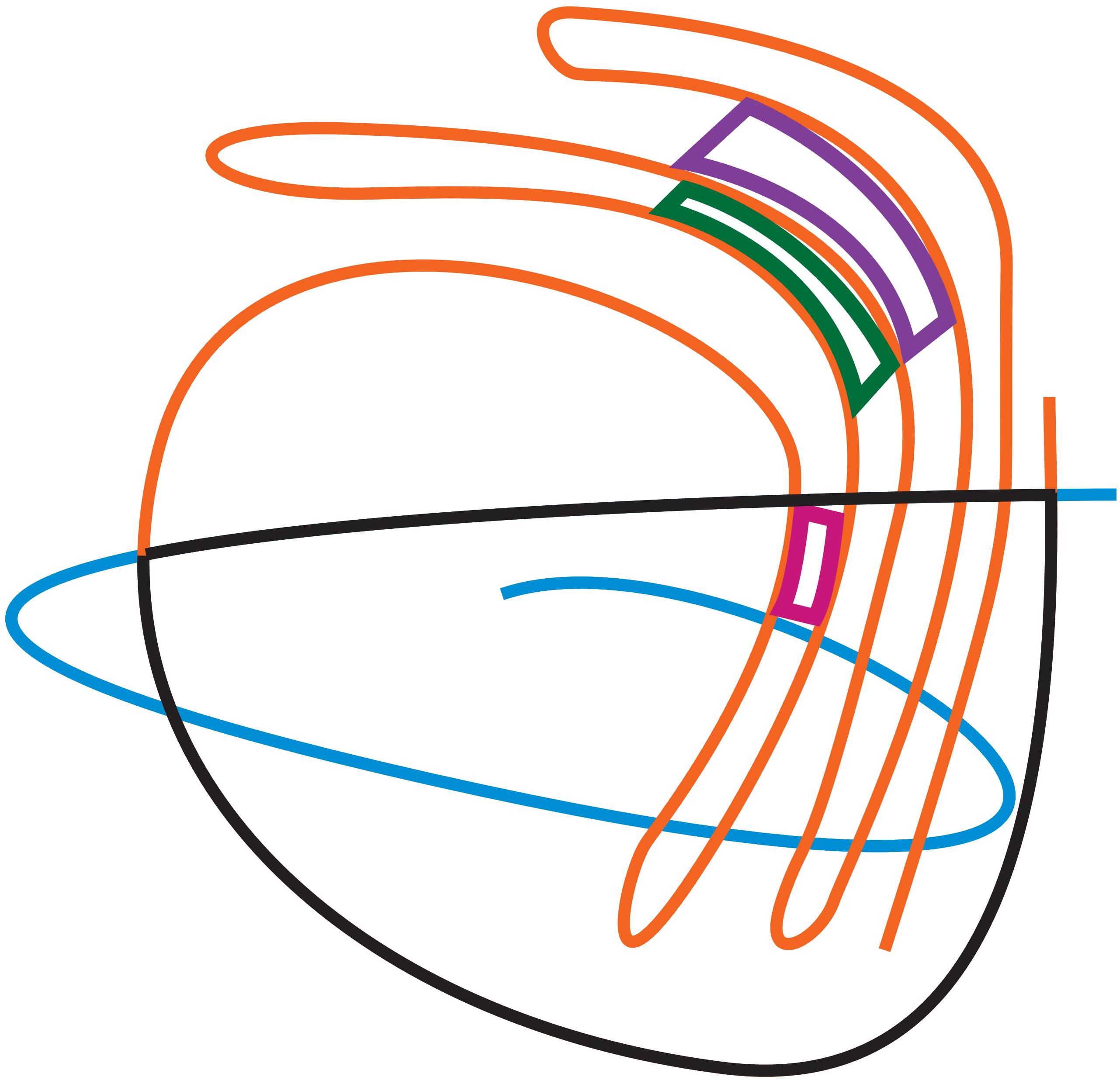
orange = repelling (stable manifold), blue = attracting (unstable manifold)

Atmospheric flows and lobe dynamics



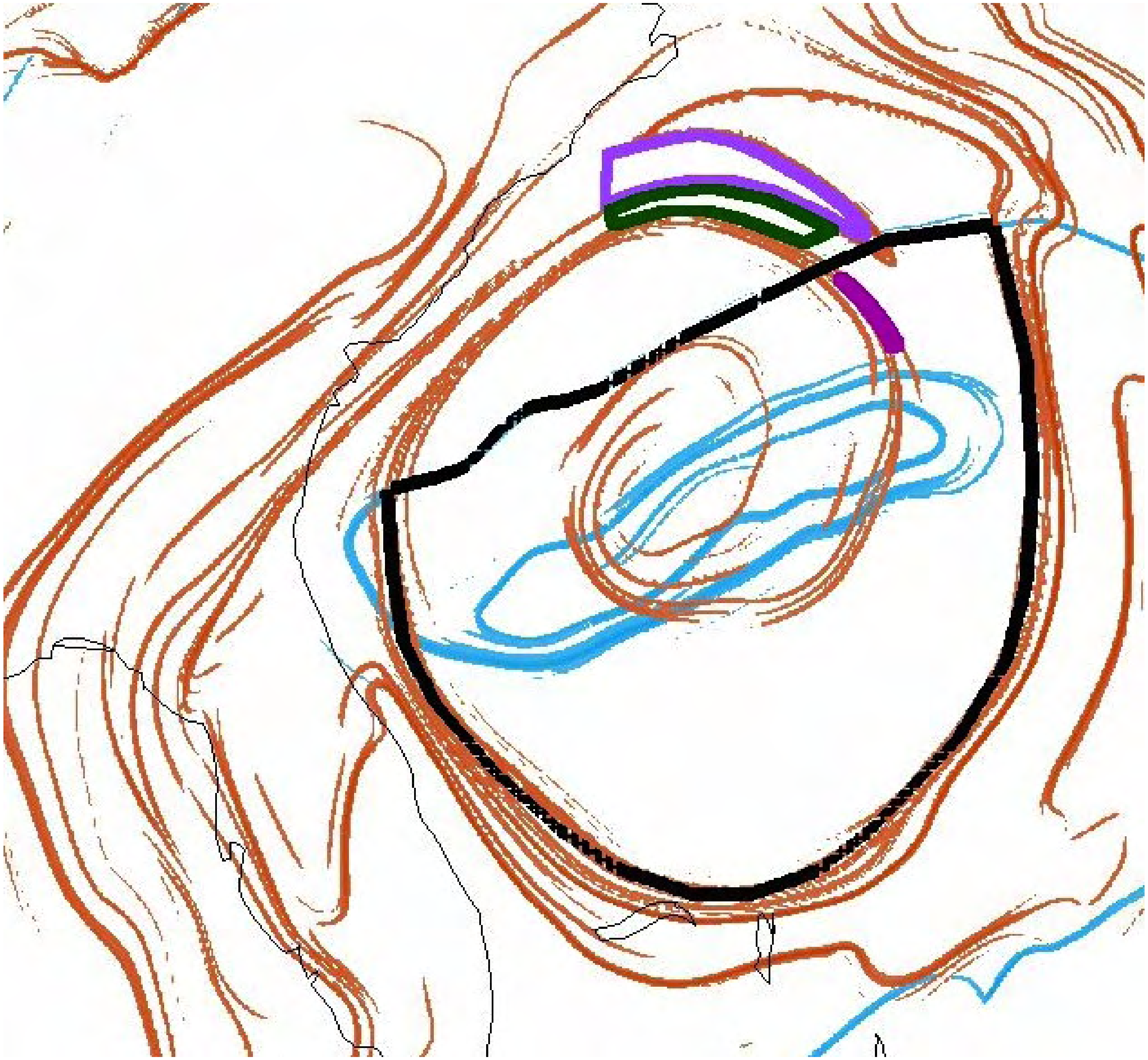
orange = repelling (stable manifold), blue = attracting (unstable manifold)

Atmospheric flows and lobe dynamics



Portions of lobes colored; magenta = outgoing, green = incoming, purple = stays out

Atmospheric flows and lobe dynamics



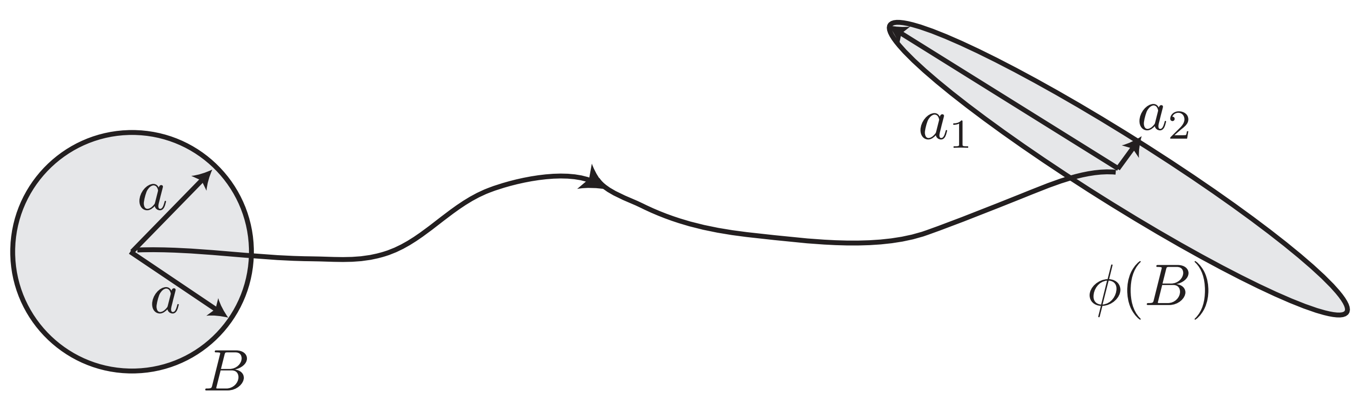
Portions of lobes colored; magenta = outgoing, green = incoming, purple = stays out

Atmospheric flows and lobe dynamics

Sets behave as lobe dynamics dictates

Coherent sets and set-based definition of FTLE

- Consider, e.g., a flow ϕ_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, $f = \frac{1}{\mu(B)}\mathcal{X}_B$, with $\mathcal{X}_B$ the characteristic function of B.
- Under the action of the flow ϕ_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.

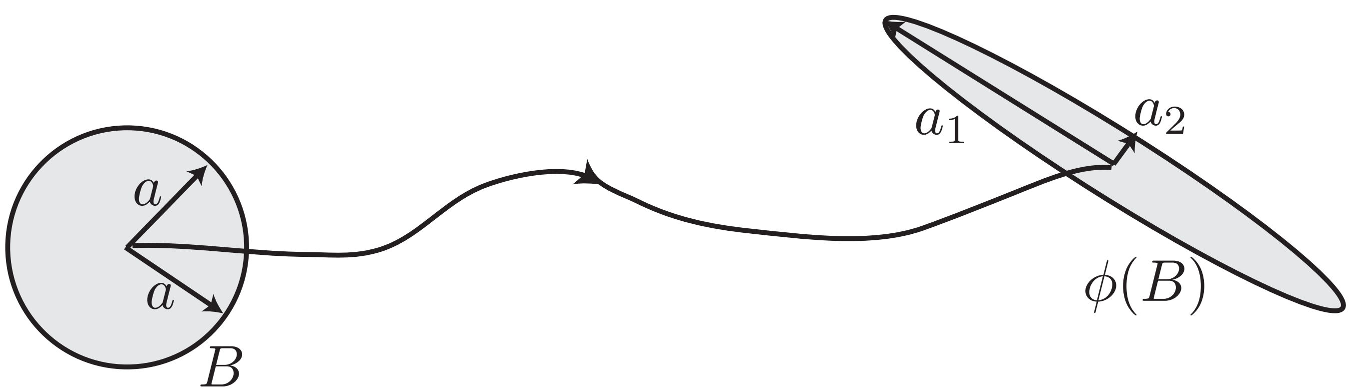


Deformation of a disk under the flow during $[t, t+T]$

Coherent sets and set-based definition of FTLE

- **Definition.** The **covariance-based FTLE** of B is
$$\sigma_I(B,t,T) = \frac{1}{|T|}\log\left(\frac{\sqrt{\lambda_{max}(I(Pf))}}{\sqrt{\lambda_{max}(I(f))}}\right).$$

- 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

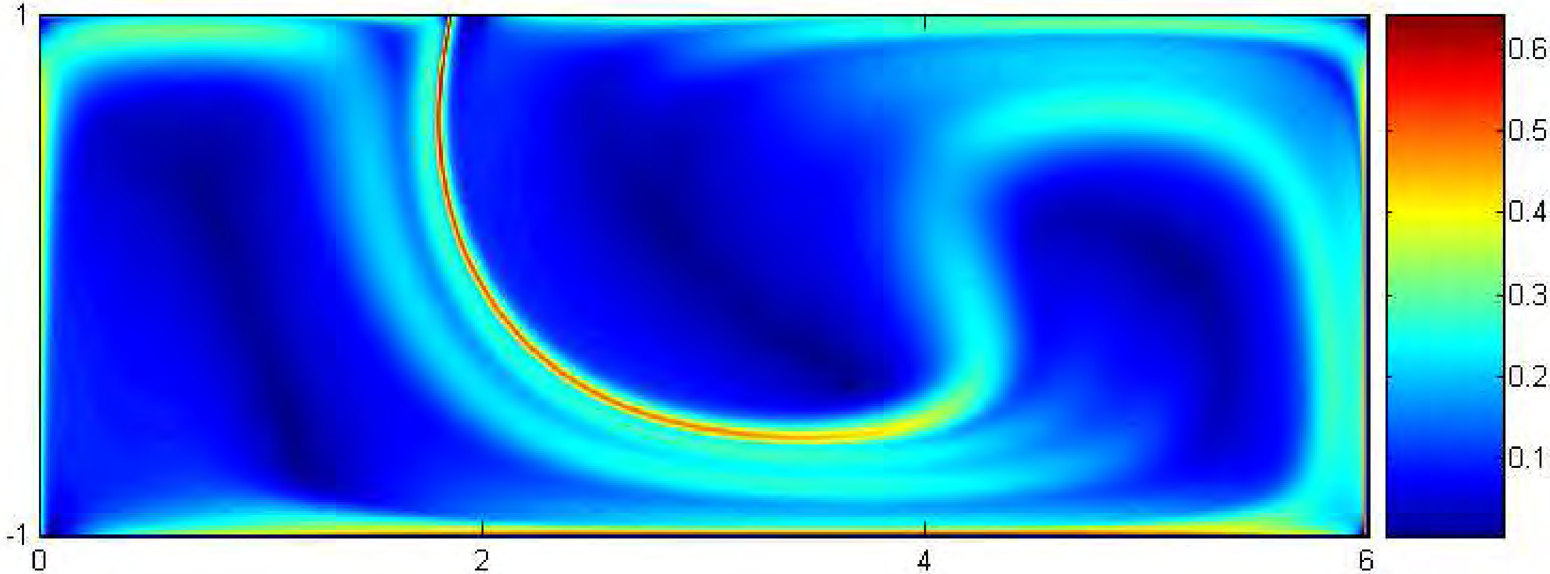
- The **coherence** of a set B during $[t, t+T]$ is $\sigma_I(B, t, T)$.
- A set B is **almost-coherent** during $[t, t+T]$ if $\sigma_I(B, t, T) \approx 0$.

- 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.

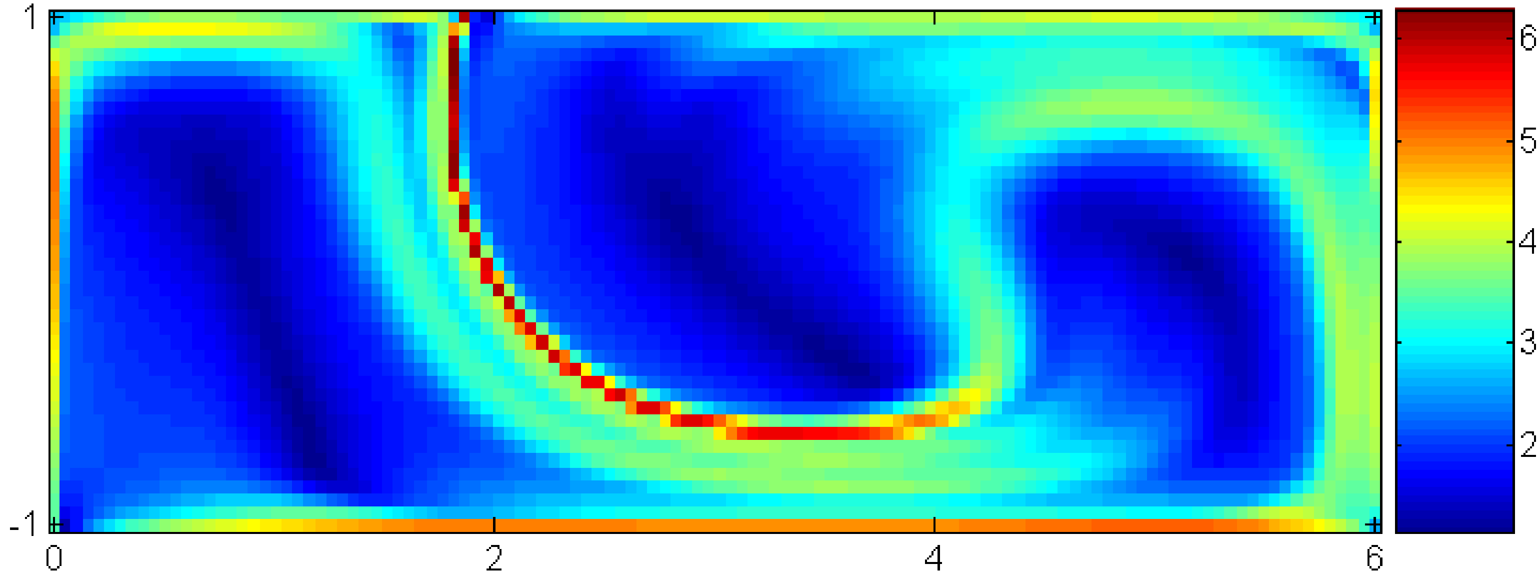
- Notice, coherent sets will be separated by ridges of high FTLE, i.e., LCS

Coherent sets in lid-driven cavity flow



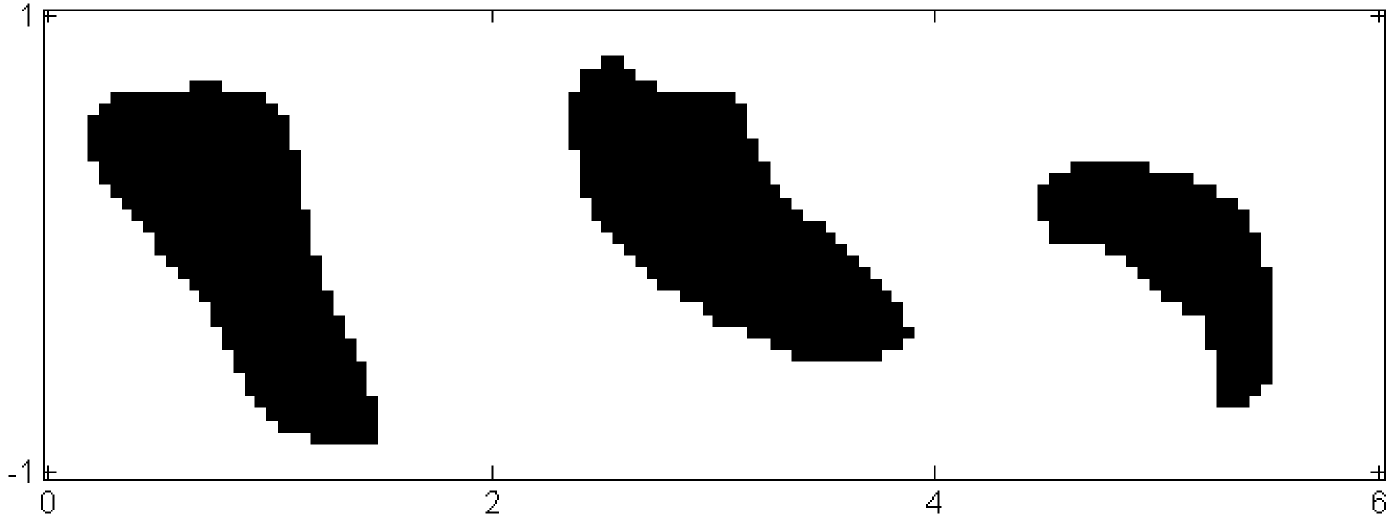
FTLE from line-stretching (conventional) during $[0, \tau_f]$

Coherent sets in lid-driven cavity flow



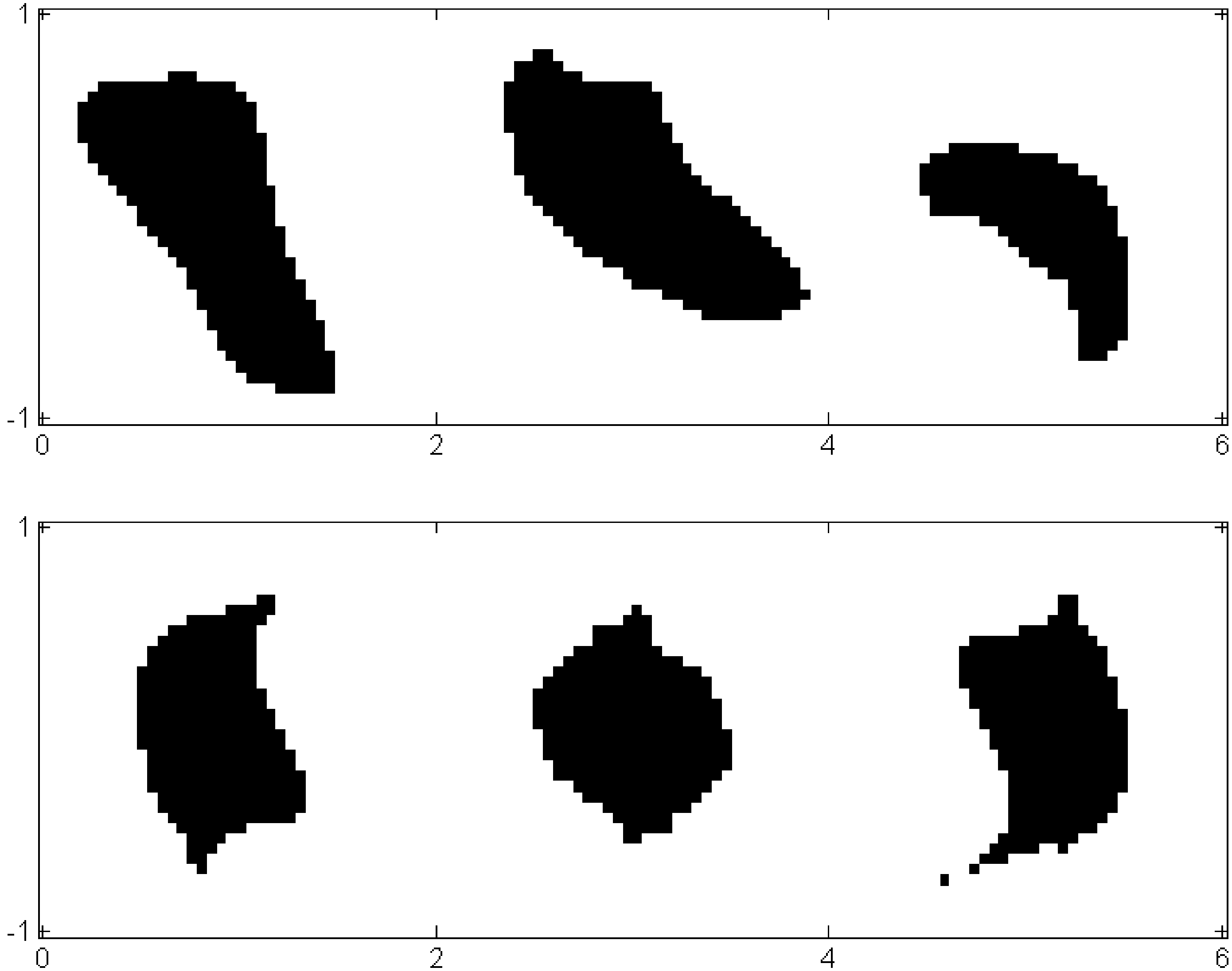
FTLE from covariance-based approach during $[0, \tau_f]$

Coherent sets in lid-driven cavity flow



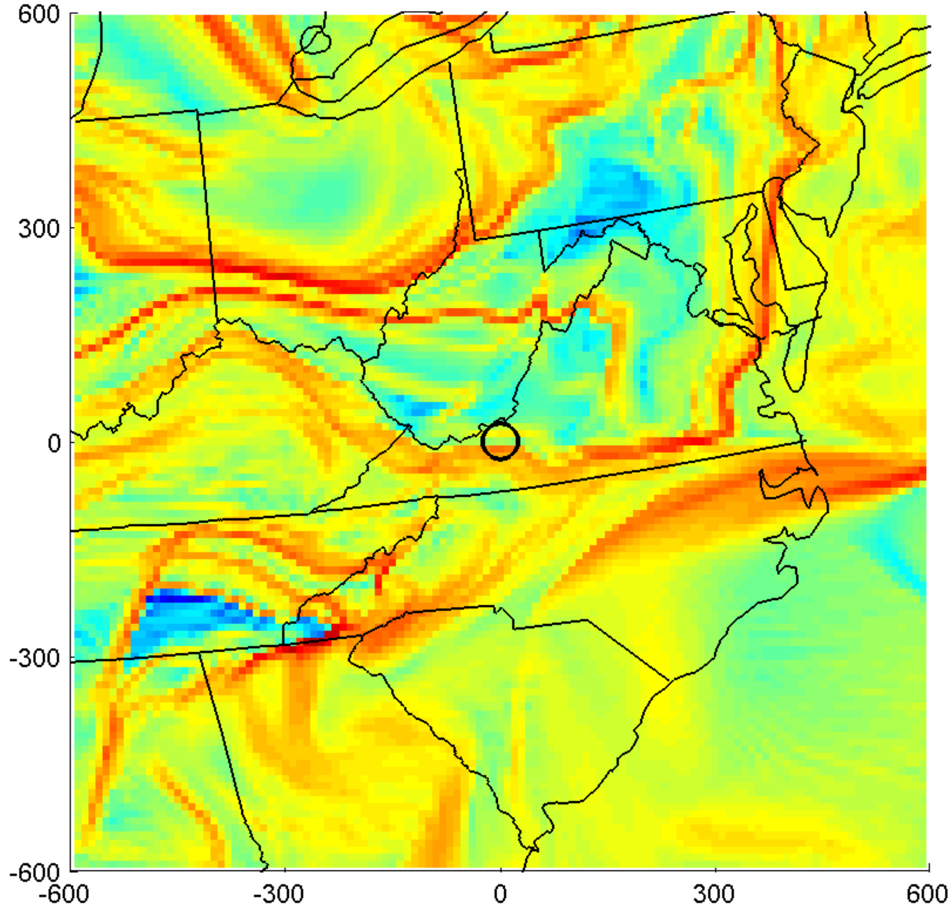
Sets of coherences $\sigma_I(0, \tau_f) < 1.6$

Coherent sets in lid-driven cavity flow



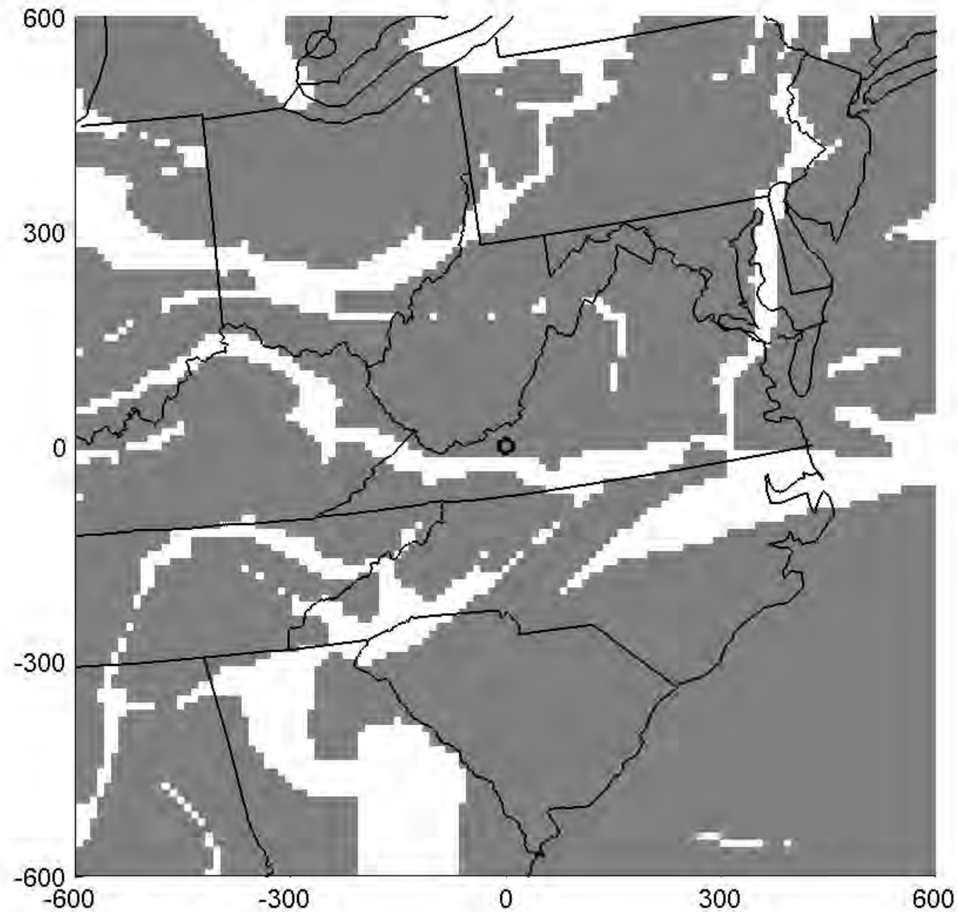
Compare with AIS from second eigenvector of P

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' $\Rightarrow$???

The End

For papers, movies, etc., visit:
www.shaneross.com

Main Papers:

- Stremler, Ross, Grover, Kumar [2011] Topological chaos and periodic braiding of almost-cyclic sets. *Physical Review Letters* 106, 114101.
- Tallapragada & Ross [2011] A geometric and probabilistic description of coherent sets. Preprint.
- Lekien & Ross [2010] The computation of finite-time Lyapunov exponents on unstructured meshes and for non-Euclidean manifolds. *Chaos* 20, 017505.
- Senatore & Ross [2011] Detection and characterization of transport barriers in complex flows via ridge extraction of the finite time Lyapunov exponent field, *International Journal for Numerical Methods in Engineering* 86, 1163.
- Grover, Ross, Stremler, Kumar [2011] Topological chaos, braiding and breakup of almost-invariant sets. Preprint.
- Tallapragada & Ross [2008] Particle segregation by Stokes number for small neutrally buoyant spheres in a fluid, *Physical Review E* 78, 036308.