Lagrangian coherent structures*

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Geometry, Mechanics and Dynamics: the Legacy of Jerry Marsden

The Fields Institute, Univ. of Toronto, July 20, 2012

(*sorry, no movies linked in this version)

MultiSTEPS: MultiScale Transport in Environmental & Physiological Systems, www.multisteps.esm.vt.edu

Motivation: application to real data

- Fixed points, periodic orbits, or other invariant sets and their stable and unstable manifolds **organize phase space**
- Many systems defined from data or large-scale simulations — experimental measurements, observations
- e.g., from fluid dynamics, biology, social sciences
- Data-based, aperiodic, finite-time, finite resolution — generally no fixed points, periodic orbits, etc. to organize phase space
- Perhaps can find appropriate analogs to the objects; adapt previous results to this setting
- Let's first look at **lobe dynamics** for analytically defined systems

Phase space transport via lobe dynamics

- Suppose our dynamical system is a discrete map[1]

$$f : \mathcal{M} \longrightarrow \mathcal{M},$$

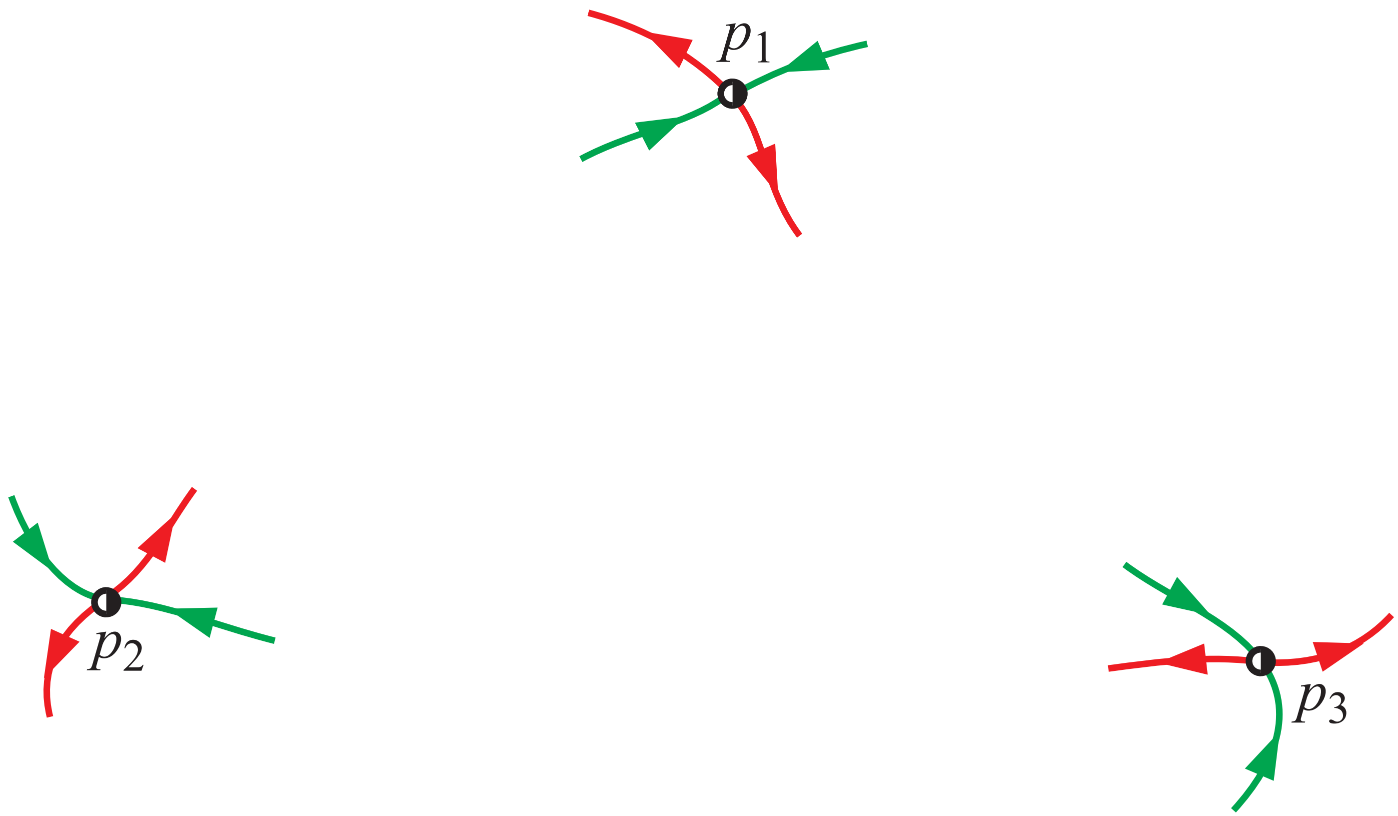
  e.g., $f = \phi_t^{t+T}$, flow map of time-periodic **vector field** and $\mathcal{M}$ is a differentiable, orientable, two-dimensional manifold e.g., $\mathbb{R}^2$, S^2

- To understand the transport of points under the f, consider **invariant manifolds of unstable fixed points**
  - Let $p_i, i = 1, ..., N_p$, denote saddle-type hyperbolic fixed points of f.

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

Partition phase space into regions

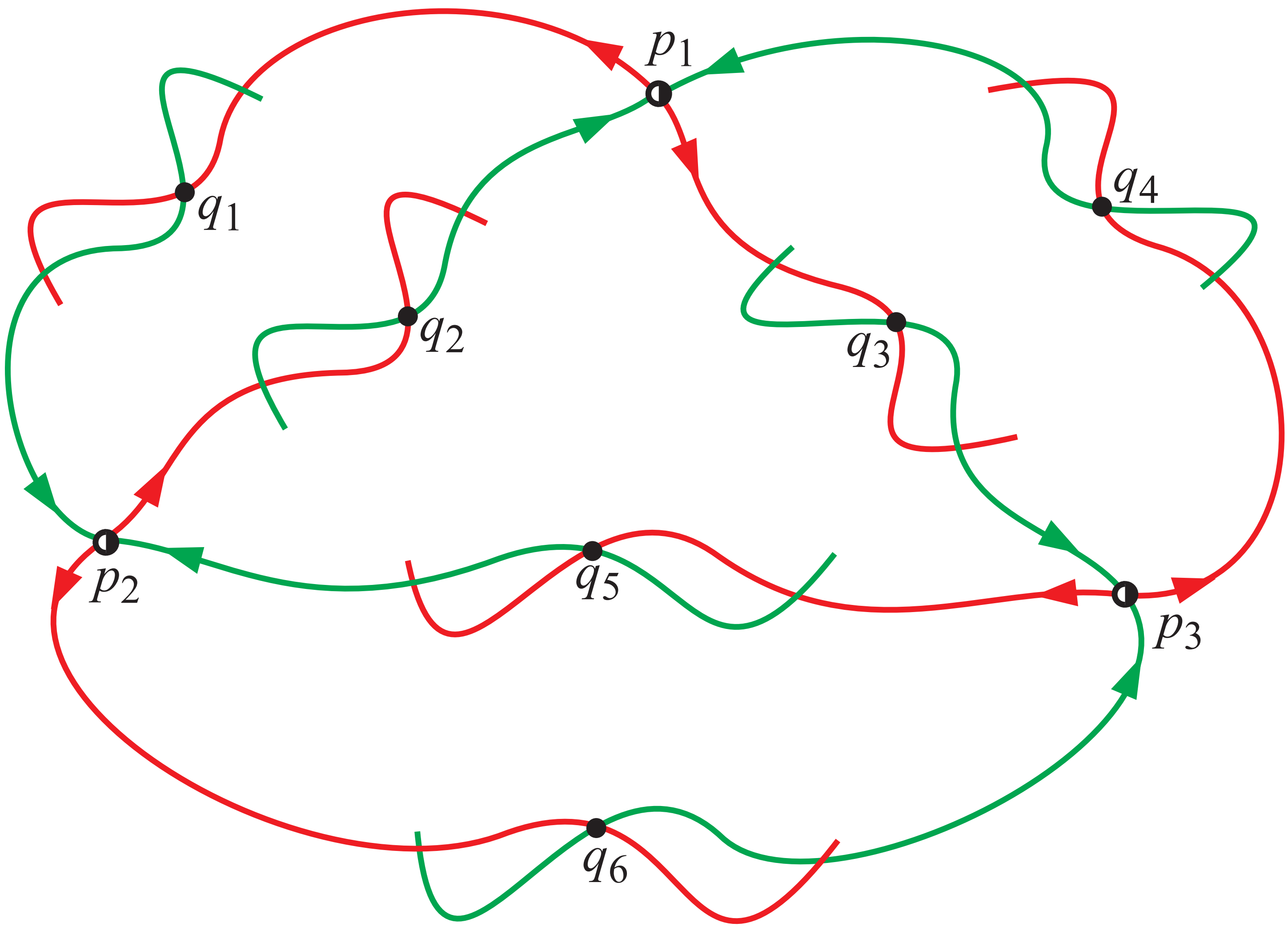
- Natural way to partition phase space
  - Pieces of $W^u(p_i)$ and $W^s(p_i)$ partition $\mathcal{M}$.



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

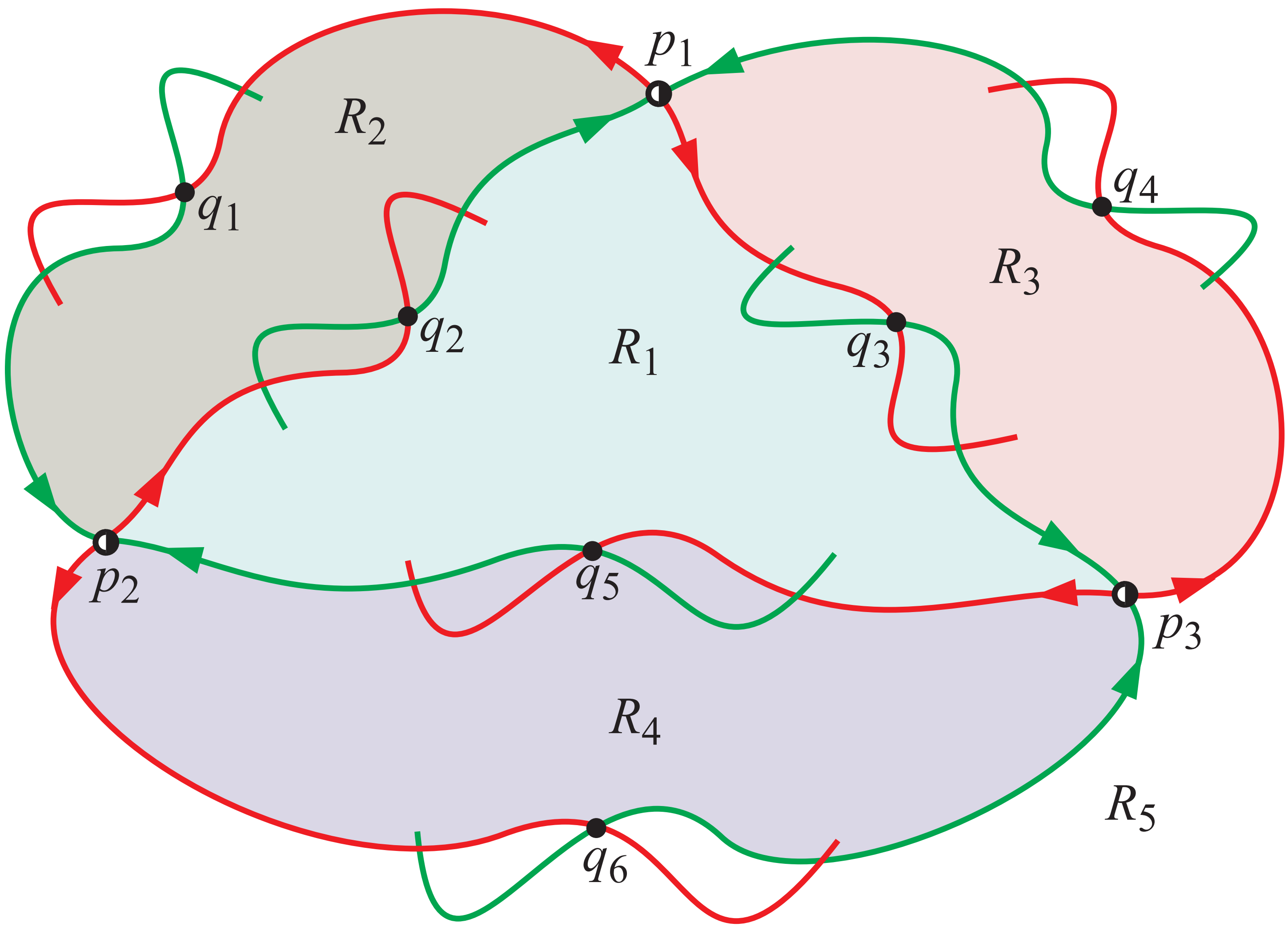
Partition phase space into regions

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



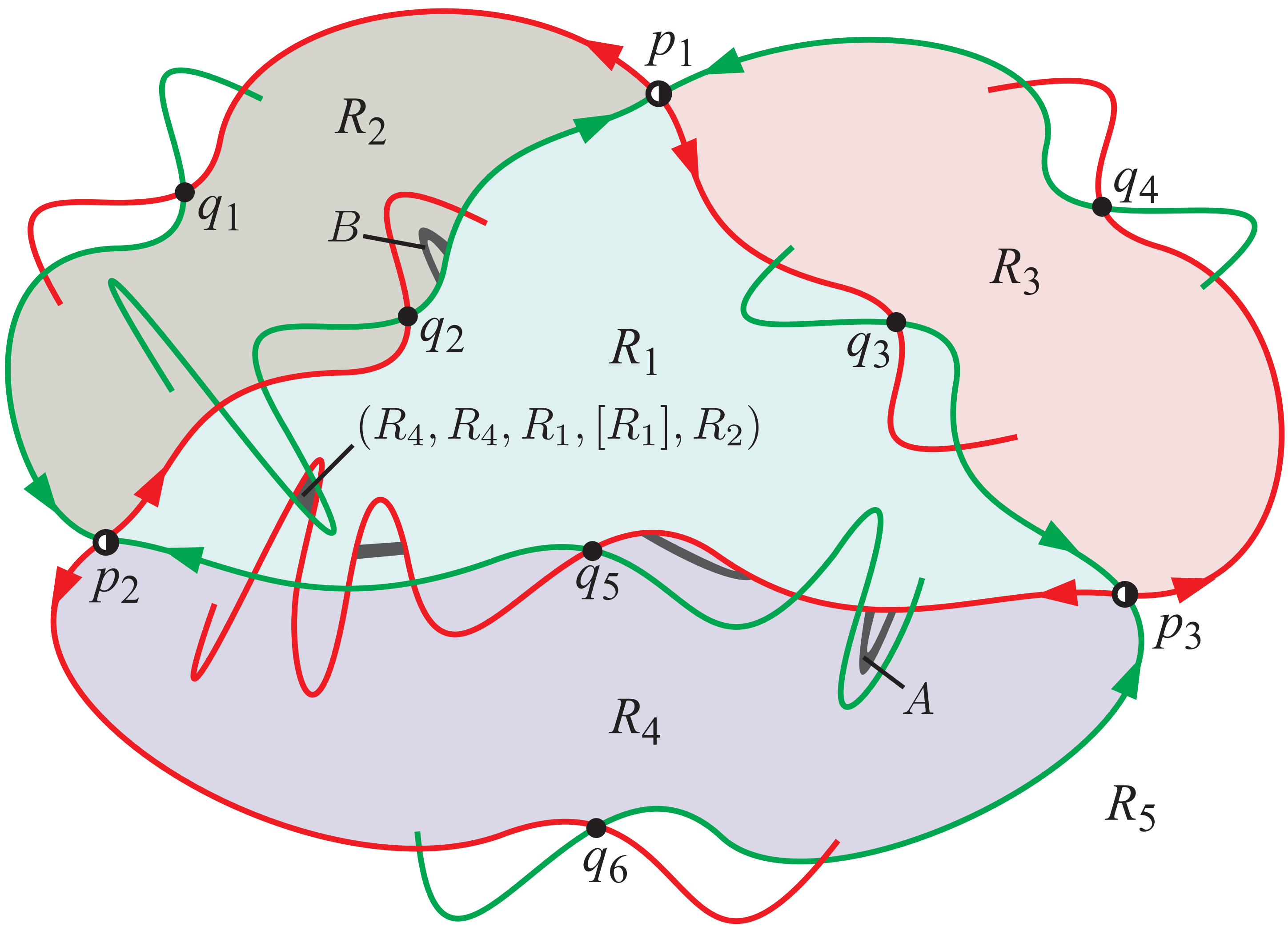
Partition phase space into regions

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



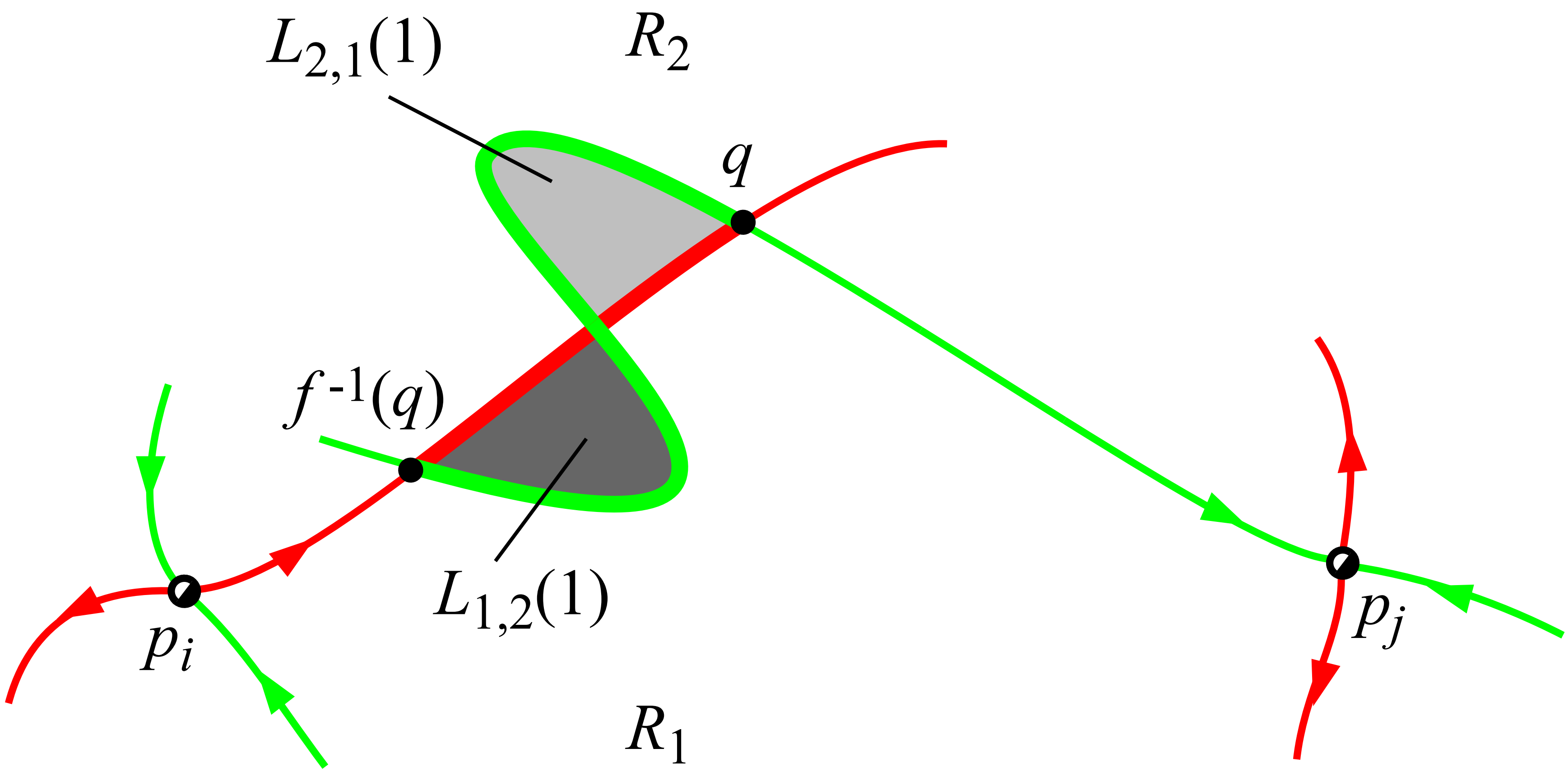
Label mobile subregions: ‘atoms’ of transport

- Can label mobile subregions based on their past and future whereabouts under one iterate of the map, e.g., $(\ldots, R_4, R_4, R_1, [R_1], R_2, \ldots)$



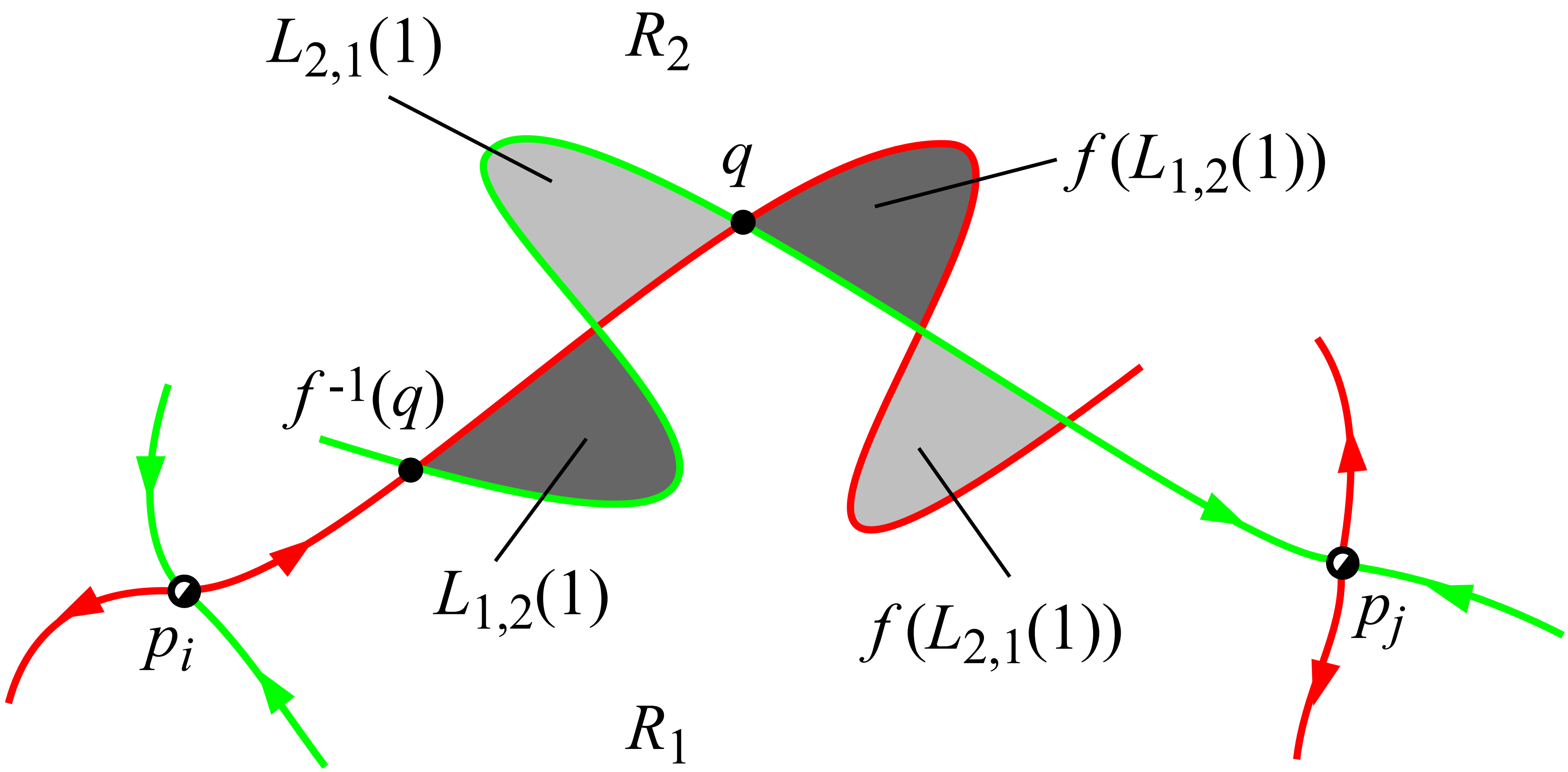
Lobe dynamics: transport across a boundary

- $W^u[f^{-1}(q), q] \bigcup W^s[f^{-1}(q), q]$ 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 $L_{2,1}(1)$



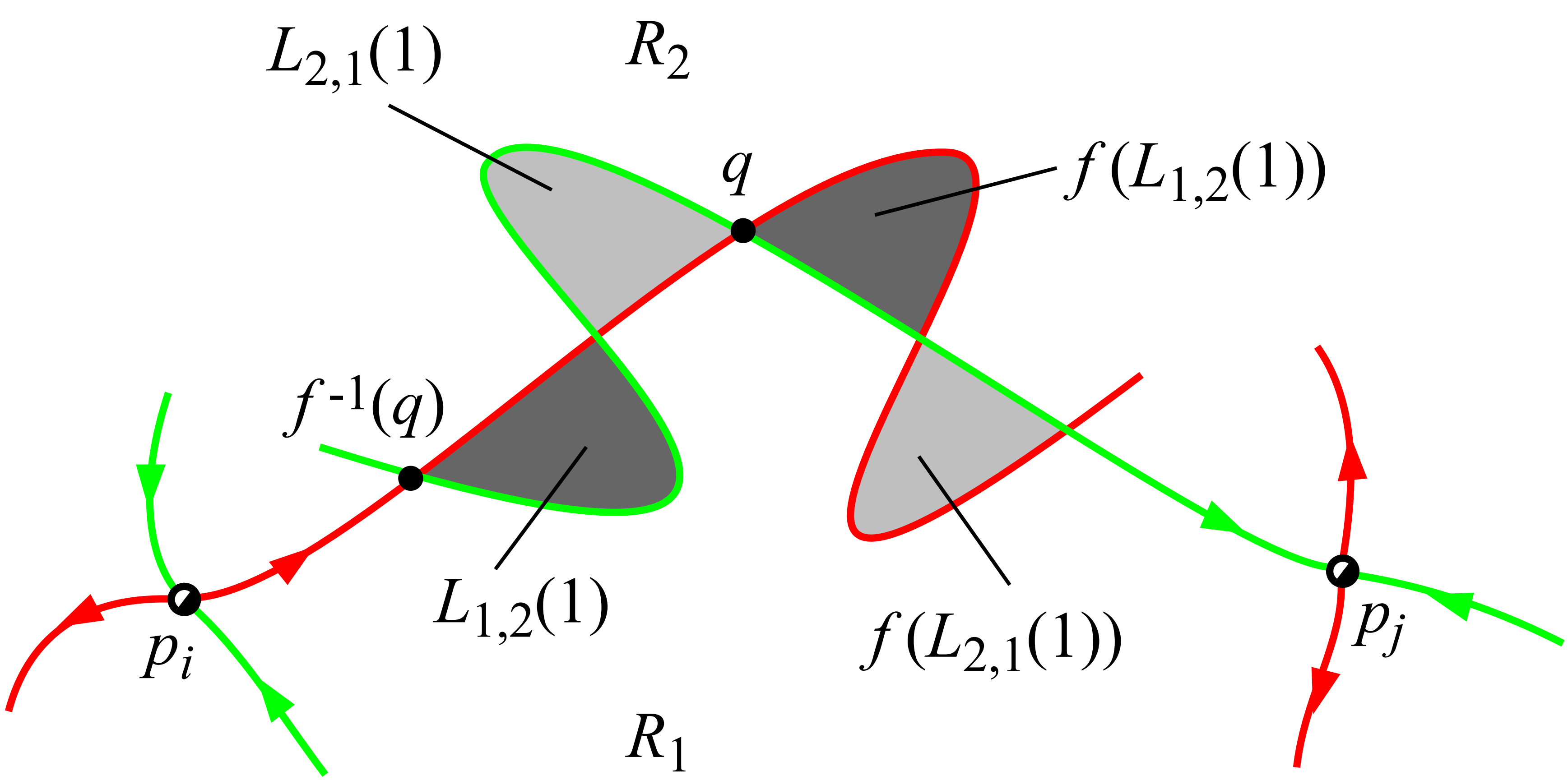
Lobe dynamics: transport across a boundary

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



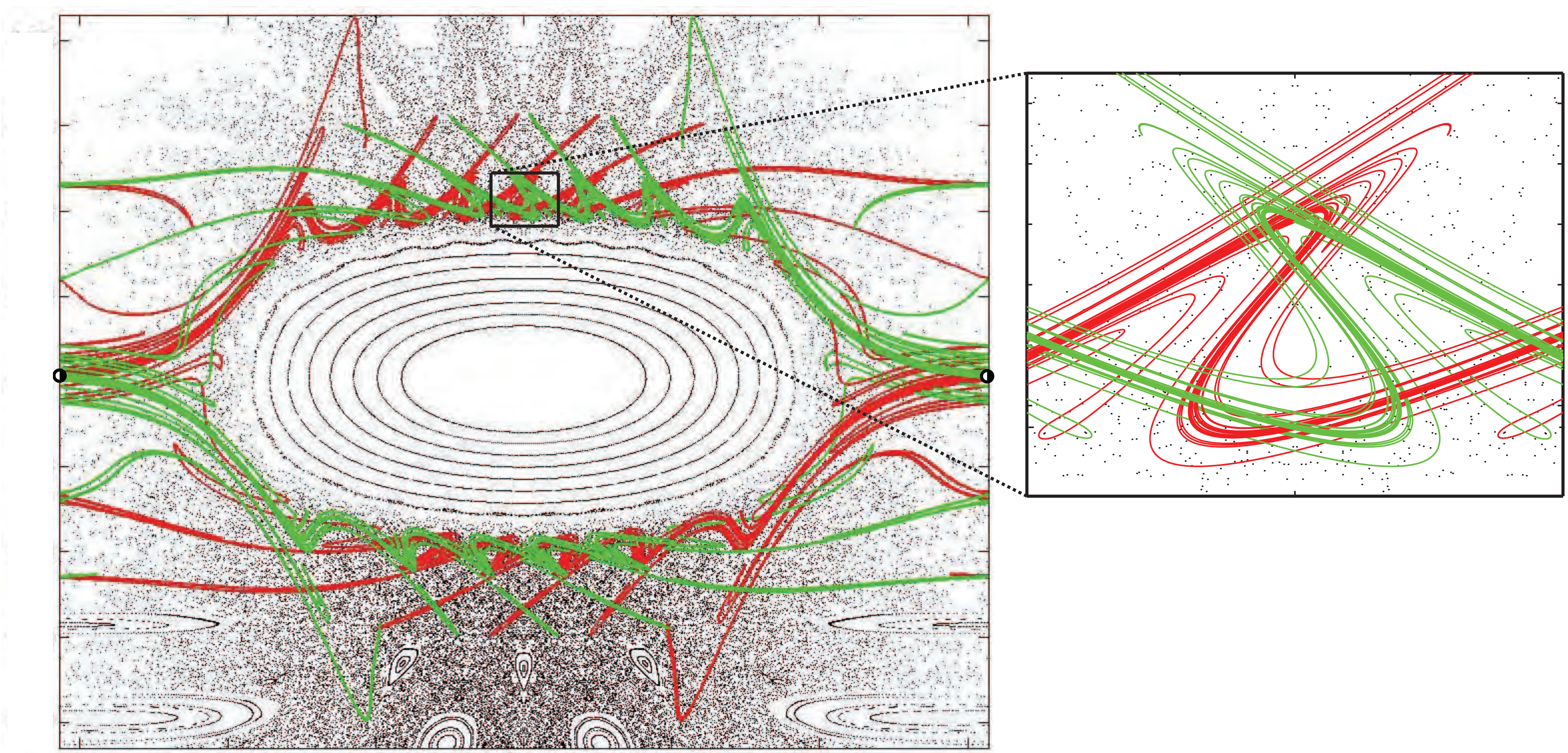
Lobe dynamics: transport across a boundary

- Essence of lobe dynamics: **dynamics associated with crossing a boundary is reduced to the dynamics of turnstile lobes associated with the boundary.**



Identifying 'atoms' of transport by itinerary

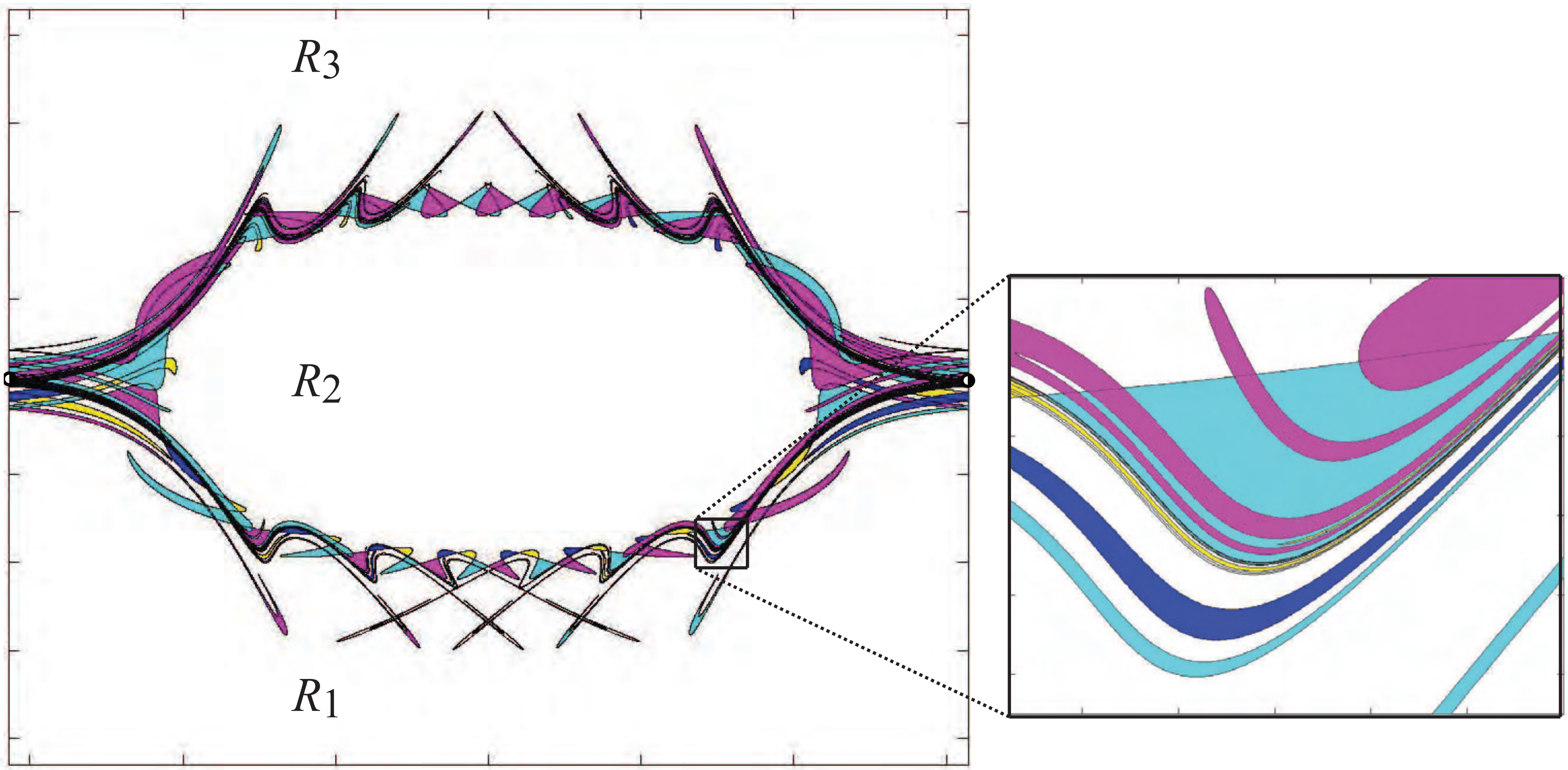
- In a complicated system, can still identify manifolds ...



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

Identifying 'atoms' of transport by itinerary

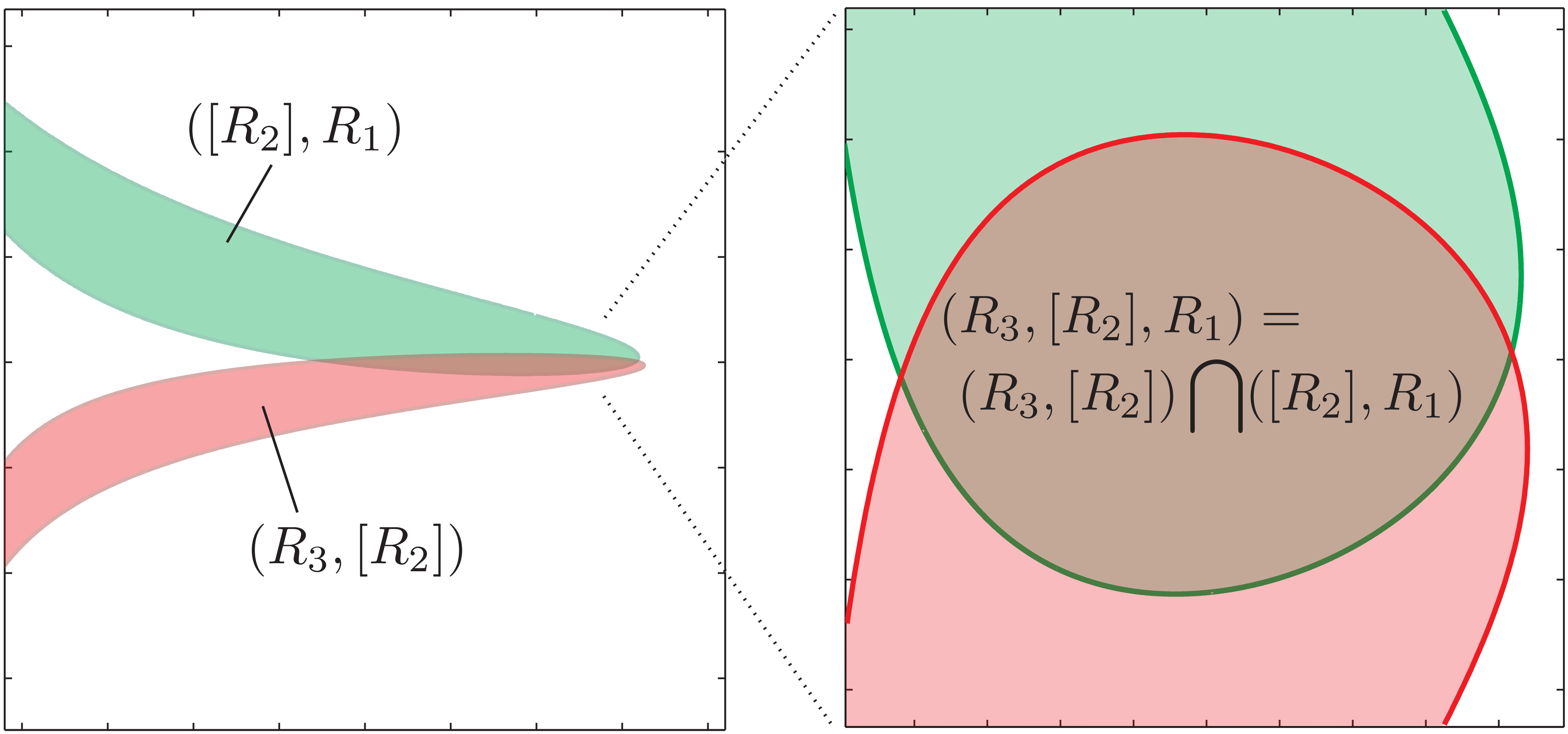
- ... and lobes



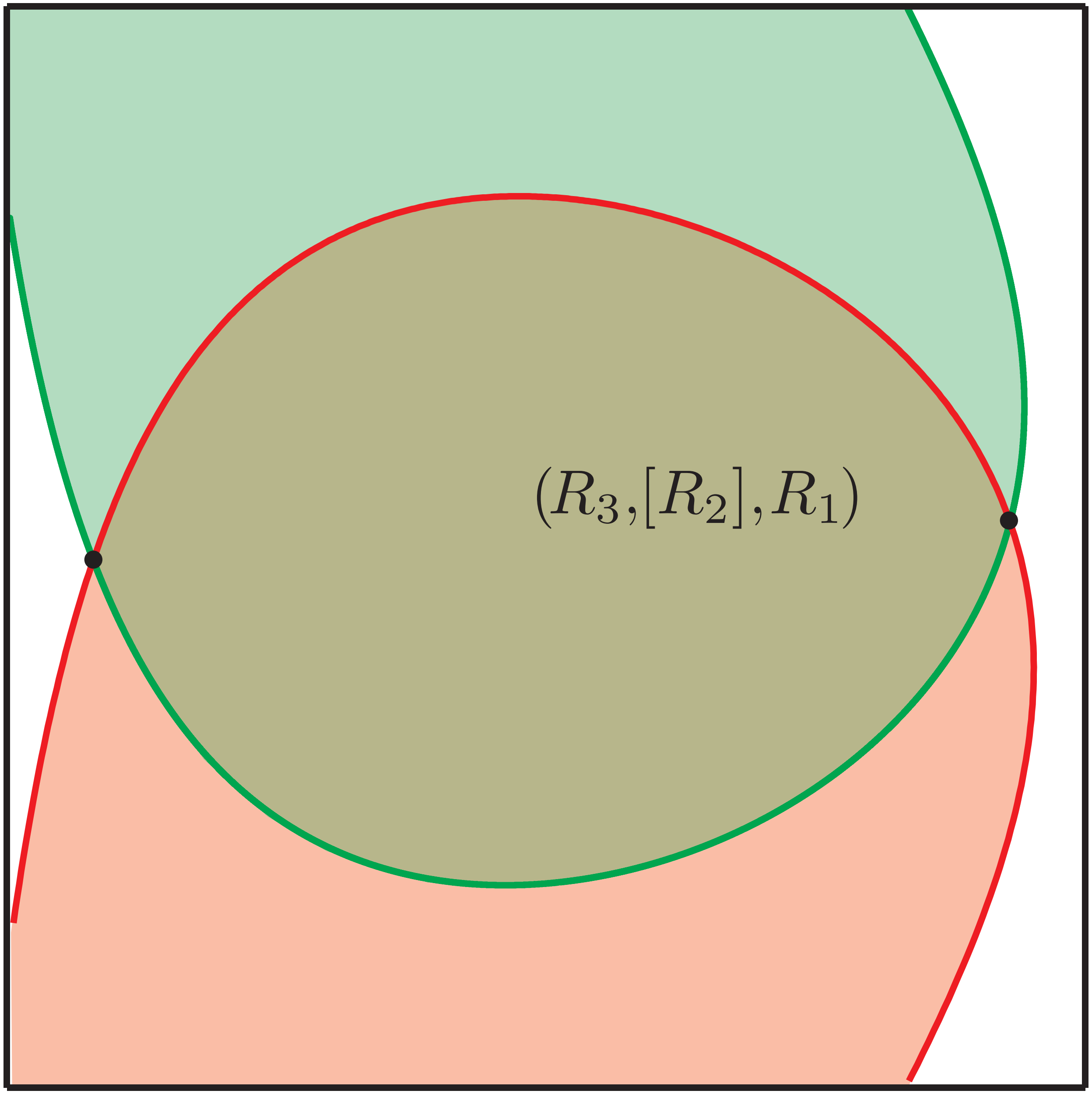
Significant amount of fine, filamentary structure.

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 $(R_3, [R_2], R_1)$

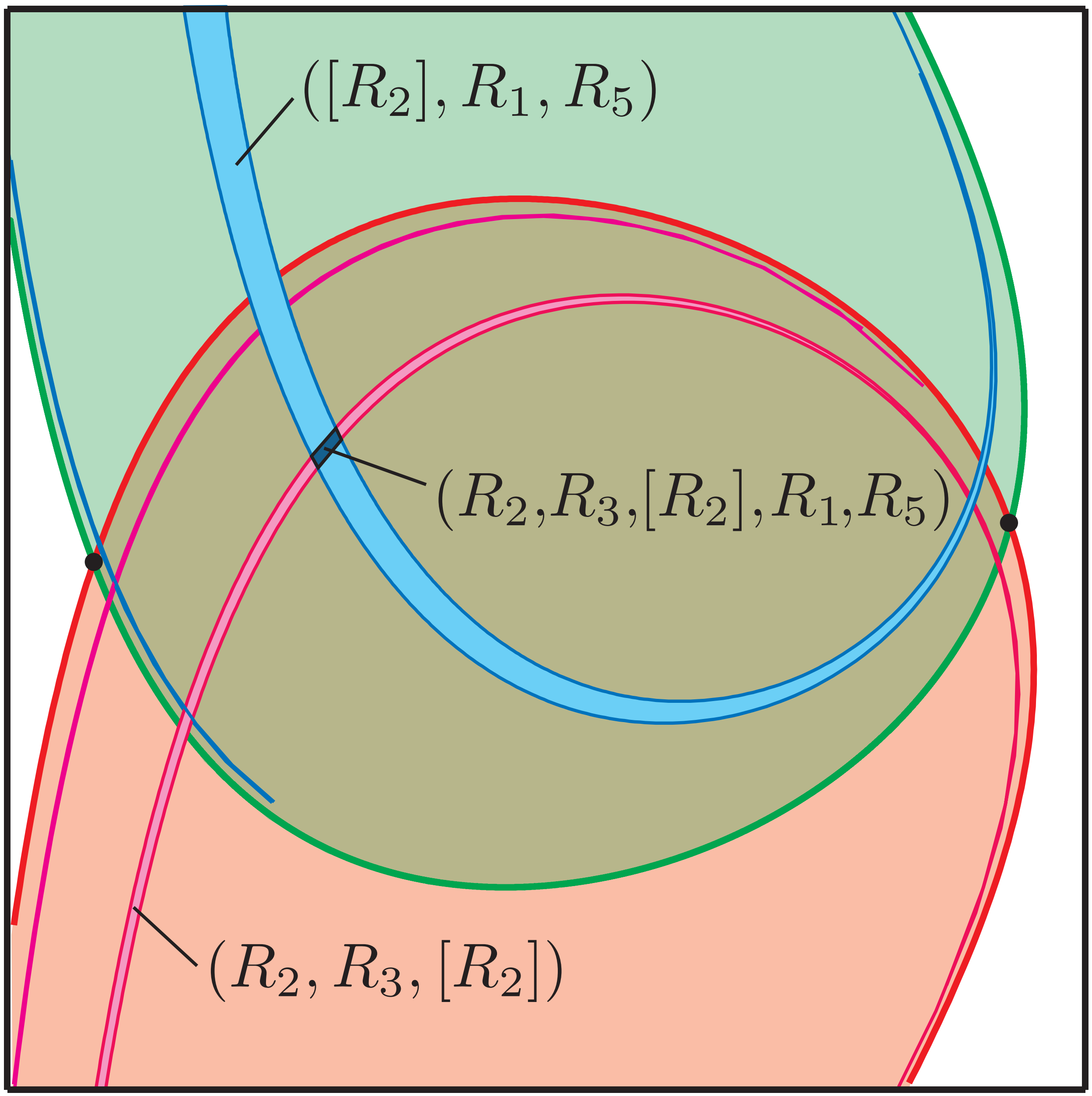


Identifying ‘atoms’ of transport by itinerary



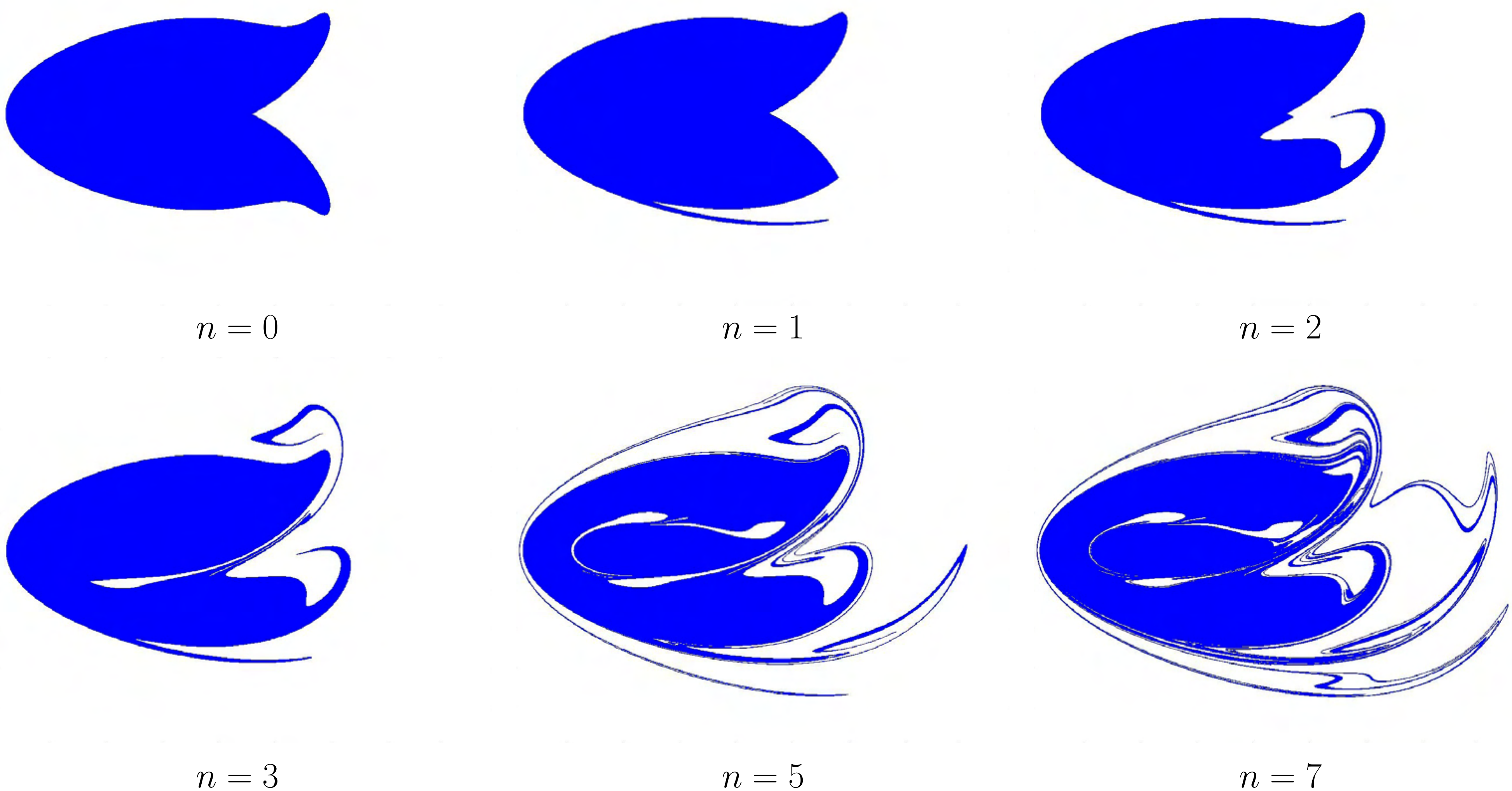
Longer itineraries...

Identifying 'atoms' of transport by itinerary



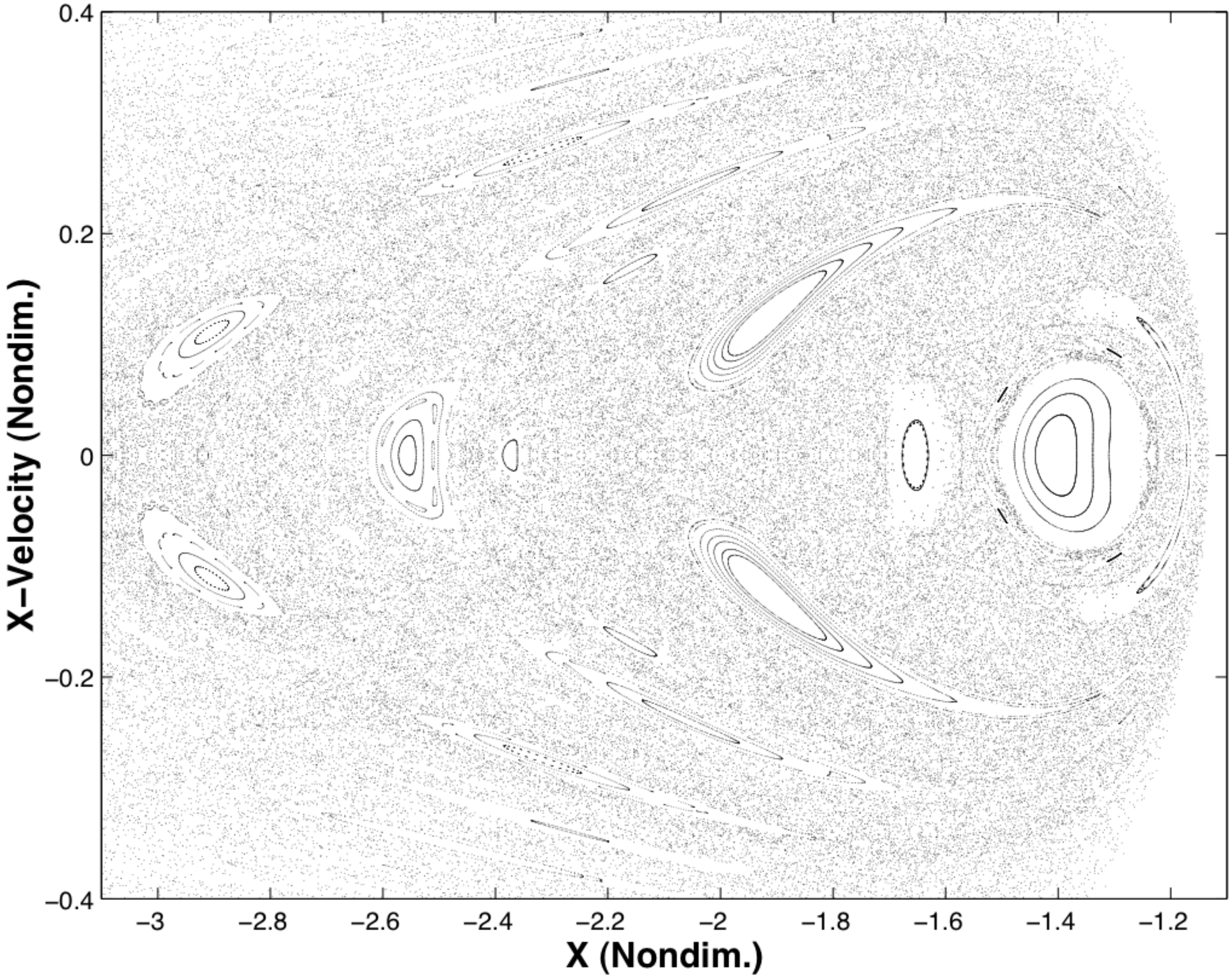
... correspond to smaller pieces of phase space; symbolic dynamics, horseshoes, etc

Lobe dynamics intimately related to transport

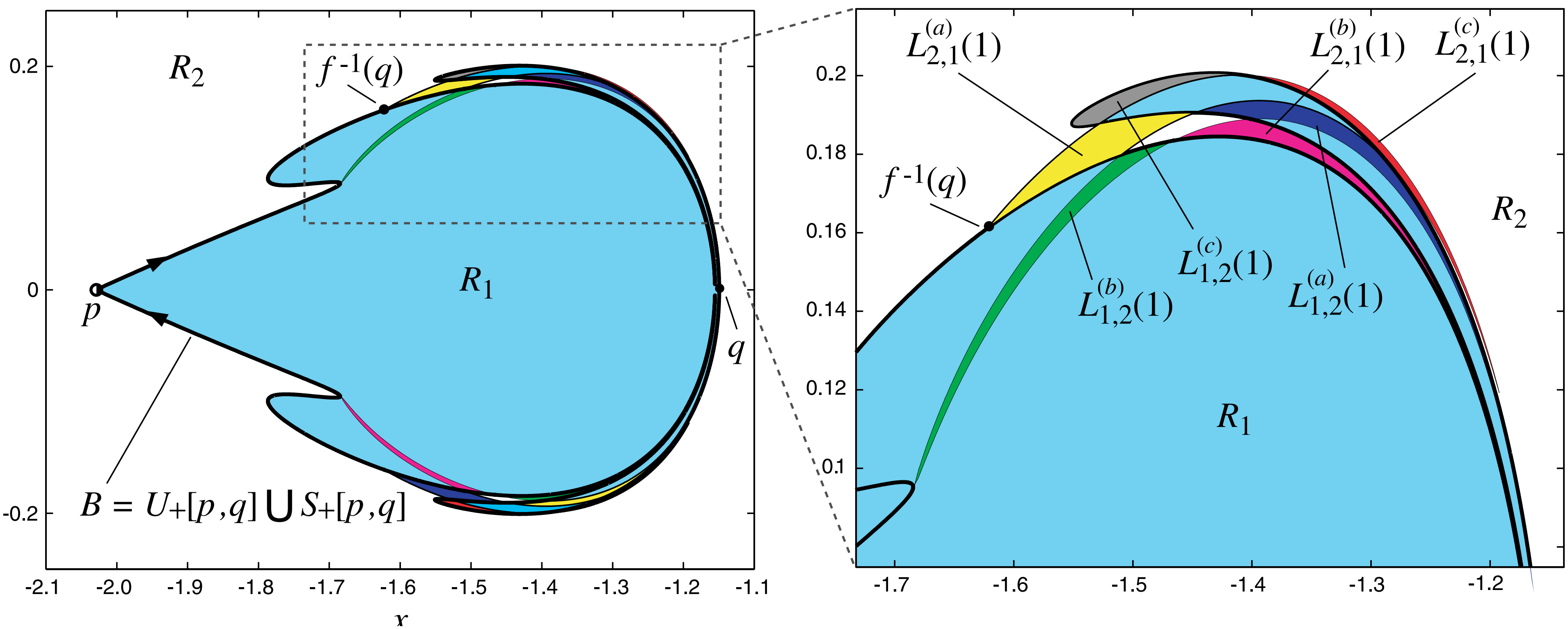


Lobe Dynamics: example

- Restricted 3-body problem: chaotic sea has unstable fixed points.



Compute a boundary

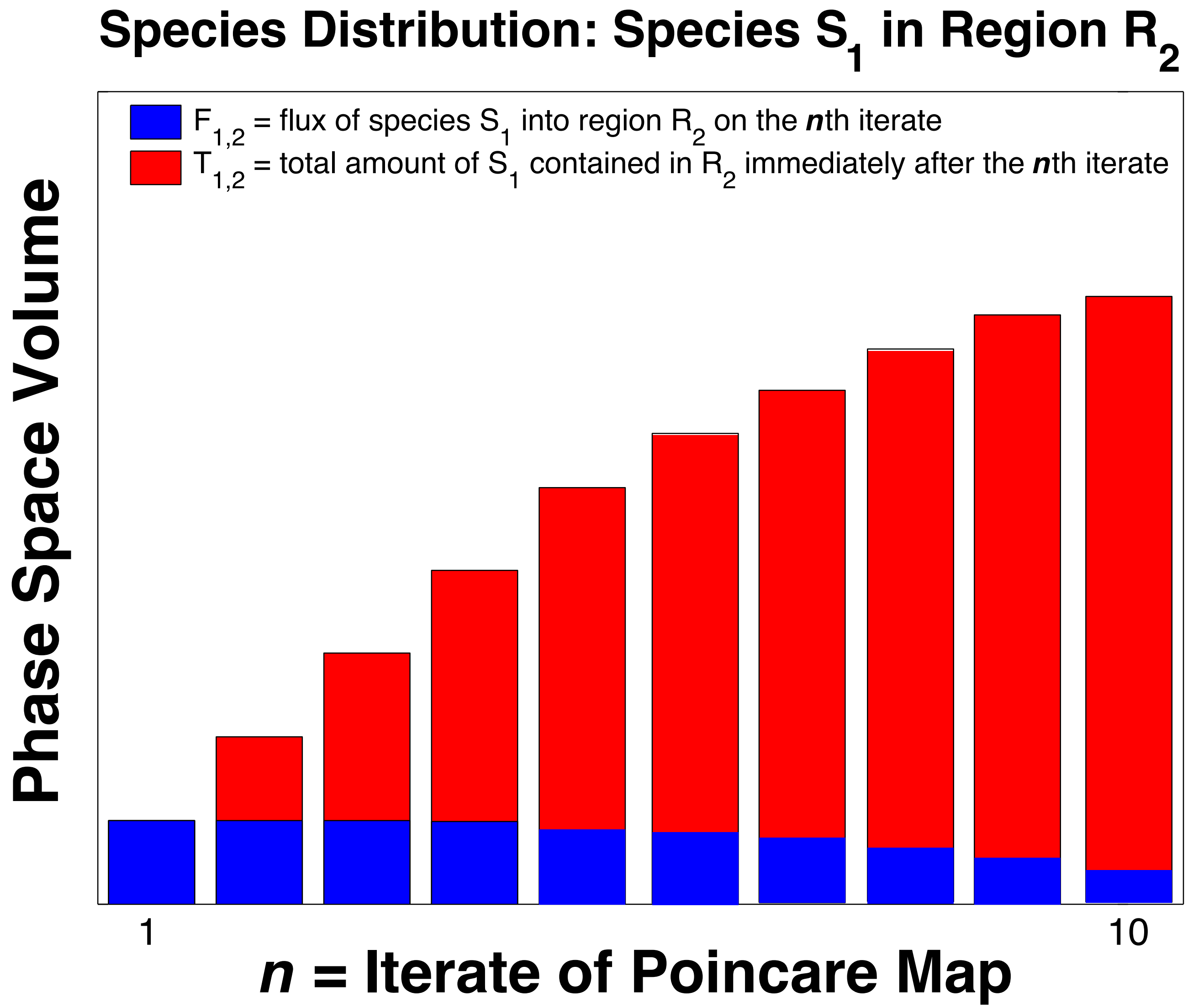


Transport between two regions

- The evolution of a lobe of species S_1 into R_2

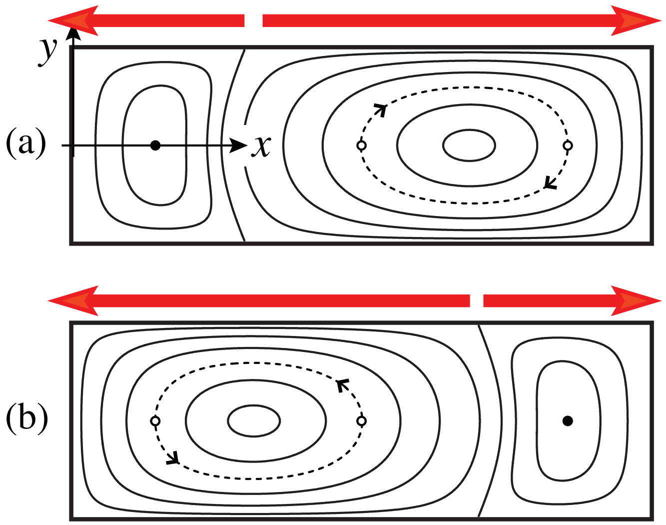
Dellnitz, Junge, Lo, Marsden, Padberg, Preis, Ross, Thiere [2005] Physical Review Letters

Transport between two regions



Lobe dynamics: fluid example

□ Fluid example: time-periodic Stokes flow



streamlines for $\tau_f = 1$

tracer blob $(\tau_f > 1)$

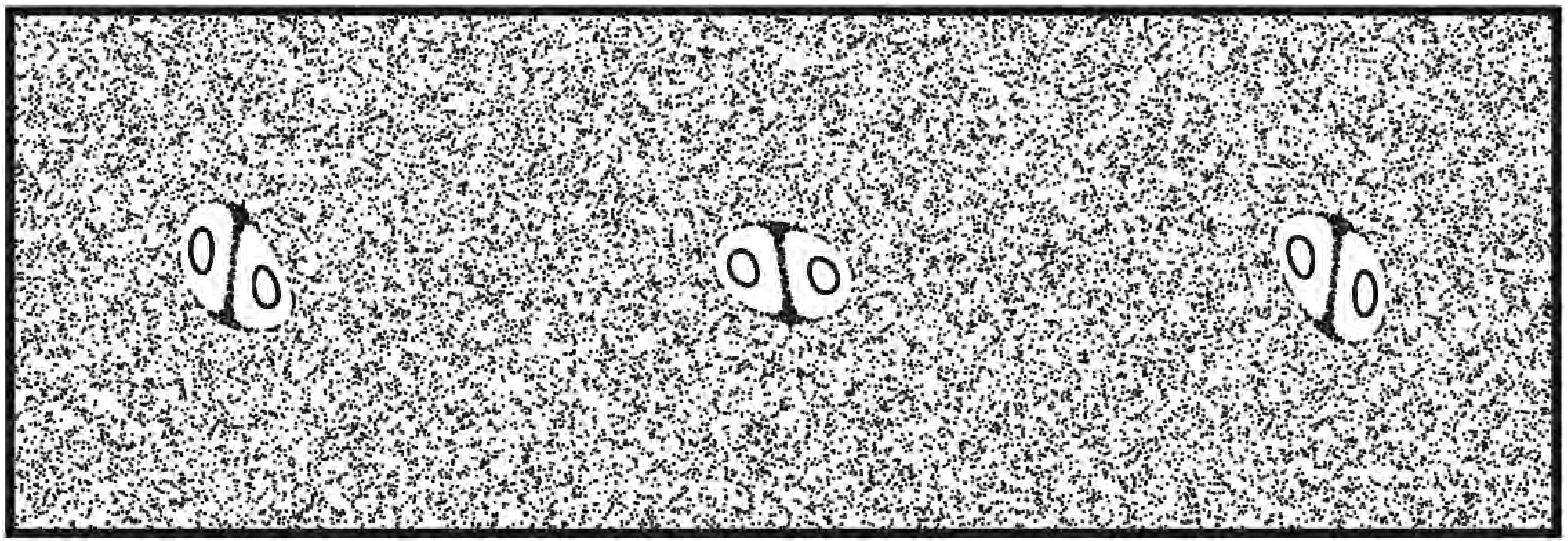
Lid-driven cavity flow

- 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

Lobe dynamics: fluid example

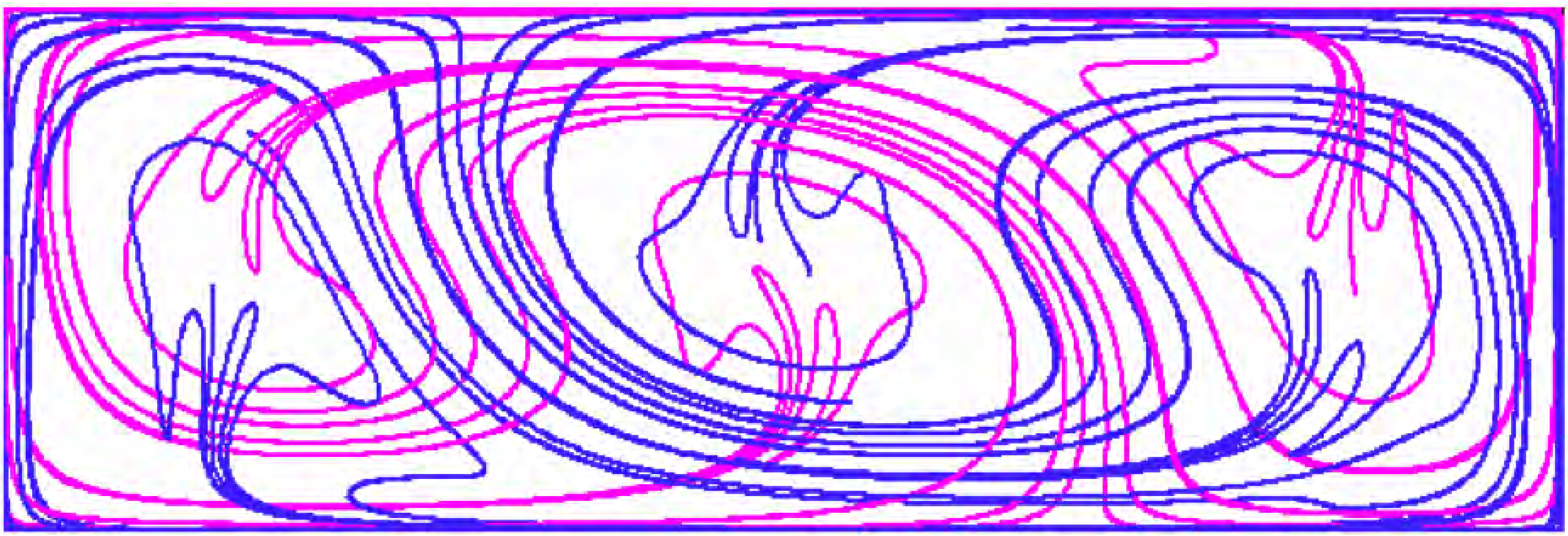
- Poincaré map for $\tau_f > 1$



period-3 points bifurcate into groups of elliptic and saddle points, each of period 3

Lobe dynamics: fluid example

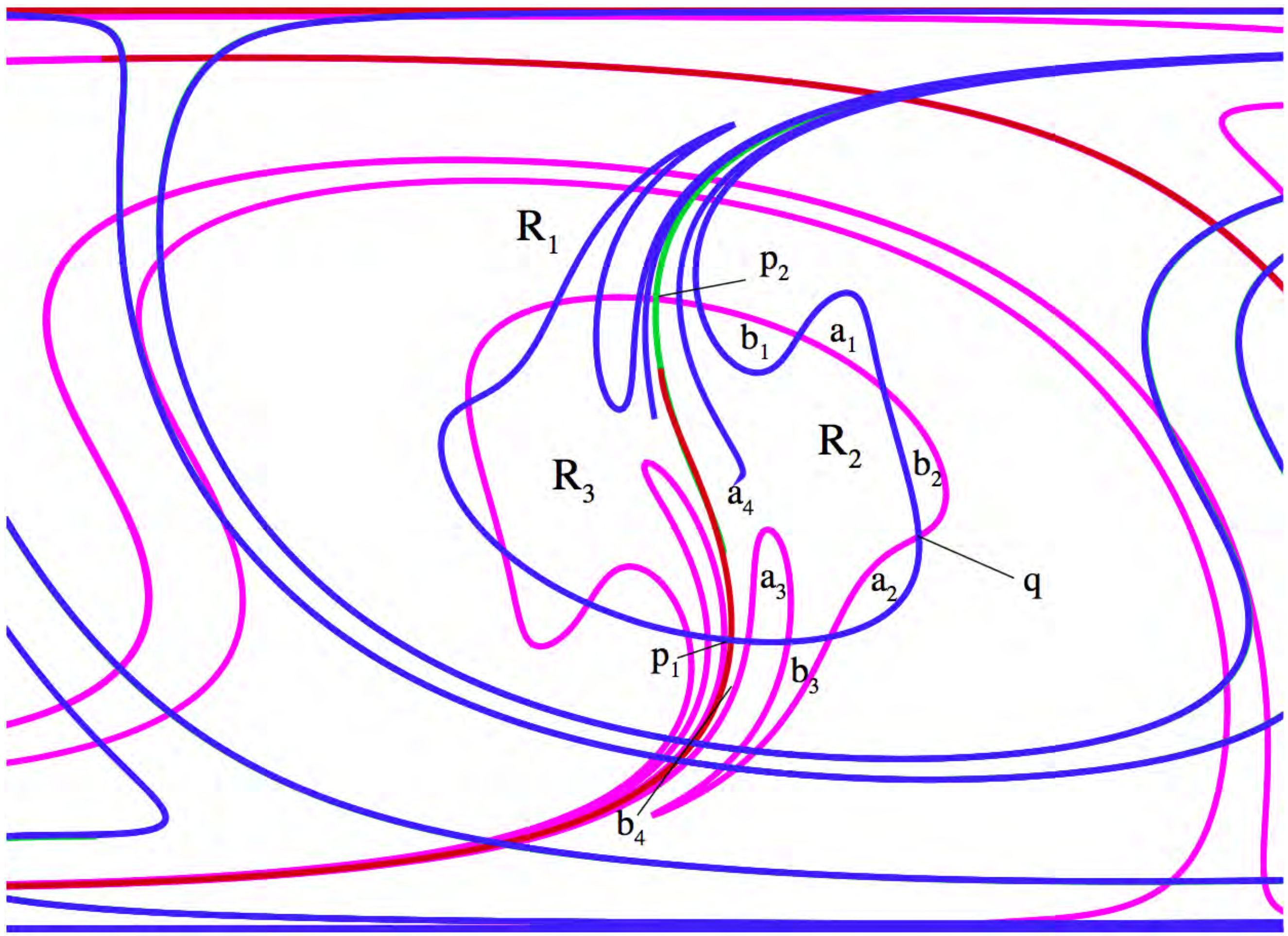
- Structure associated with saddles



some invariant manifolds of saddles

Lobe dynamics: fluid example

- Can consider transport via **lobe dynamics**

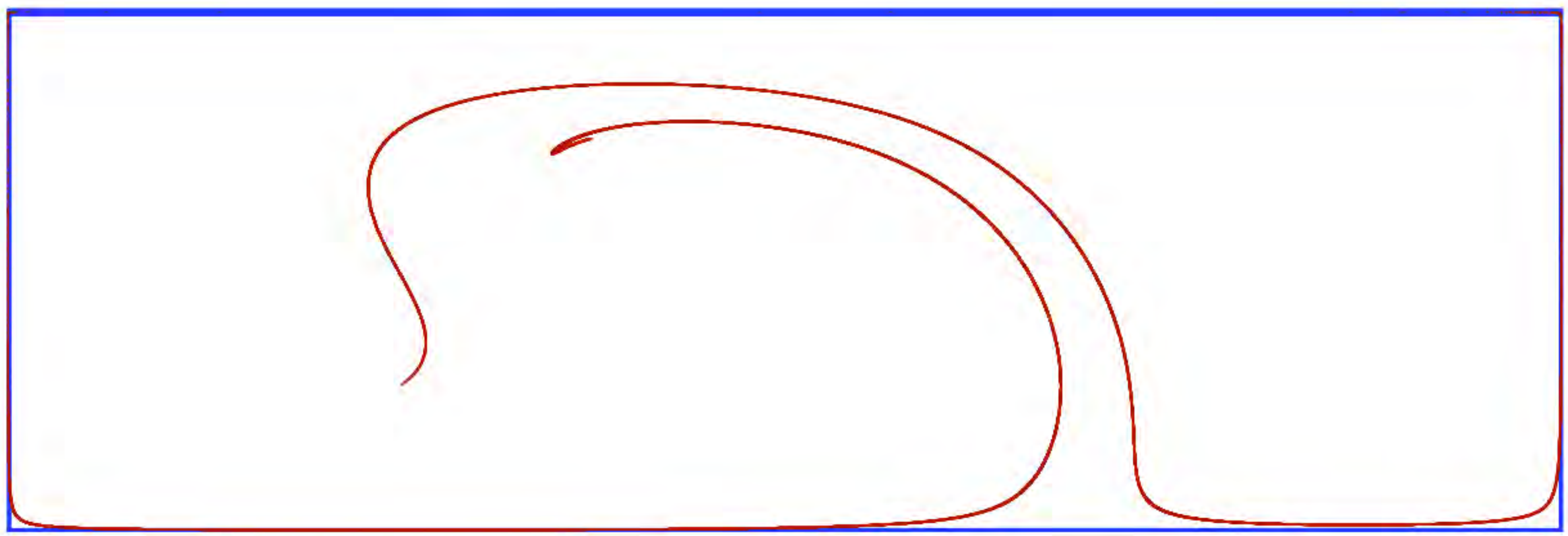


pips, regions and lobes labeled

Stable/unstable manifolds and lobes in fluids

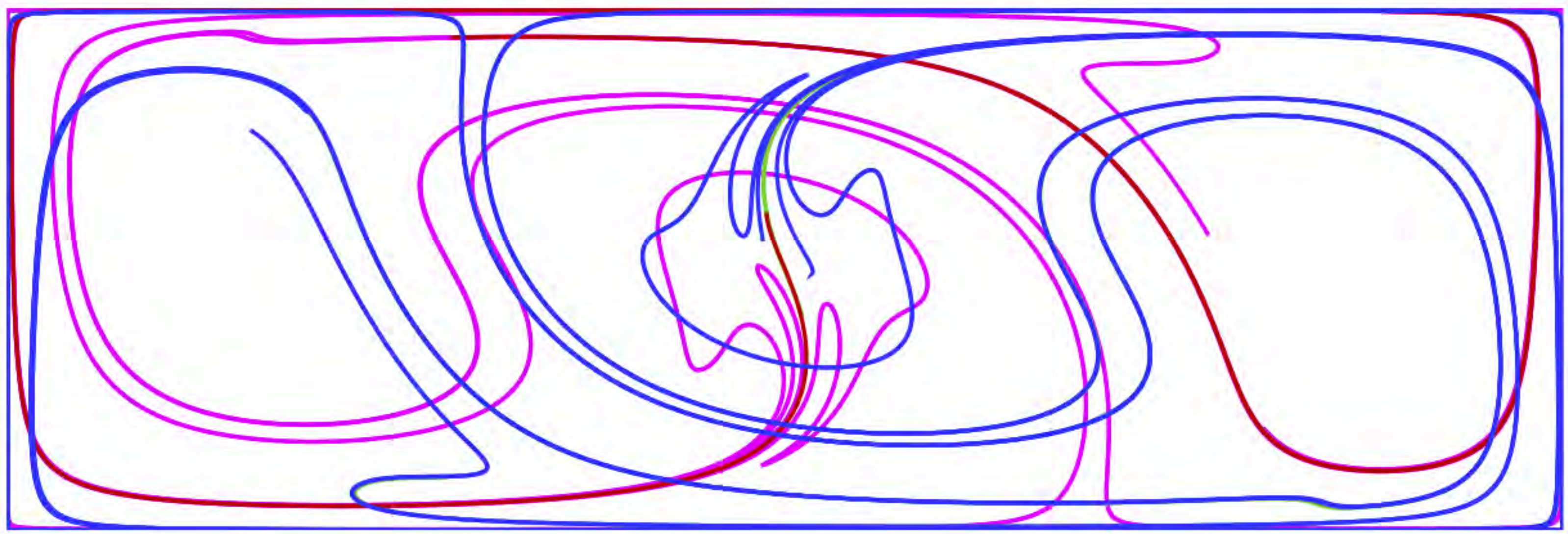
material blob at $t = 0$

Stable/unstable manifolds and lobes in fluids



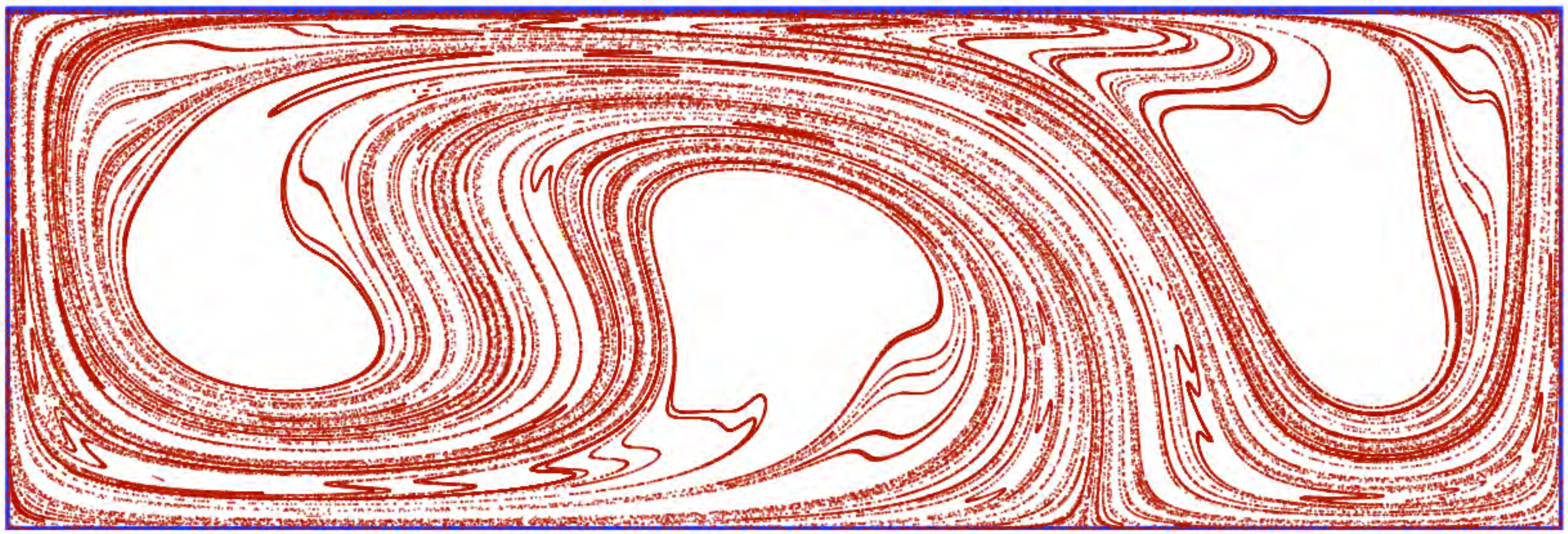
material blob at $t = 5$

Stable/unstable manifolds and lobes in fluids



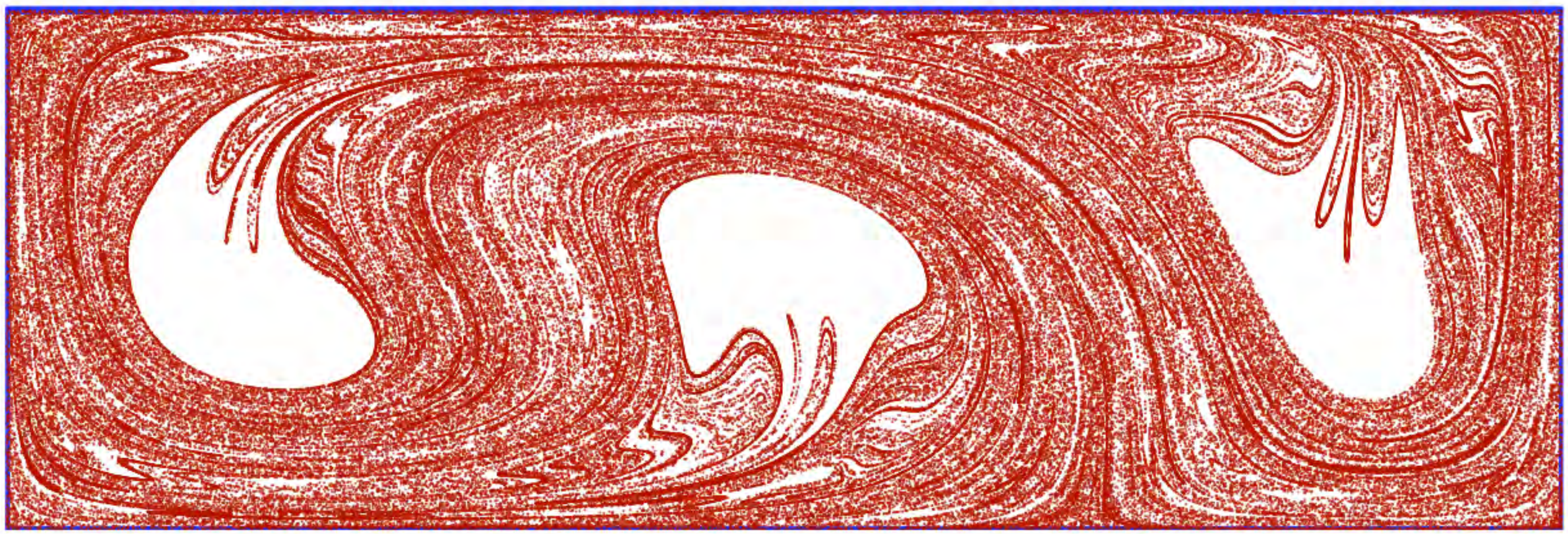
some invariant manifolds of saddles

Stable/unstable manifolds and lobes in fluids



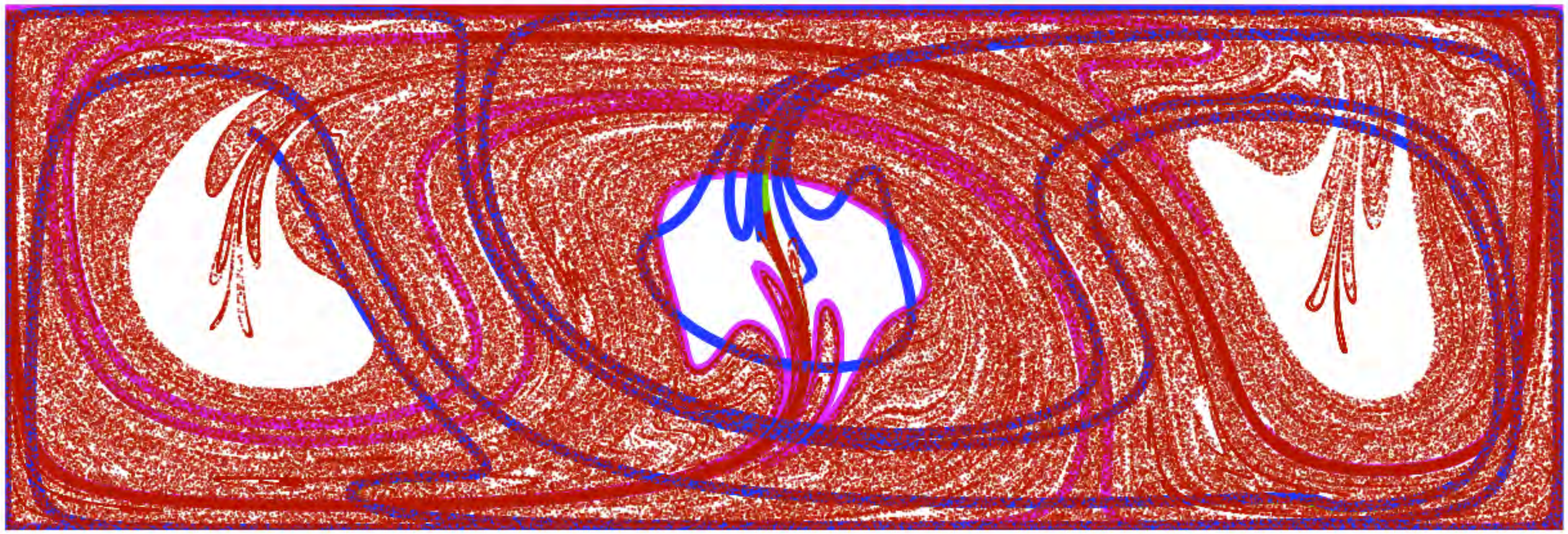
material blob at $t = 10$

Stable/unstable manifolds and lobes in fluids



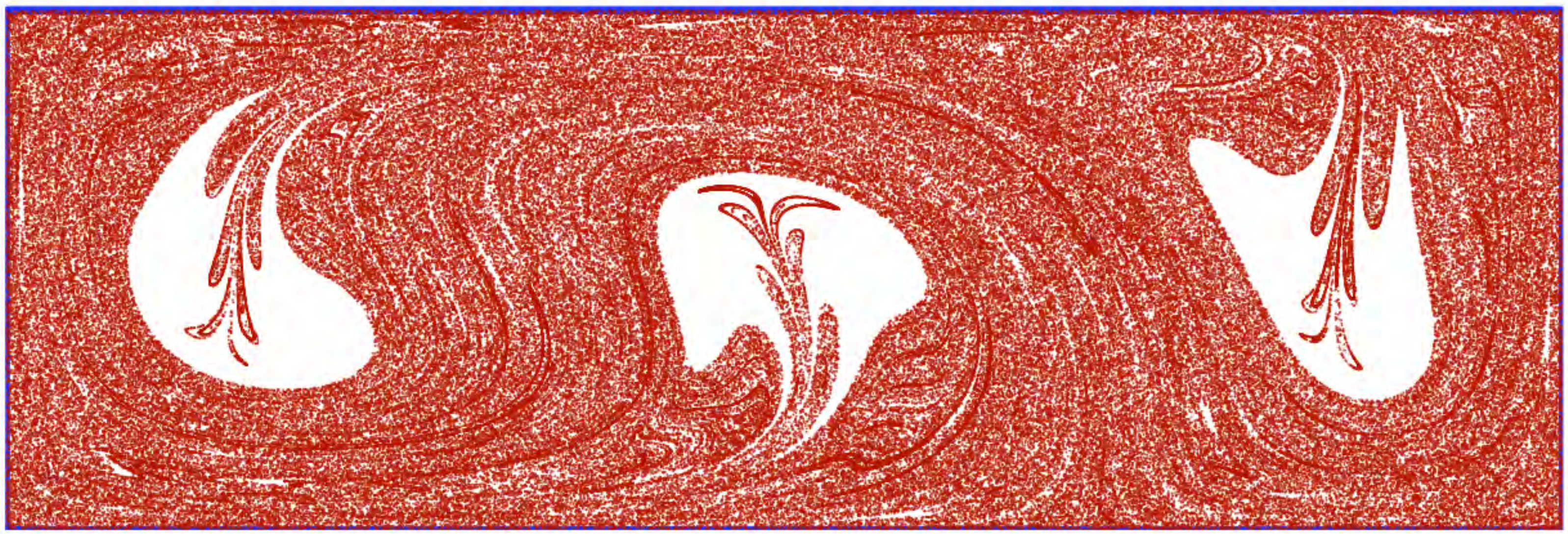
material blob at $t = 15$

Stable/unstable manifolds and lobes in fluids



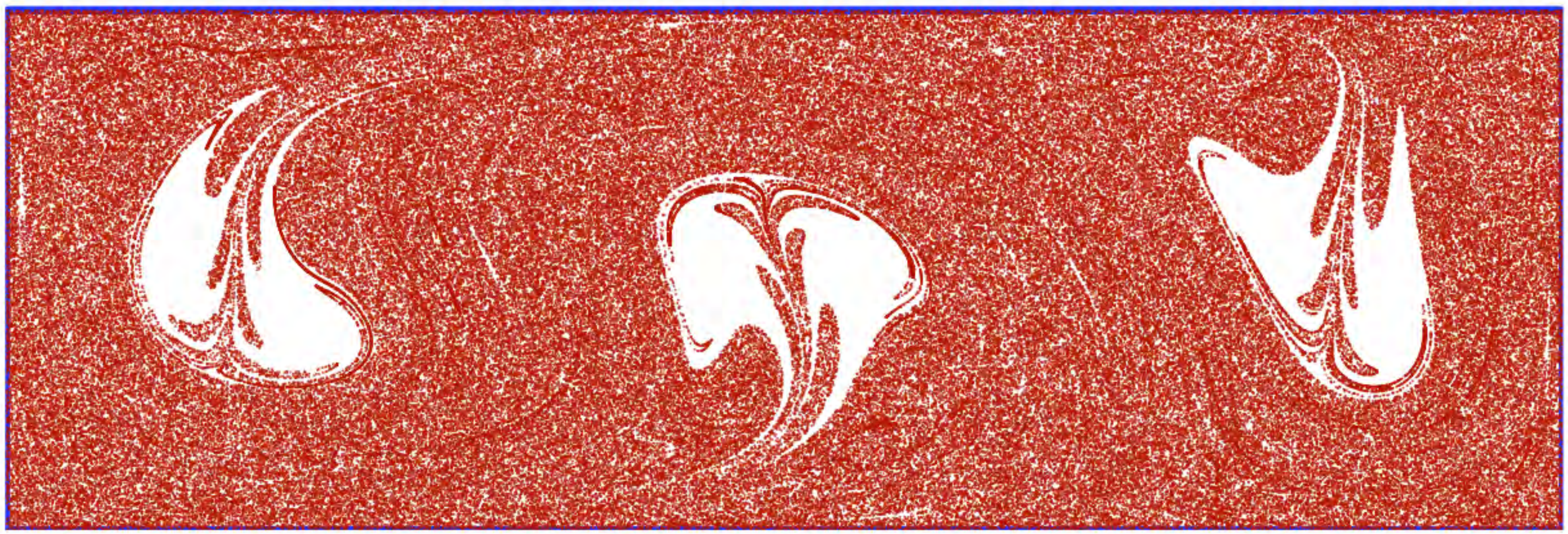
material blob and manifolds

Stable/unstable manifolds and lobes in fluids



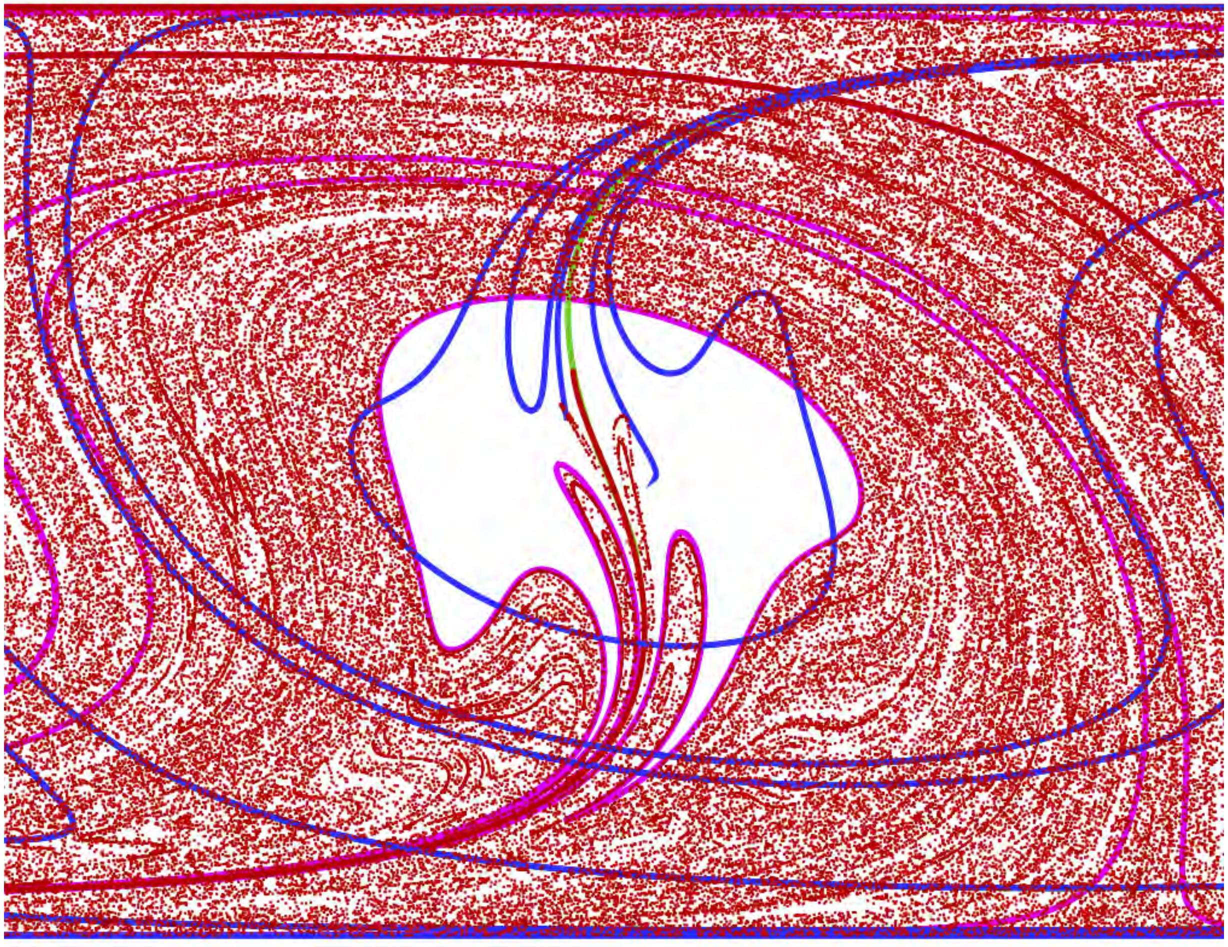
material blob at $t = 20$

Stable/unstable manifolds and lobes in fluids



material blob at $t = 25$

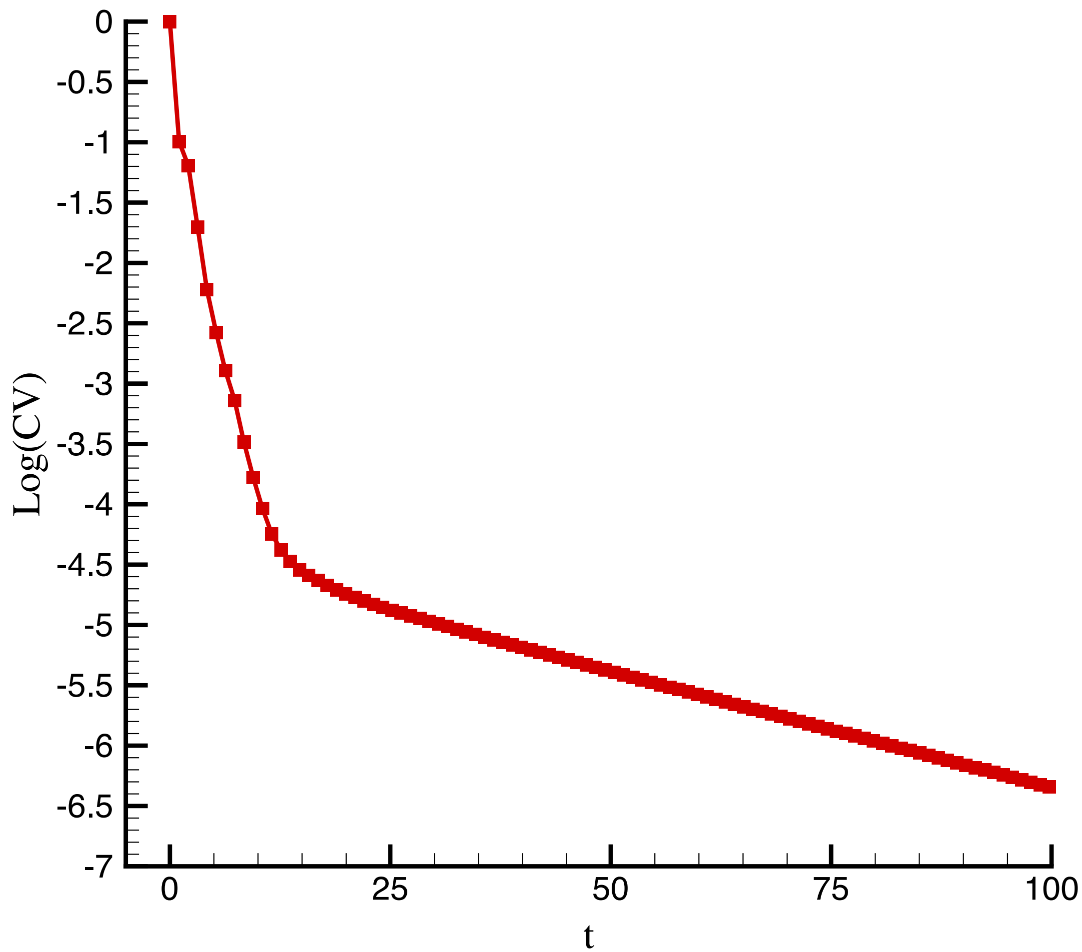
Stable/unstable manifolds and lobes in fluids



- Saddle manifolds and lobe dynamics provide template for motion

Stable/unstable manifolds and lobes in fluids

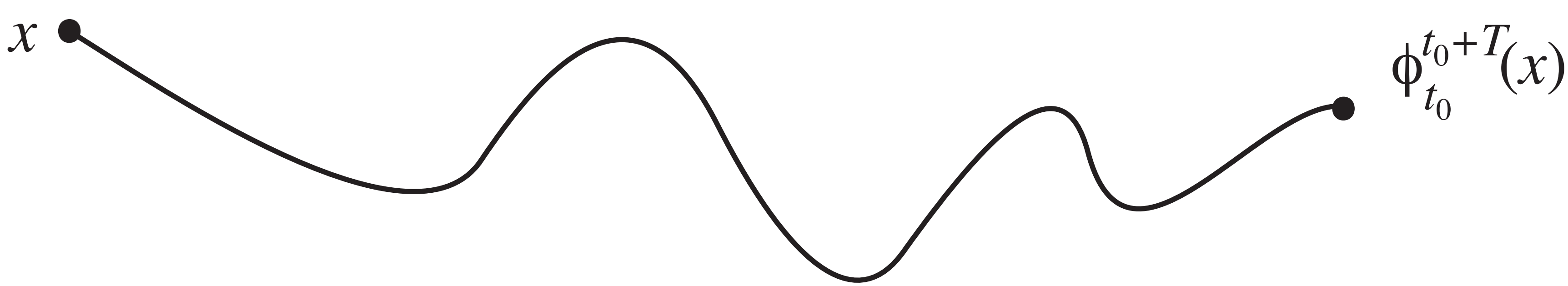
- Concentration variance; a measure of homogenization



- Homogenization has two exponential rates: slower one related to lobes
- Fast rate due to braiding of 'ghost rods' (discussed later)

Transport in aperiodic, finite-time setting

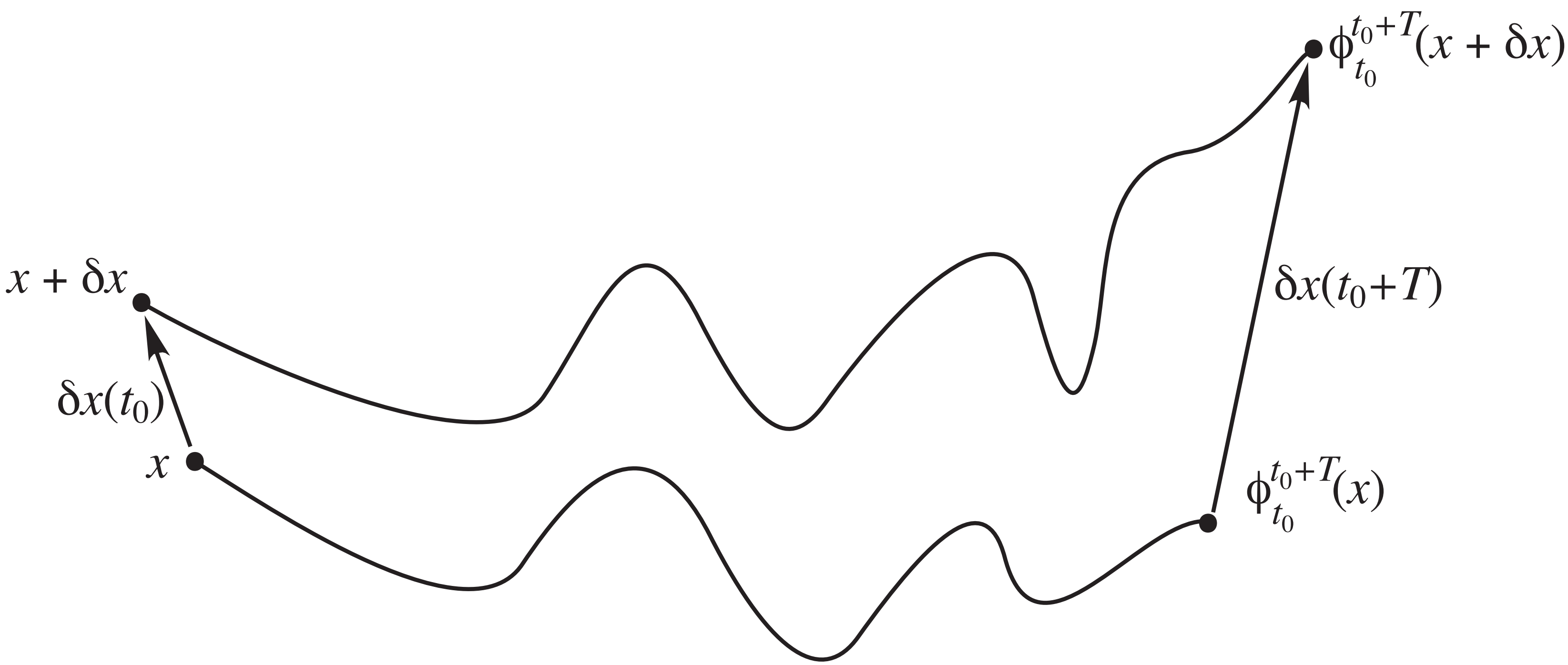
- Data-driven, finite-time, aperiodic setting
  — e.g., non-autonomous ODEs for fluid flow
- How do we get at transport?
- Recall the flow map, $x \mapsto \phi_t^{t+T}(x)$, where $\phi : \mathbb{R}^n \to \mathbb{R}^n$



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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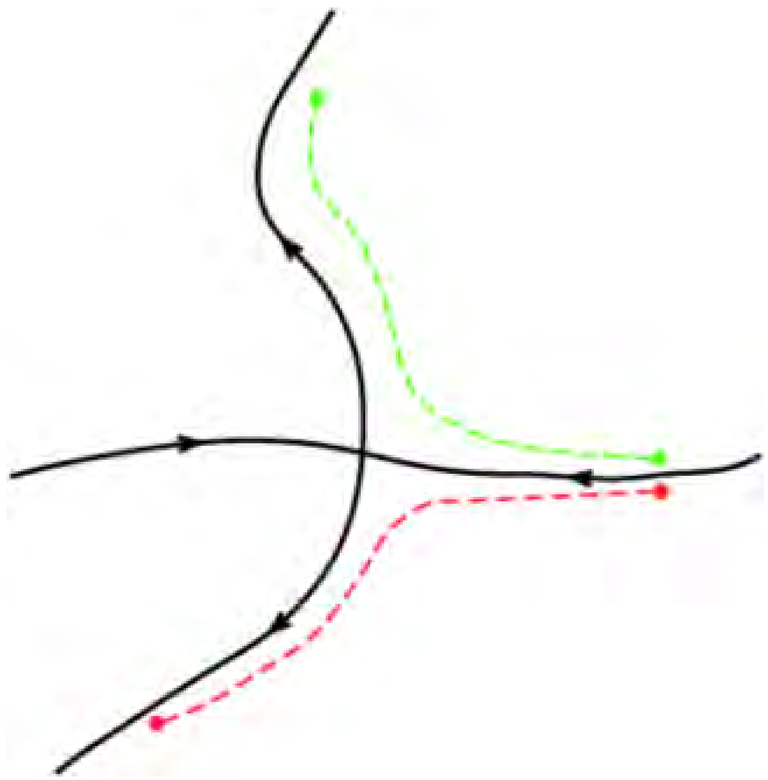


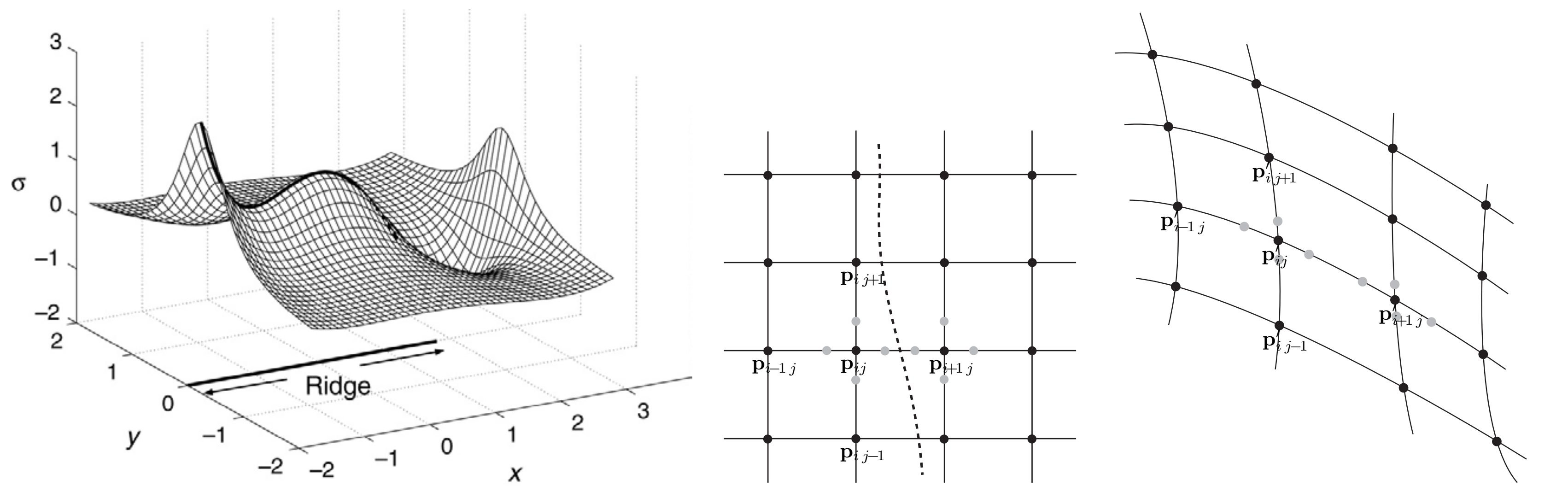
Invariant manifold analogs: FTLE-LCS approach

- The finite-time Lyapunov exponent (FTLE) for Euclidean manifolds,

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

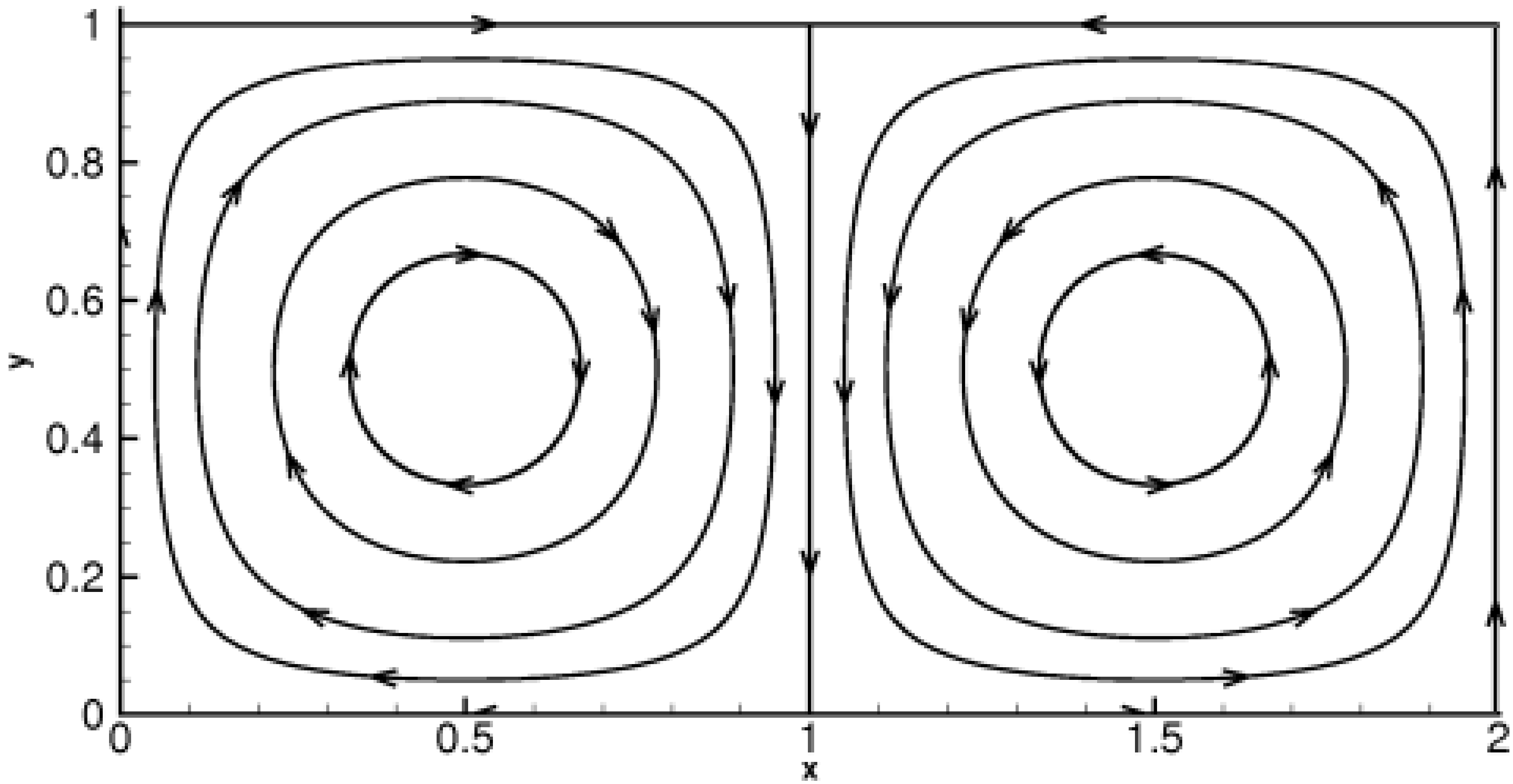
  measures maximum stretching rate over the interval T of trajectories starting near the point x at time t

- Ridges of σ_t^T are candidate hyperbolic codim-1 surfaces; analogs of stable/unstable manifolds; 'Lagrangian coherent structures' (LCS)[2]



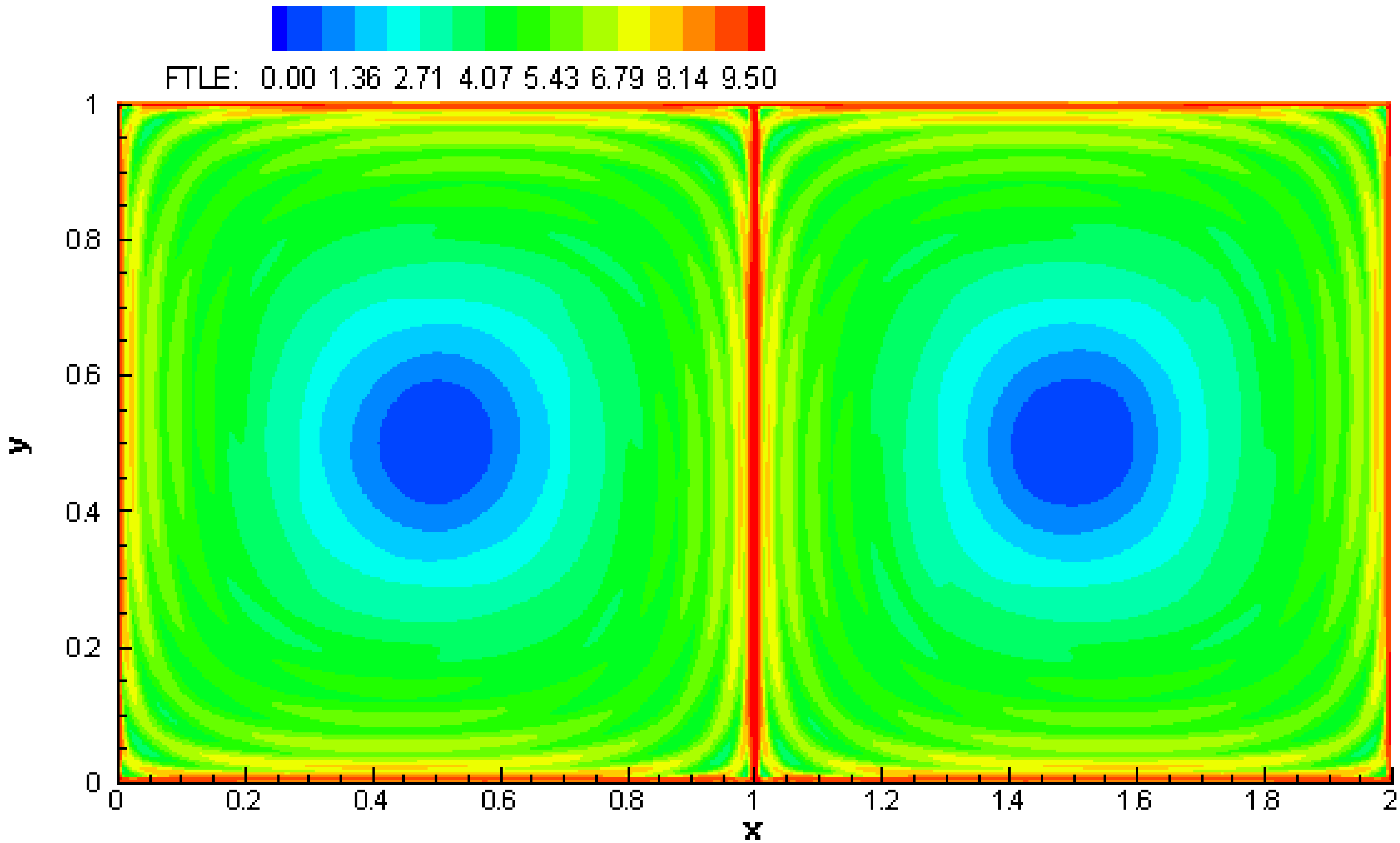
[2] cf. Bowman, 1999; Haller & Yuan, 2000; Haller, 2001; Shadden, Lekien, Marsden, 2005

Invariant manifold analogs: FTLE-LCS approach



Autonomous double-gyre flow

Invariant manifold analogs: FTLE-LCS approach

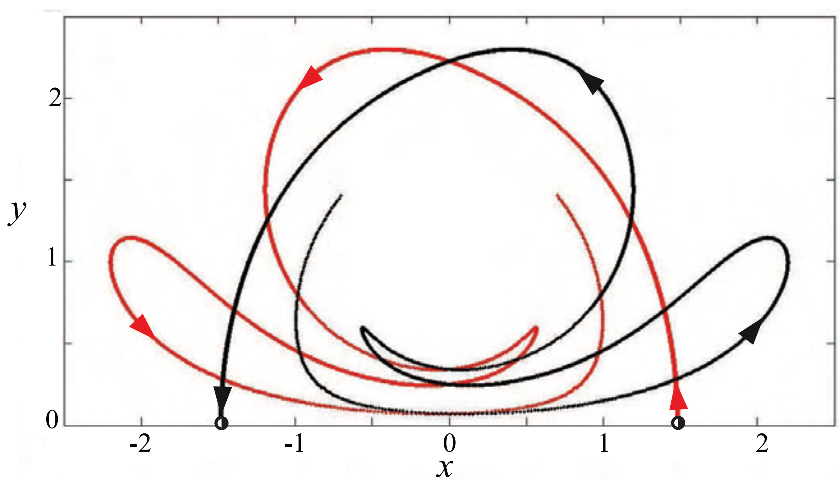


Invariant manifold analogs: FTLE-LCS approach

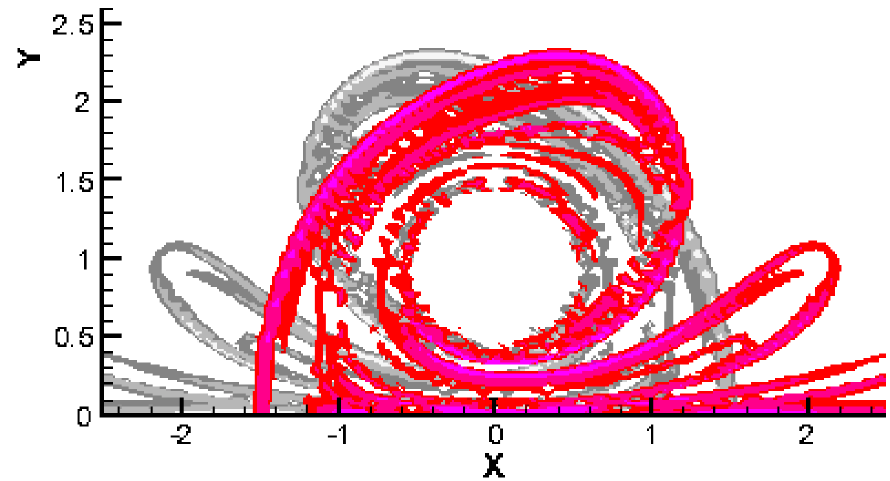
Use your intuition about ridges, e.g., a mountain ridge

Pacific Crest Trail in Oregon

Invariant manifold analogs: FTLE-LCS approach



Invariant manifolds



LCS

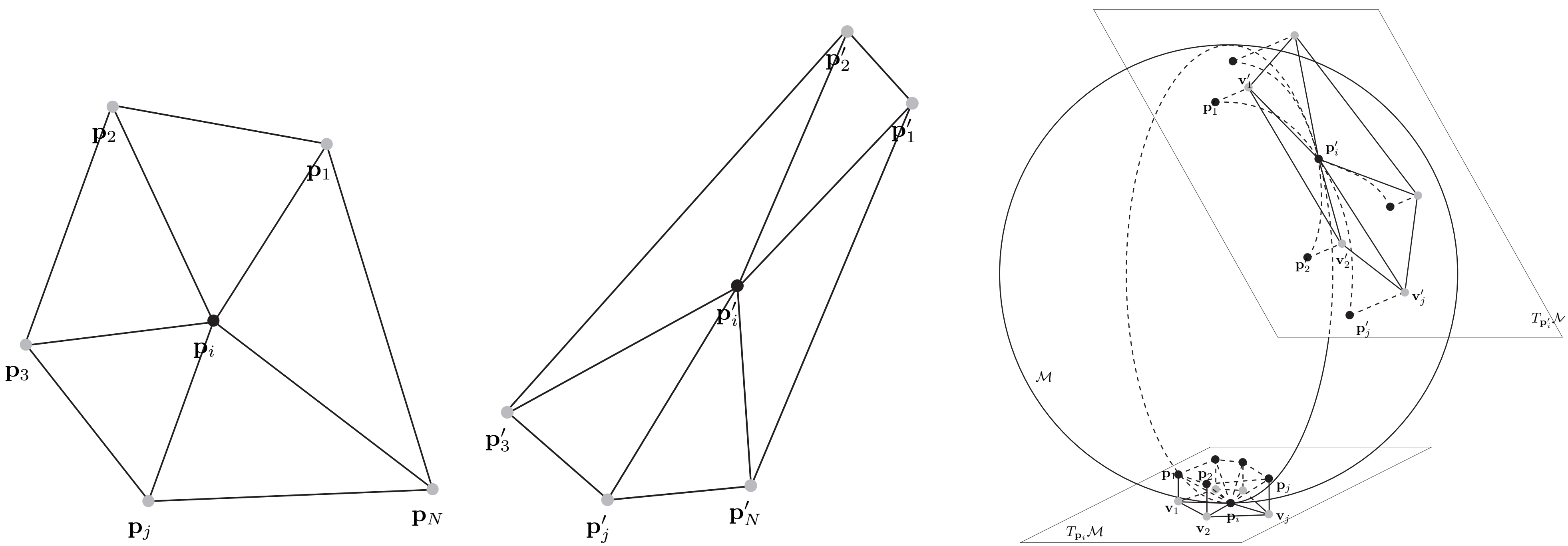
Time-periodic oscillating vortex pair flow

Invariant manifold analogs: FTLE-LCS approach

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

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

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



[3]Lekien & Ross [2010] Chaos

Transport barriers on Riemannian manifolds

- repelling surfaces for $T > 0$, attracting for $T < 0$[3]

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)

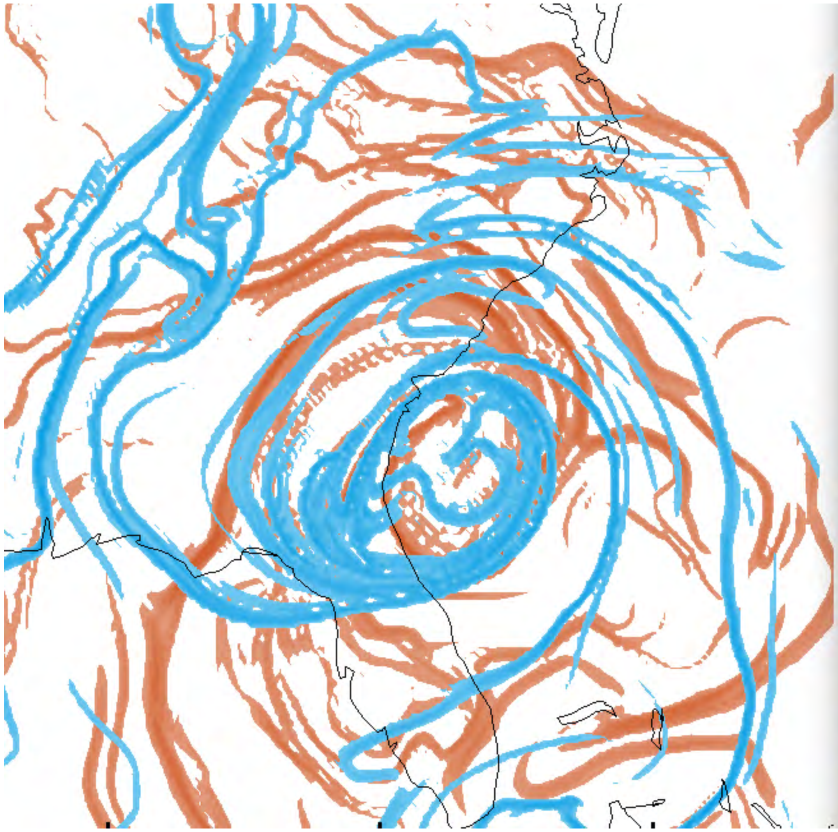
Atmospheric flows: Antarctic polar vortex

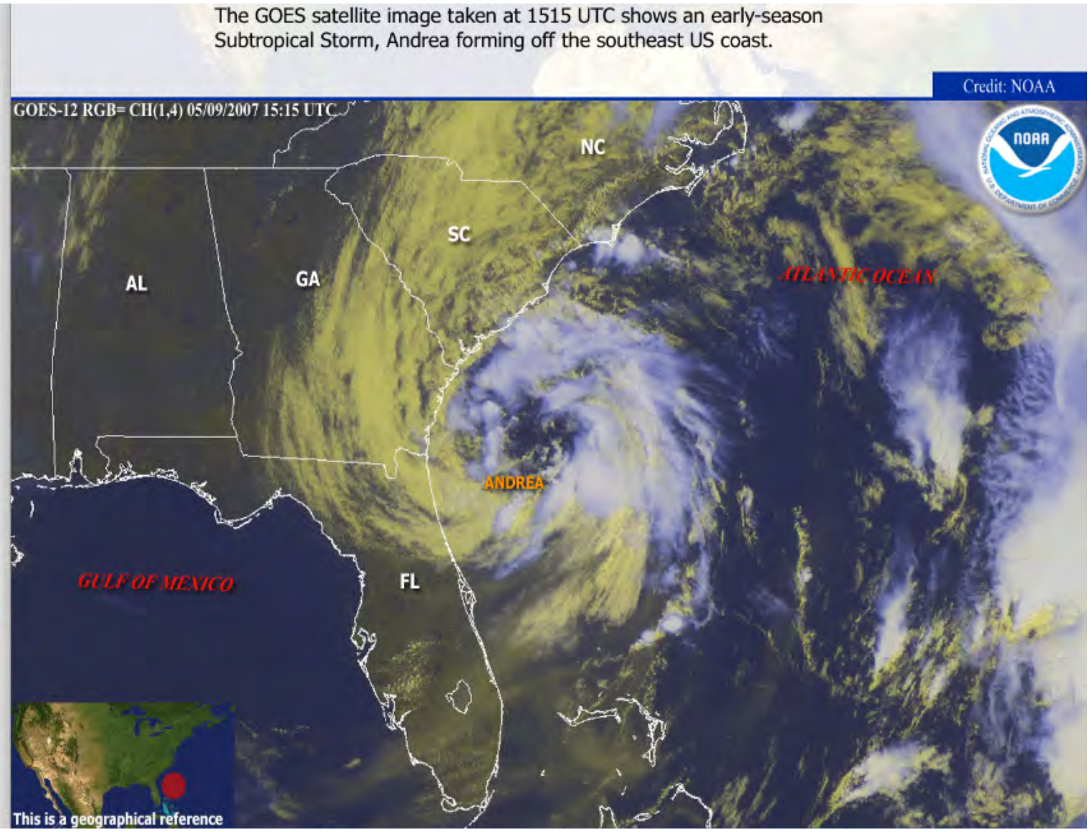
air masses on either side of a repelling LCS

Atmospheric flows: continental U.S.

LCSs: orange = repelling, blue = attracting

Atmospheric flows and lobe dynamics





orange = repelling LCSs, blue = attracting LCSs

satellite

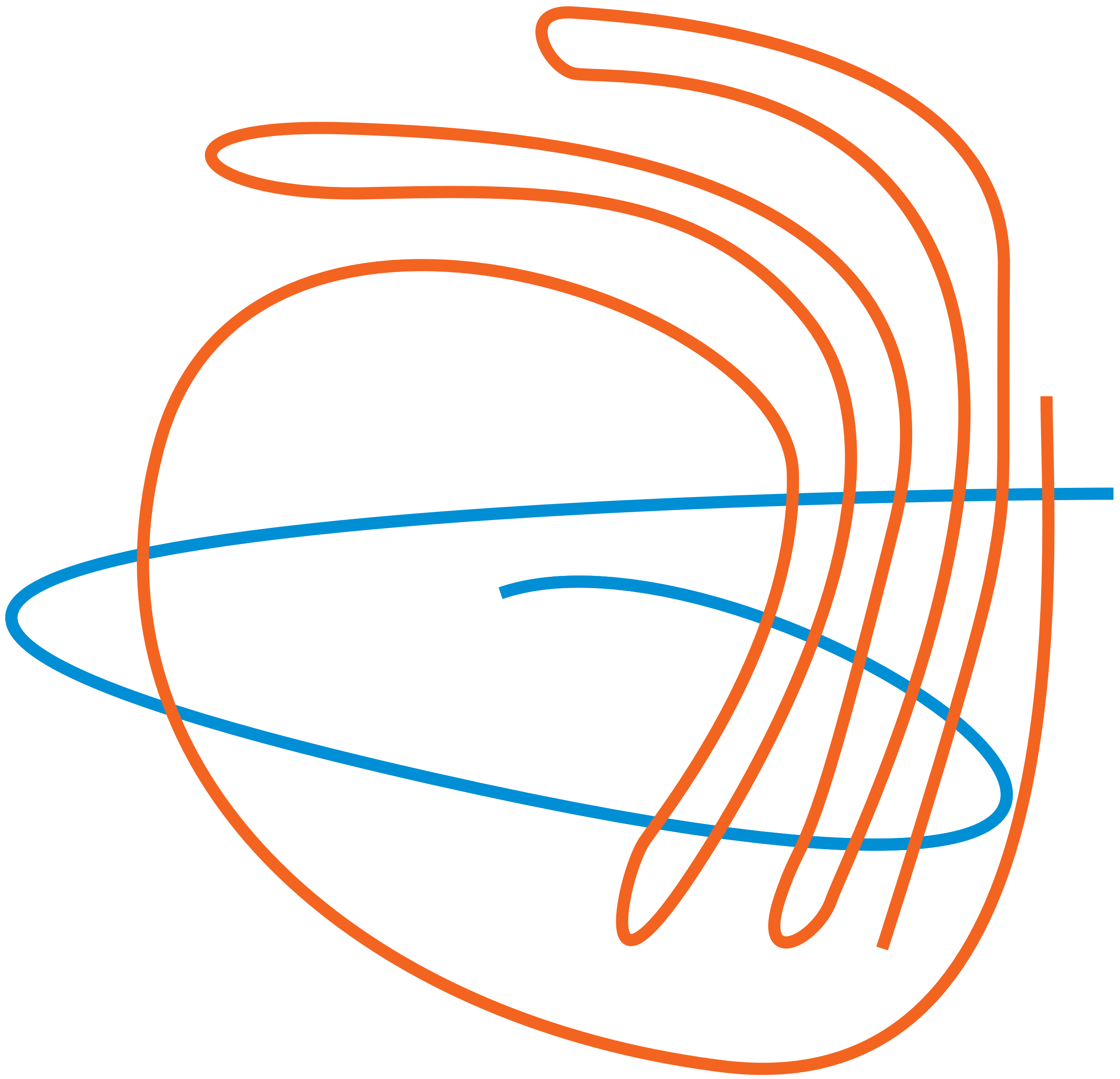
Andrea, first storm of 2007 hurricane season

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

Atmospheric flows and lobe dynamics

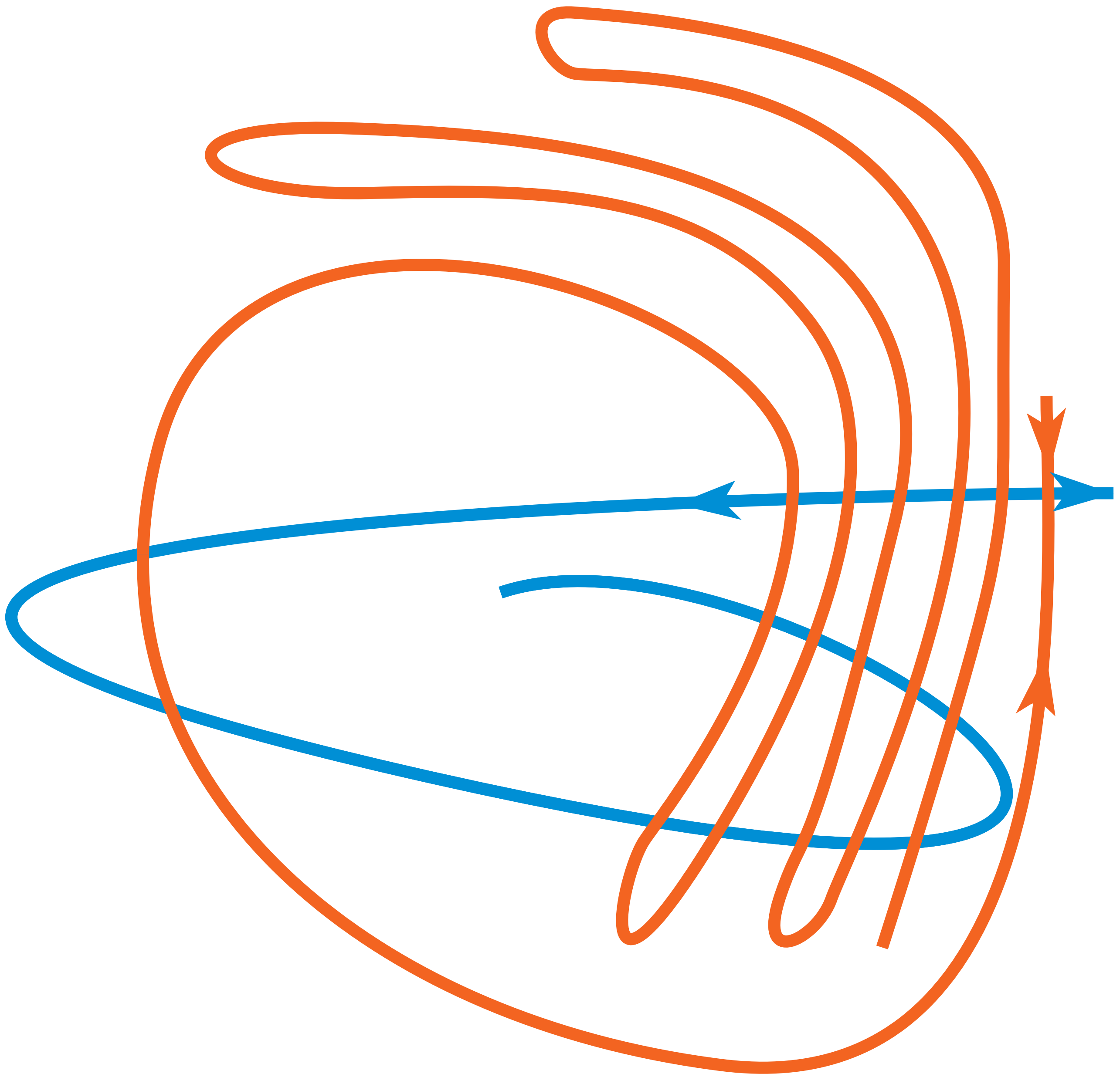
Andrea at one snapshot; LCS shown (orange = repelling, blue = attracting)

Atmospheric flows and lobe dynamics



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

Atmospheric flows and lobe dynamics



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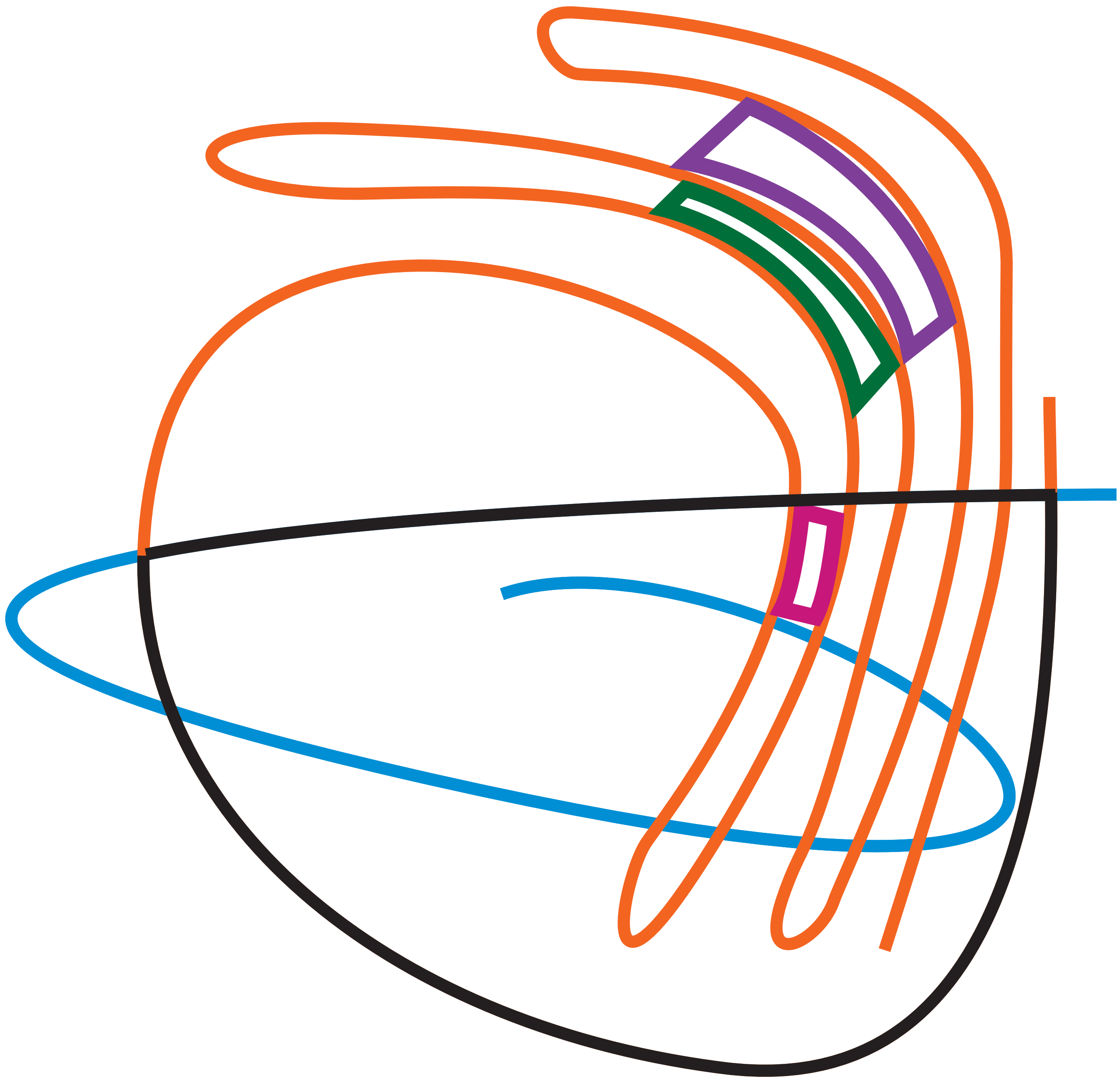
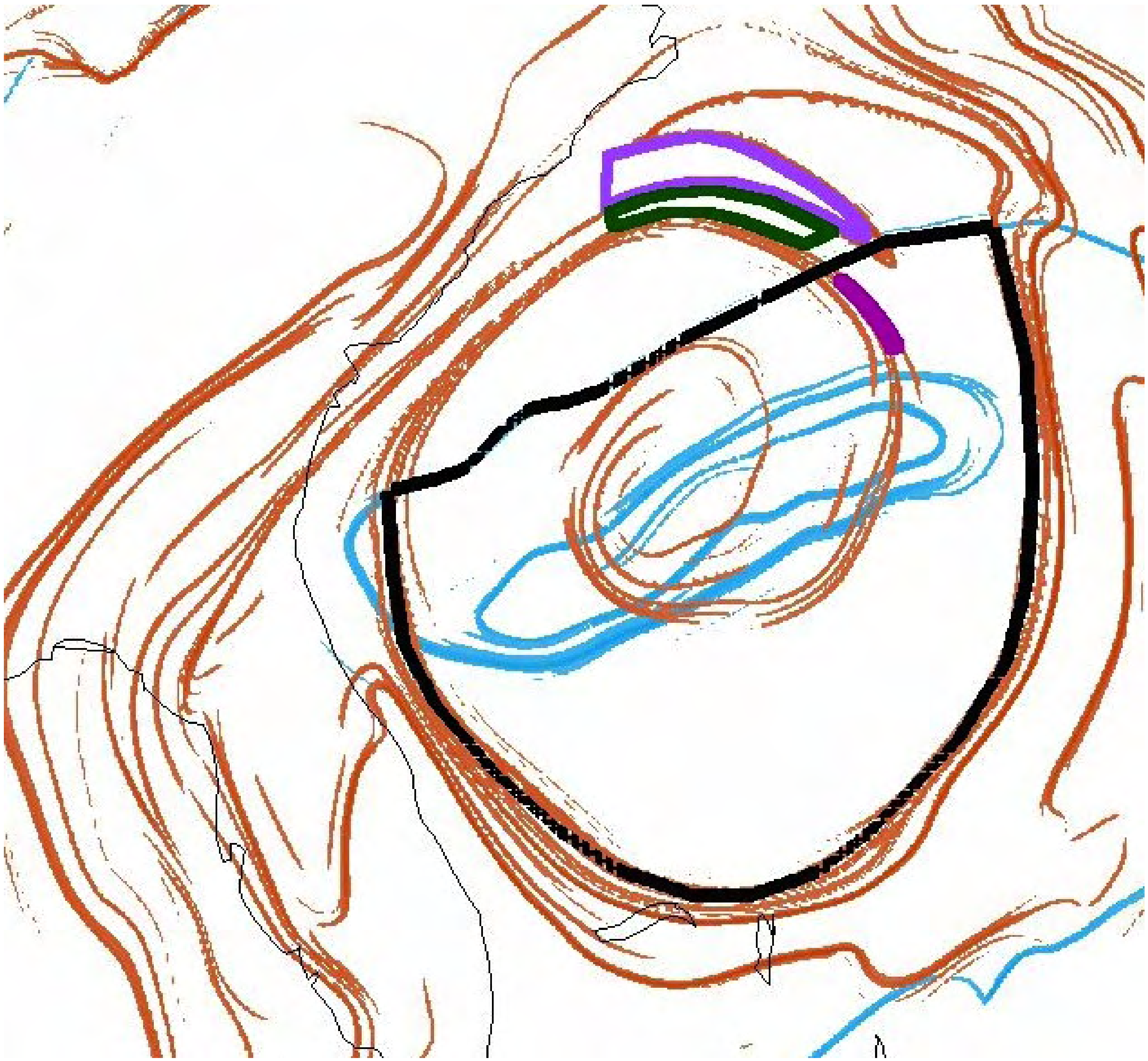
Atmospheric flows and lobe dynamics



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

Stirring fluids, e.g., with solid rods

turbulent mixing

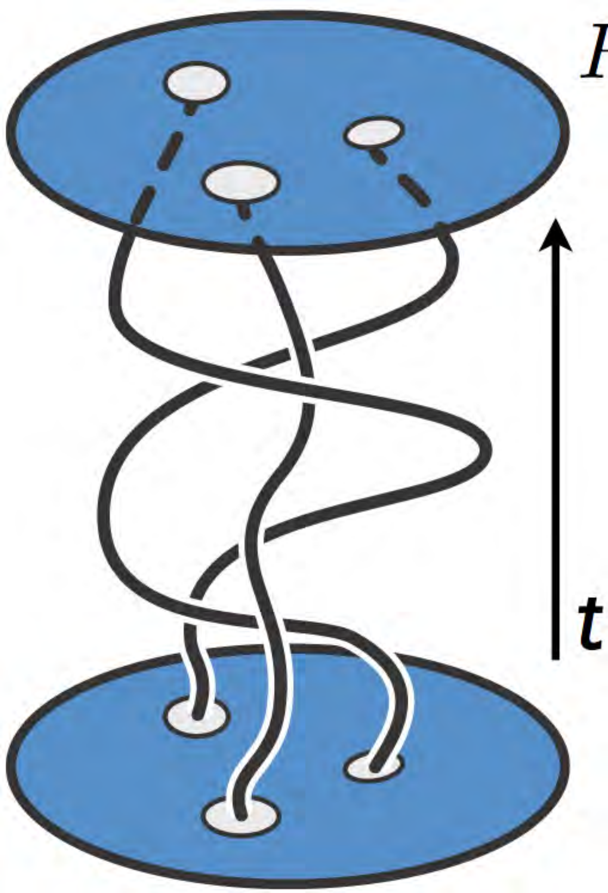
spoon in coffee

laminar mixing

3 ‘braiding’ rods in glycerin

Topological chaos through braiding of stirrers

- Topological chaos is ‘built in’ the flow due to the topology of boundary motions



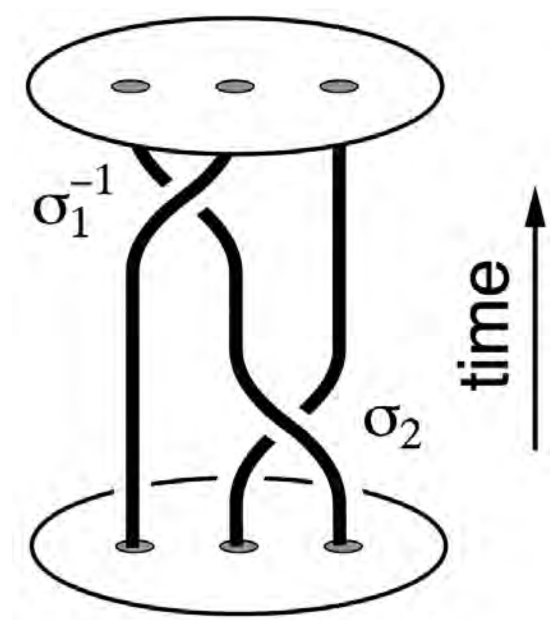
R_N : 2D fluid region with *N* stirring ‘rods’

- 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 (TNCT)

- 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 Markov partition with transition matrix A, topological entropy $h_{\mathrm{TN}}(g) = \log(\lambda_{PF}(A))$, where $\lambda_{\mathrm{PF}}(A) > 1$ (iii) reducible: g contains both f.o. and pA regions

- h_{TN} computed from 'braid word', e.g., $\sigma_1^{-1}\sigma_2$
- $\log(\lambda_{PF}(A))$ provides a **lower bound** on the true **topological entropy**



Topological chaos in a viscous fluid experiment

Move 3 rods on 'figure-8' paths through glycerin

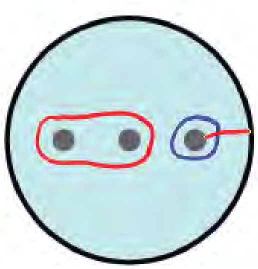
Boyland, Aref & Stremler (2000) *J. Fluid Mech.*

- stirrers move on periodic orbits in two steps

- Thurston-Nielsen theorem gives a lower bound on stretching:

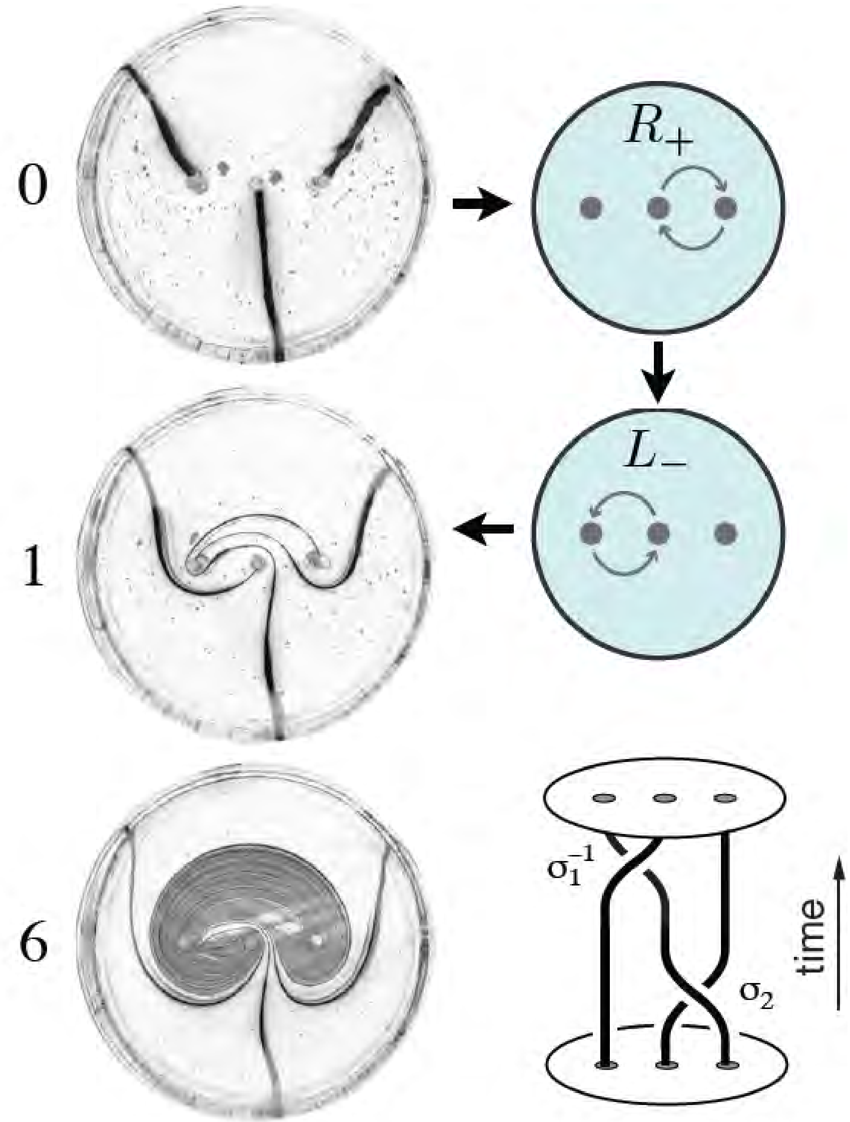
$$\lambda_{\mathrm{TN}} = \tfrac{1}{2}\left(3+\sqrt{5}\right)$$

$$h_{\mathrm{TN}} = \log(\lambda_{\mathrm{TN}}) = 0.962\ldots$$

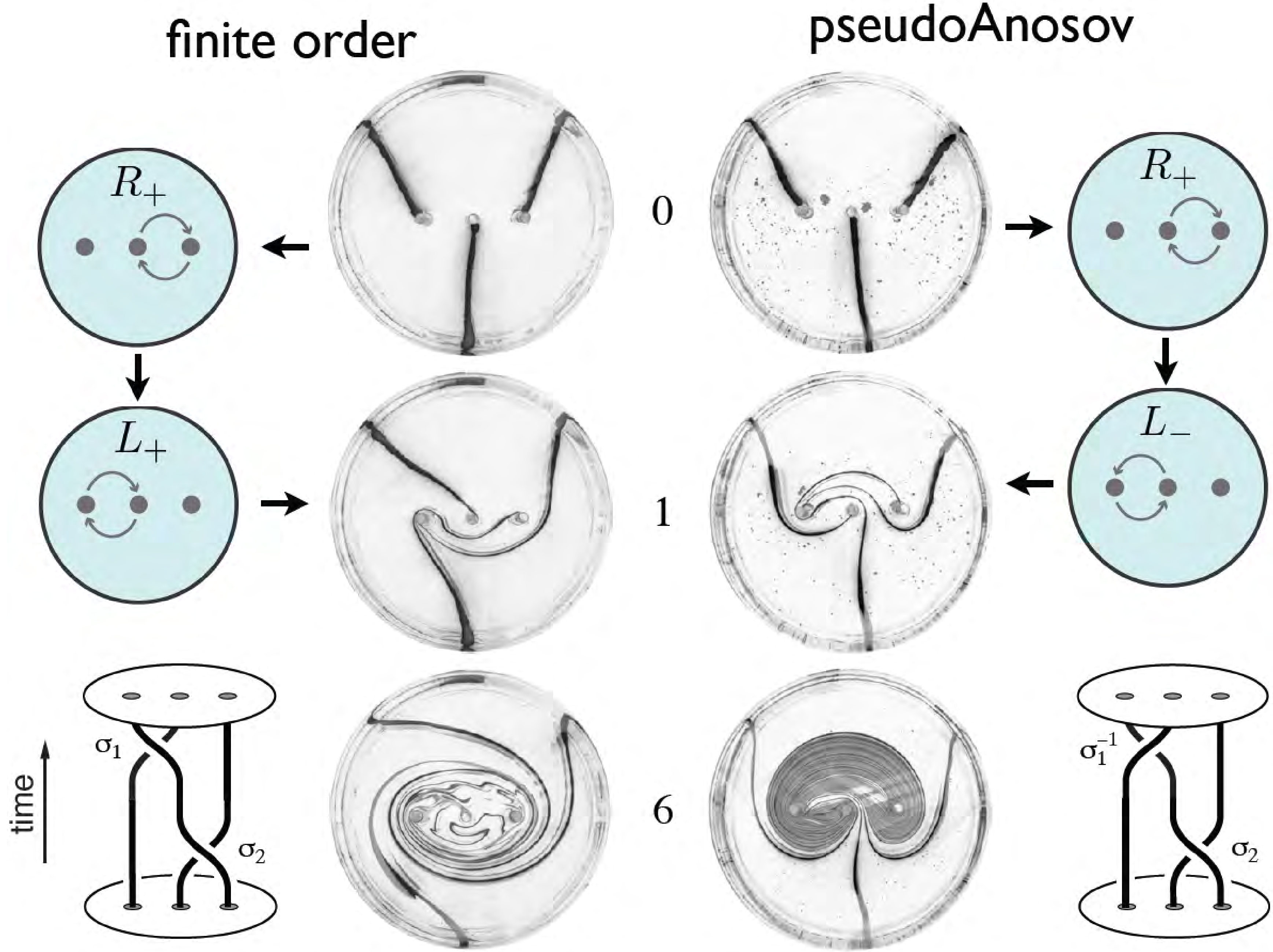


non-trivial material lines grow like $l \sim l_0\ \lambda^n$

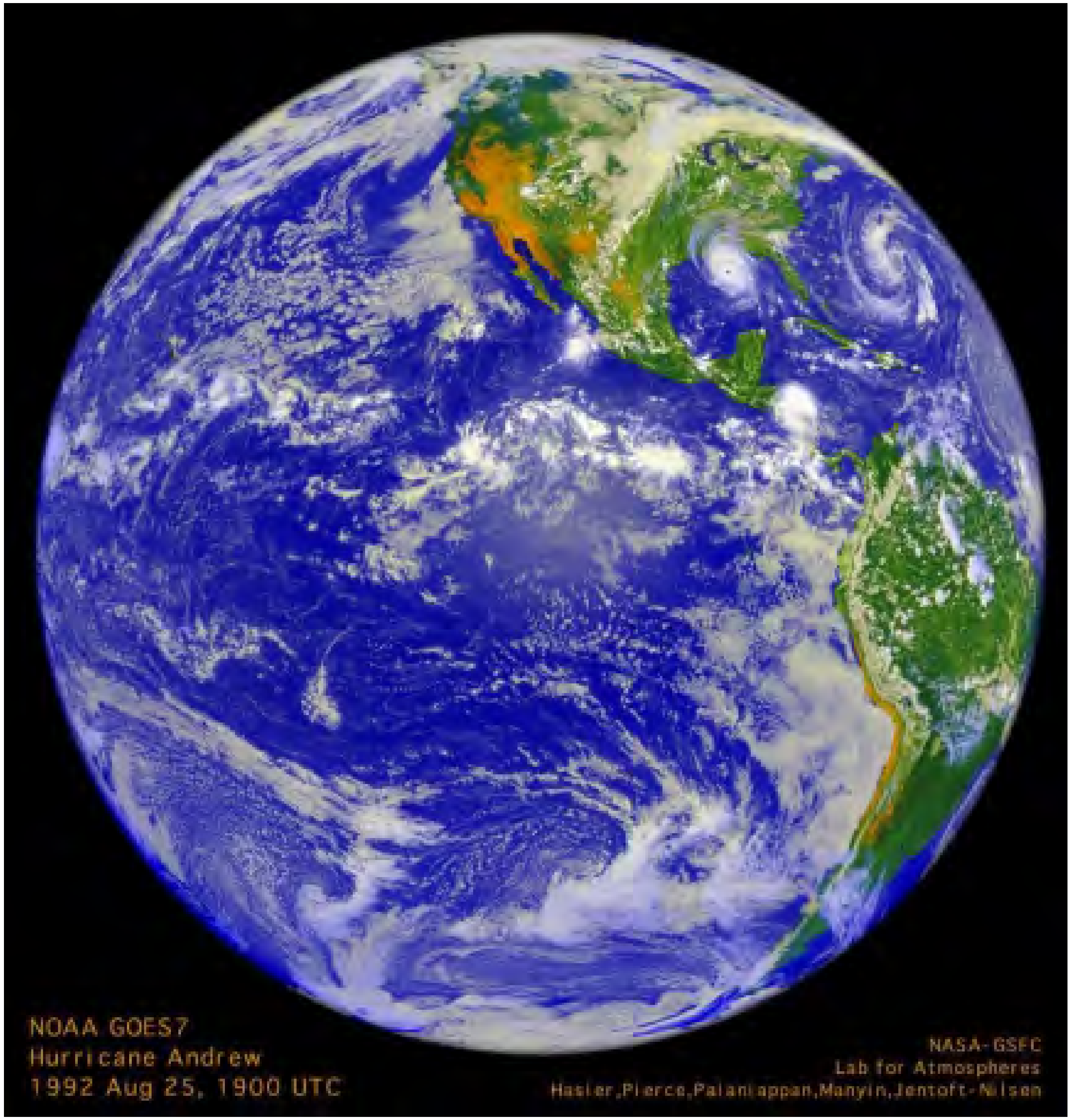
$$\lambda \geq \lambda_{\mathrm{TN}}$$



Topological chaos in a viscous fluid experiment



Stirring fluids with coherent structures (?)



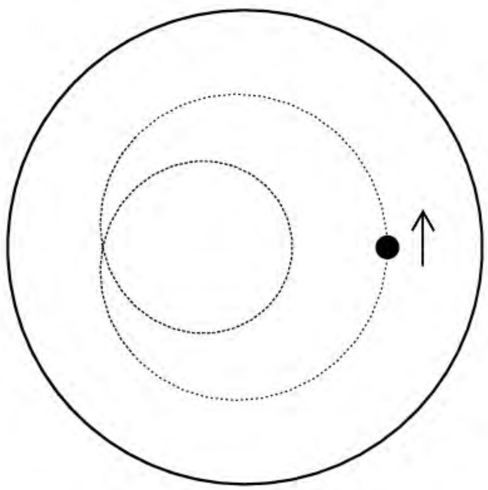
Stirring with periodic orbits, i.e., 'ghost rods'

point vortices in a periodic domain

Boyland, Stremler & Aref (2003) *Physica* D

one rod moving on an epicyclic trajectory

Gouillart, Thiffeault & Finn (2006) *Phys. Rev.* E



'ghost rods'

solid rods

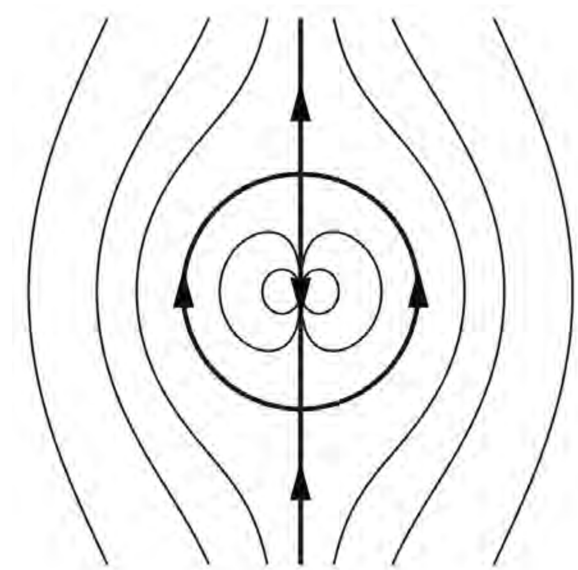
Fluid is wrapped around 'ghost rods' in the fluid

– *flow structure assists in the stirring*

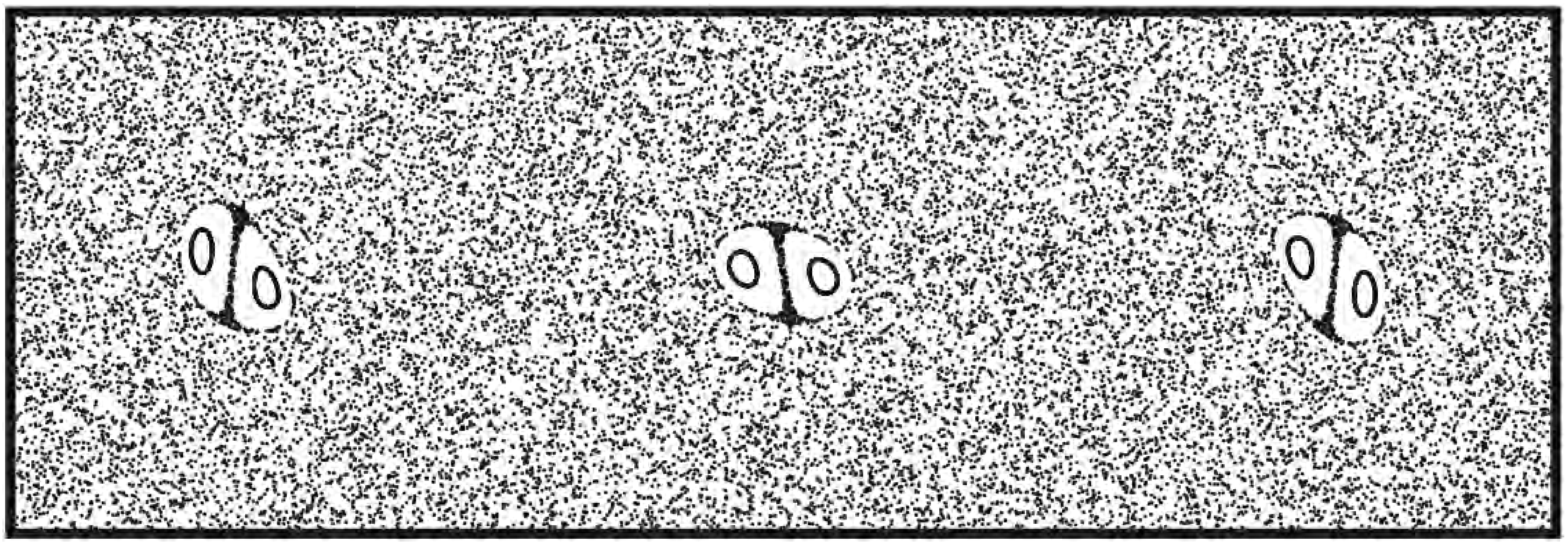
Identifying periodic points in cavity flow example

tracer blob for $\tau_f > 1$

- At $\tau_f = 1$, parabolic period 3 points of map
- $\tau_f > 1$, **elliptic / saddle points** of period 3 — streamlines around groups resemble fluid motion around a solid rod ⇒
- $\tau_f < 1$, **periodic points vanish**



Identifying periodic points in cavity flow example



period-τ_f Poincaré map for $\tau_f > 1$

- At $\tau_f = 1$, parabolic period 3 points of map
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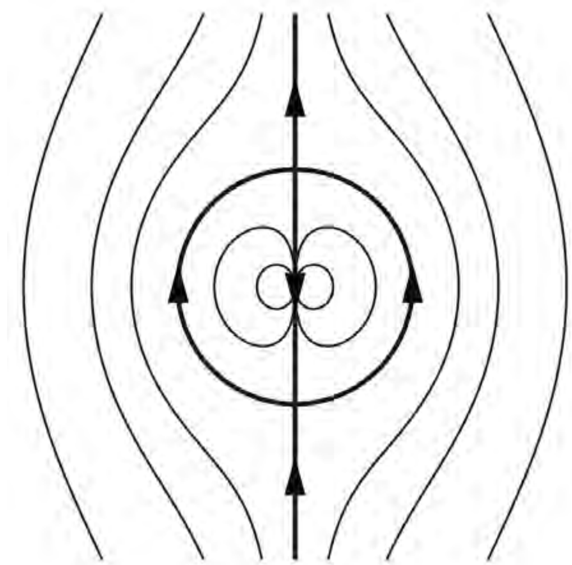
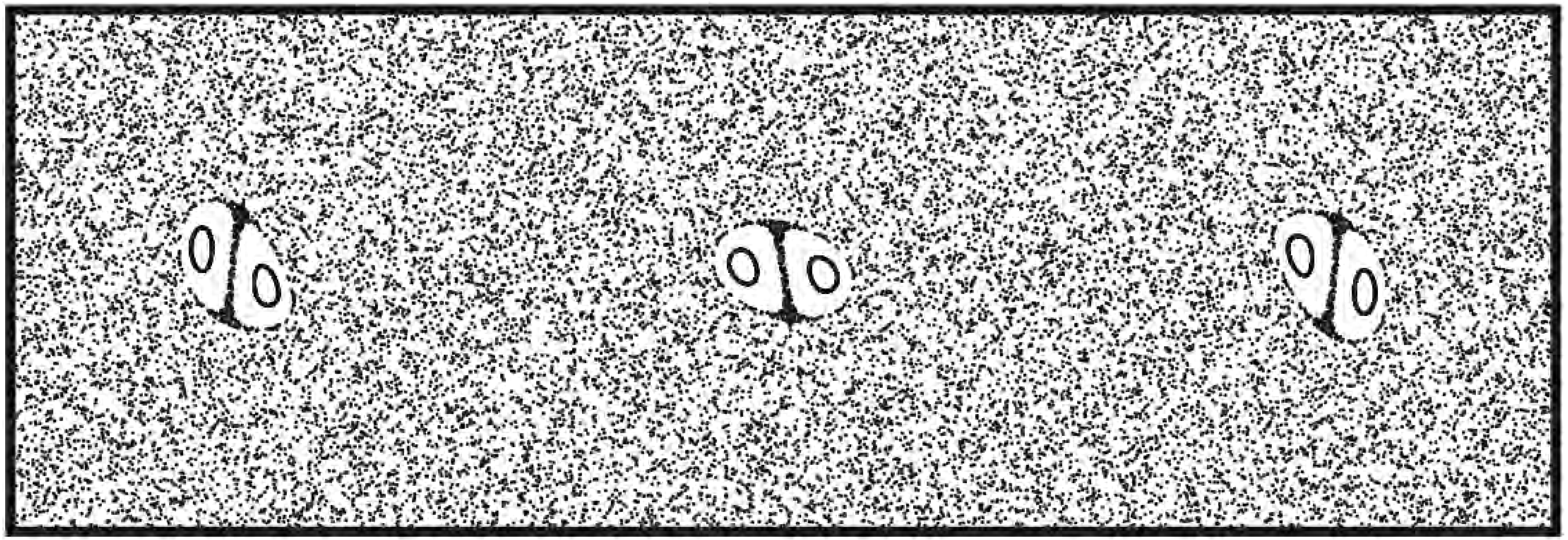
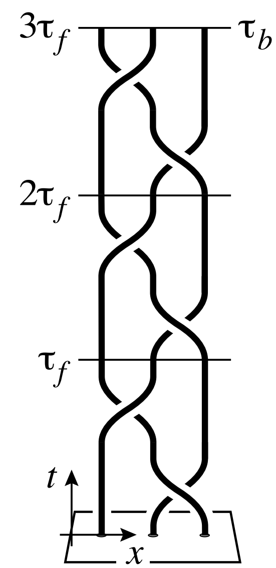


Stirring protocol ⇒ braid ⇒ topological entropy



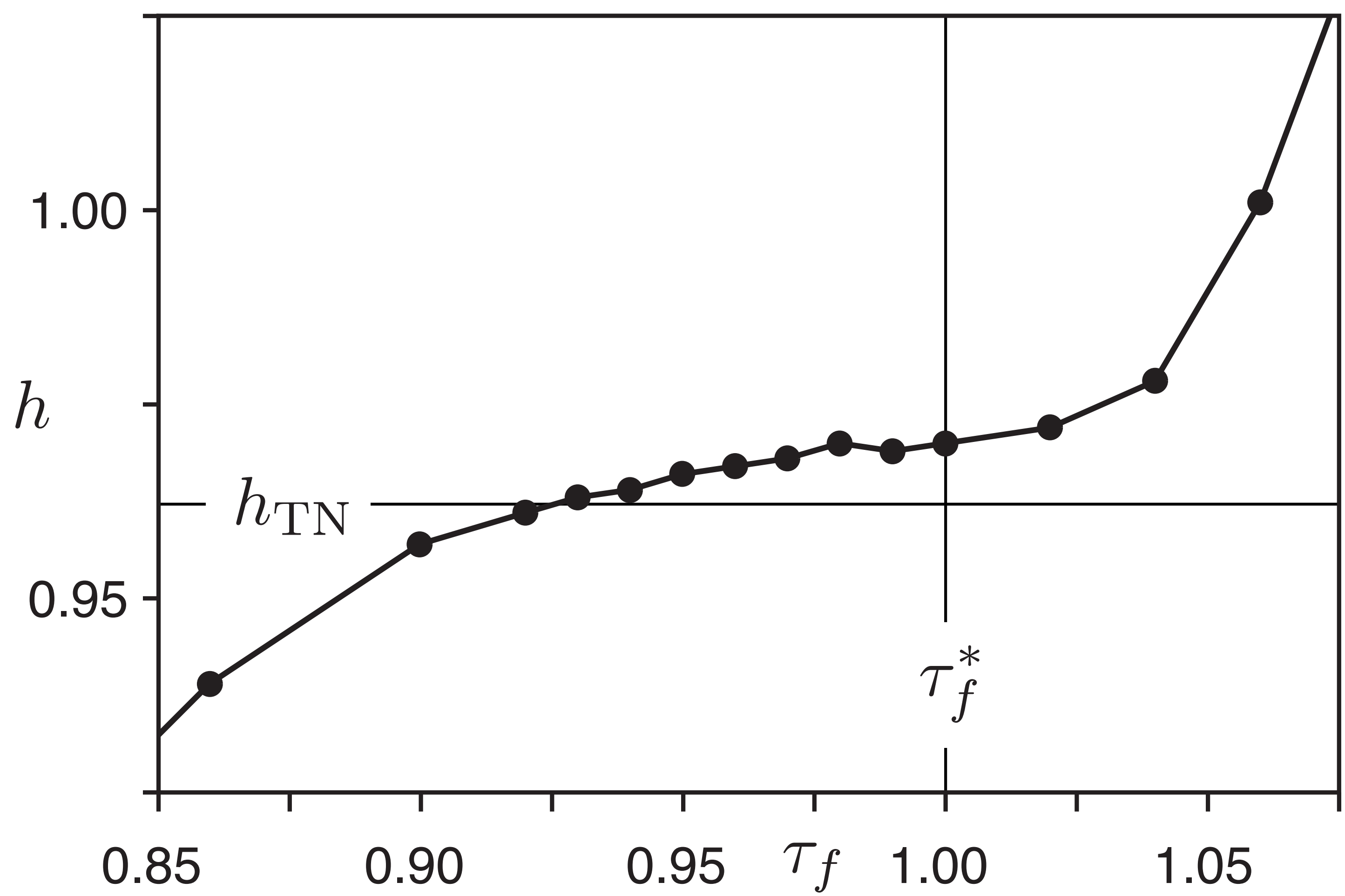
period-τ_f Poincaré map for $\tau_f > 1$

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



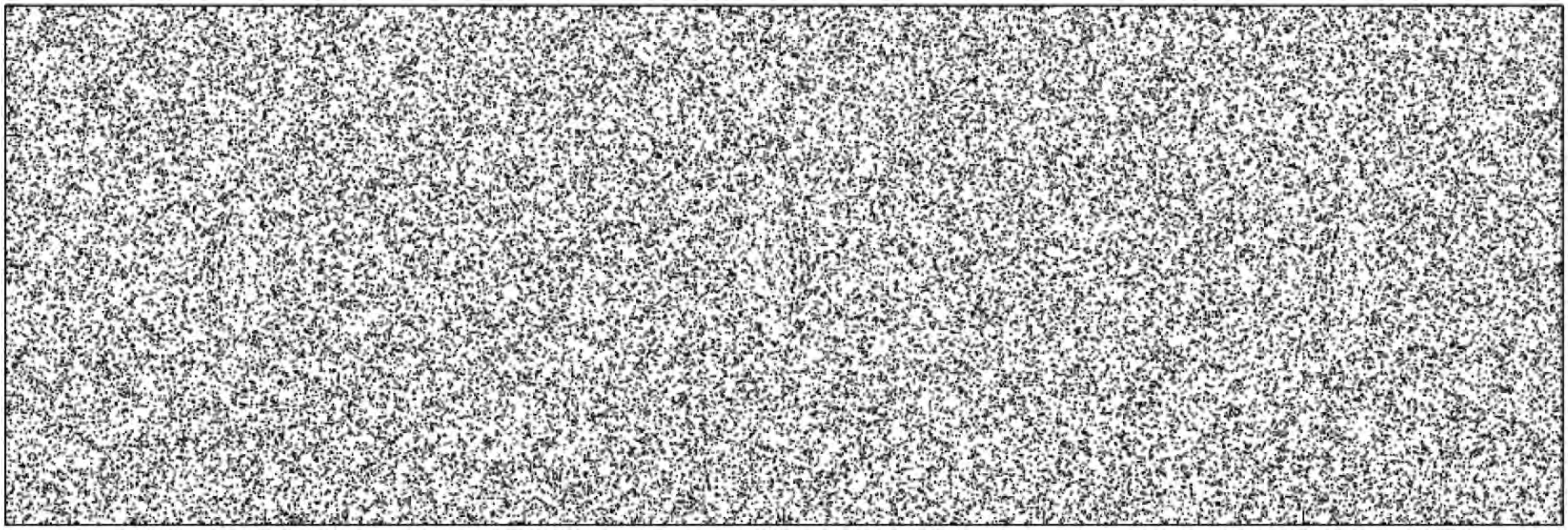
Topological entropy continuity across critical point

- Consider $\tau_f < 1$



topological entropy as a function of τ_f

Identifying 'ghost rods'?



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

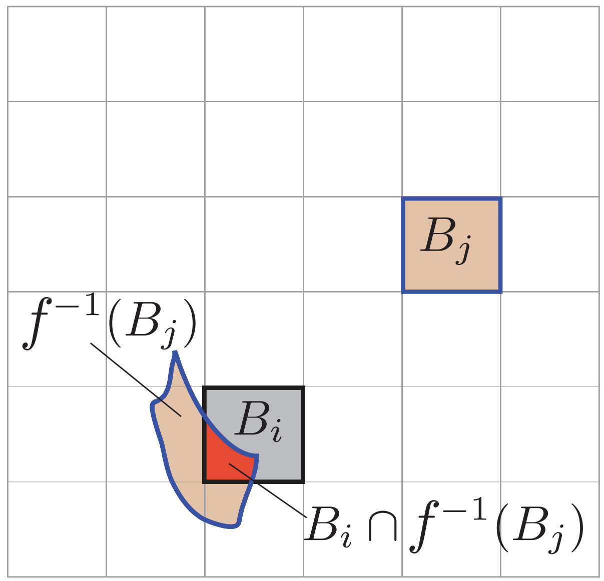
- Note the absence of any elliptical islands
- No periodic orbits of low period were found
- In practice, even when such low-order periodic orbits exist, they can be difficult to identify
- But phase space is not featureless

Almost-invariant / almost-cyclic sets

- Identify **almost-invariant sets** (AISs) using probabilistic point of view
- Relatedly, **almost-cyclic sets** (ACSs) (Dellnitz & Junge [1999])
- 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, 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., $f = \phi_t^{t+T}$, computed numerically



- Identify AISs and ACS via spectrum of P
- P approximates $\mathcal{P}$, Perron-Frobenius operator — which evolves densities, ν, over one iterate of f, as $\mathcal{P}\nu$

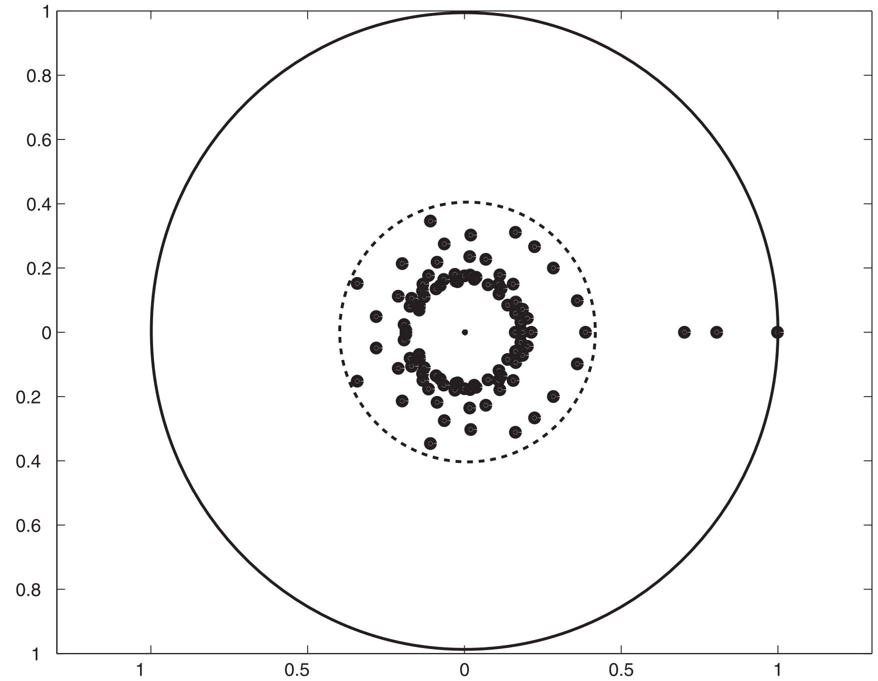
Almost-invariant / almost-cyclic sets

- A set B is called almost invariant over the interval $[t, t+T]$ if

$$\rho(B) = \frac{m(B \cap f^{-1}(B))}{m(B)} \approx 1.$$

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

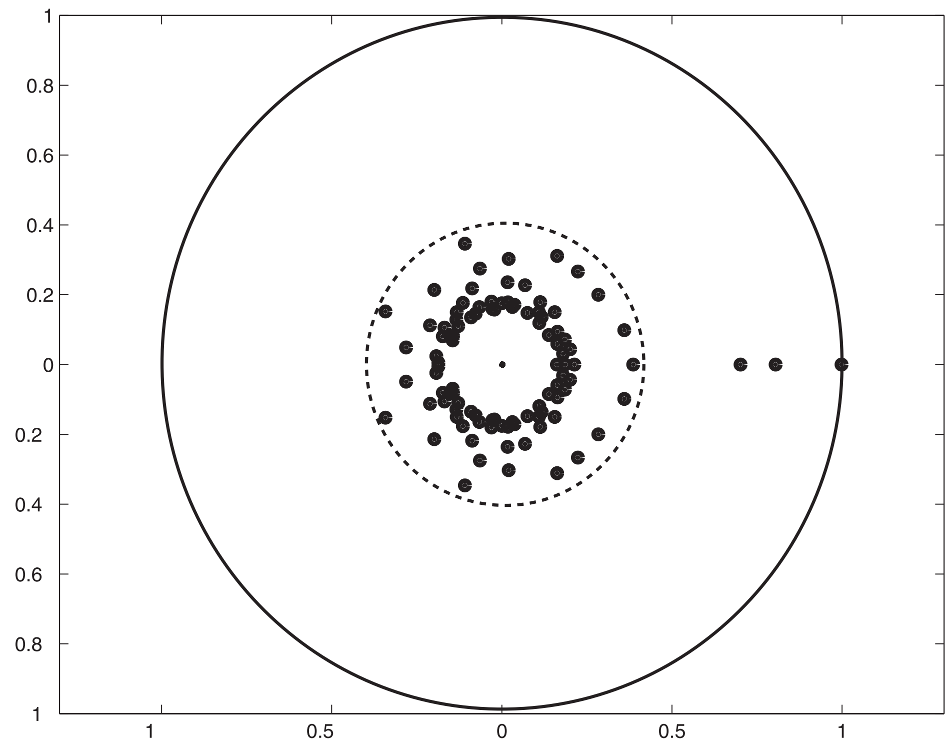
- In practice, AIS identified from spectrum of P or graph-partitioning



example spectrum of P

Dellnitz, Froyland, Sertl [2000] Nonlinearity

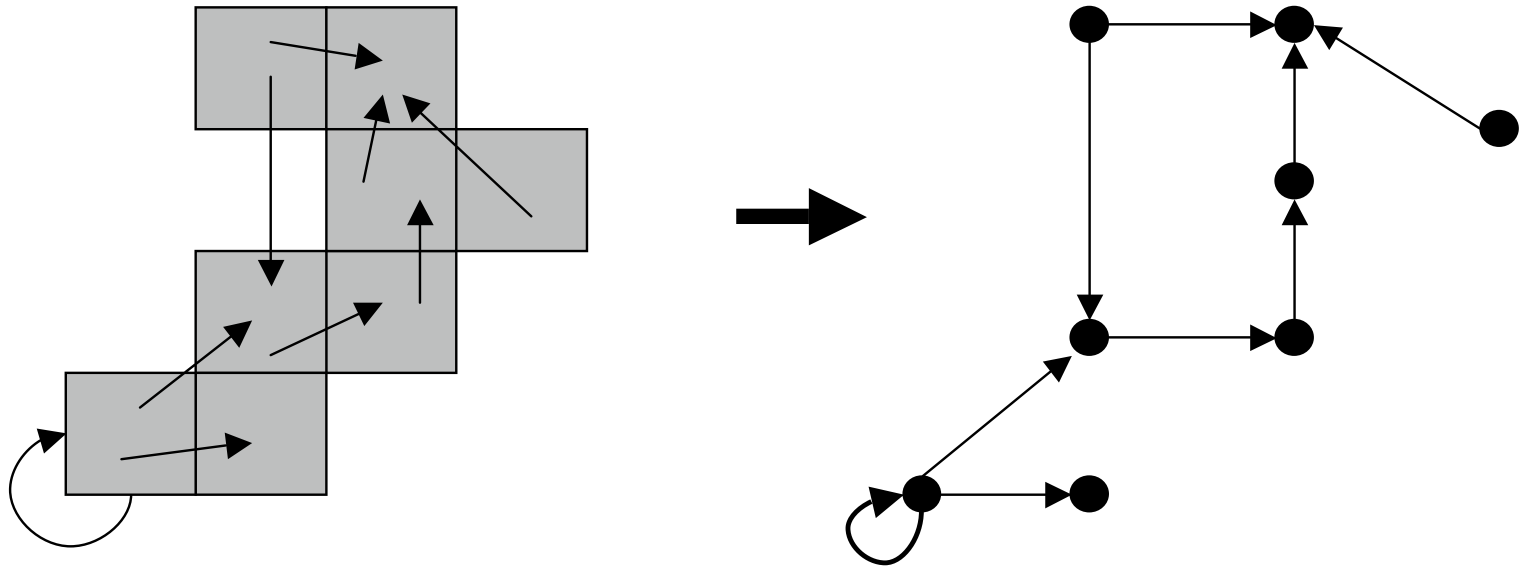
Identifying AISs by spectrum of P



- **Invariant** densities are those fixed under P, $P\nu = \nu$, i.e., eigenvalue 1
- Essential spectrum lies within a disk of radius $r < 1$ which depends on the weakest expansion rate of the underlying system.
- The other real eigenvalues identify **almost-invariant** sets

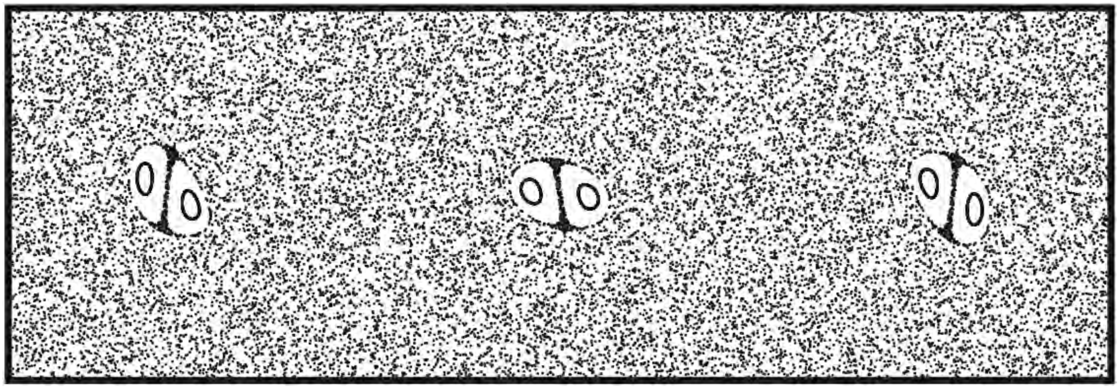
Dellnitz, Froyland, Sertl [2000] Nonlinearity

Identifying AISs by graph-partitioning



- P has graph representation where nodes correspond to boxes B_i and transitions between them are edges of a directed graph
- use graph partitioning methods to divide the nodes into an optimal number of parts such that each part is highly coupled within itself and only loosely coupled with other parts
- by doing so, we can obtain AISs and transport between them

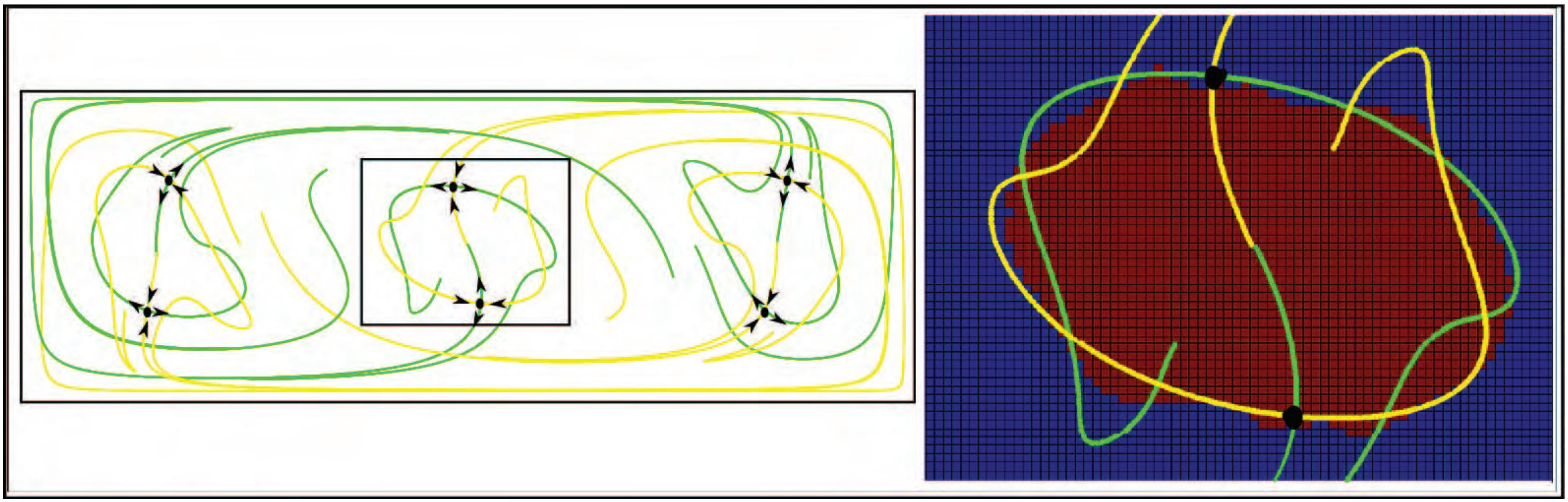
Identifying 'ghost rods': almost-cyclic sets



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

[1] 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



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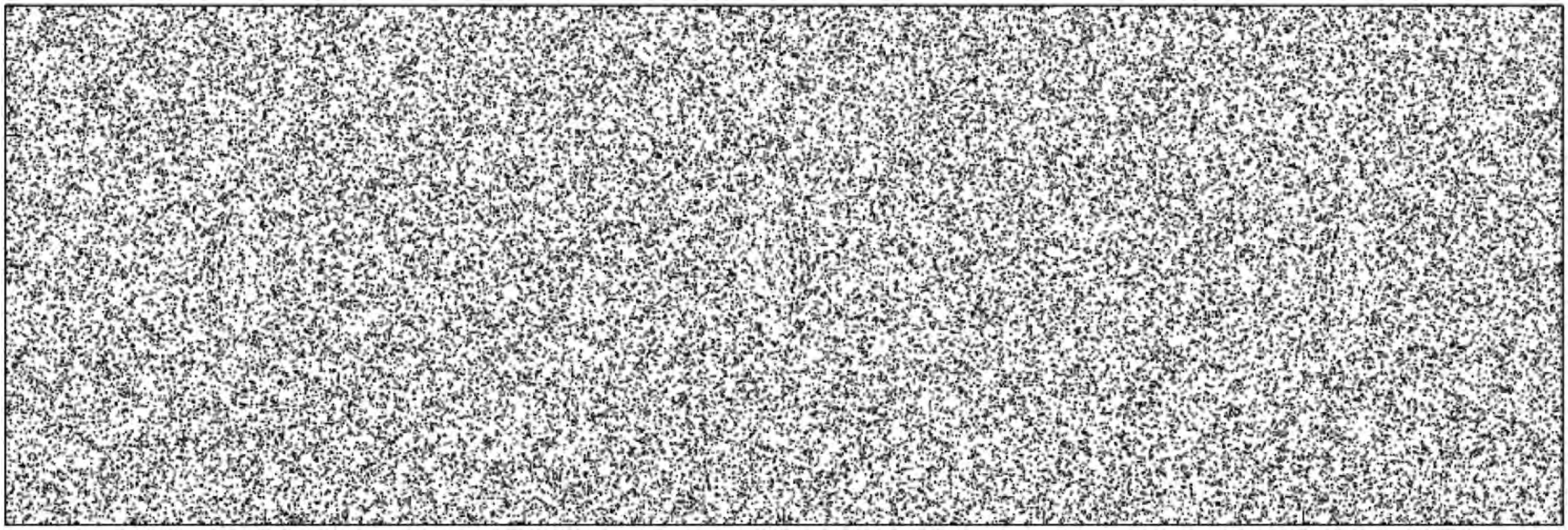
Identifying 'ghost rods': almost-cyclic sets



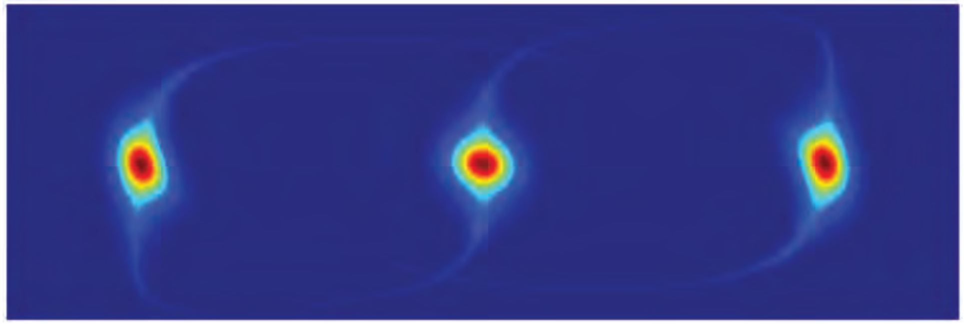
Poincaré section for $\tau_f < 1 \Rightarrow$ no obvious structure!

- Return to $\tau_f < 1$ case, where no periodic orbits of low period known
- What are the AISs and ACSs here?

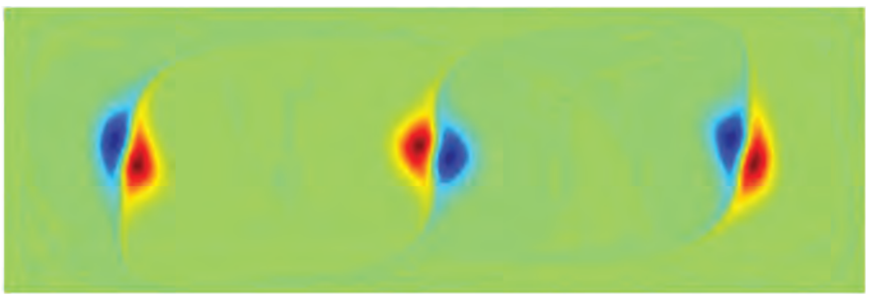
- Consider $P_t^{t+\tau_f}$ induced by family of period-τ_f maps $\phi_t^{t+\tau_f}$, $t \in [0, \tau_f)$

Identifying ‘ghost rods’: almost-cyclic sets

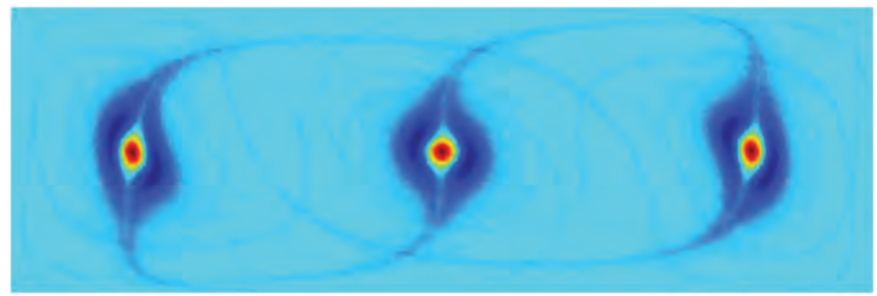
Top eigenvectors for $\tau_f = 0.99$ reveal hierarchy of phase space structures



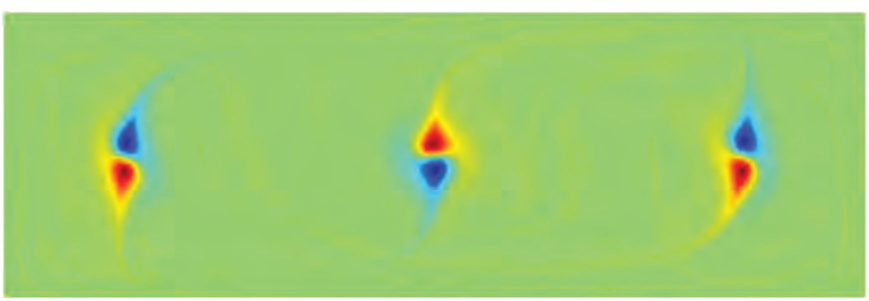
ν_2



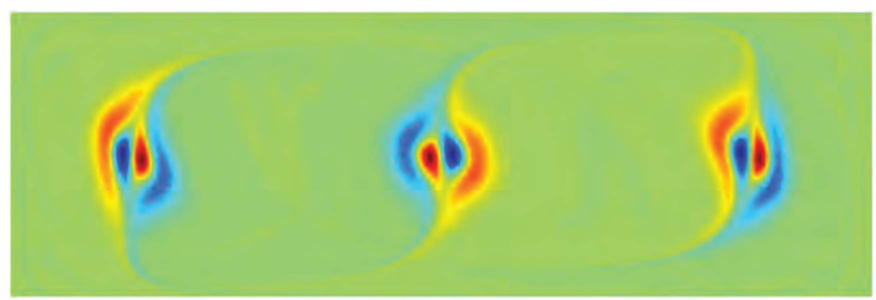
ν_3



ν_4

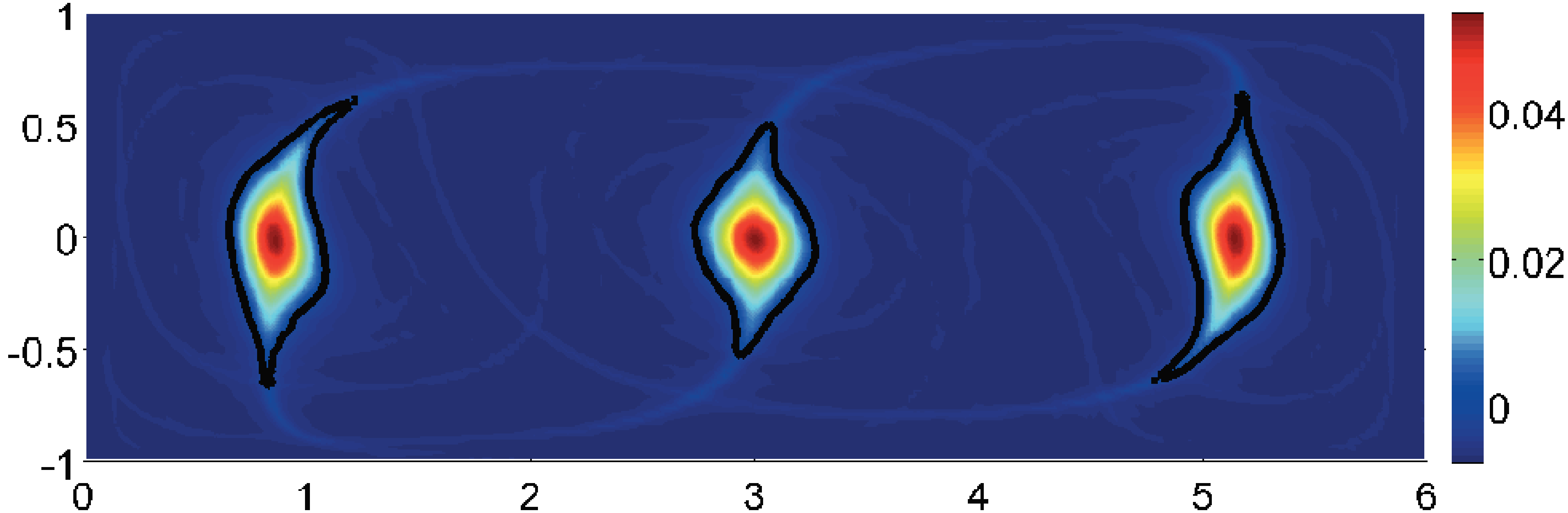


ν_5



ν_6

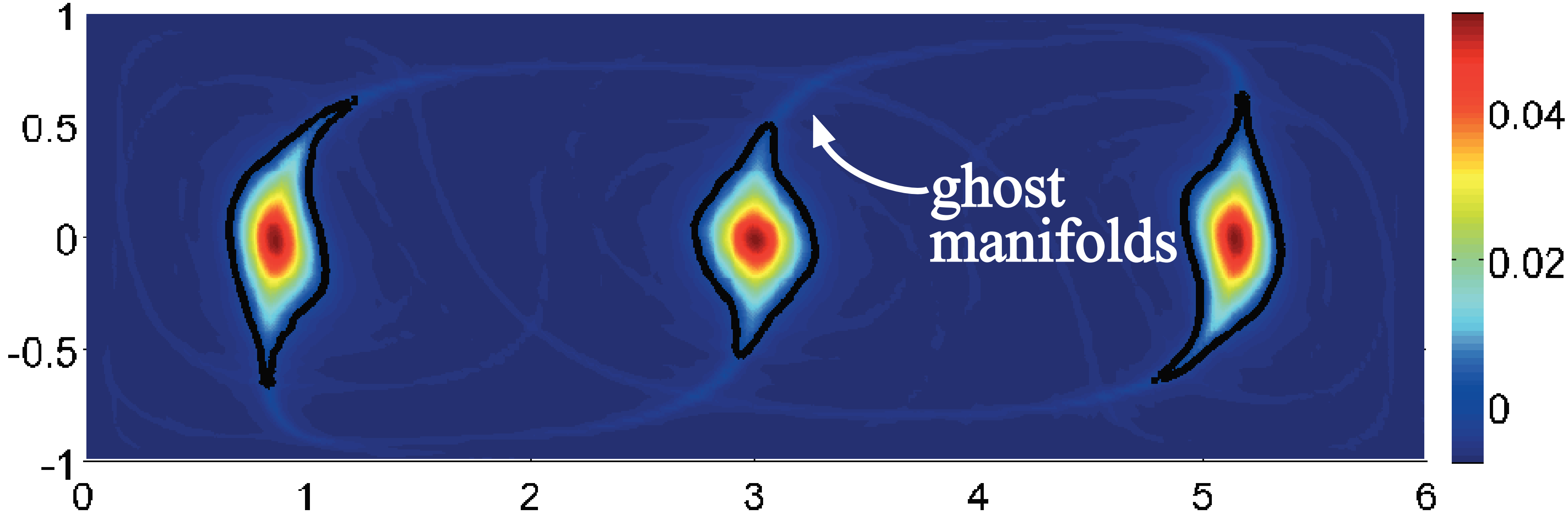
Identifying 'ghost rods': almost-cyclic sets



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

- Three-component AIS made of 3 ACSs of period 3
- ACSs, in effect, replace periodic orbits for TNCT

Identifying 'ghost rods': almost-cyclic sets



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

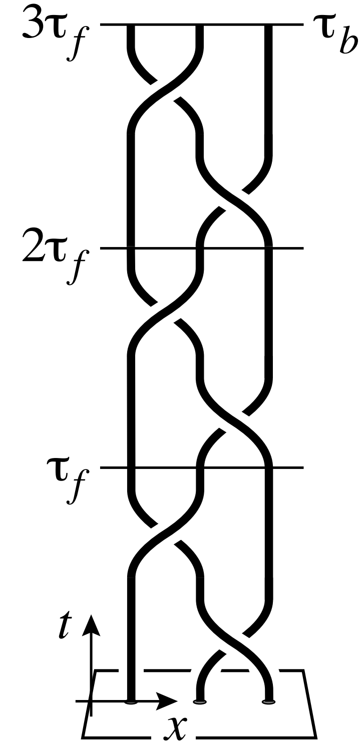
- Three-component AIS made of 3 ACSs of period 3
- ACSs, in effect, replace periodic orbits for TNCT
- Also: we see a **remnant of the 'stable and unstable manifolds' of the saddle points**, despite no saddle points – 'ghost manifolds'?

Identifying 'ghost rods': almost-cyclic sets

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

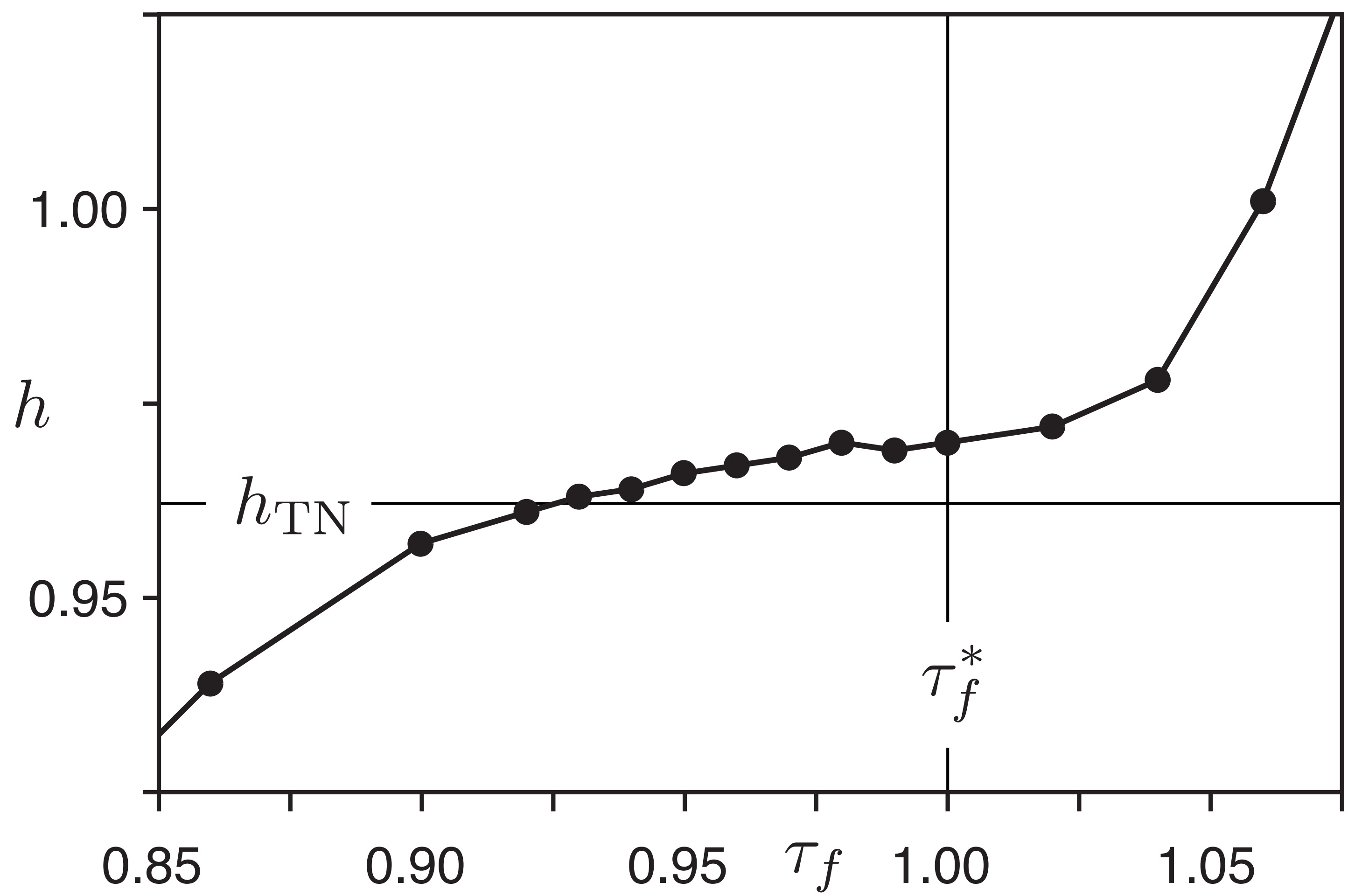
Movie shown is second eigenvector for $P_t^{t+\tau_f}$ for $t \in [0, \tau_f)$

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
— But, theorems apply only to periodic points!
— Stremler, Ross, Grover, Kumar [2011] Phys. Rev. Lett.

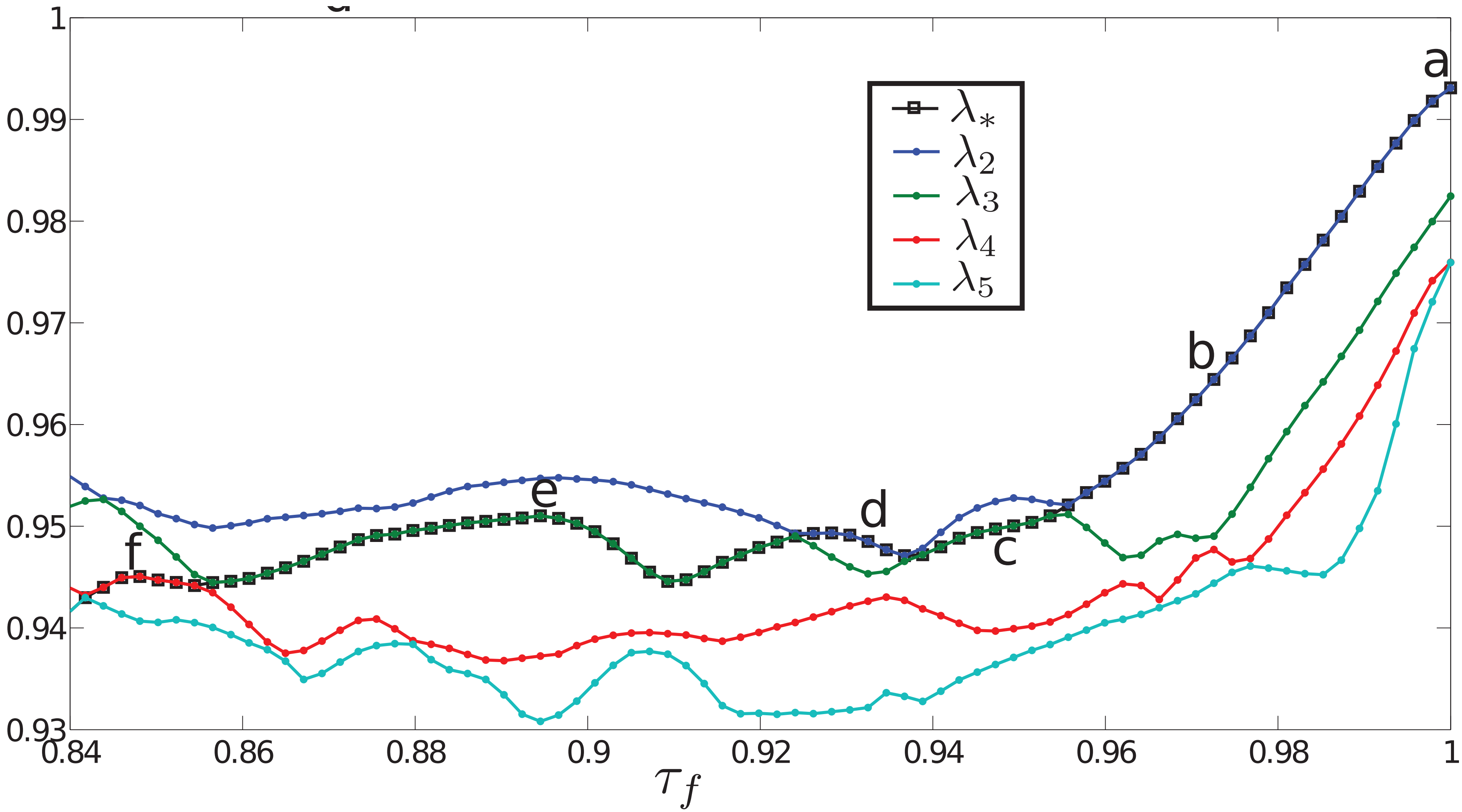
Topological entropy vs. bifurcation parameter



topological entropy as a function of τ_f

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

Eigenvalues/eigenvectors vs. bifurcation parameter



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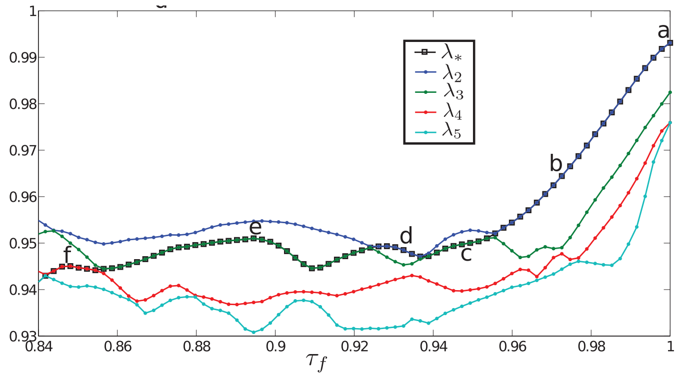
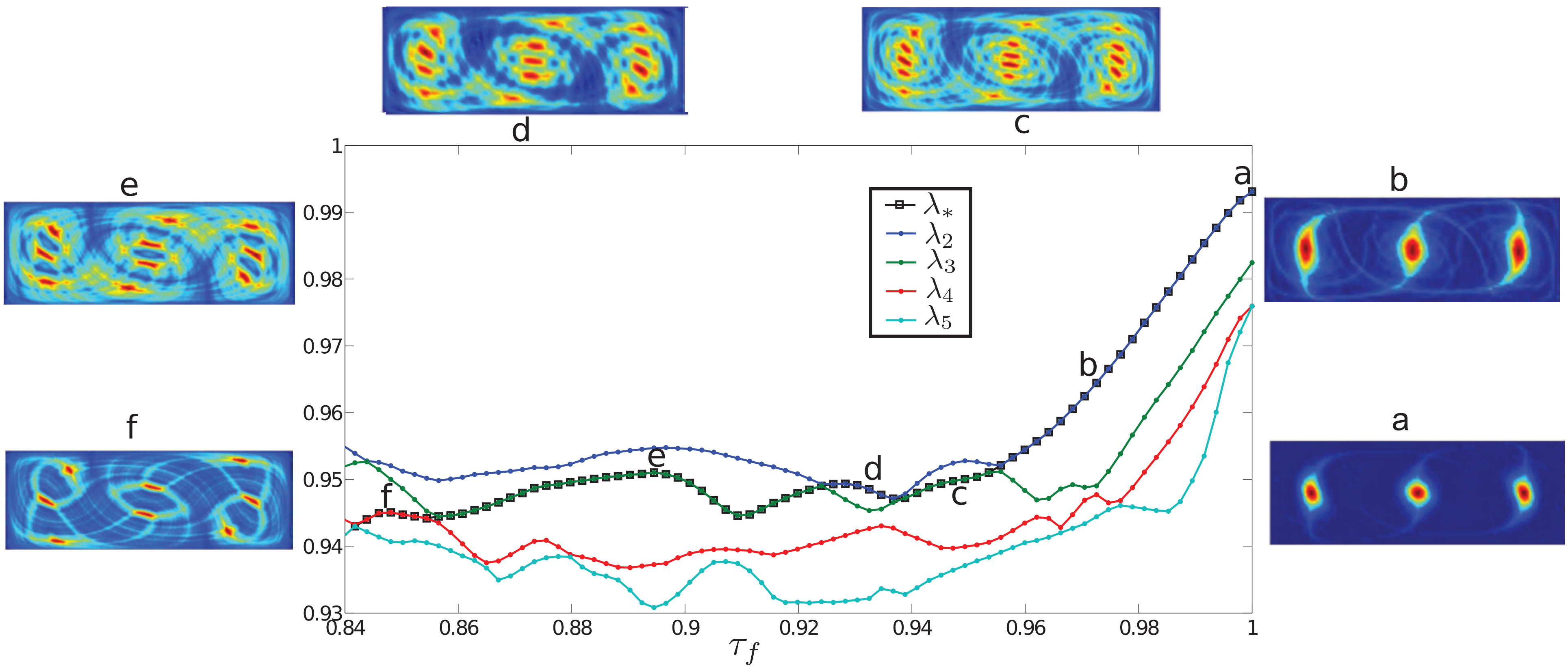


Eigenvalues/eigenvectors vs. bifurcation parameter



Movie shows change in eigenvector along branch marked with '$-\square-$' above (a to f), as τ_f decreases $\Rightarrow$

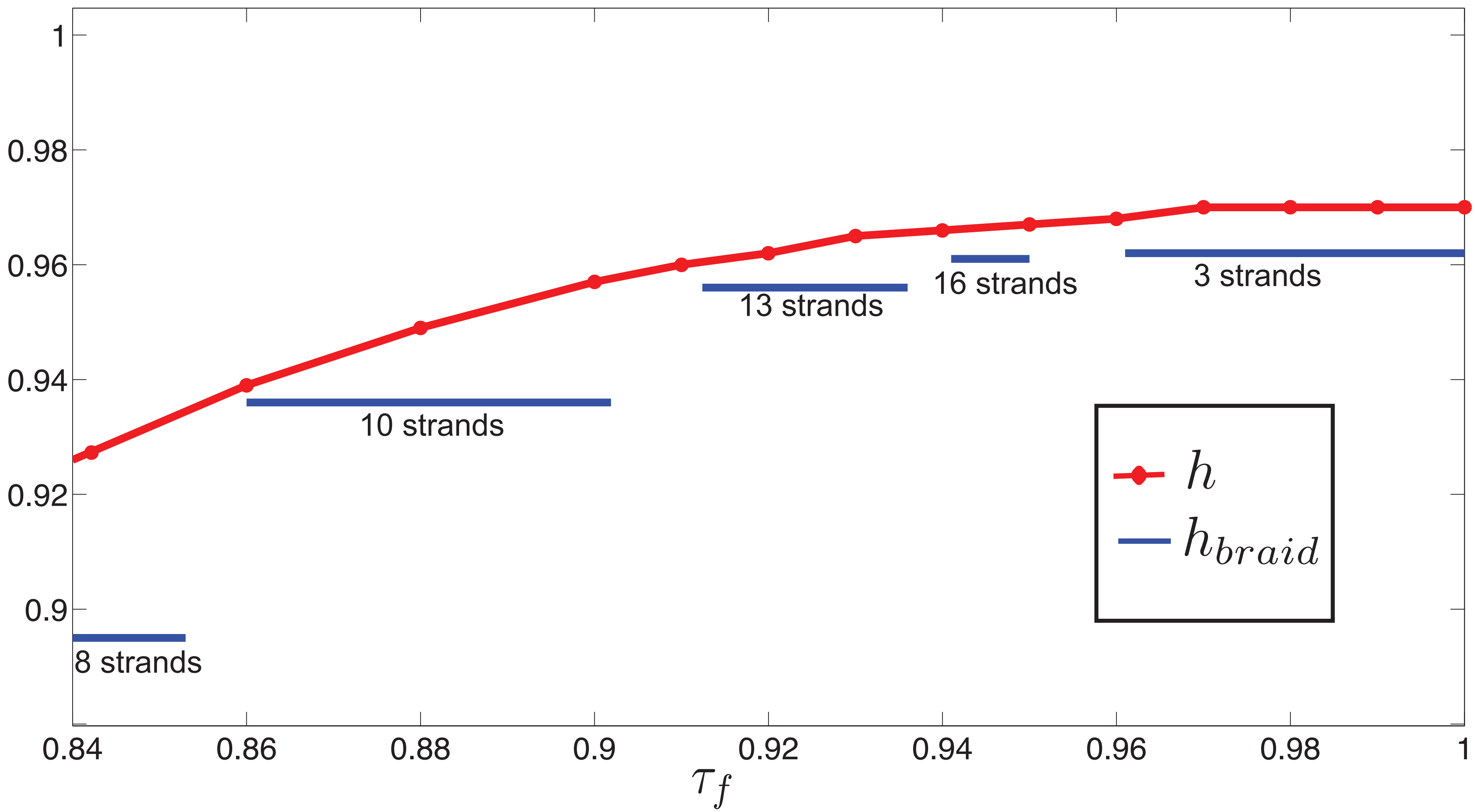
Bifurcation of ACSs

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

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

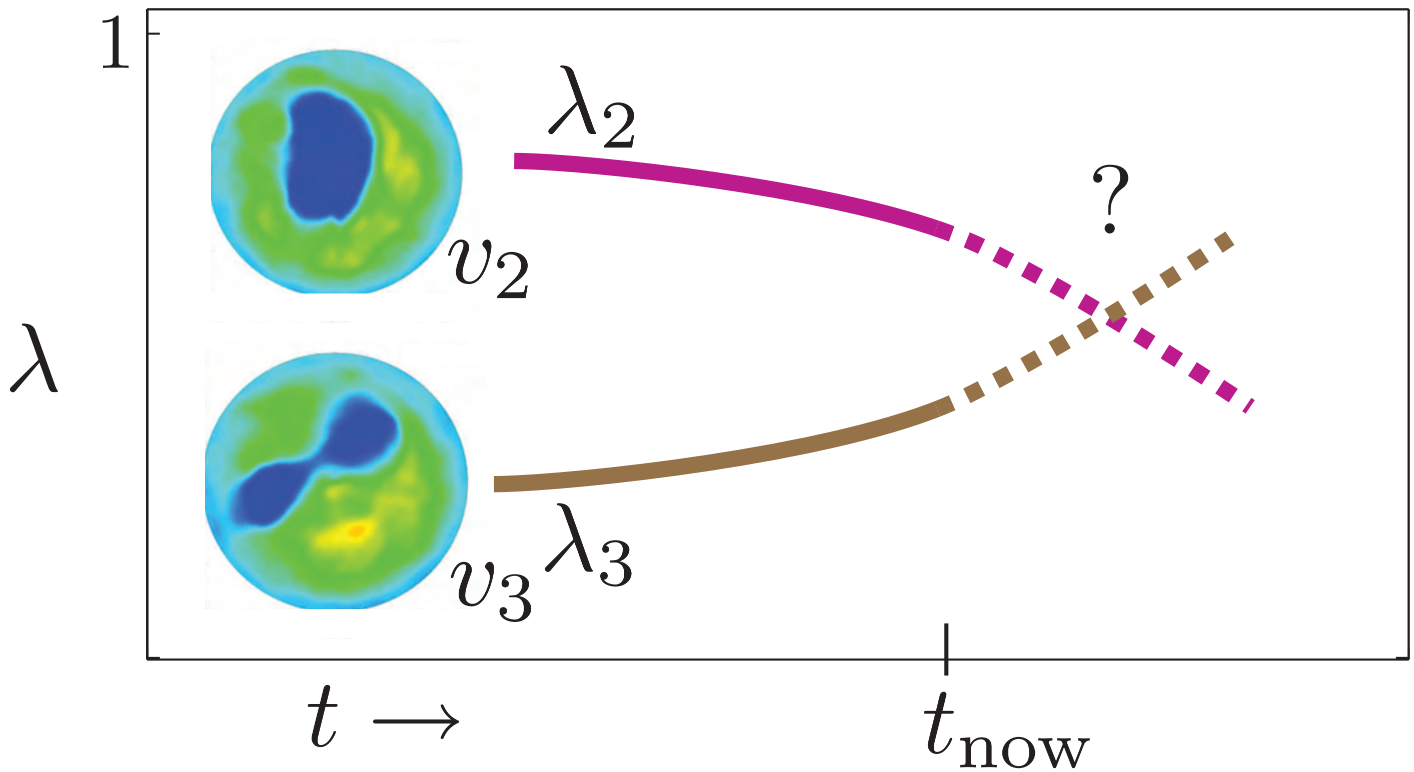
Thurson-Nielsen for this braid provides lower bound on topological entropy

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

Speculation: trends in eigenvalues/vectors for prediction



- Different eigenvectors can correspond to dramatically different behavior.
- Some eigenvectors increase in importance while others decrease
- Can we predict dramatic changes in system behavior?
- e.g., splitting of the ozone hole in 2002, using only data *before* split

Applications: Atmospheric transport networks

Skeleton of large-scale horizontal transport

relevant for large-scale

spatiotemporal patterns

of important biota

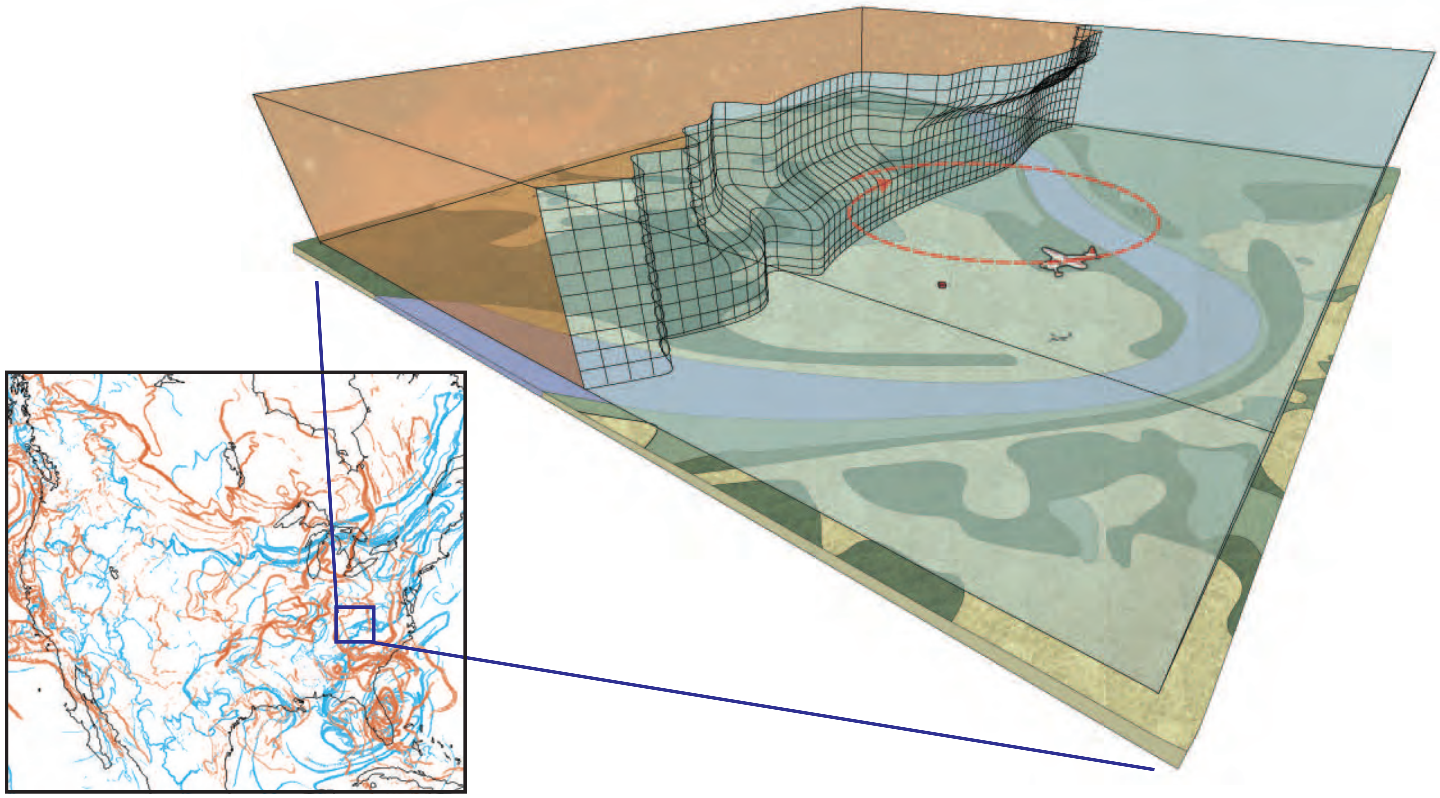
e.g., plant pathogens

orange = repelling LCSs, blue = attracting LCSs

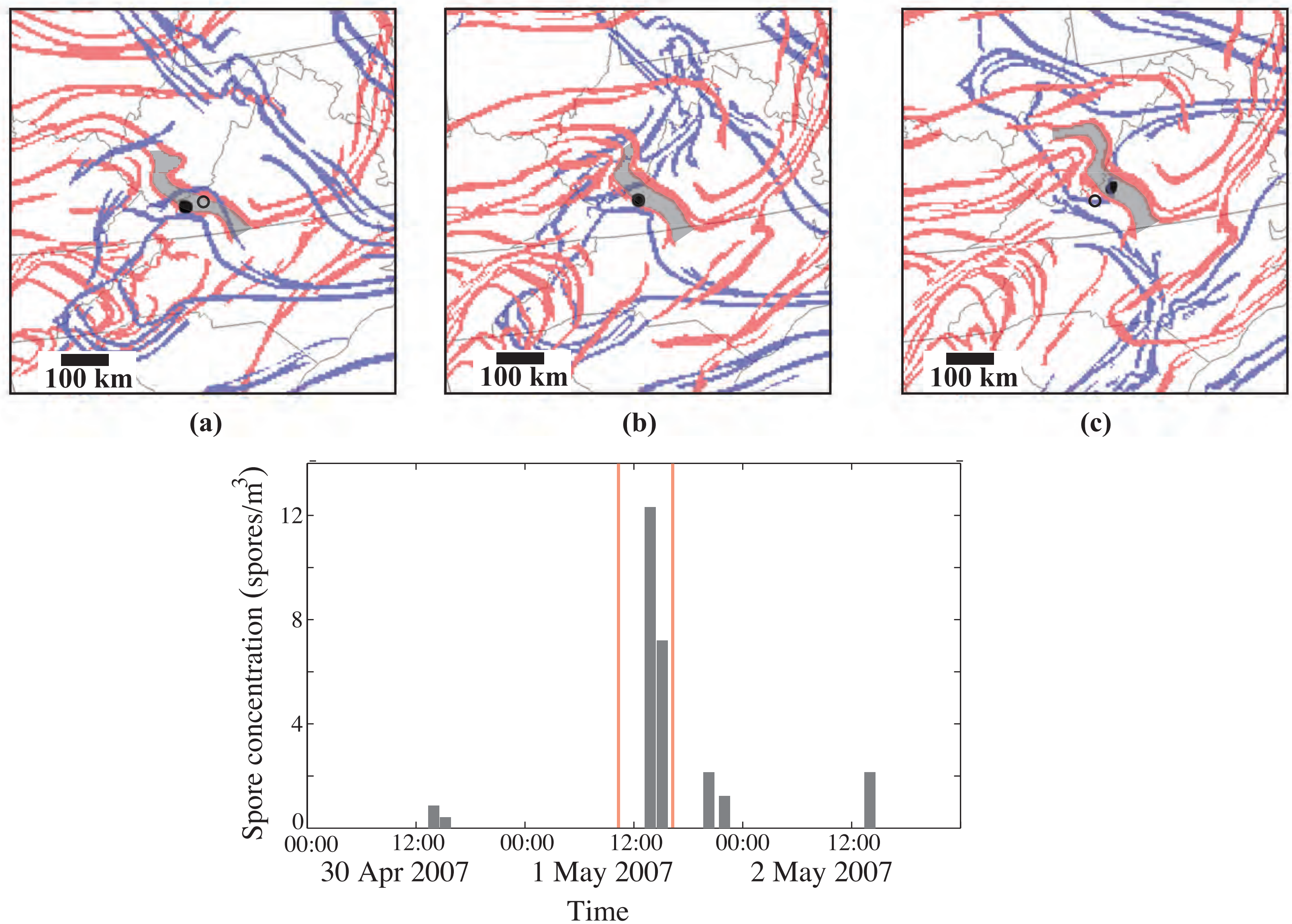
Tallapragada, Schmale, Ross [2011] Chaos

2D curtain-like structures bounding air masses

2D curtain-like structures bounding air masses

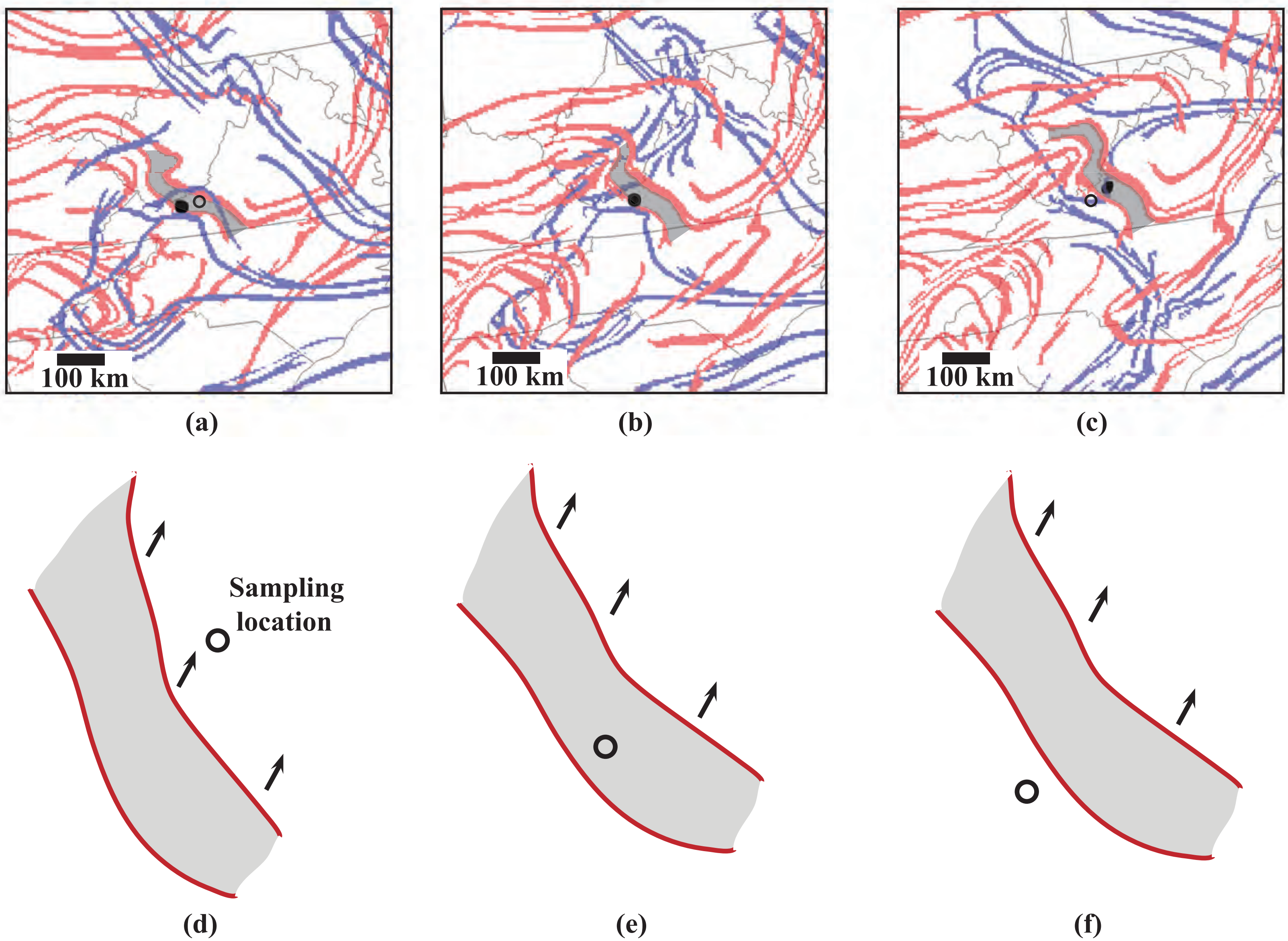


Pathogen transport: filament bounded by LCS



12:00 UTC 1 May 2007 15:00 UTC 1 May 2007 18:00 UTC 1 May 2007

Pathogen transport: filament bounded by LCS



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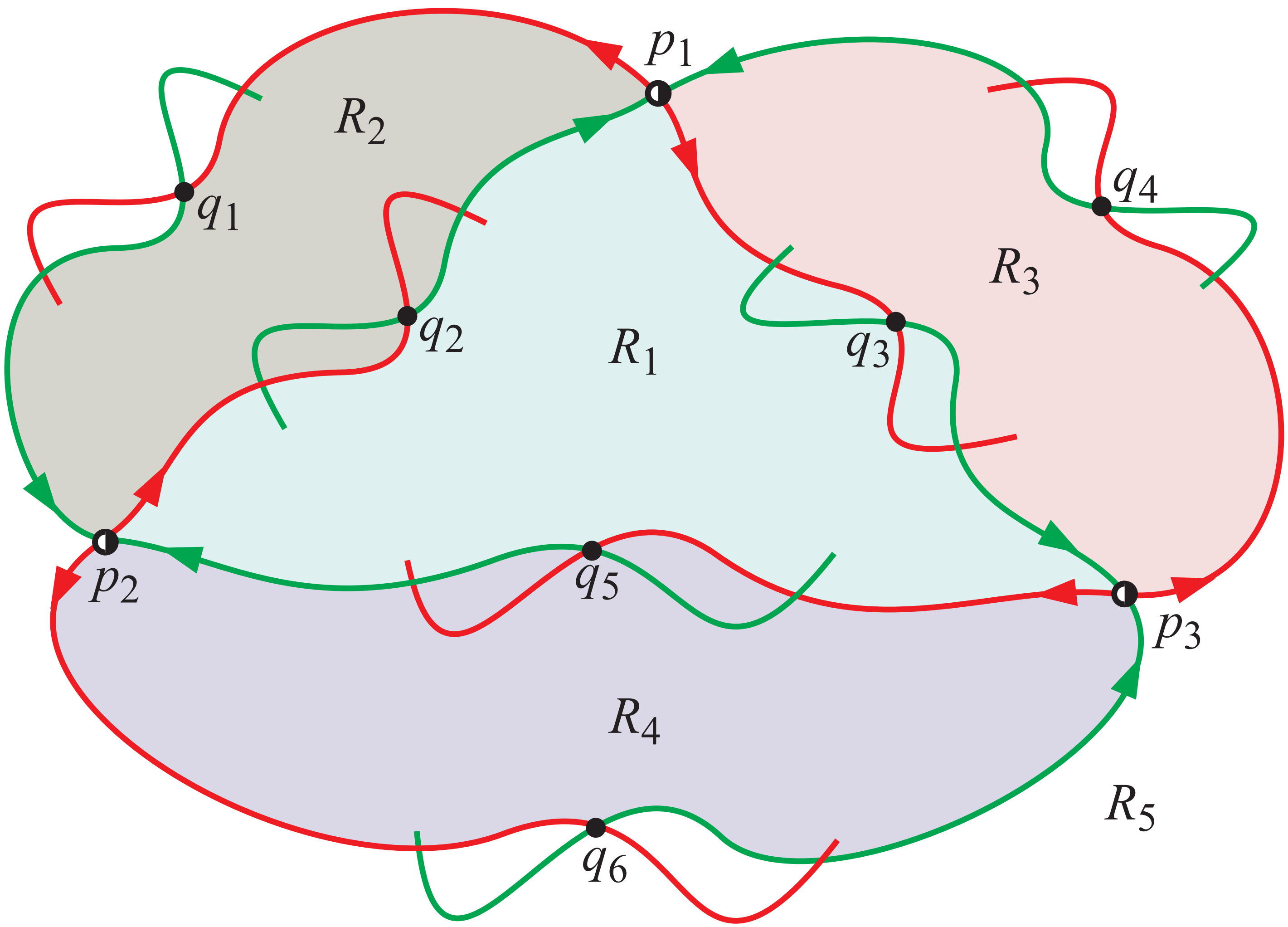
Optimal navigation in an aperiodic setting?

- Selectively 'jumping' between coherent air masses using control
- Moving between mobile subregions of different finite-time itineraries



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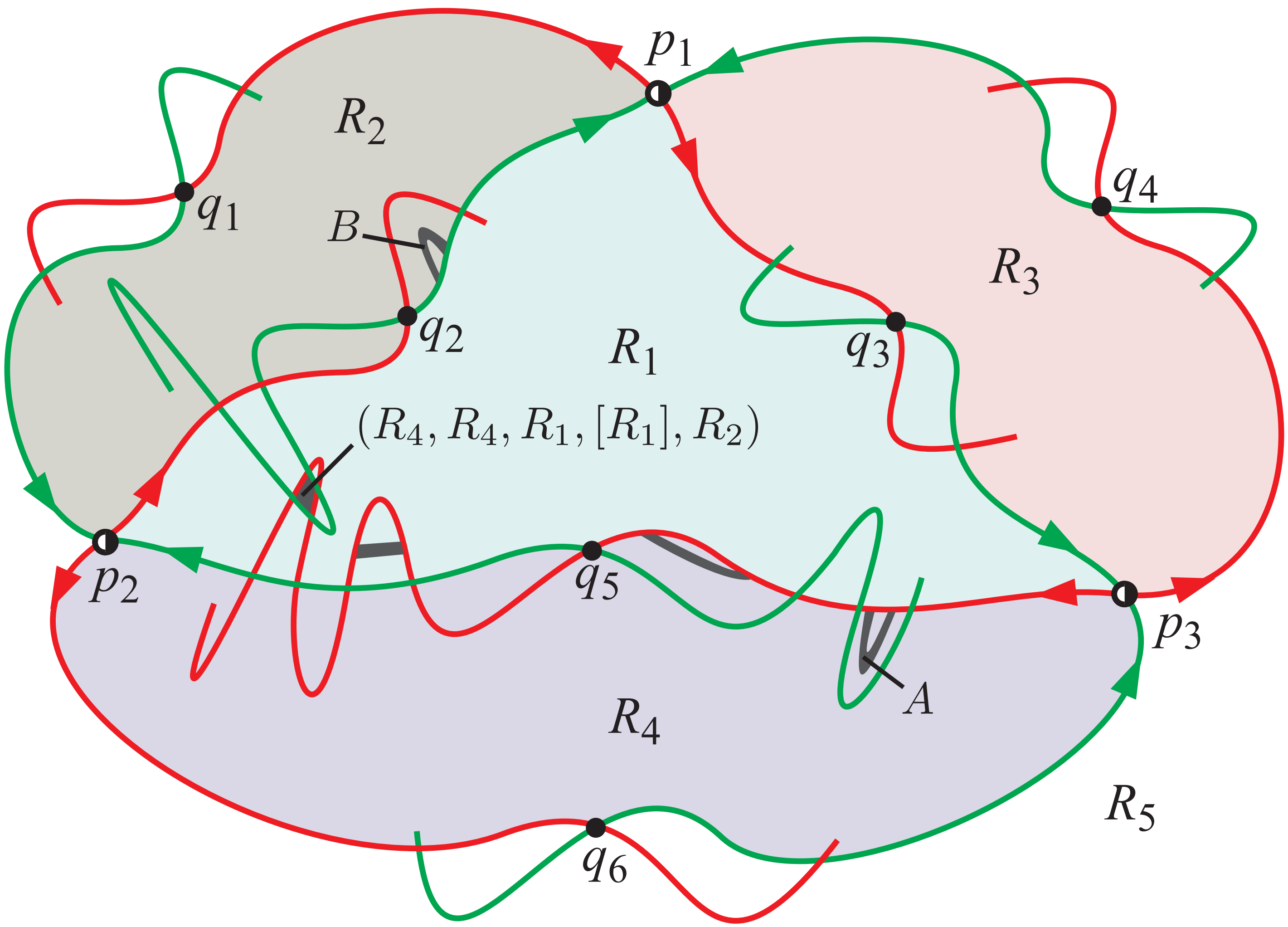

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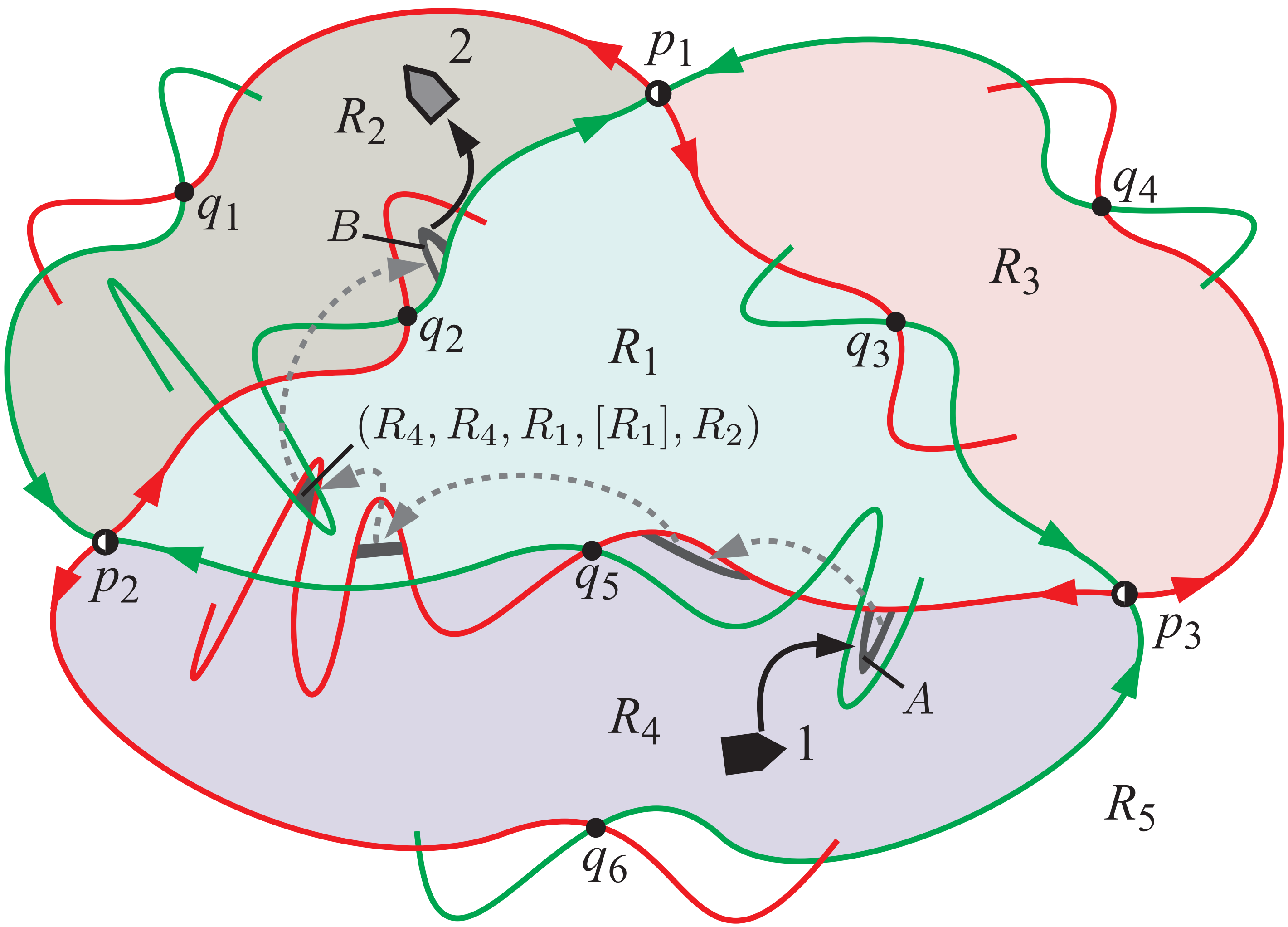

Optimal navigation in an aperiodic setting?

- Selectively 'jumping' between coherent air masses using control
- Moving between mobile subregions of different finite-time itineraries

FTLE shown in grayscale; bright lines are LCS separating coherent sets; green=passive; red=control

Final words on coherent structures

- 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 ridges/LCS

  - Many links between these notions — e.g., FTLE ridges locate analogs of stable and unstable manifolds
    — boundaries between coherent sets are FTLE ridges
    — periodic points ⇒ almost-cyclic sets for TNCT, braiding, mixing
    — their 'stable/unstable invariant manifolds' ⇒ ???

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, Schmale [2011] Lagrangian coherent structures are associated with fluctuations in airborne microbial populations. *Chaos* 21, 033122.
- 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 [2012] Topological chaos, braiding and bifurcation of almost-cyclic sets. Submitted arXiv preprint.
- Tallapragada & Ross [2012] A set oriented definition of the FTLE and coherent sets. Submitted preprint.