



Set oriented methods, invariant manifolds and transport

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Caltech/MIT/NASA: *W.S. Koon, F. Lekien, M.W. Lo, J.E. Marsden*
Uni Paderborn: *M. Dellnitz, O. Junge, K. Padberg, R. Preis, B. Thiere*

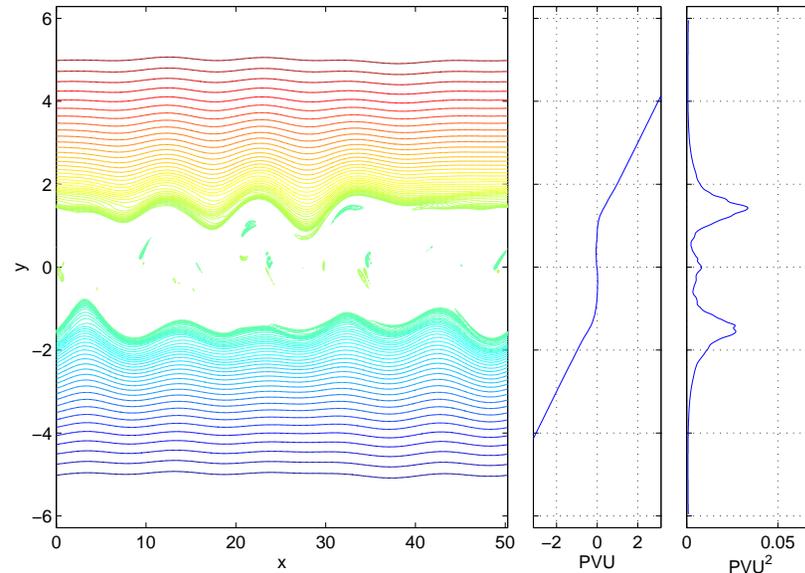
AOSN Workshop

Princeton University, October 30-31, 2003

Motivation

■ *Phase space transport*

- Many physical examples
- e.g., Geophysical fluid mixing

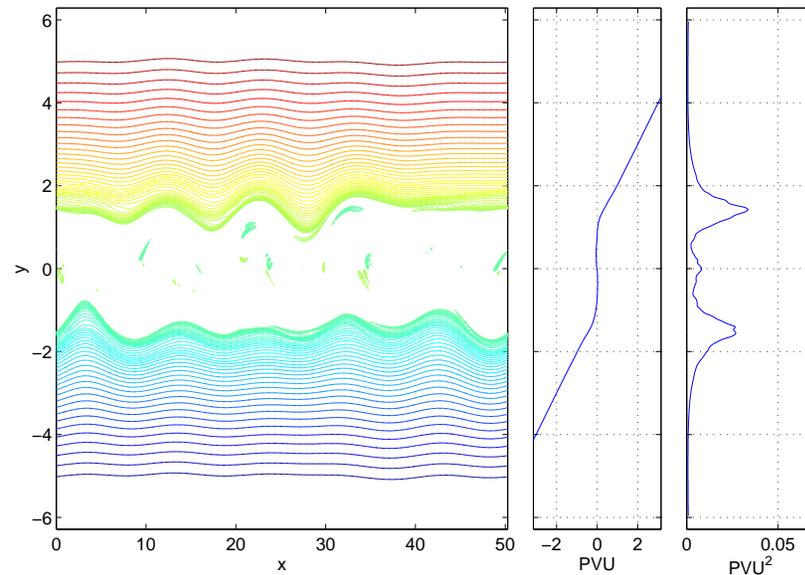


Atmospheric mixing near the equator

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Atmospheric mixing near the equator

- Qualitative understanding
- Statistical quantities

Other Examples

- Meteorite exchange between Mars & Earth

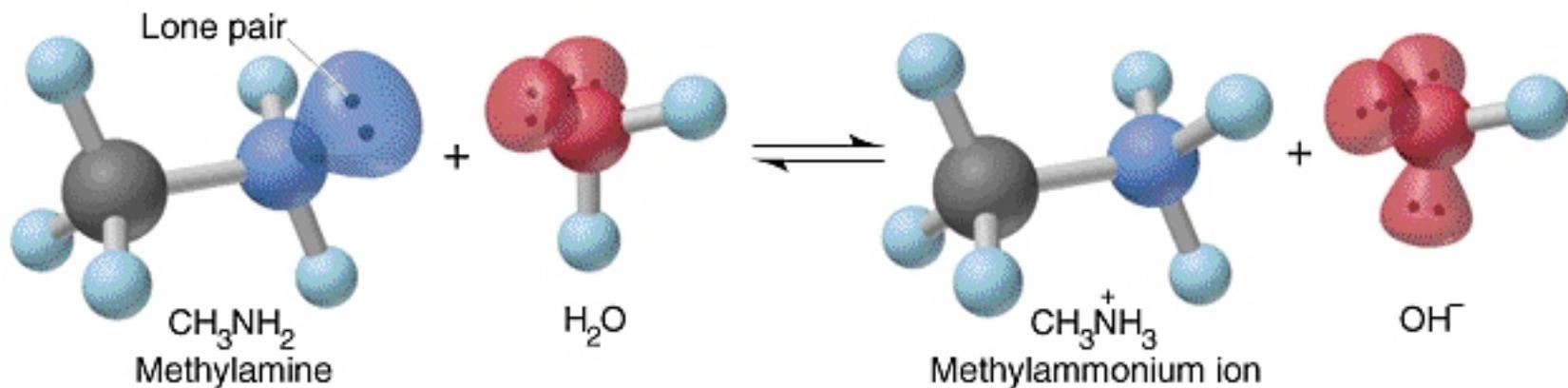


Other Examples

- Meteorite exchange between Mars & Earth



- Chemical reaction rates



In This Talk...

- Transport problem described
- Two computational techniques
 - (1) Invariant manifolds
 - (2) Almost-invariant sets
- Compare & combine
- Extensions and future work

Transport

- Describe transport of phase points on a k -dimensional manifold \mathcal{M}

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- \mathcal{M} could be, e.g., the ocean surface, an energy shell, or a Poincaré surface-of-section
- We look first at $k = 2$ for autonomous systems
- Paper: Dellnitz, Junge, Koon, Lekien, Lo, Marsden, Padberg, Preis, R., Thiere [2003]

Statement of Problem

- Consider a volume- and orientation-preserving map

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

on some compact set $\mathcal{M} \subset \mathbb{R}^2$ with volume measure μ .
e.g., f may be a discretization of an autonomous flow.

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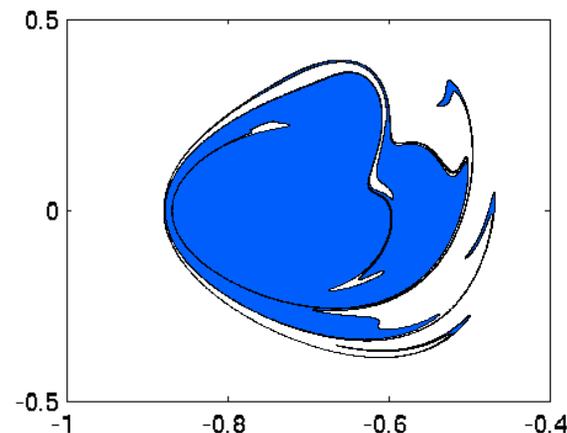
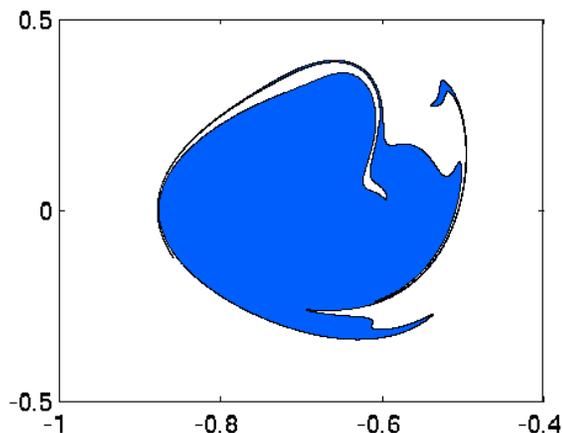
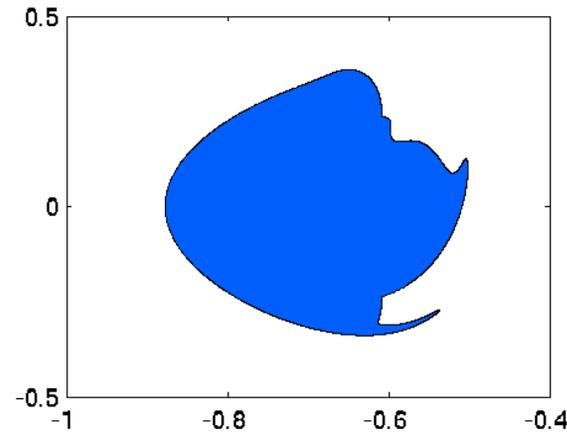
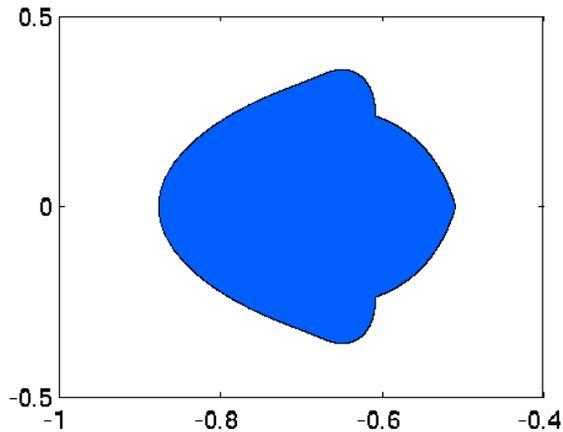
- Initially, R_i is uniformly covered with **species** S_i .
i.e., Species type indicates where a point was initially.

Statement of Problem

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Transport Quantities

□ Quantities of interest:

$T_{i,j}(n) \equiv$ the total amount of species S_i contained in region R_j immediately after the n -th iterate
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□ Our goal:

Compute the $T_{i,j}(n)$ up to some n_{\max}

Computational Approaches

- Compare & combine two computational approaches

Computational Approaches

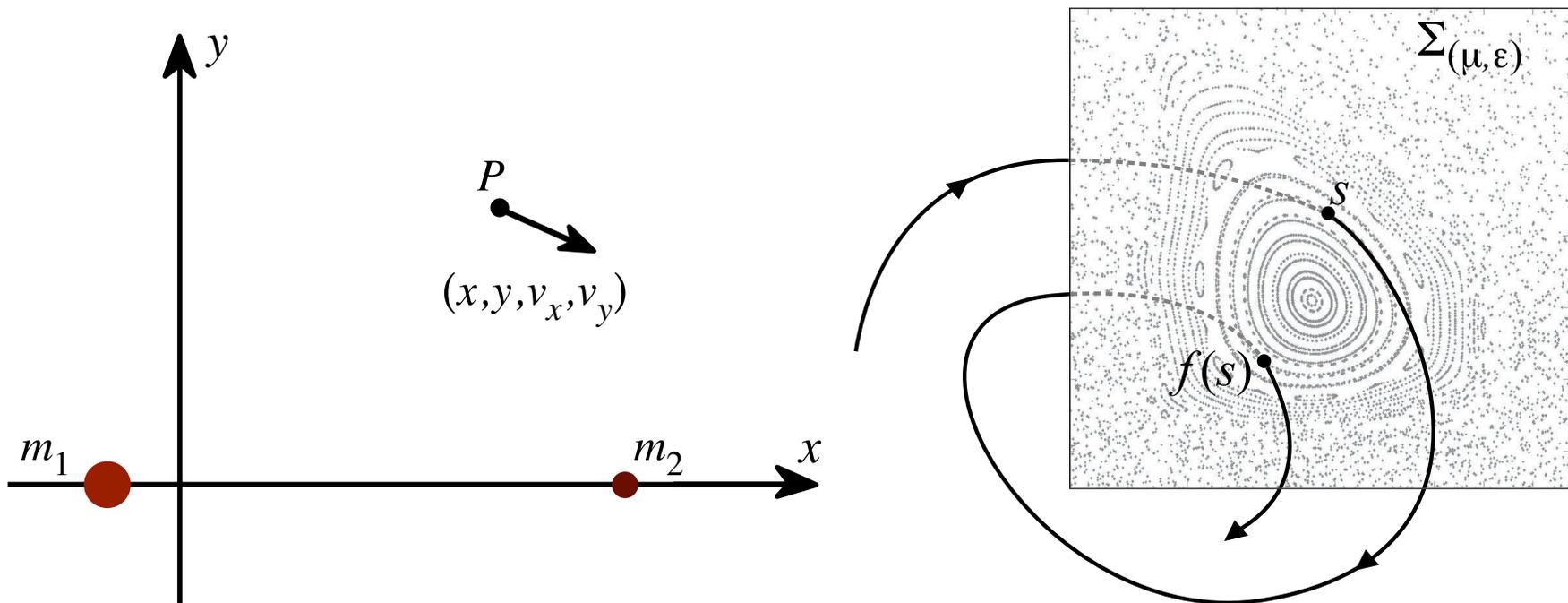
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MANGEN: Manifold Generation, Lekien etc

Computational Approaches

- Compare & combine two computational approaches
- 1) **Invariant manifolds** of fixed points, lobe dynamics; co-dimension one objects which bound regions, etc.
MANGEN: Manifold Generation, Lekien etc
- 2) **Set oriented methods**, almost-invariant sets; direct computation of regions
GAIO: Global Analysis of Invariant Objects, Dellnitz etc

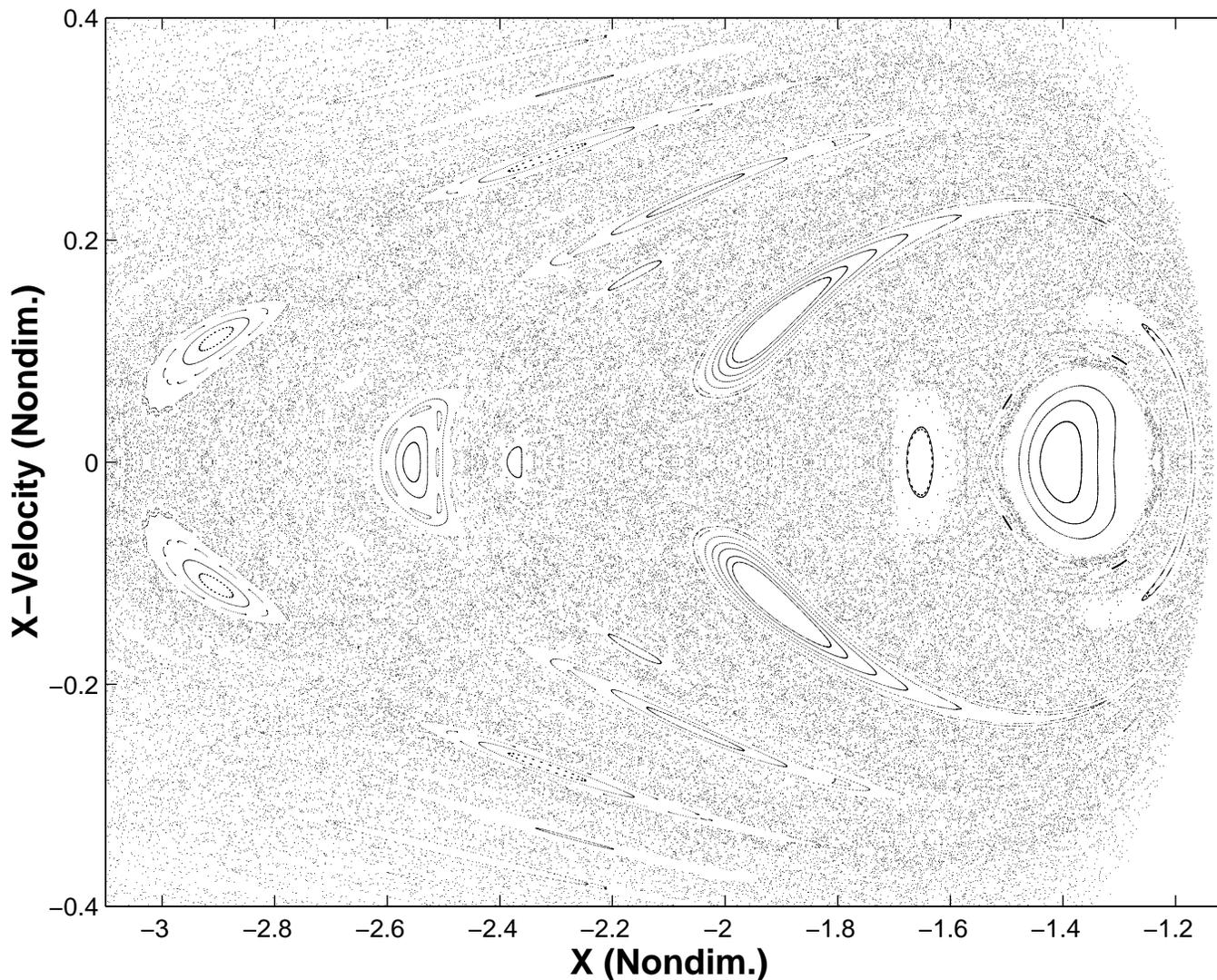
Particle in 2-Body Field

- Our chosen example problem: test particles in the gravity field of two masses, m_1 and m_2 , in circular orbit, i.e., the planar, circular restricted three-body problem with mass ratio $\frac{m_2}{m_1+m_2} \approx 10^{-3}$.
- Reduce to 2D map via Poincaré surface-of-section



Particle in 2-Body Field

- Poincaré map $f : \mathcal{M} \rightarrow \mathcal{M}$ has regular and irregular components. Large connected irregular component, the “**chaotic sea.**”

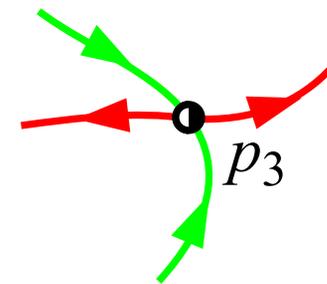
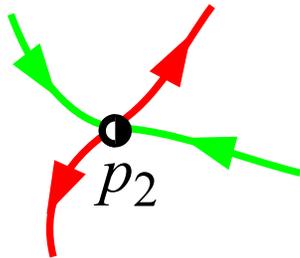
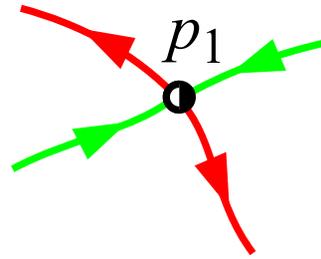


Transport on \mathcal{M}

- To understand the transport of points under the Poincaré map f , we consider the **invariant manifolds of unstable fixed points**
- Let $p_i, i = 1, \dots, N_p$, denote a collection of saddle-type hyperbolic fixed points for f .

Transport on \mathcal{M}

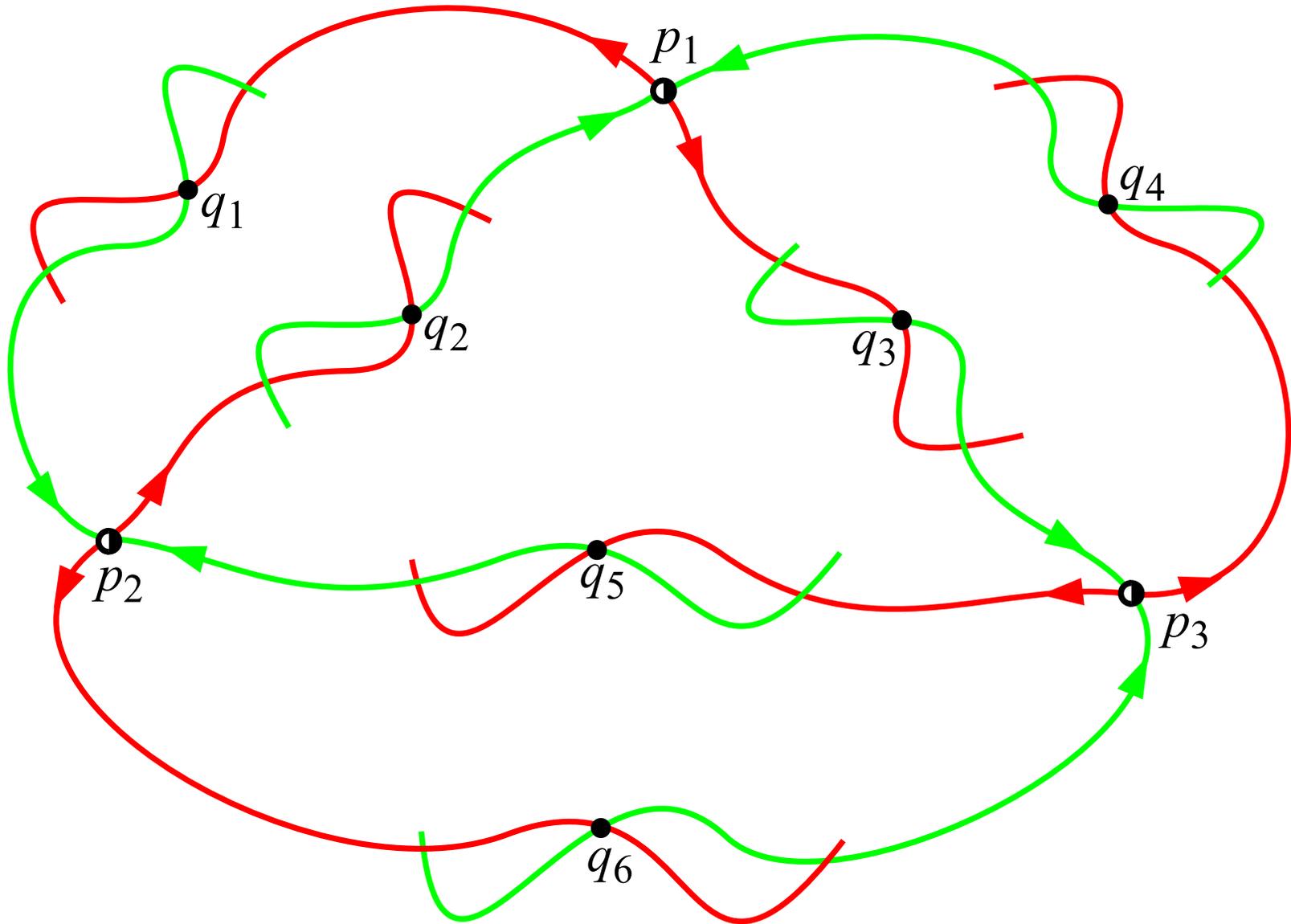
- Local pieces of unstable and stable manifolds



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

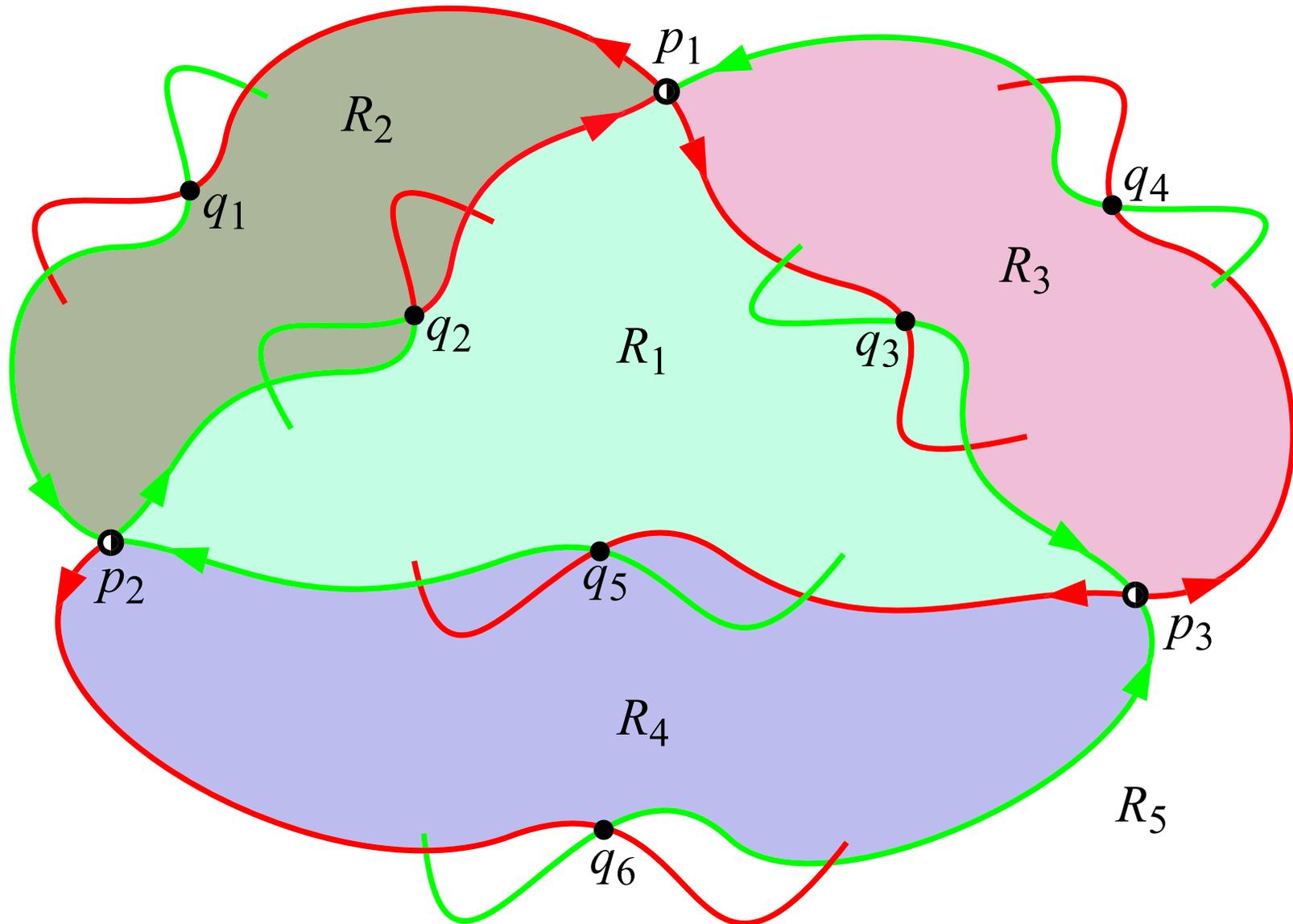
Transport on \mathcal{M}

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



Transport on \mathcal{M}

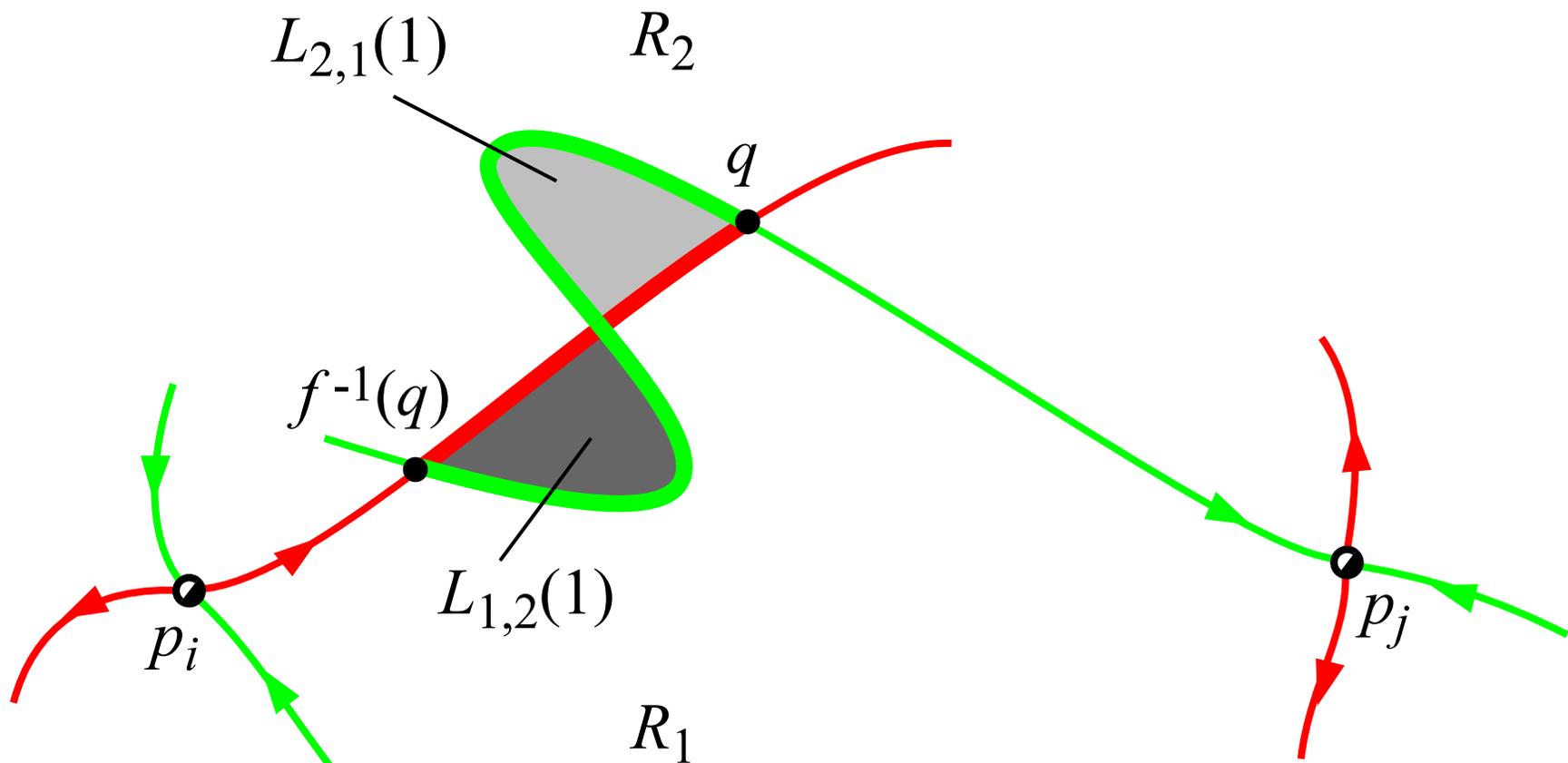
- These boundaries divide phase space into **regions**, $R_i, i = 1, \dots, N_R$



Lobe Dynamics

□ Local transport: across a boundary

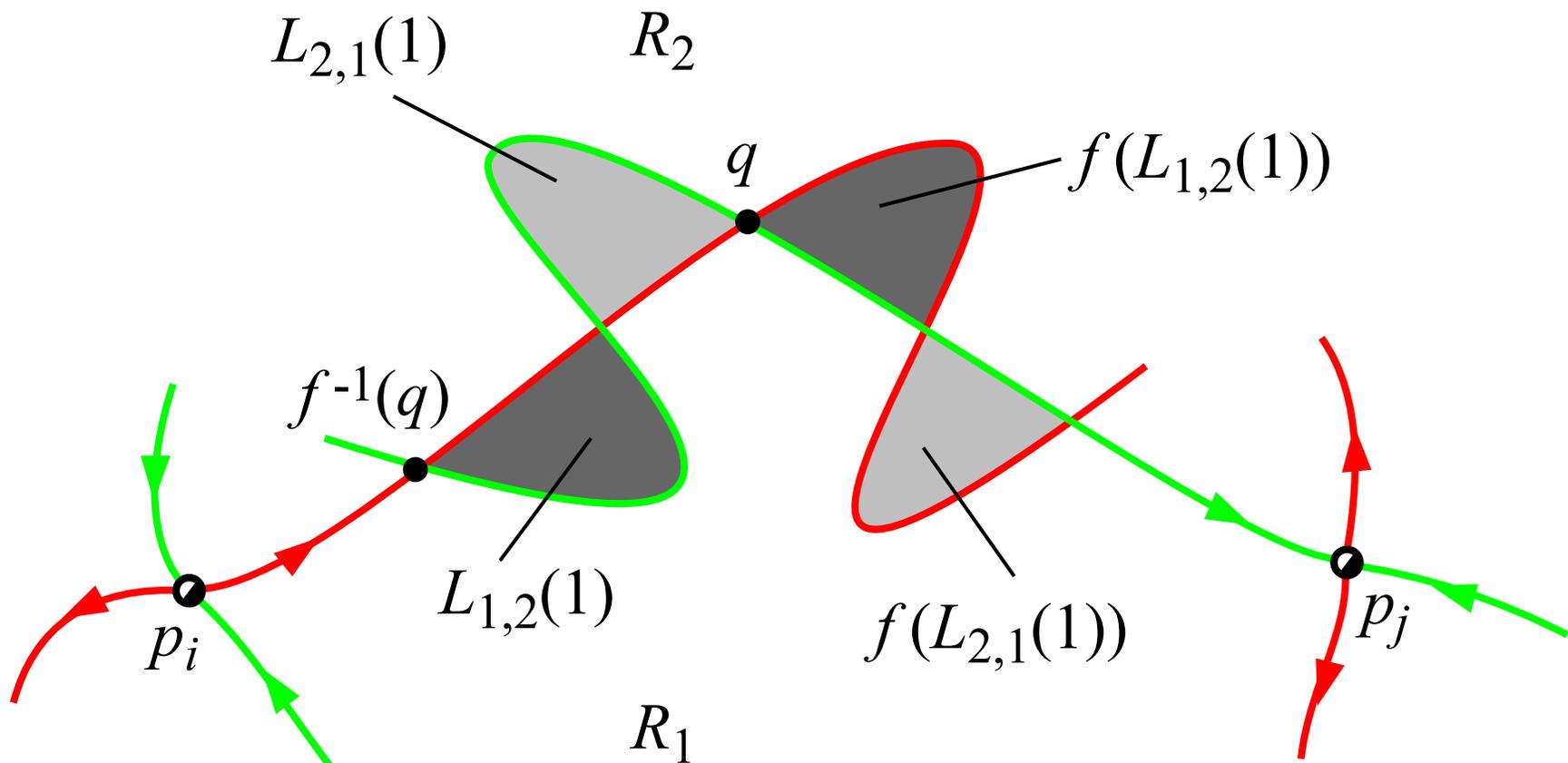
consider small sets bounded by stable & unstable mfd's



Lobe Dynamics

- They map from entirely in one region to another under one iteration of f

$L_{1,2}(1)$ and $L_{2,1}(1)$ are called turnstile **lobes**



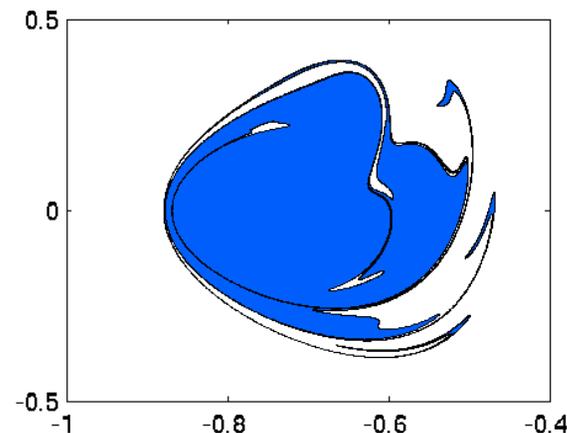
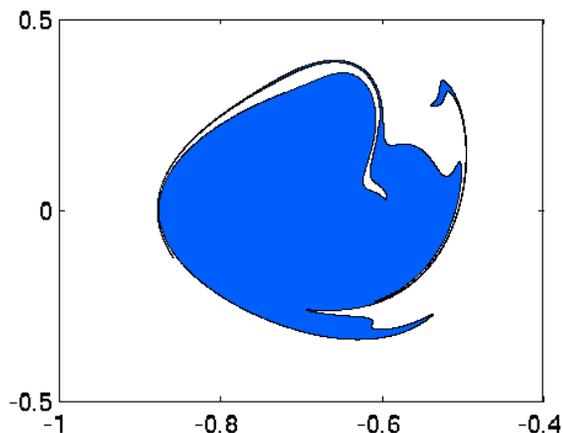
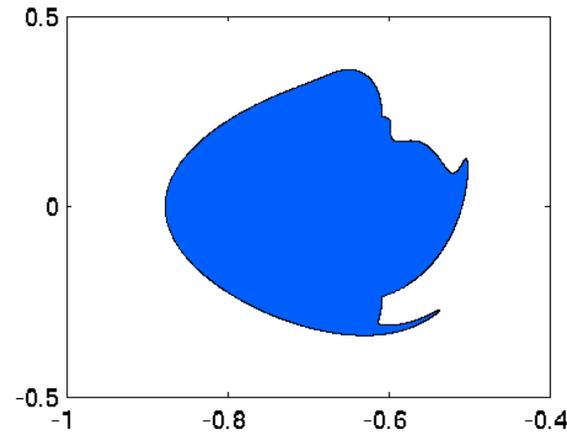
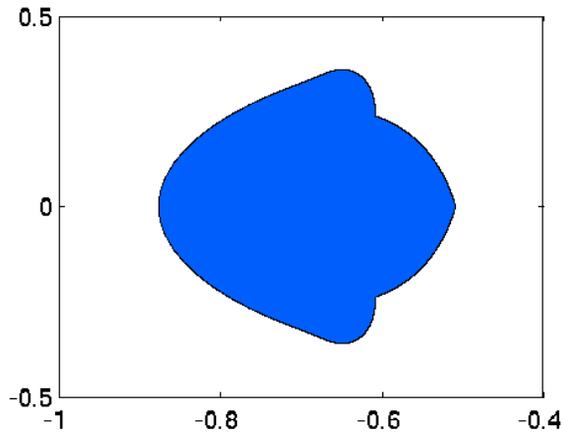
Lobe Dynamics

□ **MANGEN:** evolution of a lobe of species S_1 into R_2

insert S1 into R2 movie

Lobe Dynamics

- **Global transport** between regions ($T_{i,j}(n)$) is completely described by the dynamical evolution of lobes.



Set Oriented Approach

■ Overview

- Partition phase space into **loosely coupled regions**

$$R_i, i = 1, \dots, N_R,$$

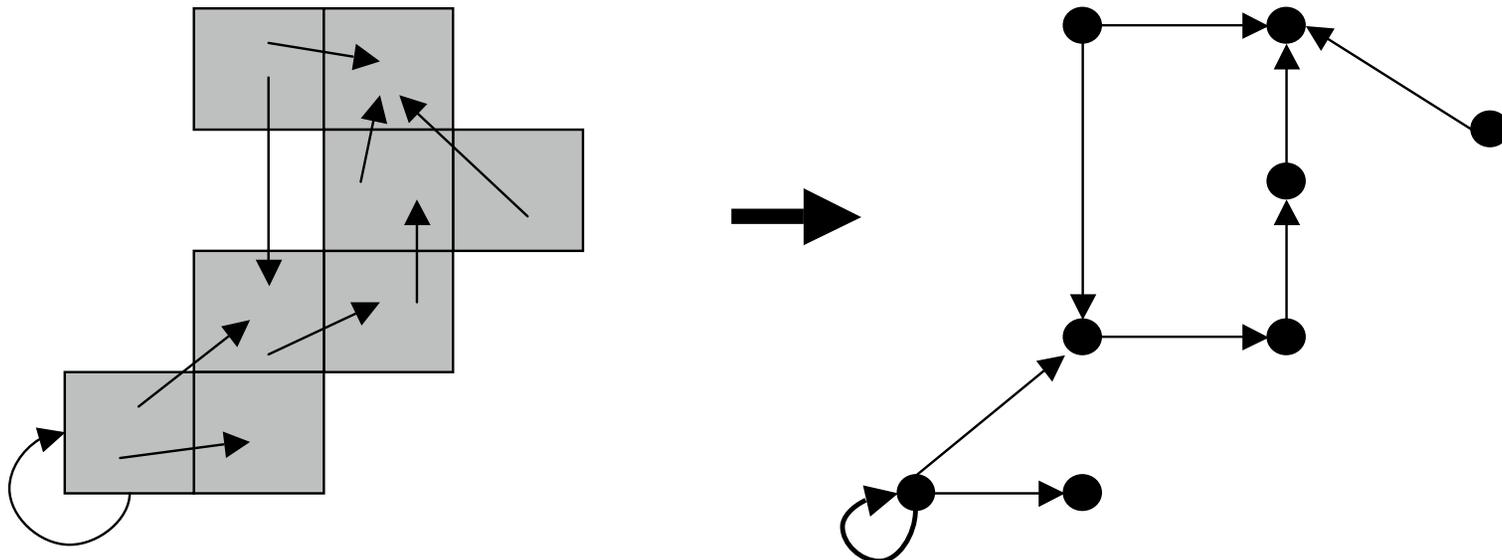
- Probability is small for a point in a region to leave in a short time under f .

- These **almost-invariant sets** (AIS's) define macroscopic structures preserved by the dynamics.

- The transport, $T_{i,j}(n)$, between almost-invariant sets can then be determined.

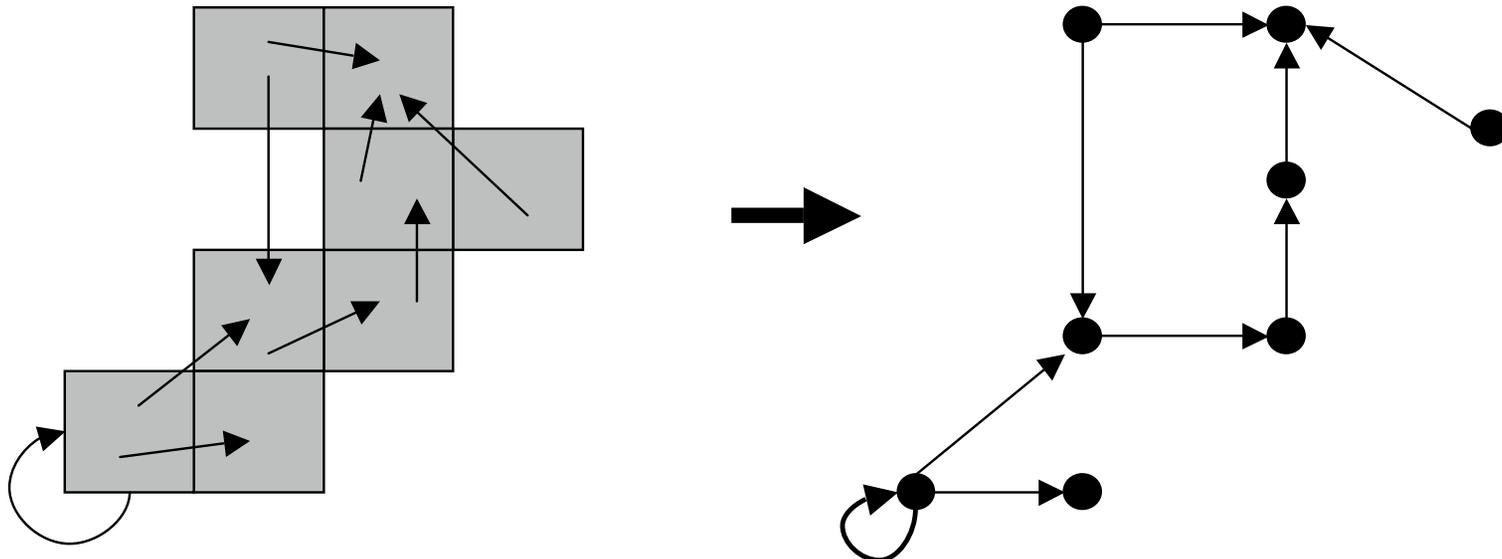
Almost-Invariant Sets

- 1) discretize the phase space into boxes; model boxes as the vertices and transitions between boxes as edges of a directed graph



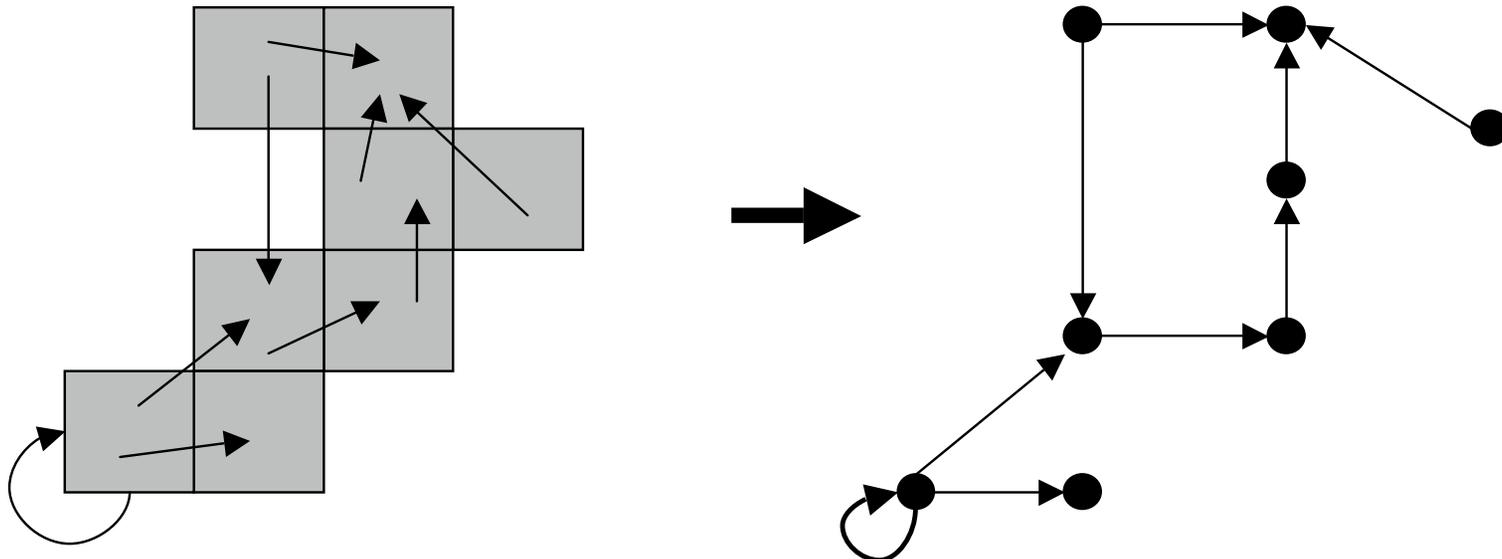
Almost-Invariant Sets

- 2) use graph partitioning methods to divide the vertices of the graph into an optimal number of parts such that each part is highly coupled within itself and only loosely coupled with other parts



Almost-Invariant Sets

- 3) by doing so, we can obtain AIS's and analyze transport between them



Almost-Invariant Sets

■ *Box Formulation*

- Create a fine box partition of the phase space

$$\mathcal{B} = \{B_1, \dots, B_q\}, \text{ where } q \text{ could be } 10^7+$$

- Consider a (weighted) q -by- q **transition matrix**, P , for our dynamical system, where

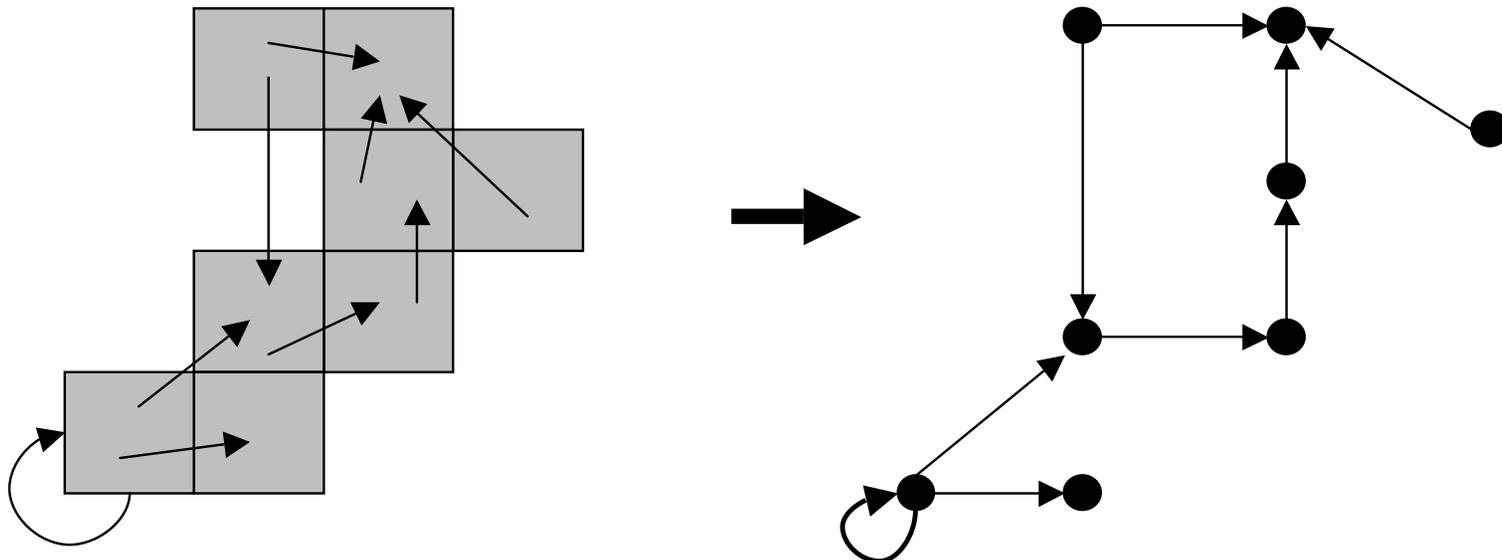
$$P_{ij} = \frac{\mu(B_i \cap f^{-1}(B_j))}{\mu(B_i)},$$

the *transition probability* from B_i to B_j

- P is an approximation of our dynamical system via a finite state Markov chain.

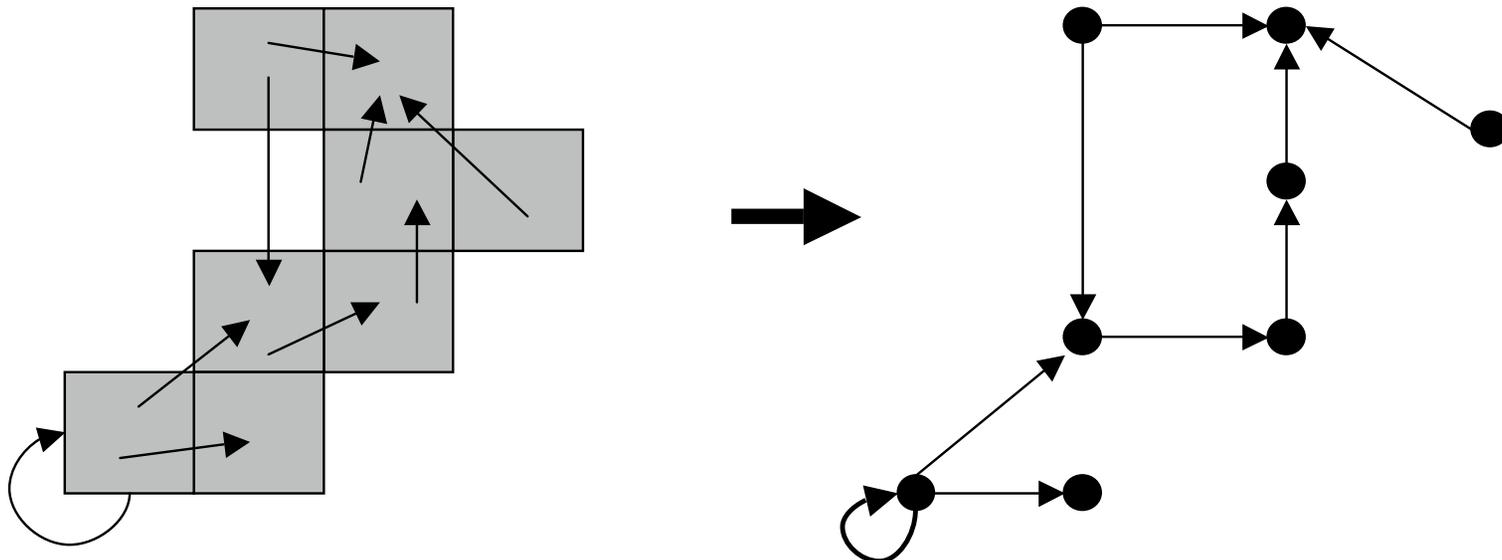
Almost-Invariant Sets

- *Graph Formulation and Partitioning*
- P has a corresponding graph representation where nodes of the graph correspond to boxes B_i .



Almost-Invariant Sets

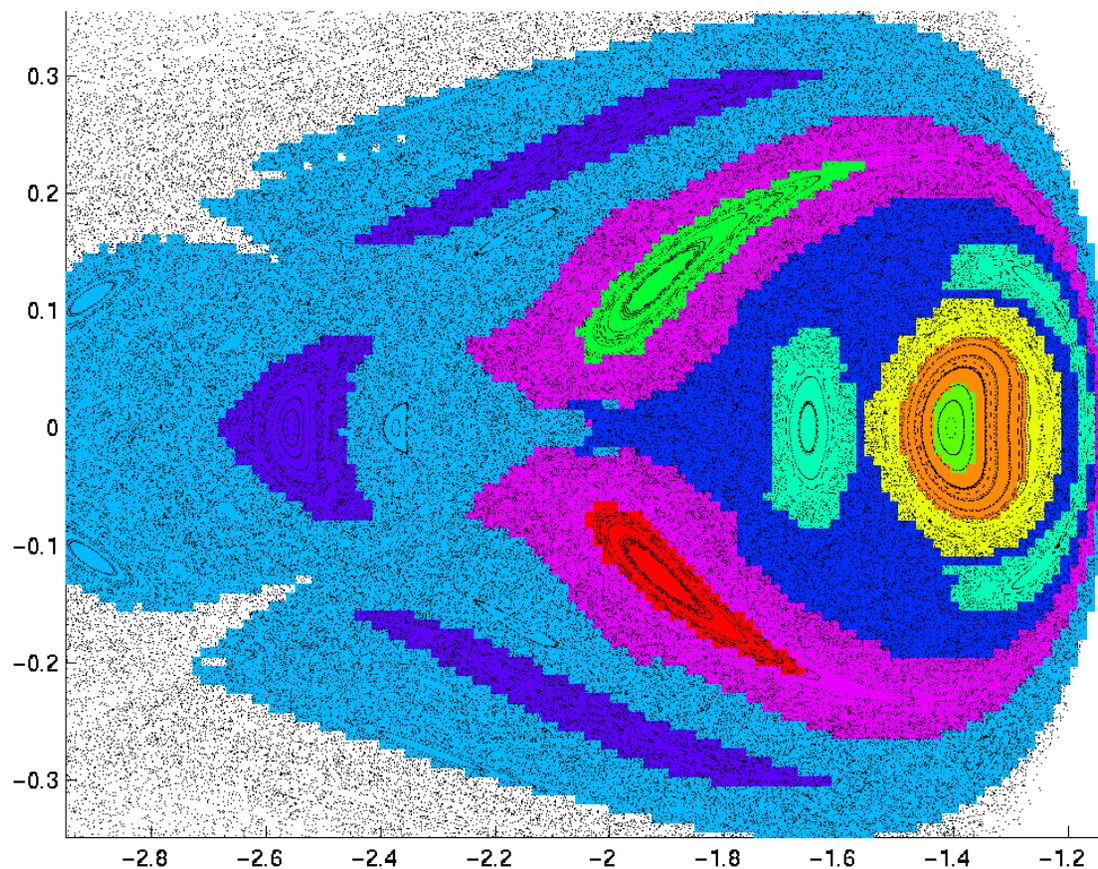
- If $P_{ij} > 0$, then there is an edge between nodes i and j in the graph with weight P_{ij} .
- Partitioning into AIS's becomes a problem of finding a minimal cut of this graph.



Almost-Invariant Sets

□ AIS's correspond with key dynamical features

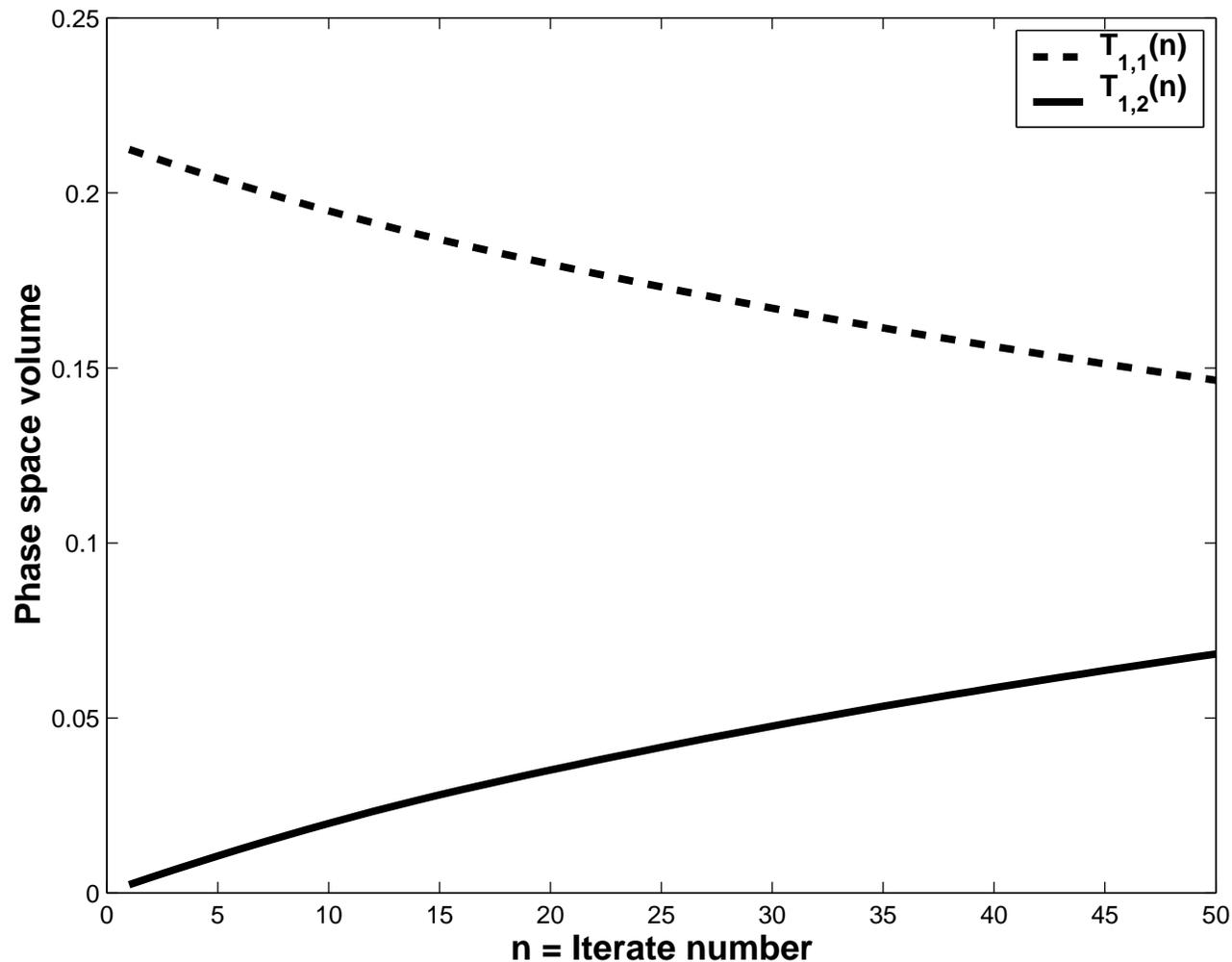
More refined methods like MANGEN can pick up details



The phase space is divided into several invariant and almost-invariant sets.

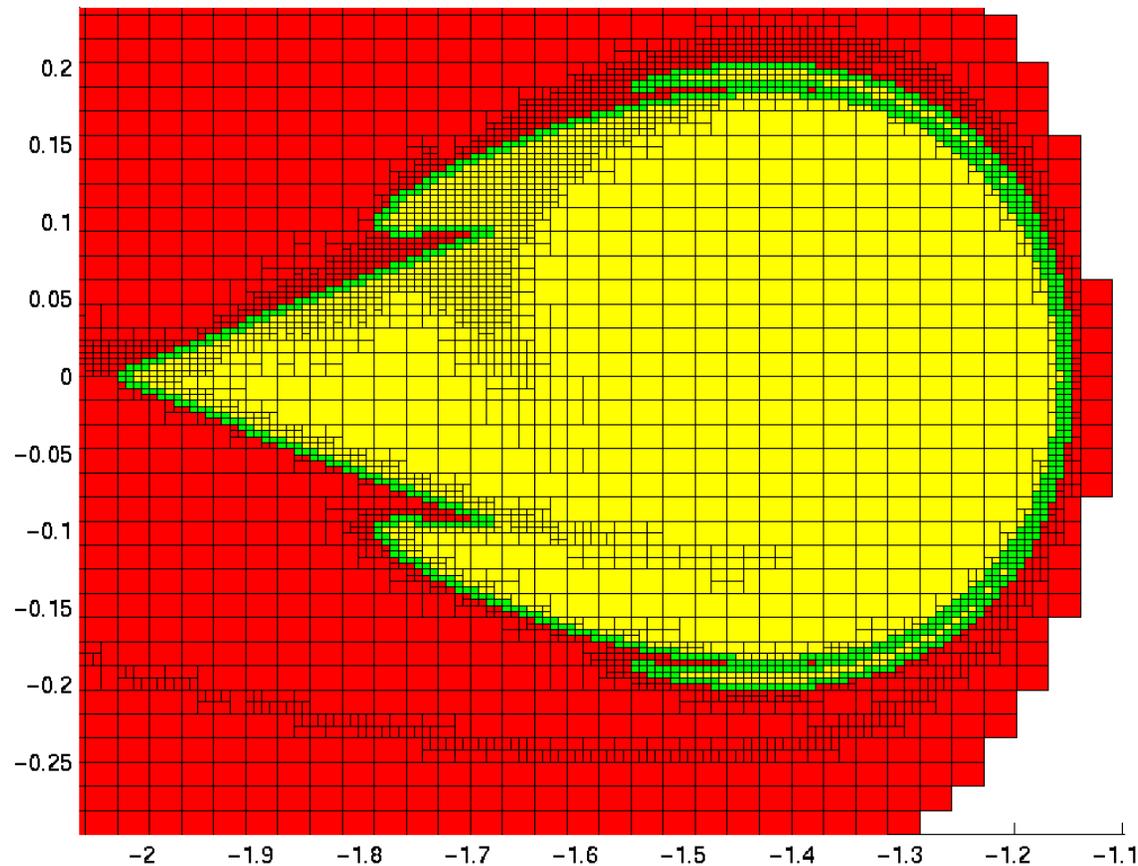
Almost-Invariant Sets

- Using the box formulation and GAIO, the $T_{i,j}(n)$ can be computed for large n . Agrees with MANGEN result.



Almost-Invariant Sets

- To speed the computation, box refinements are performed where transport related structures, e.g., lobes, are located.



Summary & Conclusion

- The merging of **statistical** and **geometric** approaches yields a very powerful tool.

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- Example problem: restricted 3-body problem.
- Both find the same regions
AIS's, statistical features, are identified with regions,
geometric features

Summary & Conclusion

- Transport between regions determined by images and pre-images of lobes.

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 $n_{\max} \approx 20$
- GAIO uses transition matrix between many boxes; Resolution limited by max box number; aided by box refinement along lobes
 $n_{\max} \approx 50$
- Both approaches in agreement for $T_{i,j}(n)$ over common domain.

Future Directions

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- Software:
GAIO for coarse grained picture, transport calculations
MANGEN to refine on regions of interest
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- Merge techniques into single package:
Box formulation, graph algorithms
Co-dimension one objects
Adaptive conditioning based on curvature

Selected References

- Dellnitz, M., O. Junge, W.S. Koon, F. Lekien, M.W. Lo, J.E. Marsden, K. Padberg, R. Preis, S. Ross, & B. Thiere [2003], *Transport in Dynamical Astronomy and Multibody Problems*, preprint.
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- Koon, W.S., M.W. Lo, J.E. Marsden and S.D. Ross [2000] *Heteroclinic connections between periodic orbits and resonance transitions in celestial mechanics*. *Chaos* **10**(2), 427–469.

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