Dynamics, Mixing, and Coherence

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Outline

1. Complicated flows are often a combination of turbulent, random-looking, behaviour and more regular or predictable (in the medium-term) behaviour.
2. The aim of this talk is to describe some of the tools that can be used to study these types of dynamics, and to separate these different types of behaviour.

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Key tool: the transfer operator

- Suppose I have a dynamical system $T : X \to X$.
- The transformation T tells me how to evolve points, or more generally, sets of points.
- One can canonically identify a subset $A \subset X$ with its indicator function $\mathbf{1}_A$ contained in some function space $\mathcal{B}(X)$ $(= \mathcal{B})$.
- For simplicity, if T is invertible and volume preserving, then the **transfer operator** (or Perron-Frobenius operator), $\mathcal{P} : \mathcal{B} \to \mathcal{B}$ is defined by $\mathcal{P}f = f \circ T^{-1}$ for all $f \in \mathcal{B}$.
- Why composition with T^{-1} and not with T?

	Set	Function
Object	A	$\mathbf{1}_A$
Evolved object	$T(A)$	$\mathcal{P}(\mathbf{1}_A) = \mathbf{1}_A \circ T^{-1} = \mathbf{1}_{T(A)}$

More generally, the transfer operator is designed to be the **natural push forward of a density under T to another density**.

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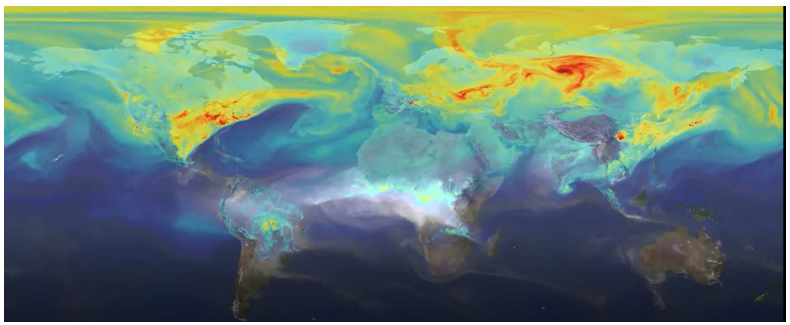
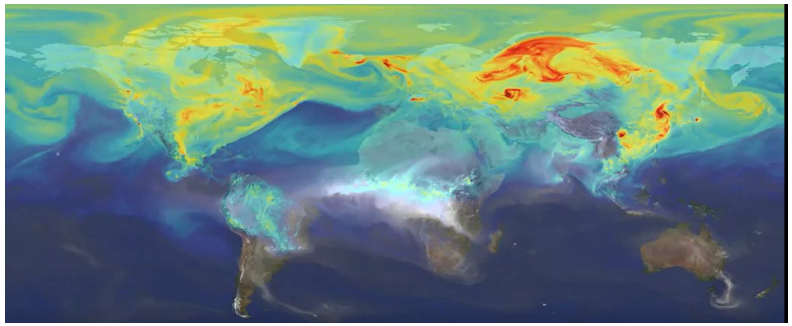
Temporal correlations of CO_2

$X =$ A 2D slice of the atmosphere, $T : X \to X$ is 1-day evolution, $f(x) = CO_2$ concentration at location $x \in X$ on April 2, 2006.

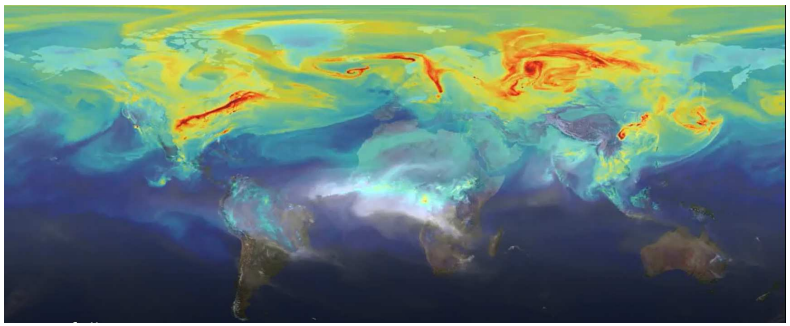
Measure temporal (auto-)correlation by
$cov(\mathcal{P}^k f, f) = \int_X \mathcal{P}^k f \cdot f \; d\mu - \left(\int_X f \; d\mu\right)^2$.



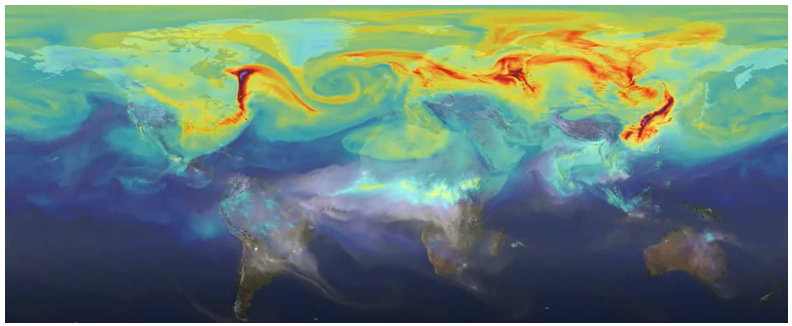
April 2, 2006, (Graph of f);



April 4, 2006, (Graph of $\mathcal{P}^2 f$)



April 6, 2006, (Graph of $\mathcal{P}^4 f$);



April 10, 2006, (Graph of $\mathcal{P}^8 f$)

What properties of T will guarantee that $cov(\mathcal{P}^k f, g) \to 0$ "quickly" as $k \to \infty$?

Theorem (Sinai'72, Bowen'75, Ruelle'76)

If T is C^2 and uniformly hyperbolic, f is C^1, and g is bounded, then there is a $0 < \lambda < 1$ such that

$$cov(\mathcal{P}^k f, g) \leq C(f, g)\lambda^k \text{ for all } k \geq 0.$$

*That is, T has "**exponential decay of correlations**".*

- **Q:** What is driving this decay of correlation?
- **A:** The exponential separation of nearby trajectories caused by the strict local expansion of T.
- Local expansion is a common feature in many dynamical systems. *Rapidly decaying correlation is why the weather is hard to predict far in advance using observations from the present.*

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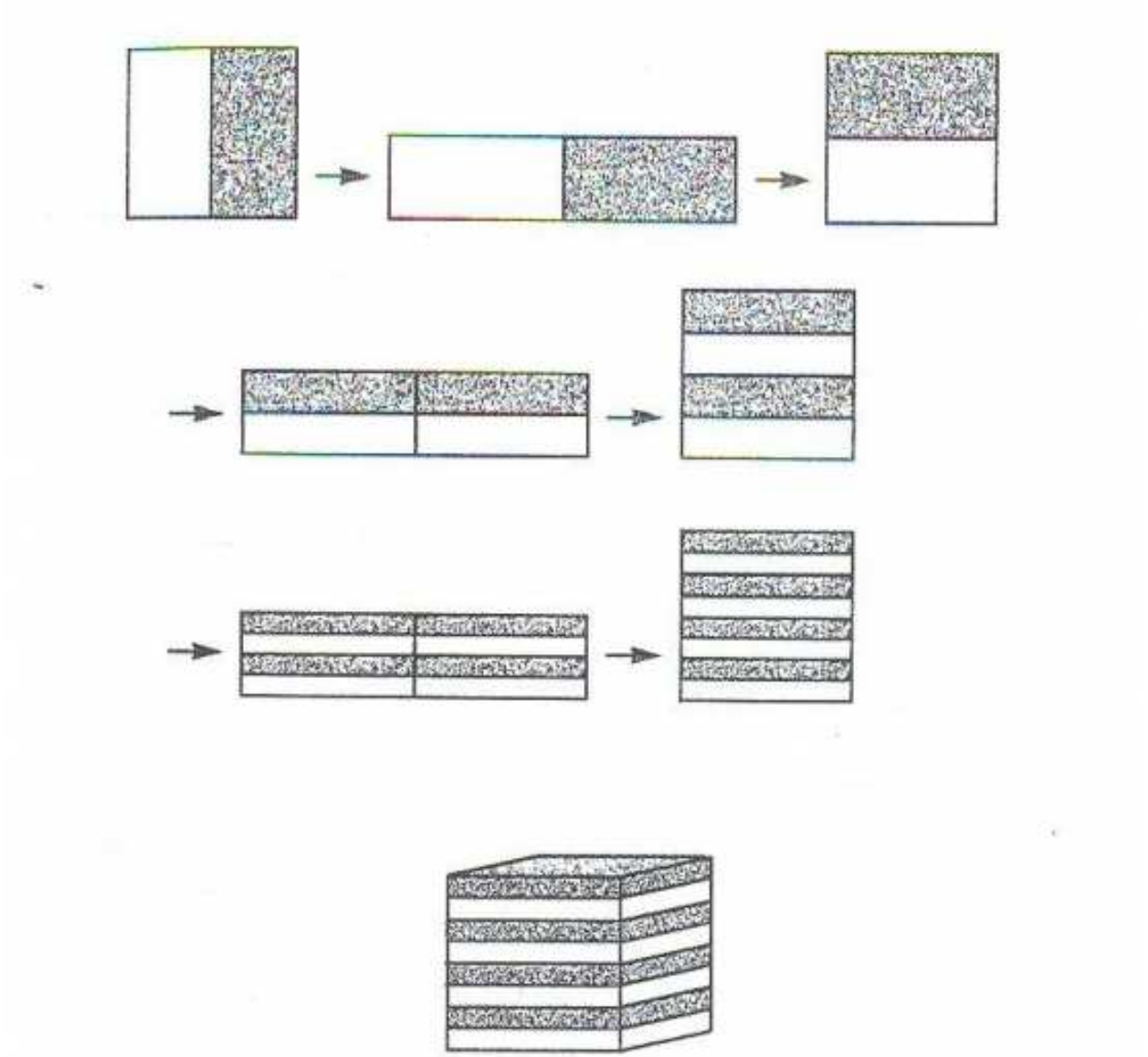
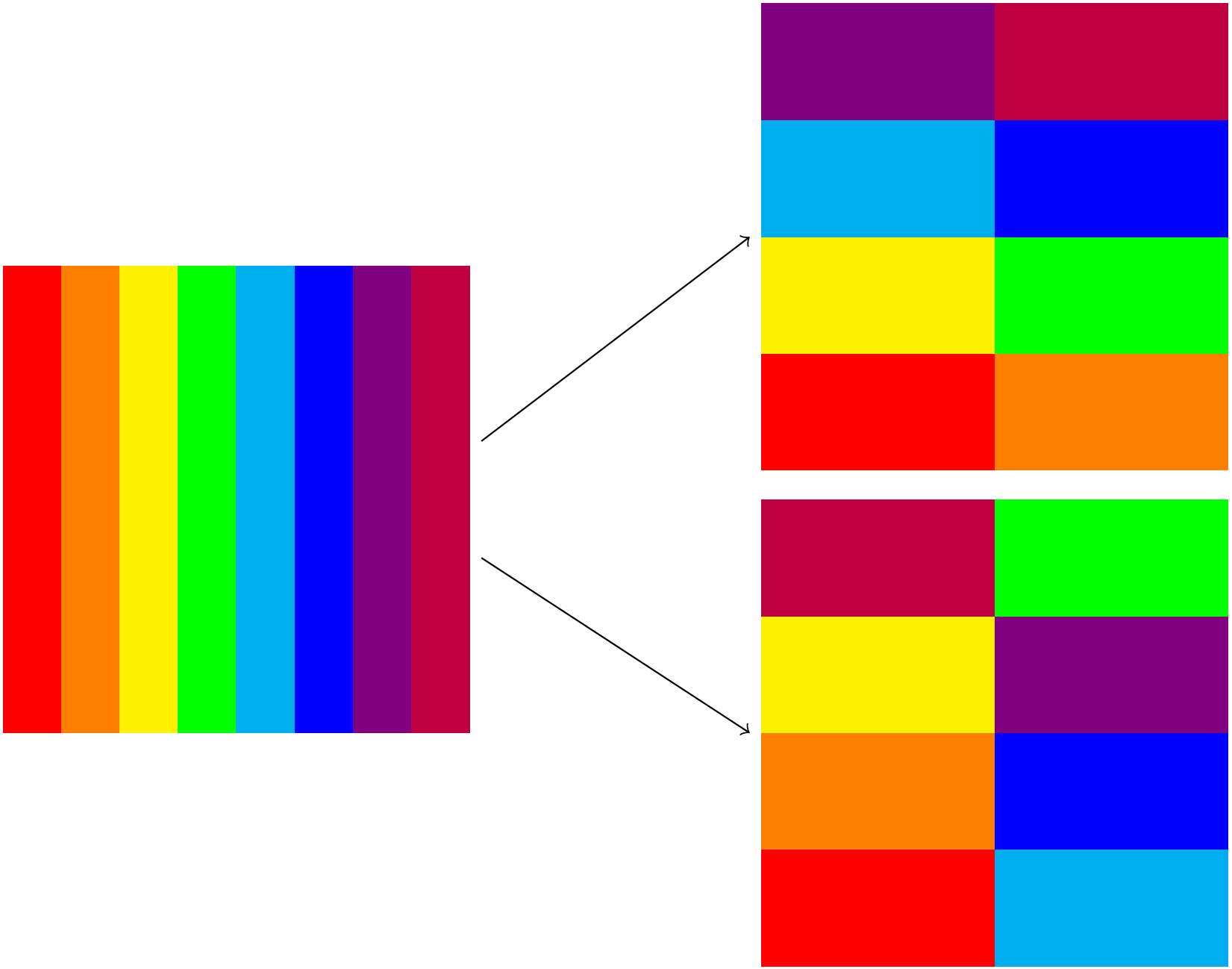
A uniformly hyperbolic dynamical system



A uniformly hyperbolic dynamical system

So what is this rate of decay?



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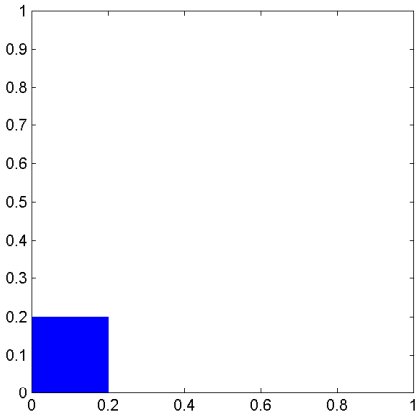
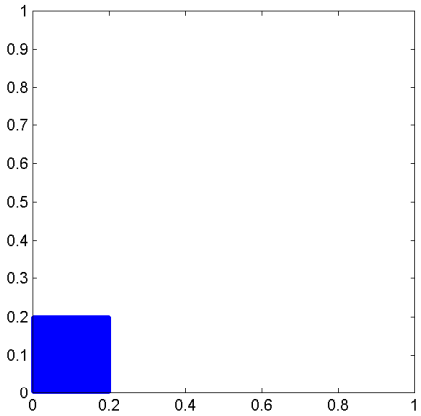




- The figure on the left shows the evolution of a small square of points under the "standard" 4-fold lamington map.
- The figure on the right is the tweaked lamington map.
- **Both lamington maps have expansion factors of 4**, meaning nearby trajectories separate by a factor 4 at each iteration.
- However, the "standard" version (on the left) **appears to mix faster**. What's going on?

Spectrum controls decay rate

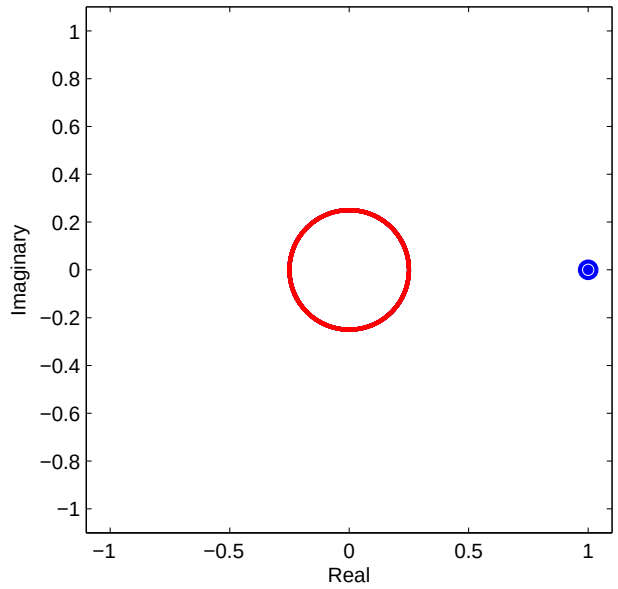
- For $f \in \mathcal{B}, g \in L^\infty(X)$, if $\mathbb{E}_\mu(f) = 0$,

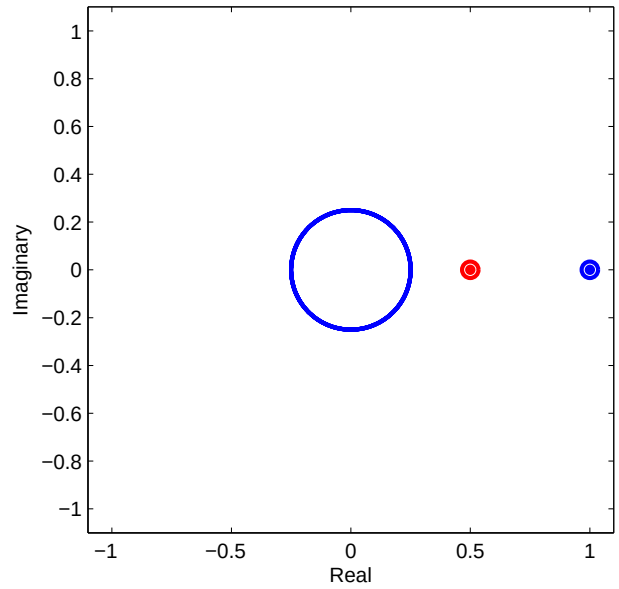
$$|cov(\mathcal{P}^k f, g)| = \left| \int_X \mathcal{P}^k f \cdot g \; d\mu \right| \leq \|\mathcal{P}^k f\|_{\mathcal{B}} \cdot \|g\|_{L^\infty}, \quad k \geq 0.$$

- Thus, the **spectrum of** $\mathcal{P}$ is important for controlling covariances and upper bounds of rates of decay of correlations.
- Typically, one considers $\mathcal{P} : \mathcal{B} \circlearrowleft$, where $\mathcal{B}$ is a Banach space of suitably regular functions, with norm stronger than L^1.

Spectrum controls decay rate

Left: Spectrum of $\mathcal{P}$ for the "standard" lamington map;
Right: Spectrum of $\mathcal{P}$ for the tweaked lamington map.





The rate of decay of correlations λ is controlled by the size of the spectral gap, which is **not necessarily related to expansion rates or Lyapunov exponents**. "More chaotic" does not necessarily equal "faster mixing" (Dellnitz/F/Sertl'00, Collet/Eckmann'04, F'07)

Visualising an eigenfunction of $\mathcal{P}$

- Experiments of dye-mixing in periodically forced fluids (eg. [Voth *et al.* '02]) have shown that intricate, persistent patterns can develop from an initial dye distribution.

- You are watching convergence to f_2, where $\mathcal{P}f_2 = \lambda_2 f_2$ and λ_2 is the second largest eigenvalue of $\mathcal{P}$.
- f_2 known as *strange eigenmodes* [Pierrehumbert'94, Liu/Haller'04], *persistent patterns* [Pikovsky/Popovych'03] and used to find *almost-invariant sets* [Dellnitz/Junge'99, Deuflhard *et al.*'00].

Optimizing mixing by manipulating the spectrum

Numerical strategy

Original vector field
↓
Original transfer operator
↓
Optimized transfer operator
↓
Optimized velocity field

Numerically approximate transfer operator

Optimization to increase spectral gap

Infer optimized velocity field

Mixing optimisation work includes [Ottino/Wiggins'04, Balasuriya'05/'10, Mathew *et al.*'07, Cortelezzi *et al.*'08, Thiffeault/Pavliotis'08, Gubanov/Cortelezzi'10, Forgoston *et al.*'11, Lin *et al.*'11, Ober-Blöbaum/Padberg-Gehle'15, F/González-Tokman/Watson'16, Grover/Elamvazhuthi'17].

Here we address the question of **computing a general small perturbation of the vector field that most enhances mixing**. We do this by *transforming the nonlinear flow into a linear representation*.

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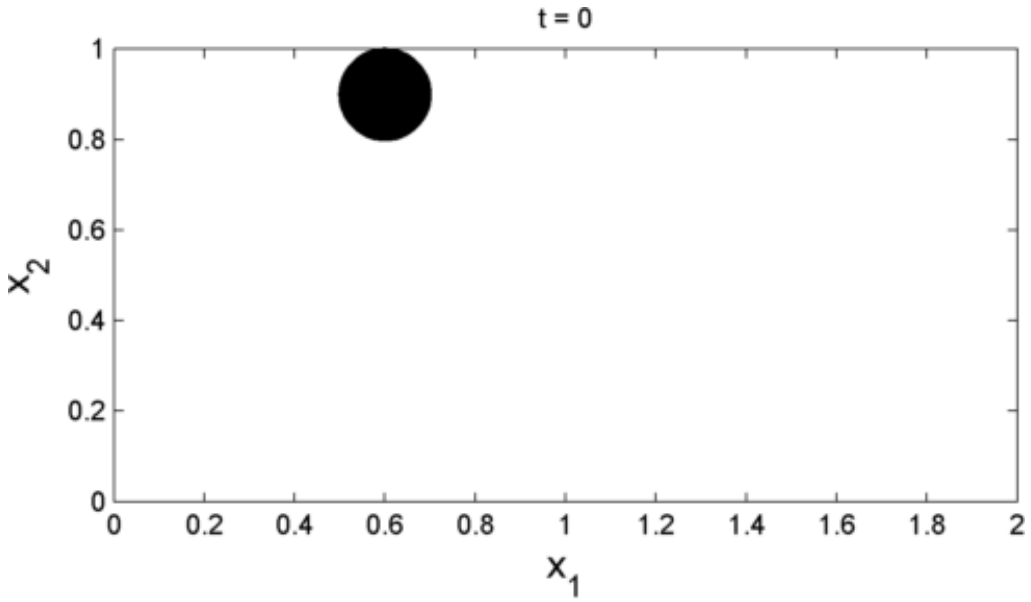
The double gyre

Consider a periodically driven flow on $[0, 2] \times [0, 1]$ with vector field

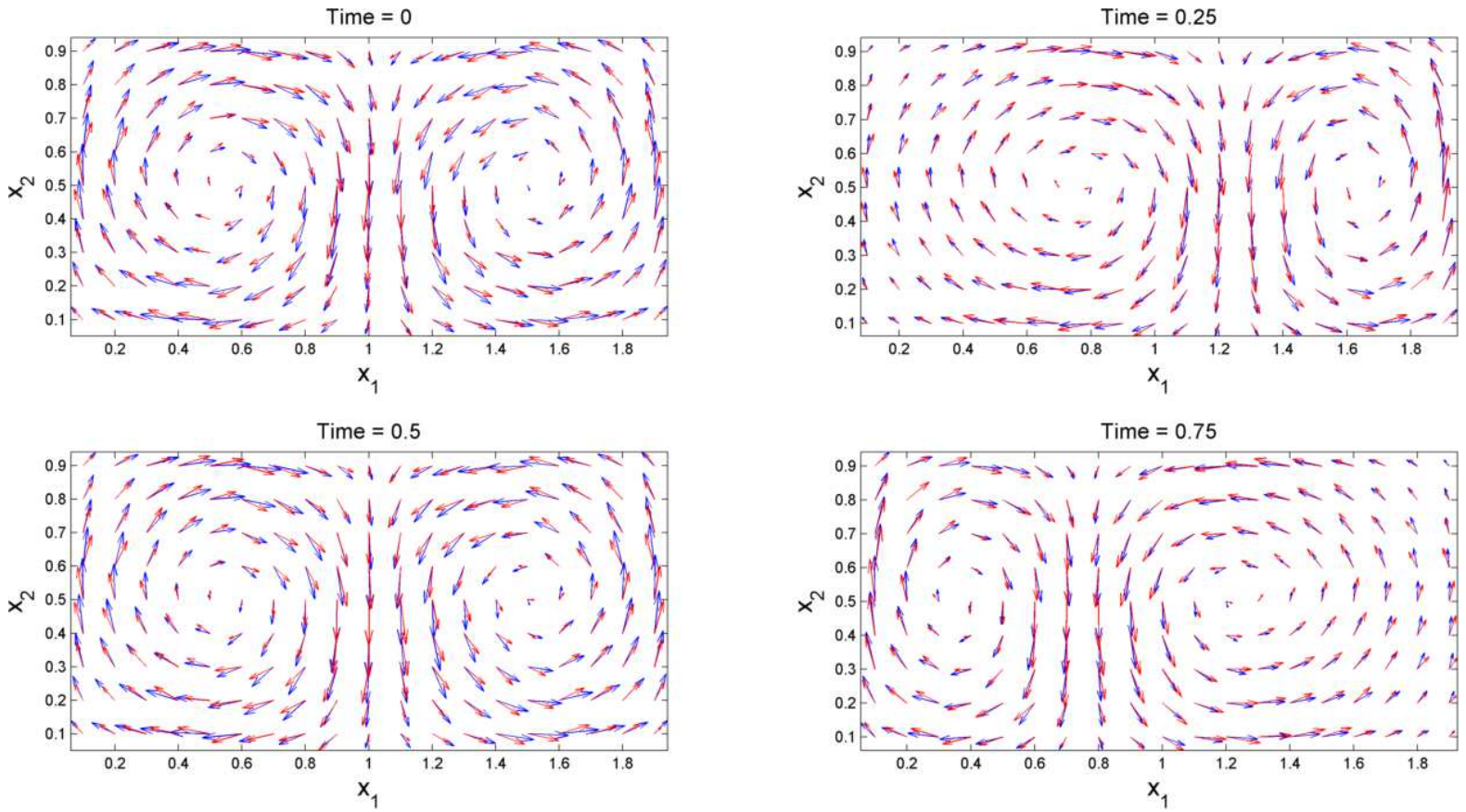
$$v(t, x) = (-(\pi/4)\sin(\pi f(t, x_1))\cos(\pi x_2),$$
$$(\pi/4)\cos(\pi f(t, x_1))\sin(\pi x_2) \cdot (df/d_{x_1})(t, x_1))$$

where $f(t, x_1) = \sin(2\pi t)x_1^2/4 + (1 - \sin(2\pi t)/2)x_1$.

Parameters used as in [Shadden *et al.*'05].



Original and optimized vector fields

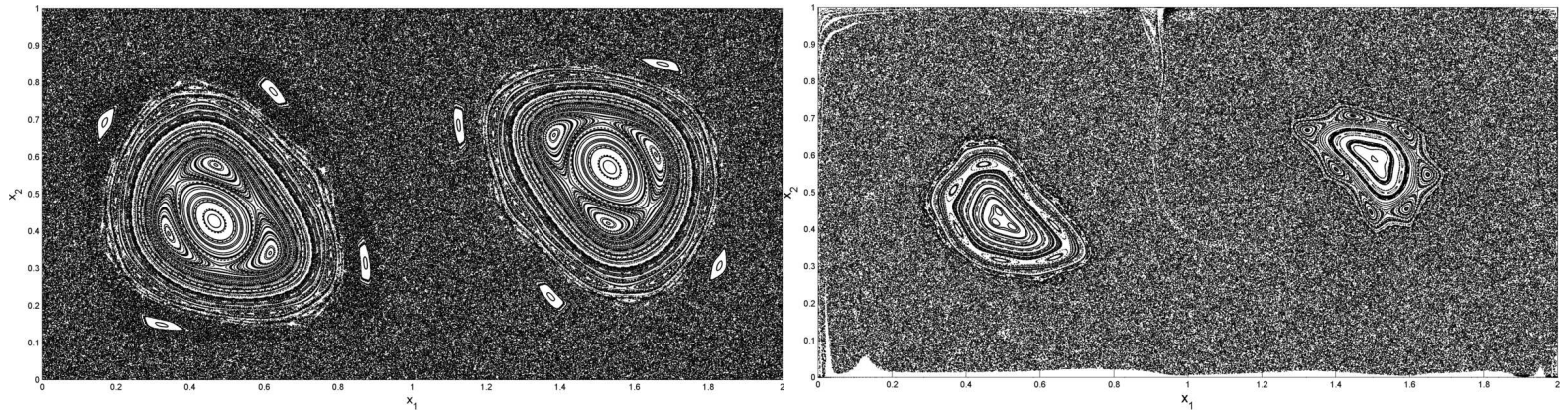


Original vector field, Optimally perturbed vector field

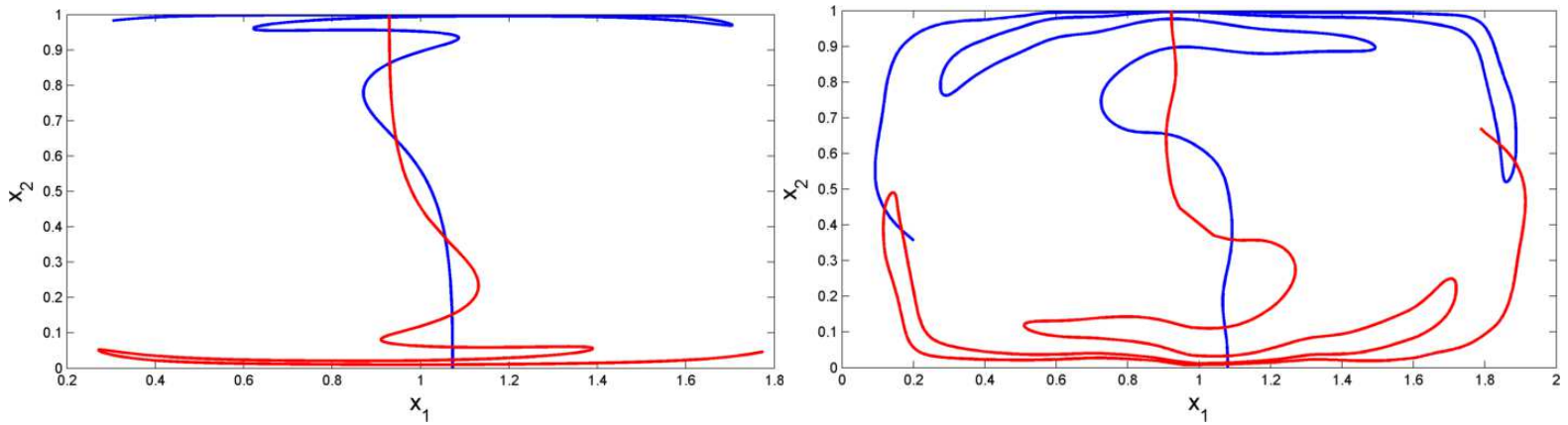
See [F/Santitissadeekorn, subm.], computations done using the time derivative of the transfer operator (the infinitesimal generator), based on constructions in [F/Junge/Koltai'13,F/Koltai'17].

The double gyre (Left: original; Right: optimized)

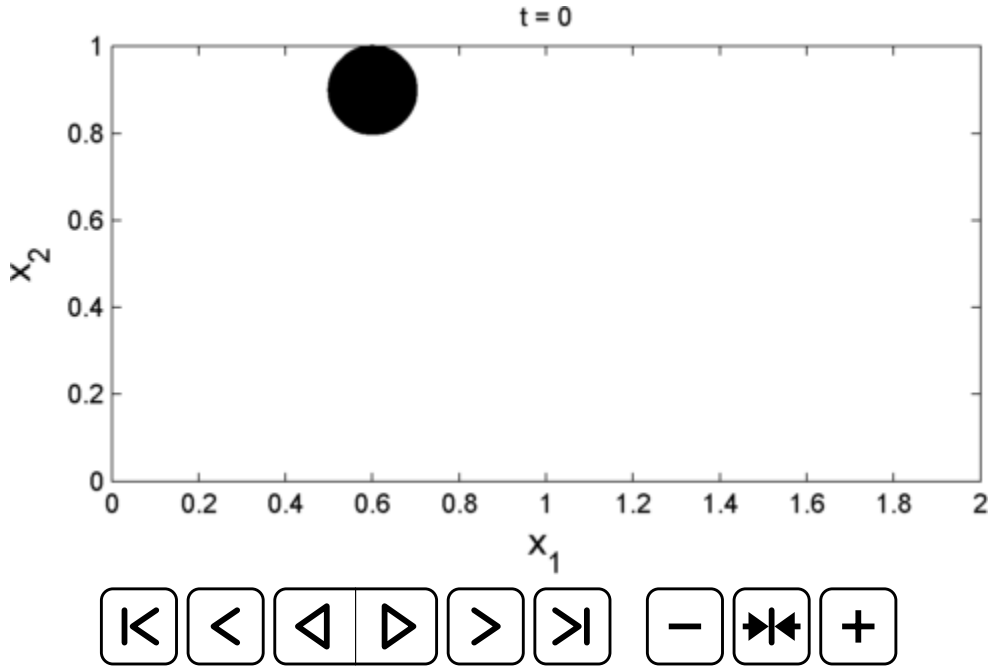
The double gyre has both regular and chaotic dynamics.

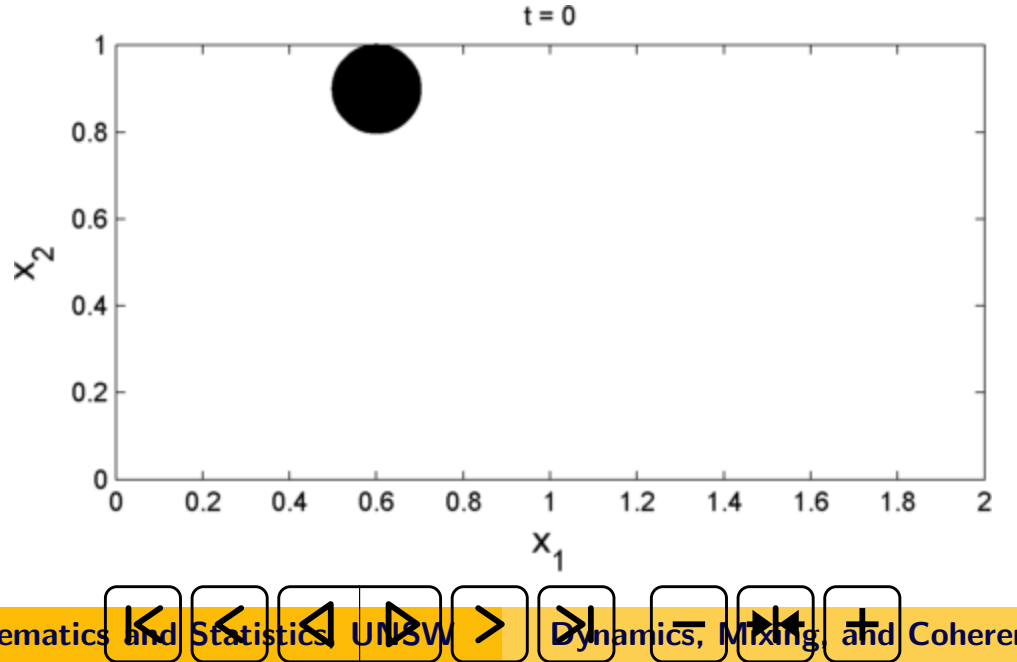


The chaotic dynamics is controlled by the intersection of the stable (blue) and unstable (red) manifolds of periodic points on the lower and upper boundaries, respectively (Lobe dynamics [Rom-Kedar/Wiggins '90]).



Evolution (Upper: original; Lower: optimized)





Time-dependent dynamics

- In applications, many systems are time-dependent, meaning that the **underlying dynamical rules change over time**.
  - **Continuous time:** A time-dependent ODE $\dot{x} = f(x, t)$ rather than $\dot{x} = f(x)$.
  - **Discrete time:** A concatenation $\cdots T_k \circ T_{k-1} \circ \cdots \circ T_2 \circ T_1$, where $T_i, i = 1 \ldots, k$ are **different maps**, rather than T^k, iteration of a single map T.

Slow mixing structures in time-dependent systems

- There is no reason to expect the slowly-mixing structures to be **fixed in space** (like almost-invariant sets) in time-dependent systems.
- In fact, they can be **highly mobile**, making their detection considerably more difficult.

Decay in time-dependent systems

- **Time-independent case**
  - We found the eigenfunction f_2 corresponding to the second largest eigenvalue λ_2. Thus,

$$\|\mathcal{P}^k f_2\| \leq C(f_2)\lambda_2^k, \quad \text{for all } k \geq 0.$$

  - *But what are "eigenvalues" and "eigenfunctions" in the time-dependent setting?*
- **Time-dependent case**
  - The analogous growth rate expression is

$$\|\mathcal{P}_{T_k} \circ \cdots \circ \mathcal{P}_{T_2} \circ \mathcal{P}_{T_1} f\| \leq C(f)\lambda_2^k.$$

  - Or:

$$\lim_{k\to\infty} \frac{1}{k} \log \|\mathcal{P}_{T_k} \circ \cdots \circ \mathcal{P}_{T_2} \circ \mathcal{P}_{T_1} f\| \leq \log \lambda_2.$$

  - Note that the $\mathcal{P}_{T_i}$ are *linear* operators (or in numerical experiments, matrices), so $\log \lambda_2$ is a **Lyapunov exponent**.
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Decay in time-dependent systems

- The Oseledets Multiplicative Ergodic Theorem (MET), proven in Oseledets' thesis in 1965, **creates time-dependent generalisations of eigenvalues and eigenvectors for compositions of matrices**.
- Building on the work of Ruelle, Mañé, Thieullen, extensions of Oseledets' MET have been developed (Blumenthal, F, González-Tokman, Lloyd, Quas, Young,...) to **enable application to time-dependent dynamical systems**.
- The Oseledets vectors corresponding to the second Lyapunov exponent λ_2 are the **unique collection of fs that decays as slowly as possible and evolve consistently with the time-dependent dynamics**:

$$\lim_{k\to\infty} \frac{1}{k} \log \|\mathcal{P}_{T_k} \circ \cdots \circ \mathcal{P}_{T_2} \circ \mathcal{P}_{T_1} f\|$$

  is exactly $\log \lambda_2$.
- See e.g. [F/Lloyd/Santitissadeekorn'10] for an applied description.

Slowly decaying structures in finite time

- What about finite time durations (finite k)?
- We want to find an f_2 so that $\|\mathcal{P}_{T_k} \circ \cdots \circ \mathcal{P}_{T_2} \circ \mathcal{P}_{T_1} f_2\| = \lambda_2 \|f_2\|$ with $\lambda_2 < 1$ as large as possible.
- This is accomplished by selecting f_2 to the be **singular vector** corresponding to the 2nd largest **singular value** λ_2 of $\mathcal{P}_{T_k} \circ \cdots \circ \mathcal{P}_{T_2} \circ \mathcal{P}_{T_1}$, and
- This leads to the **slowest decay in finite time** [F'13].

Stratospheric polar vortex

- In the stratosphere over each pole, there is huge whirlpool of cold air centred over the pole.
- The boundary of the vortex (the polar front jet stream) is a barrier that stops polar air and subtropical air from mixing.
- The polar vortex and this mixing interface is constantly changing.

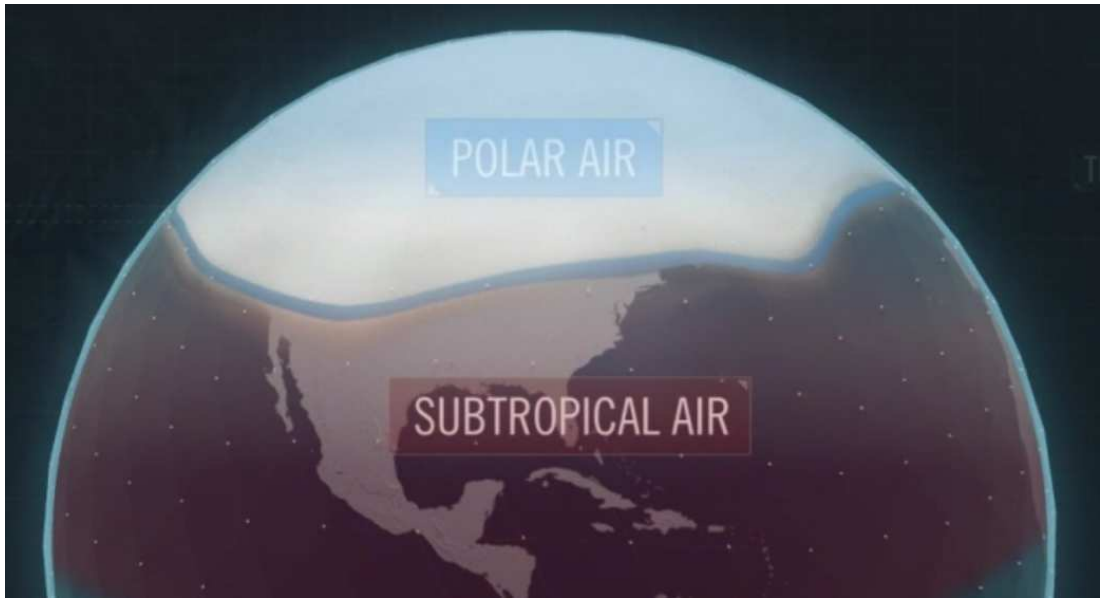
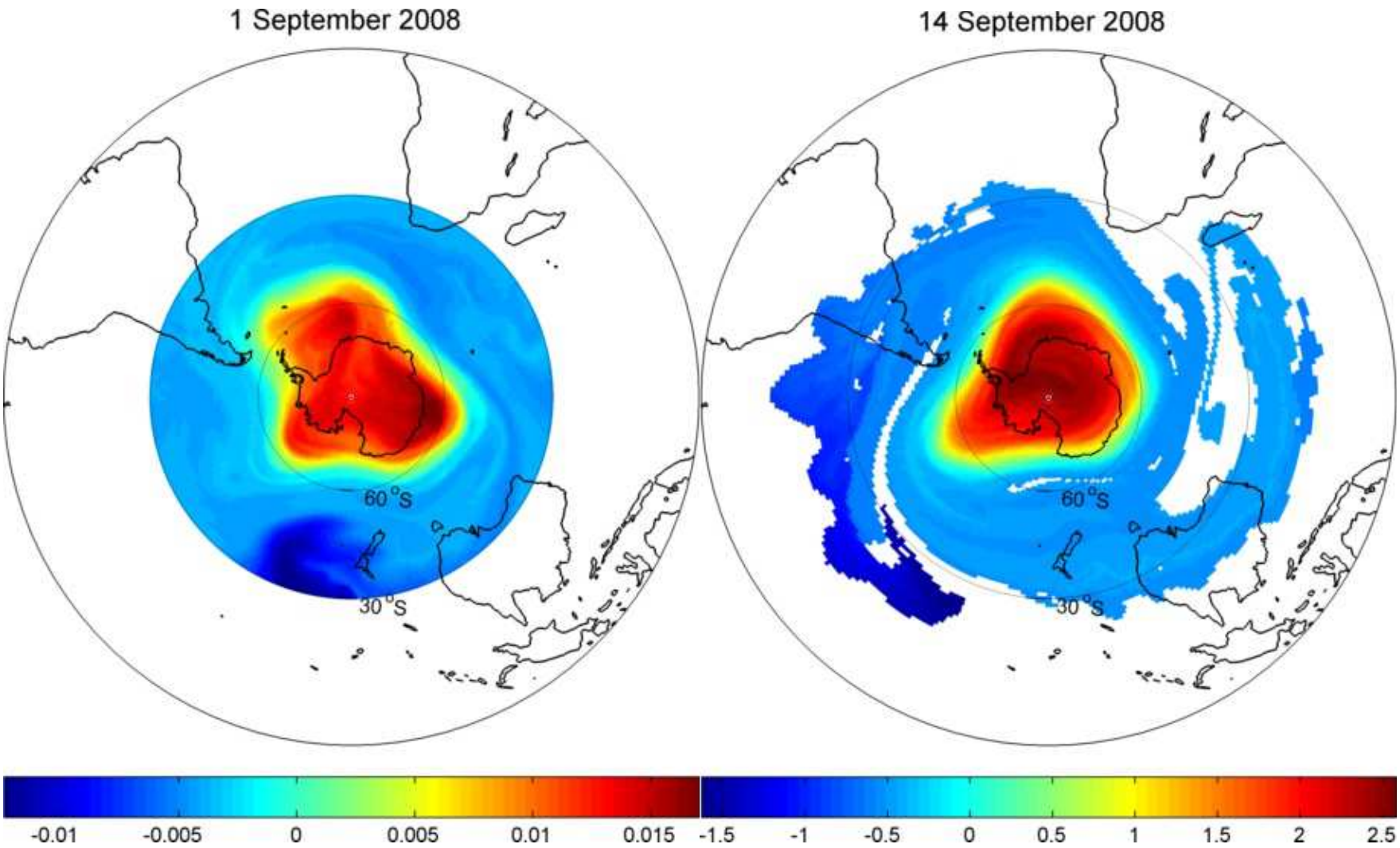


Image: National Geographic.

The polar vortex is a slowly mixing object

- We wish to **resolve the polar vortex as the slowest decaying object** in the vicinity of the pole.
- We do this by **numerically approximating transfer operators** $\mathcal{P}$ using ECMWF vector fields, and computing the second singular vectors (left and right).
- Our initial domain is a 475K isentropic surface and we **follow the flow for two weeks** from September 1, 2008 until September 14, 2008.
- Other work on resolving the polar vortex includes Boffetta *et al.* '01, Koh/Legras '02, Rypina *et al.* '07, Lekien/Ross '10, de la Cámara *et al.* '12, Padberg-Gehle/Schneide'17, Serra *et al.*'17

The left & right second singular vectors f_2 & $\mathcal{P}f_2$



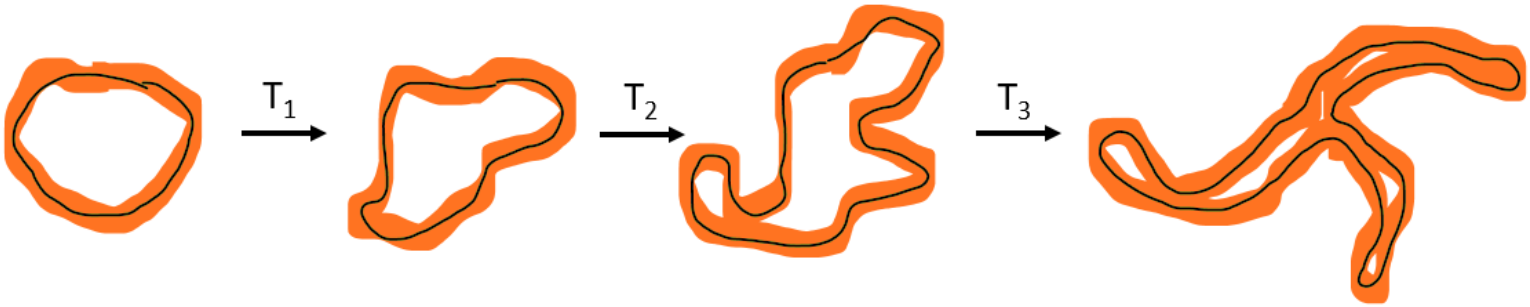
See [F/Santitissadeekorn/Monahan, 2010.]

Particle simulation demonstrating the identified vortex inhibits global mixing

Methods for detecting coherent structures

- *Lagrangian (trajectory-following) scalar fields.* e.g. FTLE, FSLE, mesohyperbolicity, M-function,... (Budišić, Haller, Mancho, Mezić, Pratt, Rom-Kedar, Ross, Rypina, Scott, Shadden, ...).
- *Spatially local continuum-mechanical ideas* (Blazevsky/Beron-Vera/Hadjighasem/Haller/Huhn/Farazmand/Karrasch, Bollt/Ma,...).
- *Topological methods and trajectory grouping ideas* (Allshouse/Thiffeault, F/Padberg-Gehle, Hadjighasem/Haller/Karrasch/Teramoto, Schlueter-Kuck/Dabiri,...)
- *Probabilistic transfer operator methods* (F/González-Tokman/Junge/Padberg-Gehle/Santitissadeekorn, Bollt/Ma, Rowley/Rypina/Williams, Banisch/Koltai,...).
- *Geometric transfer operator methods* (F/Junge/Kwok, Karrasch/Keller,...)

Probabilistic mixing vs. geometric mixing



- In the presence of small diffusion, the only region in which mixing across the boundary can occur is in the orange neighbourhood of the boundary.
- The probability of this mixing occurring is proportional to the **area of the orange region**. This area is minimised by the probabilistic transfer operator method.
- In the **pure advection limit**, as the diffusion amplitude goes to zero, (the orange band narrows), the **boundary length determines the amount of "mixing"**. ([Mathew *et al*'05, Thiffeault'12]).
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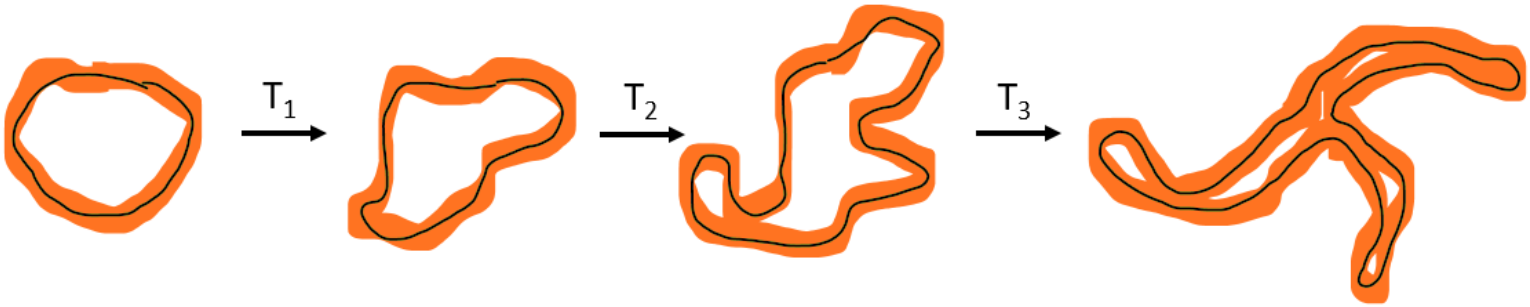
Probabilistic mixing vs. geometric mixing



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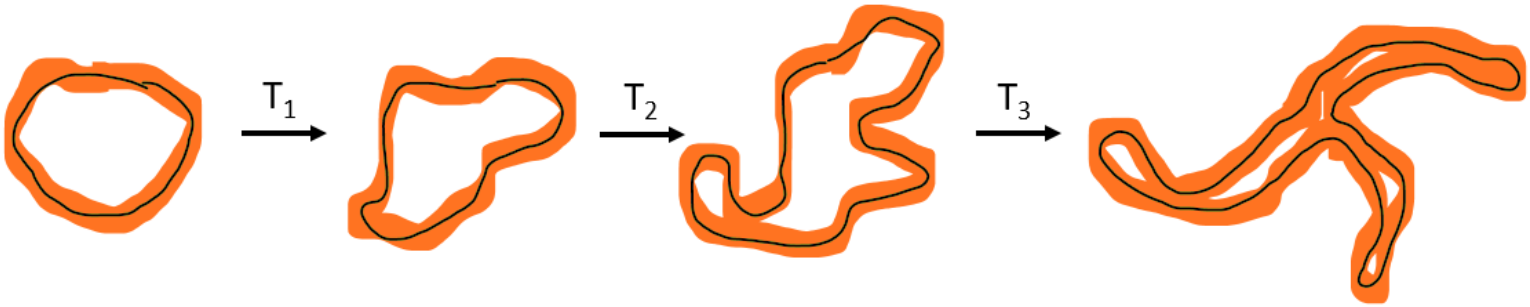

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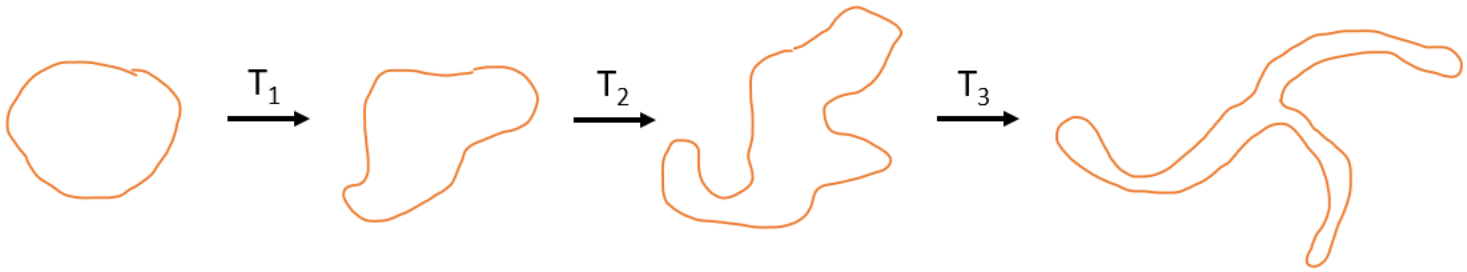

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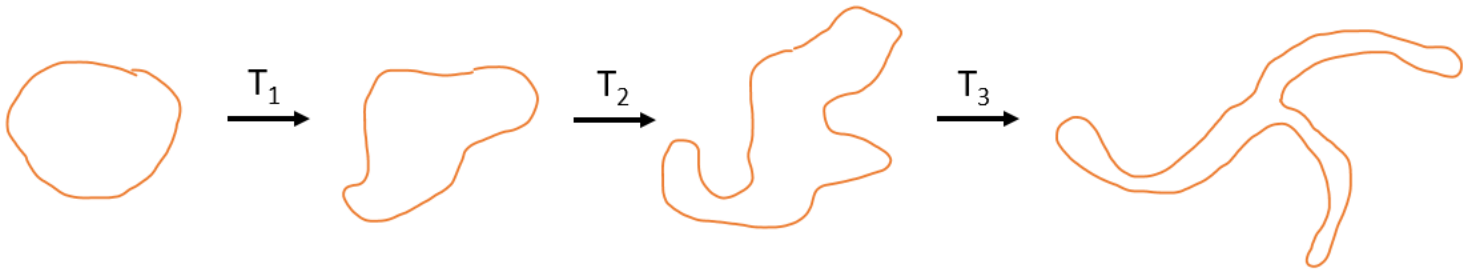
Probabilistic mixing vs. geometric mixing



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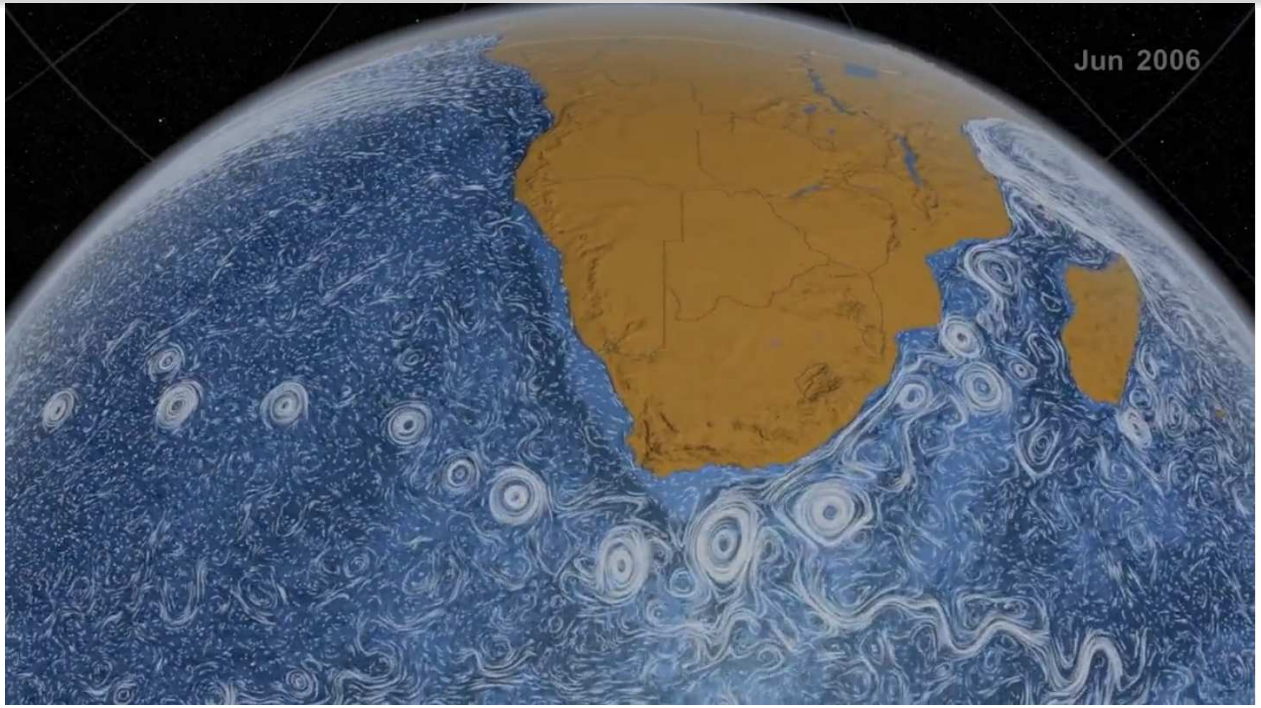
Application 2: Tracking Agulhas Rings



- How much heat and salt an Agulhas Ring transports, and how far into the North Atlantic the Ring transports these tracers, is sensitive to **how long the water remains within a Ring** as well as **its path** [Treguier *et al.* 2003].
- Previous LCS-based studies include Poje/Haller '99, Beron-Vera *et al.* '08, Bettencourt *et al.* '11, Beron-Vera *et al.* '13, Karrasch *et al.* 15, Wang *et al.* '16.

Tracking ocean eddies

Use AVISO ocean surface velocity data to track Agulhas rings over a 90 day period: 11 November 2006 to 9 February 2007. The initial domain is $M = [-4, 6] \times [-34, 28]$ in degrees longitude by latitude; domain as in [Hadjighasem/Haller'16]

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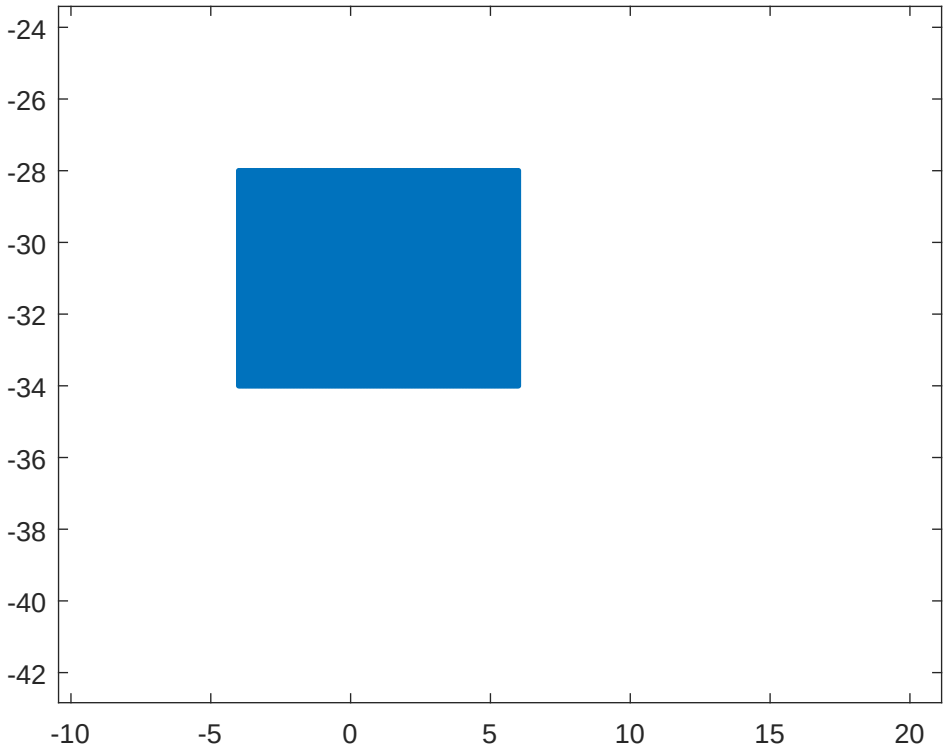
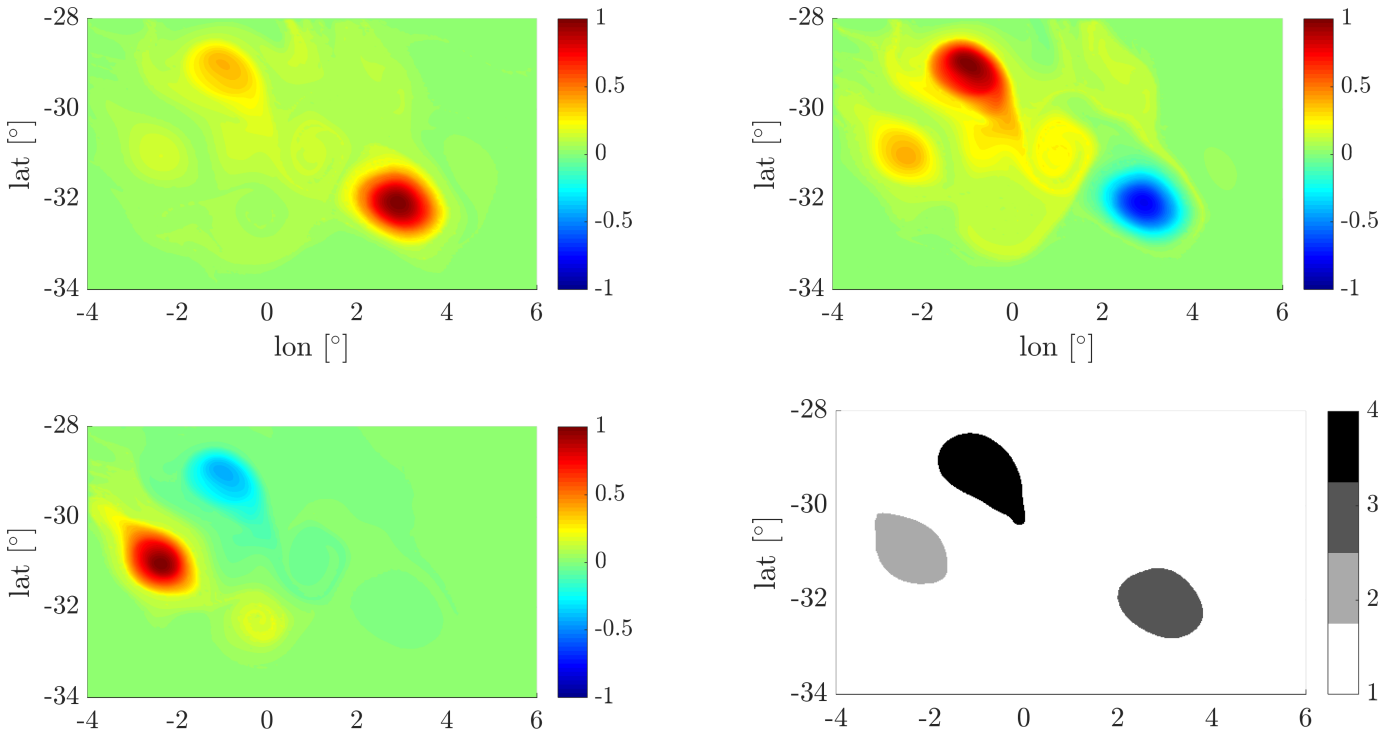


Tracking ocean eddies

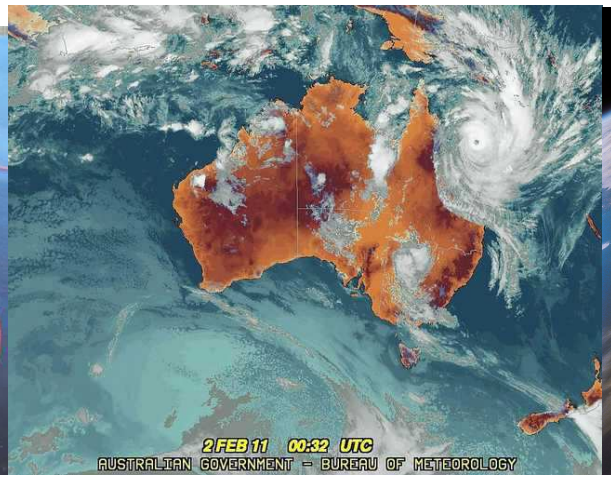
- We approximate the dynamic Laplacian Δ^{DYN} using a bespoke finite-element method, combined with collocation [F/Junge, subm.].
- Below, we use a grid of 250×150 points and **only their positions at the initial date 11 Nov 2006 and at the final date 9 Feb 2007**; in particular, no derivatives need to be calculated.



Evolution of identified eddies

Summary

- The **spectrum(s) of the transfer operator** are a powerful tool to quantify mixing, to reveal slow mixing structures, and even to manipulate those structures.
- These ideas also apply to e.g. **evolution operators of time-dependent advection-diffusion PDEs**.
- Accurately mapping and tracking slowly decaying structures is of great importance in models of geophysical flows because these structures are the **predictable components of often highly unpredictable dynamics**.
- Aim is to produce automated algorithms to process input and present results **in near-real time for predictive use**.



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N. Santitissadeekorn (Surrey),