An overview of transfer operator methods in nonautonomous dynamics: geometry, spectrum, and data

Gary Froyland

School of Mathematics and Statistics
University of New South Wales, Sydney

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Status

- This talk
  - Autonomous
  - Nonautonomous
  - Nonautonomous (finite-time)
  - Nonautonomous (finite-time) – advective limit

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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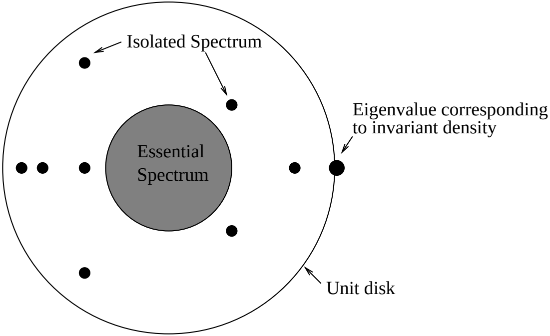
Spectrum of the transfer operator

Typically one wants $\mathcal{P}$ to act on a Banach space $\mathcal{B}$:

1. containing $L^1(X)$ (which itself contains densities),
2. for which the spectral radius of the transfer operator is 1,
3. and on which the transfer operator is *quasi-compact*, meaning that there is an *essential spectral radius* $r_{ess} \geq 0$ outside which there are finitely many eigenvalues of finite multiplicity.



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Eigenfunctions of the transfer operator

- The most important eigenfunction of $\mathcal{P}$ is the (often unique) fixed point h satisfying $\mathcal{P}h = h$, which is the **invariant density** of T.
- The eigenfunction h defines a probability measure $\mu(A) = \int_A h\ dLeb$, which is the **absolutely continuous invariant measure** of T, and satisfies $\mu = \mu \circ T^{-1}$.
- The eigenfunction h describes the **time-asymptotic distribution of trajectories** of T. That is, for an arbitrary $g \in L^1(X)$, by Birkhoff $\lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} g \circ T^k = \int_X g \cdot h\ dLeb = \int_X g\ d\mu$, μ-a.e.
- There is a long history of **rigorous numerical approximation of** h beginning with [Li'76] and Didier will talk about this shortly.

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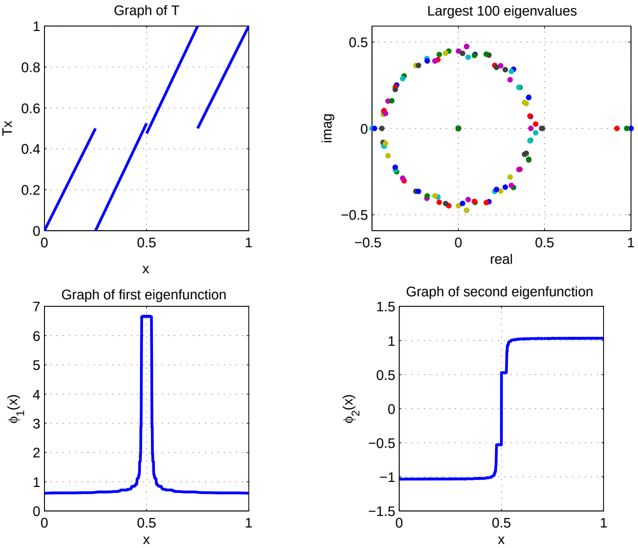
Example


Graph of T
Tx
x
0
0.2
0.4
0.6
0.8
1
0.5
Largest 100 eigenvalues
imag
real
0.5
0
−0.5
−0.5
0
0.5
1
Graph of first eigenfunction
$\phi_1(x)$
x
0
1
2
3
4
5
6
7
0.5
Graph of second eigenfunction
$\phi_2(x)$
x
1.5
1
0.5
0
−0.5
−1
−1.5
0
0.5
1

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The second eigenfunction

- The next most important eigenvalue of $\mathcal{P}$ is the one with second largest magnitude denoted by Λ_2.
- One reason for its importance is that it quantifies the **rate at which functions** f **in** $\mathcal{B}$ **converge to** h as they are pushed forward by the dynamics, i.e.

$$\left\| \mathcal{P}^n f - \left(\int f \ dLeb \right) h \right\| \leq C(f)|\Lambda_2|^n, \text{with } |\Lambda_2| < 1.$$

- Further, the eigenfunction f_2 of $\mathcal{P}$ corresponding to Λ_2 is the **non-equilibrium distribution** of (signed) mass in phase space that **mixes most slowly** to the equilibrium distribution given by h.
- Indeed, the sign [Dellnitz/Junge'99] (or more generally, extreme values) of this signed mass distribution describe **almost-invariant sets**.

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Nonautonomous dynamical systems

- **Driving system:** let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and assume that $\sigma\colon \Omega \to \Omega$ is invertible, ergodic transformation preserving $\mathbb{P}$.
- One thinks of Ω as a configuration space, evolving with the passage of time (iteration of σ).
- **ω-dependent maps:** Consider a collection $\{T_\omega\}_{\omega\in\Omega}$ of maps.
- **Map cocycle:** for $\omega \in \Omega$ and $n \in \mathbb{N}$, set $T_\omega^n = T_{\sigma^{n-1}\omega} \circ \ldots \circ T_{\sigma\omega} \circ T_\omega$.

Some trivial warm-up examples:

1. *Autonomous dynamics:* $\Omega = \{\omega\}$, σ is the trivial map, $\mathbb{P}$ is the probability measure supported on ω, $T_\omega = T$.
2. *Periodic dynamics:* $\Omega = \{\omega_0, \ldots, \omega_{p-1}\}$, $\sigma(\omega_i) = \omega_{i+1}$ (mod p), $\mathbb{P}(\omega_i) = 1/p, i = 0, \ldots, p-1$, $T_{\omega_i} = T_i, i = 0, \ldots, p-1$.

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Nonautonomous examples

The types of driving we can model are extremely general, e.g.:

1. $\Omega = [0,1]^{\mathbb{Z}}$, σ is the left shift, $\mathbb{P} = \Pi_{i=-\infty}^{\infty}\mathrm{Leb}$, $T_\omega : \mathbb{R} \circlearrowleft$ is given by $T_\omega = T + 2\epsilon(\omega_0 - 1/2)$. This setup models **iid** uniformly distributed noise in the range $[-\epsilon, \epsilon]$.
2. $\Omega = S^1$, $\sigma(\omega) = \omega + \alpha$, $\alpha \notin \mathbb{Q}$, $\mathbb{P} = \mathrm{Leb}$, $T_\omega : \mathbb{R} \circlearrowleft$ is given by $T_\omega = T + 2\epsilon(\omega - 1/2)$. This setup models **highly correlated** uniformly distributed noise in the range $[-\epsilon, \epsilon]$.
3. $\Omega =$ Lorenz attractor, $\sigma =$ time-1 map of Lorenz flow, $\mathbb{P} =$ SRB measure of Lorenz flow, $T_\omega(\cdot) = T(\omega, \cdot)$ a family of general measurable maps parameterised in some general way by the (three-dimensional) parameter $\omega \in \mathbb{R}^3$.

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Nonautonomous/Random ACIMS

- Clearly, for a general nonautonomous system, one cannot expect a **fixed** invariant density. Instead, the natural object is a random invariant density, **parameterised by the driving configuration ω.**
- From the map cocycle, one builds a **transfer operator cocycle:** $\mathcal{P}_\omega^n = \mathcal{P}_{\sigma^{n-1}\omega} \circ \ldots \circ \mathcal{P}_{\sigma\omega} \circ \mathcal{P}_\omega$
- An ω-measurable family of densities $\{h_\omega\}_{\omega\in\Omega}$ satisfying $\mathcal{P}_\omega h_\omega = h_{\sigma\omega}$ will be called a **(quenched) random absolutely continuous invariant measure (ACIM)** [Buzzi'99,'00]; see also [Bogenschuetz/Gundlach'95,Khanin/Kifer'96,Baladi'97].
- In terms of probability measures, define a family $\{\mu_\omega\}_{\omega\in\Omega}$ by $\mu_\omega(A) = \int_A h_\omega\ dLeb$; this family is **equivariant**: $\mu_{\sigma\omega} = \mu_\omega \circ T_\omega^{-1}$.

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Quenched vs Physical vs Annealed

- Our quenched random ACIMs $\{h_\omega\}_{\omega\in\Omega}$ describe **limiting distributions after pushing forward to time** ω e.g. Lebesgue from the distant past. They are equivariant: $\mathcal{P}h_\omega = h_{\sigma\omega}$.
- Define a **non-random physical invariant measure** [Buzzi'99] $\mu := \lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n-1} \delta_{T_\omega^{(i)}(x)}$ for *Leb* a.e. $x \in [0,1]$ and $\mathbb{P}$ a.e. $\omega \in \Omega$ where weak convergence is meant.
  The density of μ *is* $\int h_\omega \; d\mathbb{P}(\omega)$.
- IF $\sigma : \Omega \circlearrowleft$ were Bernoulli, it would make sense to form an averaged transfer operator $\bar{\mathcal{P}} = \int_\Omega \mathcal{P}_\omega \; d\mathbb{P}(\omega)$. An **annealed invariant density** is a fixed point of $\bar{\mathcal{P}}$; [Ohno'83, Pelikan'84, Morita'85].

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- Our quenched random ACIMs $\{h_\omega\}_{\omega\in\Omega}$ describe **limiting distributions after pushing forward to time** ω e.g. Lebesgue from the distant past. They are equivariant: $\mathcal{P}h_\omega = h_{\sigma\omega}$.
- Define a **non-random physical invariant measure** [Buzzi'99] $\mu := \lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n-1} \delta_{T_\omega^{(i)}(x)}$ for *Leb* a.e. $x \in [0,1]$ and $\mathbb{P}$ a.e. $\omega \in \Omega$ where weak convergence is meant. *The density of* μ *is* $\int h_\omega \, d\mathbb{P}(\omega)$.
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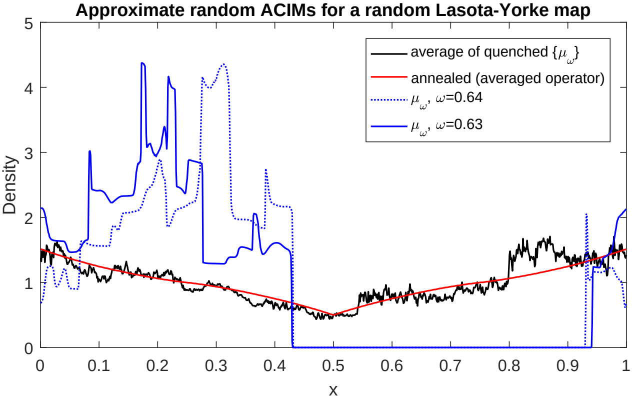
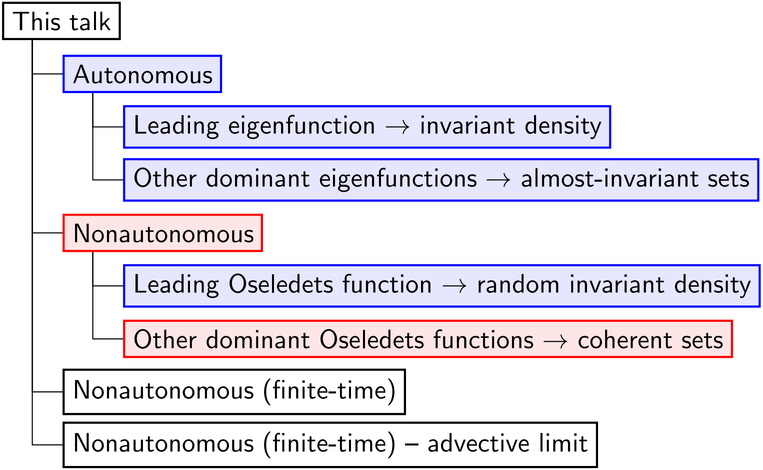
Quenched vs Physical vs Annealed

- Quenched random ACIMs, the non-random physical measure, and the annealed measure are **all different** in general.
- The physical measure encodes fluctuations **not captured by the annealed measure**.



(see [F/González-Tokman/Quas'14,F/GT/Murray'18] for random ACIM stability)

Status



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Spectrum for nonautonomous systems

- **Autonomous case**
  - We found the eigenfunction f_2 corresponding to the second largest eigenvalue Λ_2. Thus,

$$\|\mathcal{P}^n f_2\| \leq C(f_2)|\Lambda_2|^n, \quad \text{for all } n \geq 0.$$

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

$$\|\mathcal{P}_{T_{\sigma^{n-1}\omega}} \circ \cdots \circ \mathcal{P}_{T_{\sigma\omega}} \circ \mathcal{P}_{T_\omega} f\| \leq C(f)|\Lambda_2|^n.$$

  - Or:

$$\lim_{n\to\infty} \frac{1}{n} \log \|\mathcal{P}_{T_{\sigma^{n-1}\omega}} \circ \cdots \circ \mathcal{P}_{T_{\sigma\omega}} \circ \mathcal{P}_{T_\omega} f\| \leq \log|\Lambda_2|.$$

  - Note that the $\mathcal{P}_{T_\omega}$ are *linear* operators (or in numerical experiments, matrices), so $\lambda_2 := \log|\Lambda_2|$ is a **Lyapunov exponent**.
  - Thus, eigenvalues are replaced with Lyapunov exponents, and the eigenspectrum is replaced with the Lyapunov spectrum.

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Equivariant (not eigen-) functions in nonautonomous dynamics

- Because the nonautonomous driving is aperiodic, it **does not make sense to talk about eigenfunctions** of the transfer operator cocycle.
- In the quasi-compact setting [Thieullen'87, F/Lloyd/Quas'10&'13, Gonzalez-Tokman/Quas'14, Blumenthal'16] one can show (via a Multiplicative Ergodic Theorem) that there is a finite or countable set of Lyapunov exponents $0 = \lambda_1 > \lambda_2 > \cdots$ associated with the transfer operator cocycle and a family of **Oseledets (covariant) functions** $\{f_\omega\}_{\omega\in\Omega}$ satisfying:

$$\lim_{n\to\infty} \frac{1}{n} \log \|\mathcal{P}_\omega^n f_{k,\omega}\| = \lambda_k.$$

- Moreover, the $f_{k,\omega}$ are **equivariant**: $\mathcal{P}_\omega(f_{k,\omega}) = \lambda_{k,\omega} f_{k,\sigma\omega}$.
- The λ_k correspond to the Λ_k in the autonomous setting ($\lambda_k = \log|\Lambda_k|$).
- The $\{f_{k,\omega}\}_{\omega\in\Omega}$ are the nonautonomous family corresponding to the (single) k^{th} eigenfunction f_k in the autonomous setting.

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Coherent sets

Similar to the autonomous case, extreme values (red/yellow) of the ω-dependent family of Oseledets functions for large Lyapunov spectral values indicate **spatially mobile "coherent sets"**.

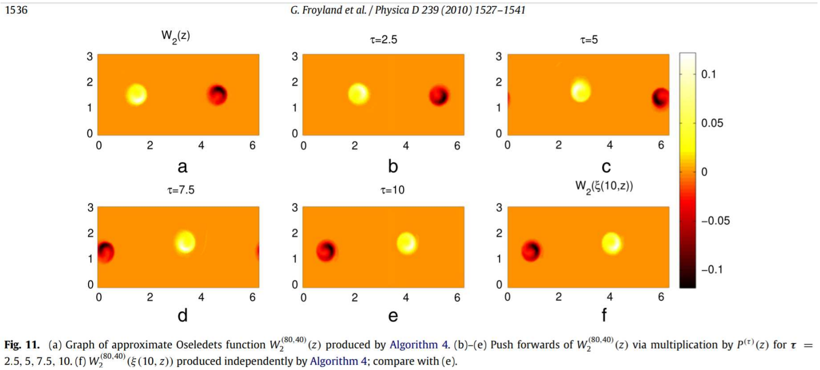

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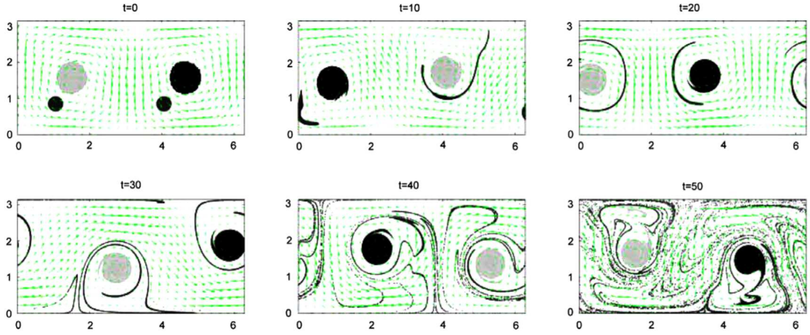
Fig. 11. (a) Graph of approximate Oseledets function $W_2^{(80,40)}(z)$ produced by Algorithm 4. (b)–(e) Push forwards of $W_2^{(80,40)}(z)$ via multiplication by $P^{(\tau)}(z)$ for $\tau = 2.5, 5, 7.5, 10$. (f) $W_2^{(80,40)}(\xi(10,z))$ produced independently by Algorithm 4; compare with (e).

Oseledets functions $f_{2,\omega}$, for a travelling wave flow with a perturbation that is driven aperiodically by the Lorenz equations.

Coherent sets



Evolution of coherent sets (and randomly chosen nearby sets) by the Lorenz-driven perturbation of a travelling wave flow (from [F/Lloyd/Santitissadeekorn'10]).

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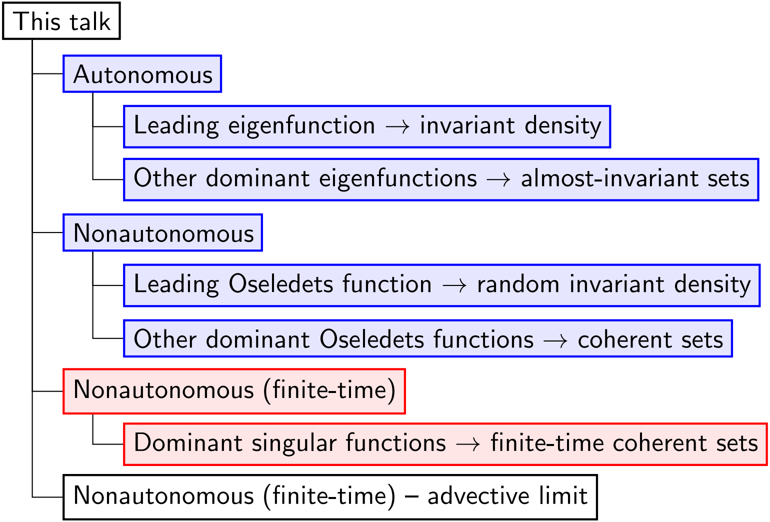

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Slowly decaying structures in finite time

- What about finite time durations (finite k)?
- We want to find a sequence of Λ_k and f_k so that $\|\mathcal{P}_{T_n} \circ \cdots \circ \mathcal{P}_{T_2} \circ \mathcal{P}_{T_1} f_k\| = \Lambda_k^n \|f_k\|$ with $\Lambda_k \leq 1$ **as large as possible**.
- This is accomplished by setting $1 = \Lambda_1 > \Lambda_2 > \cdots \geq 0$ to be **singular values** of (a suitably weighted version of) $\mathcal{P}_{T_n} \circ \cdots \circ \mathcal{P}_{T_2} \circ \mathcal{P}_{T_1}$, and $\mathbf{1} = f_1, f_2, \cdots$ to be the corresponding **singular vectors**.
- This leads to the **slowest decay in finite time** [F/Santitissadeekorn/Monahan'10,F'13].
- In particular, the singular value Λ_2 **exactly quantifies the slowest decay from time 1 to** n for the nonautonomous dynamics.

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Coherent transport in the presence of diffusion

- Consider a vector field $v(x, t)$ on a domain $X \subset \mathbb{R}^d$.
- For small $\epsilon > 0$ the SDE $dx = v(x, t)dt + \epsilon dW$ models paths of an advection-diffusion process.
- The corresponding advection-diffusion (or Fokker-Planck) equation for this SDE is

$$\frac{\partial f}{\partial t}(x, t) = -\nabla \cdot (f(x, t)v(x, t)) + \frac{\epsilon^2}{2}\Delta f(x, t) \qquad (1)$$

- **Solutions of the above PDE are given by the corresponding transfer operator:**

$$f(x, t) = \mathcal{P}^t_{t_0,\epsilon} f(x, t_0),$$

where $\mathcal{P}^t_{t_0,\epsilon} : L^2(X) \to L^2(X)$ is the transfer operator evolving a mass distribution $f(x, t_0)$ at t_0 to the future distribution at t.

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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.

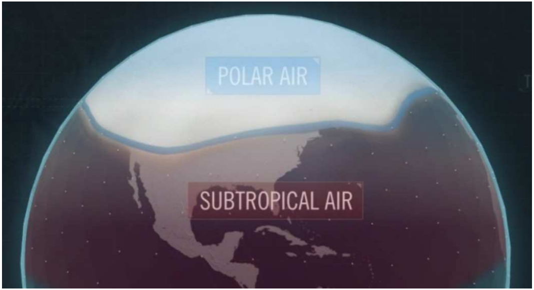
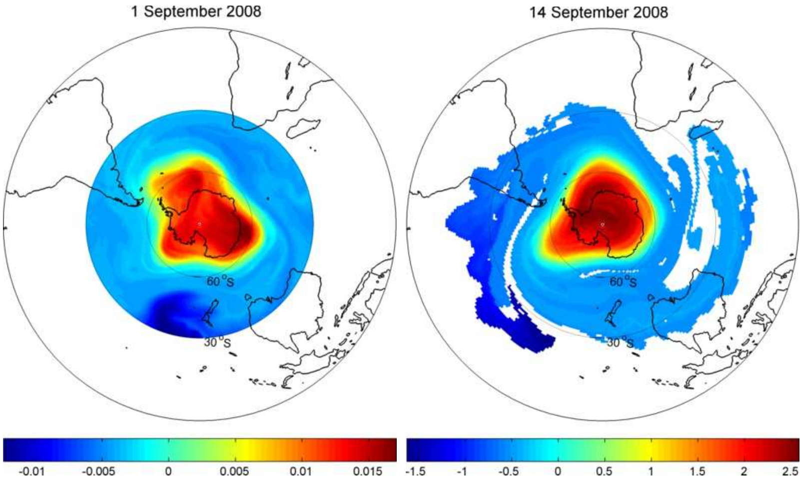


Image: National Geographic.

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'10].

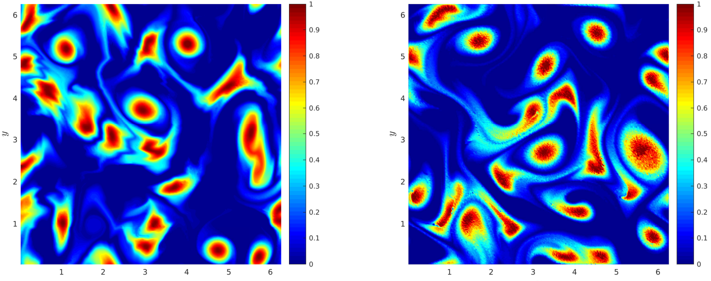
Particle simulation demonstrating the identified vortex inhibits global mixing

Multiple sets: 2D turbulence

Consider the velocity field $u : \mathbb{T}^2 \times \mathbb{R} \to \mathbb{R}^2$ that solves

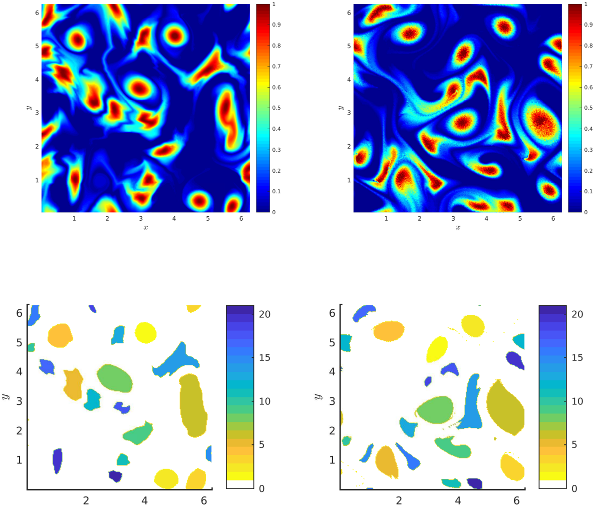
$$\partial_t u + u \cdot \nabla u = -\nabla p + \nu \Delta u + f; \qquad \nabla \cdot u = 0$$

where the toral domain $\mathbb{T}^2 = [0, 2\pi] \times [0, 2\pi]$.
Using data from [Hadjighasem *et al.*'17] and techniques from [F/Rock/Sakellariou, subm.]: a superposition of 21 rotated singular vectors of the transfer operator are shown below (left singular vector, $t = 0$; right singular vector $t = 50$).



2D turbulence

From these singular vectors we can extract individual sets that are coherent under 50 time units of turbulent flow.



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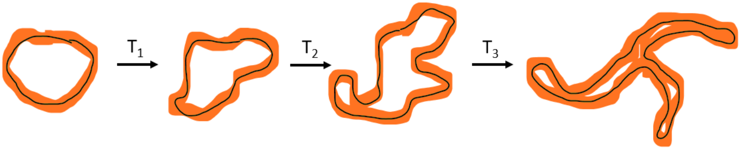
  - Nonautonomous (finite-time) – advective limit
    - Dominant eigenfunctions of Dynamic Laplacian → finite-time CS

Small diffusion regime

- In geophysical flow, one is often interested in the regime where advection plays a stronger role than diffusion.
- 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 interface.



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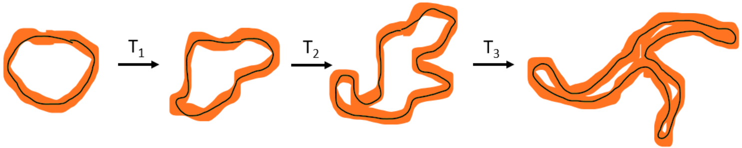

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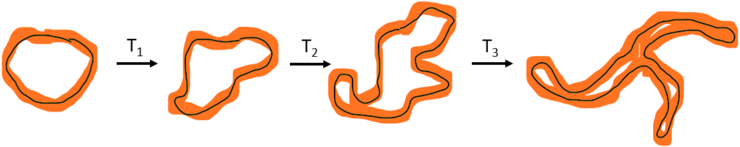

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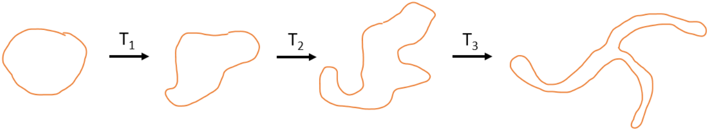


- The amount of mixing occurring is proportional to the **area of the orange region**. This area is minimised by the singular vectors of the transfer operator.
- In the **pure advection limit**, as the diffusion amplitude goes to zero, (the orange band narrows), the **length of the boundary/interface determines the amount of "mixing"**. ([Mathew *et al*'05, Thiffeault'12])

Small diffusion regime

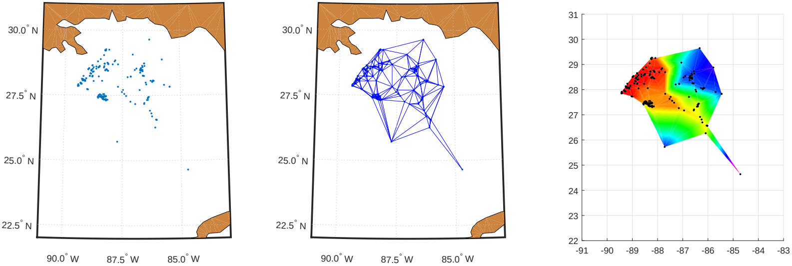
- A limiting form of the earlier transfer operator constructions yields the **dynamic Laplace operator** $\Delta^D_{t_0,t}$ [F'15,F/Kwok'17]:

$$\lim_{\epsilon\to 0}\frac{((\mathcal{L}^t_{t_0,\epsilon})^*\mathcal{L}^t_{t_0,\epsilon}-\mathrm{Id})f}{\epsilon^2}=c\,\underbrace{\left(\Delta+(T^t_{t_0})^*\circ\Delta\circ(T^t_{t_0})_*\right)}_{:=\Delta^D_{t_0,t}}f,$$

  where $\mathcal{L}^t_{t_0,\epsilon}$ is a weighted version of $\mathcal{P}^t_{t_0,\epsilon}$, c is a constant, $(T^t_{t_0})^*f=f\circ T^t_{t_0}$, and $(T^t_{t_0})_*f=f\circ(T^t_{t_0})^{-1}$.
- The **orthogonal eigenfunctions of the dynamic Laplacian** $\Delta^D_{t_0,t}$ provide independent solutions to the **persistently smallest interface (isoperimetric) problem**.
- In the small diffusion regime, eigenvectors of $\Delta^D_{t_0,t}$ correspond to singular vectors of $\mathcal{L}_\epsilon$ and the two approaches coincide.
- There is a **formal dual interpretation of coherent sets** in terms of **mixing properties** and **small interfaces** [F'15,F/Kwok'17], (also [Karrasch/Keller,subm.]).

Implementation

- A convenient, flexible, and accurate way to approximate the operator Δ^D is using a specialised **finite element method** [F/Junge'18] (see Oliver's talk on Friday).
- The **only input data are the positions of trajectories**; these can be **sparse**, **scattered**, and have **missing elements**.
- As in the transfer operator approaches, **no derivative information is required**, but if present, it can be used. There are **no free parameters** to select, and estimates of mixing barriers and persistently small interfaces are provided on the **full phase space**.

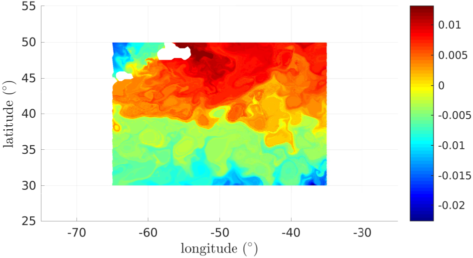


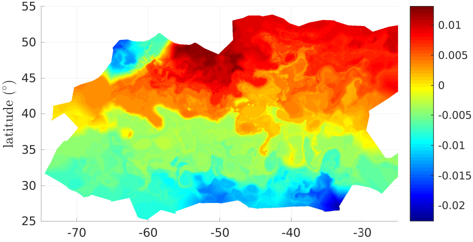
SST in the North Atlantic

North Atlantic flow

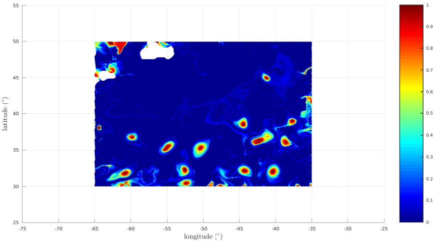
- The following movies use AVISO satellite altimetry to derive time-dependent velocity fields.
- I used 56205 nonautonomous trajectories (positions only, no derivatives!) over a flow period from 15 January 2015 to 15 April 2015 (90 days) [trajectory data courtesy of Irina Rypina].
- The movies show daily evolution.
- Techniques from [F/Junge'18] combined with [F/Rock/Sakelleriou, subm.].

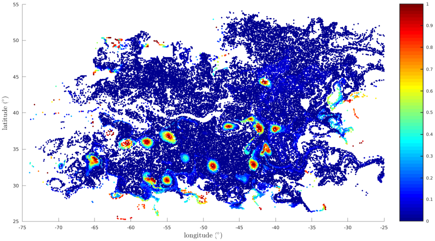
Large-scale features



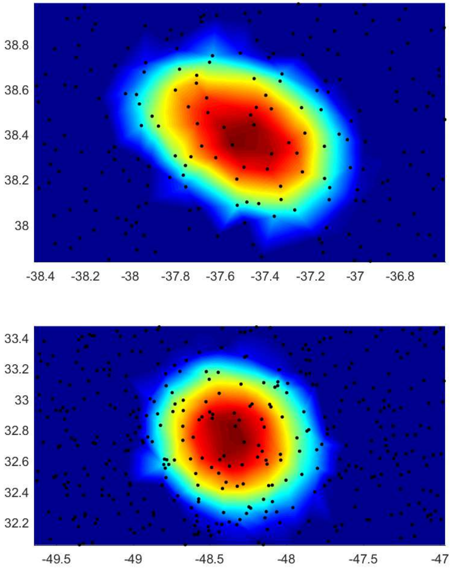


Small-scale features





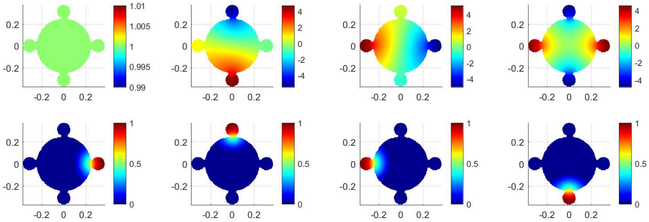
High-resolution eddies vs sparse data



Status

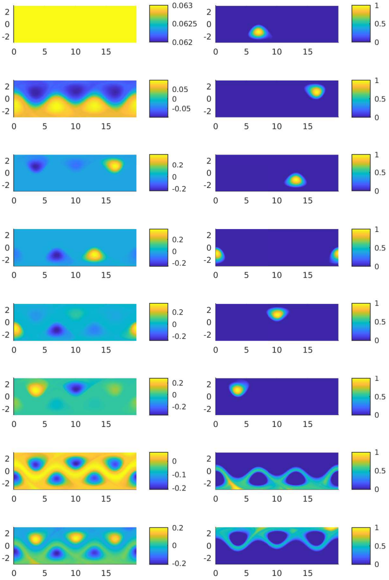
- This talk
  - Autonomous
    - Leading eigenfunction → invariant density
    - Other dominant eigenfunctions → almost-invariant sets
  - Nonautonomous
    - Leading Oseledets function → random invariant density
    - Other dominant Oseledets functions → coherent sets
  - Nonautonomous (finite-time)
    - Dominant singular functions → finite-time coherent sets
  - Nonautonomous (finite-time) – advective limit
    - Dominant eigenfunctions of Dynamic Laplacian → finite-time CS
  - Automatic feature separation – Sparse Eigenbasis Approximation (SEBA)

SEBA – Sparse Eigenbasis Approximation



- The **features captured in extreme values** of eigen-(singular-)(Oseledets-) vectors of transfer operators, eigenvectors of the Koopman operator, and eigenvectors of the (Dynamic) Laplace operator, are often **"mixed" between different eigenvectors** *(first row, standard Laplace eigenfunctions)*.
- We would like to highlight the 4 geometric "knobs" on the outside of the large disk, *(second row)*.
- The second row is a solution of a sparse eigenbasis approximation problem, where **one rotates the (four-dimensional) eigenbasis** to find the **best-approximating sparse basis**; see [F/Rock/Sakellariou].

SEBA – Sparse Eigenbasis Approximation



(Left:) SEBA applied to leading 8 eigenfunctions of Dynamic Laplacian of Bickley jet.

See also [F/Rock/Sakellariou] for:

1. **automatic feature separation** procedure based on SEBA,
2. a **rescaling of the spectrum** to better identify eigengaps,
3. **determining natural spatial scales** from eigenfunctions, in contrast to temporal scales given by eigengaps.

See my webpage for code.

Other nonautonomous analysis with transfer operators

- **(Quenched)** statistical limit laws for **nonautonomous** systems, e.g. (Quenched) Central Limit Theorem, (Quenched) Local Central Limit Theorem, (Quenched) Large Deviation Principle.
- Obtained by differentiating leading Lyapunov of twisted transfer operator cocycles wrt the twist parameter [Dragicevic/F/Gonzalez-Tokman/Vaienti'18].

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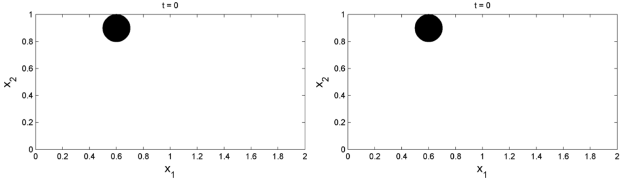
- Mixing optimisation – **manipulating the transfer operator spectrum** to **optimally perturb time-dependent vector fields** to enhance mixing.
- Periodic case treated in [F/Santitissadeekorn'17] and nonautonomous case to be submitted shortly with P. Koltai and M. Plonka.



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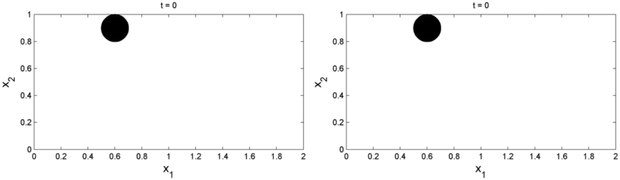

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