A perspective on set-oriented and transfer operator techniques for quantifying transport and coherence in flows

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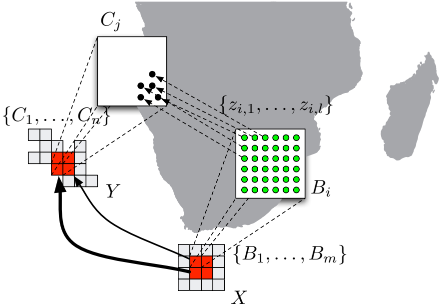
AUTONOMOUS AND/OR PERIODICALLY DRIVEN DYNAMICS.

Elementary transport questions

- Consider an autonomous flow $\dot{x} = F(x)$ or discrete-time map $x \mapsto T(x)$, where $x \in X \subset \mathbb{R}^d$. **Note** $1 \leq d < \infty$**.**
- **Question 1:** Determine a decomposition of X into invariant sets (a set A is *invariant* if points in A do not leave A in forward and backward time).
- **Question 2:** Suppose there are no nontrivial invariant sets. Determine a decomposition of X into sets that are as *close to invariant* as possible.

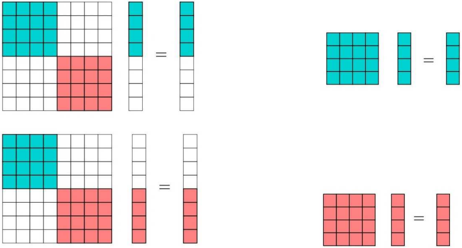
"Transfer operator" approach

Lay a grid over X and construct a large Markov chain based on intersections of grid cells with their images (see figure). Compute transient (open) sets, absorbing sets, and invariant sets as unions of grid cells [Hsu'81]. This idea was revitalised in the late 90s, including efficiencies in grid construction, and importantly, the recognition that the **eigenvectors of the eigenvalues of the Markov chain that are close to 1 yield "almost-invariant" sets** [Dellnitz/Junge'99]. I'll call this approach **Ulam's method**.



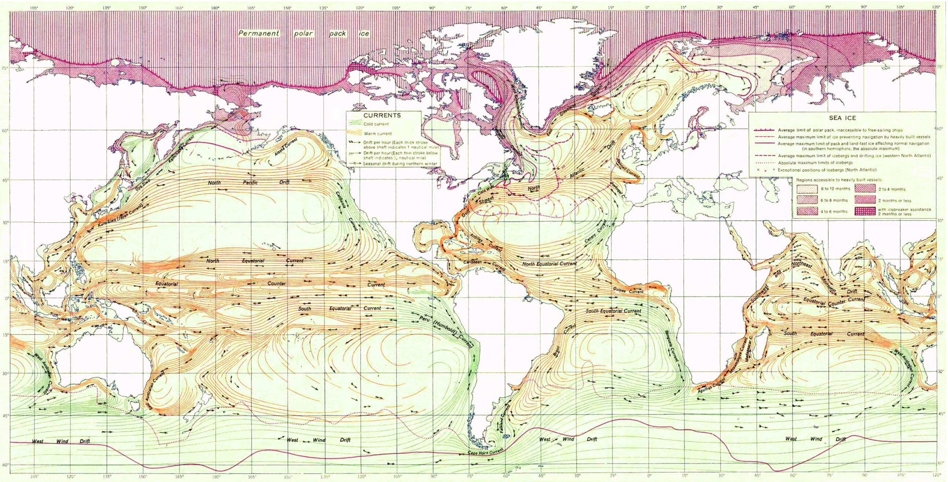
“Almost-invariant” regions and eigenvectors of P

Suppose that the collection of cells can be neatly partitioned into 2 pieces so that the transition matrix P has the following block structure (possibly after relabelling).



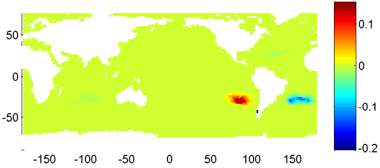
- Then the matrix P has **two eigenvalues 1** and the **two spatial regions corresponding to the two collections of cells are dynamically invariant**.
- In practice, one may observe several blocks (several regions) and the eigenvalues may be close to 1, not exactly 1.
- A modified transition matrix is used for **finite-time** almost-invariant sets [F'05].

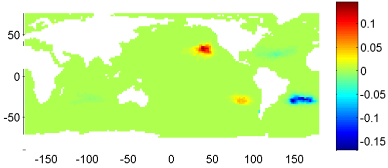
The global ocean, circa 1943

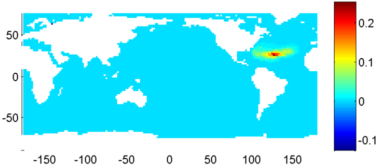


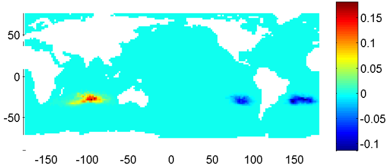
Application 3: Gyre cores as left eigenvectors

Based on OFES ($1/10^o$) and 2^o grid cells, and the year 2001. The following leading eigenvectors, highlight the gyre cores.



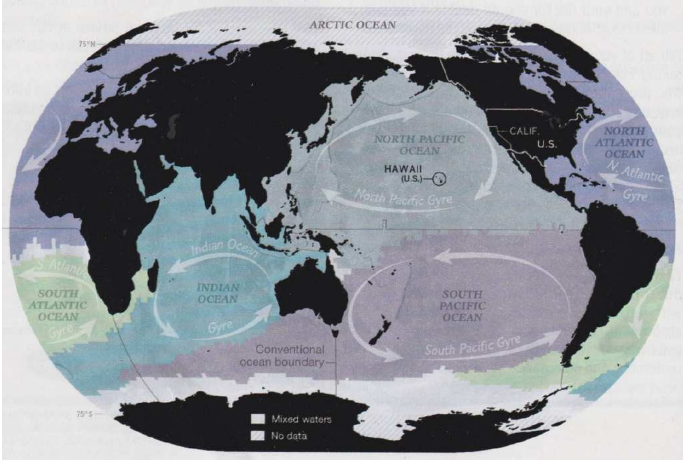






Basins of attraction of gyre cores

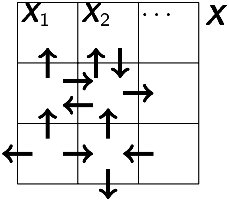
By combining information from 4 of these eigenvectors, we can separate the ocean surface into **5 domains of attraction**, one for each of the 5 garbage patches. [F/Stuart/van Sebille '14 and Nat.Geo.]. (See also [Hsu'81, Koltai'11]).



Implementation

All of these grid-based methods are particular implementations of transfer operator methods, where the transfer operator describes the linear action of the flow on function space. One needs to **approximate** this transfer operator (*see Oliver's talk next*).

- Classical, most common method is based on sampling several initial conditions per grid cell and numerically integrating in time (Ulam's method). Can be expensive, but highly parallelisable.
- In the autonomous [F/Junge/Koltai'13] and periodically driven case [F/Koltai, subm.], one can **replace time integration of many trajectories with spatial integration on box boundaries** (which are one dimension lower). Can also use *spectral collocation*.



NONAUTONOMOUS, APERIODIC DYNAMICS

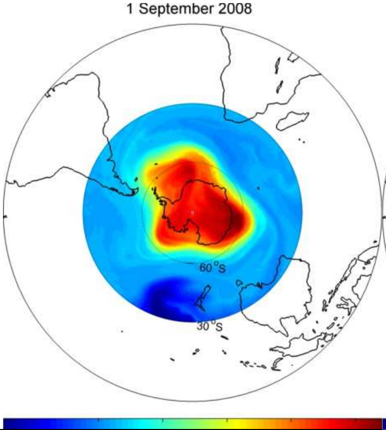
Finite-time coherent sets as minimally mixing regions

- Consider an aperiodic flow $\dot{x} = F(x,t)$ and a given finite time horizon $t \in [t_0, t_f] \subset \mathbb{R}$, where $x \in X \subset \mathbb{R}^d$.
- Because the flow is aperiodic, it is **highly unlikely that truly invariant sets exist**. However one can search for finite-time almost-invariant sets using similar techniques to those just discussed [F'05].
- Also of interest are **finite-time coherent sets**, which have a **minimal mixing (or minimal inter-communication) property** over the finite time duration [F/Santitissadeekorn/Monahan'10,F'13]. Mixing relies on a **small amount of diffusion/stochasticity**.
- The strategy and computation is similar to the computation of almost-invariant sets, except **singular vectors** of the gridcell-to-gridcell transition matrix are used in place of **eigenvectors**. This amounts to searching for blocks **off** the diagonal, rather than **on** the diagonal.

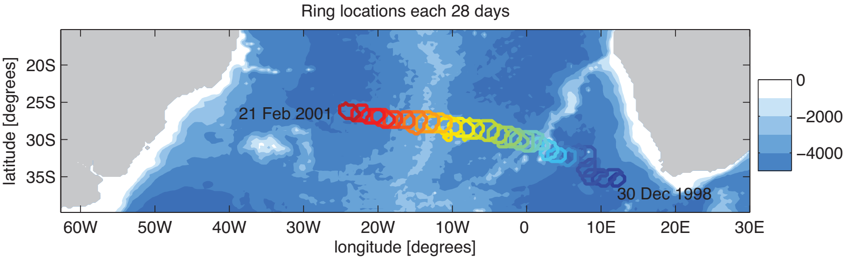
Example: finite-time coherent sets in an idealised stratospheric flow

Example: southern polar vortex from singular vectors

Computation on a 475K isentropic surface in the stratosphere over 14 days using ECMWF velocity fields. The **southern polar vortex is revealed as the strongest finite-time coherent set in the domain** from the second singular vectors [F/Santitissadeekorn/Monahan'10].



Agulhas ring as a coherent set transports mass



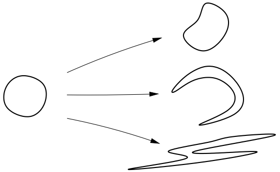
- We use velocity fields derived from satellite sea-surface height data to identify and track a surface ring for 26 months.
- Agulhas ring identified as a coherent set carries surface water mass over a 26-month period [F/Horenkamp/Rossi/SenGupta/vanSebille'15, *Chaos*]. See also [F/Horenkamp/Rossi/Santitissadeekorn/SenGupta'12, *Ocean Modelling*] for a 6-month 3D study.

Implementation

- Gridcell-to-Gridcell approach [F/Santitissadeekorn/Monahan'10,F/Padberg-Gehle'14] (Ulam's method, most common).
- Approximate Galerkin projection onto a basis of thin-plate splines [Williams/Rypina/Rowley'15].
- Spectral collocation [Denner/Junge/Matthes].
- Diffusion map [Banisch/Koltai'16].

Finite-time coherent sets as regions with persistently small boundary

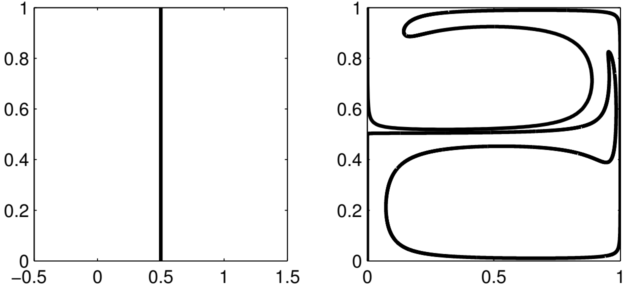
Instead of considering coherent sets as regions with that minimally mix over a finite time, one can instead consider coherent sets as regions with **persistently small boundary** [F'15,F/Kwok subm.,Keller/Karrasch subm.]. In particular, this is a **purely deterministic notion**.



- Uses **eigenvectors of a "dynamic Laplace operator"**.
- In fact, because mixing under small diffusion occurs at the boundary, there is a **tight relationship between these two notions**. The target of persistently small boundary is also consistent with some of the work of Haller, *discussed by Nick*.

Implementation

- Gridcell-to-Gridcell approach [F'15,F/Kwok subm.] (Ulam).
- Radial basis function collocation [F/Junge'15] (exploits smoothness to achieve large reduction in number of trajectories, but careful choice of RBF centres and radii).
- Finite element methods [F/Junge/Karrasch, in prep.] (**many**



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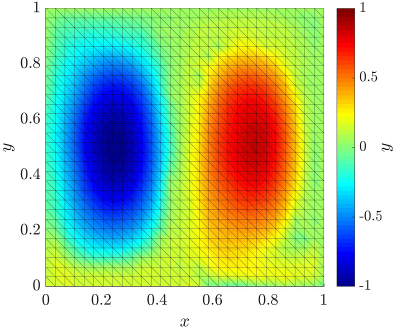

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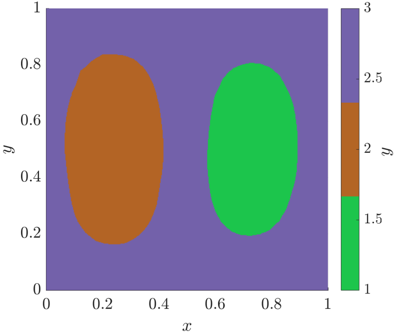

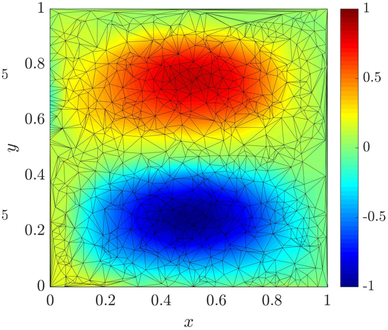

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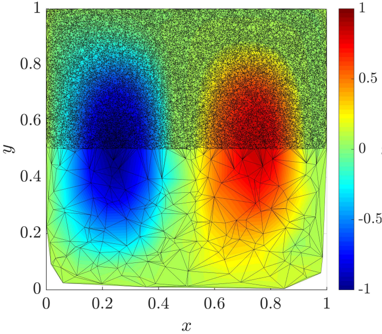
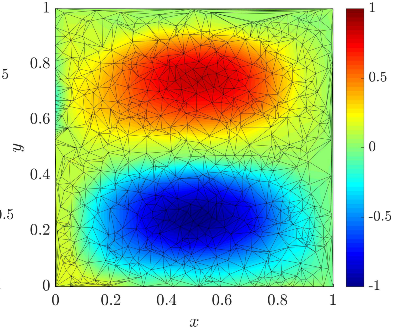
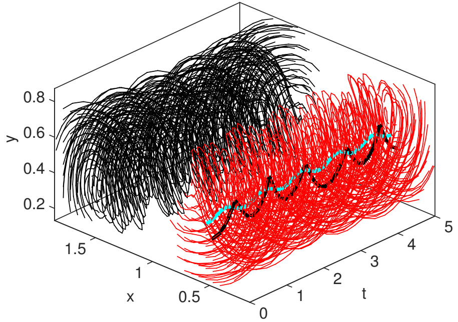




Groups of trajectories that remain proximal

One may also try to find groups of trajectories that "remain proximal" by performing clustering with a space-time distance, e.g. [F/Padberg-Gehle'15] (fuzzy clustering, *see Kathrin Padberg's talk*), [Hadjighasem/Karrasch/Teramoto/Haller'16] (spectral clustering – with strong connection to the previous "dynamic Laplace operator").

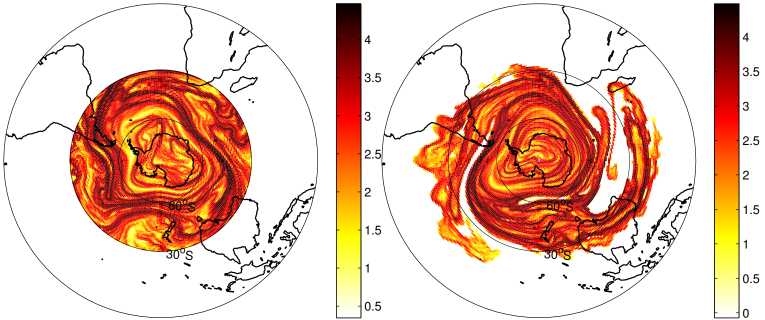


Fuzzy clustering application

Application to global ocean surface circulation from buoy data (Global drifter program, NOAA, AOML), [F/Padberg-Gehle'15].

Local spreading methods

- Methods based on how quickly particular grid cells are distributed over phase space and interact with other grid cells (*see Irina Rypina's talk*: complexity, trajectory encounter).
- Finite-time entropy [F/Padberg-Gehle'12], measures the spread of a grid cell under advective-diffusive flows and converges to FTLE in the zero diffusion limit.



Discussion

- I have (very briefly) outlined some techniques that identify important structures in time-dependent flows, particularly those that control global transport properties of the flow.
- Questions –
  1. What are the current important questions from oceanography, atmospheric science, climate, weather? e.g. what sort of transport, of which quantities, on what sort of spatial/temporal scales?
  2. Which of these questions are being addressed by coherent set approaches and which aren't (or aren't well addressed)?

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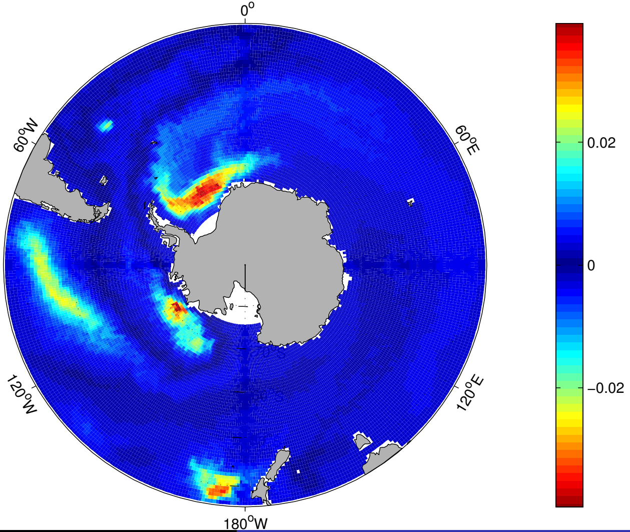
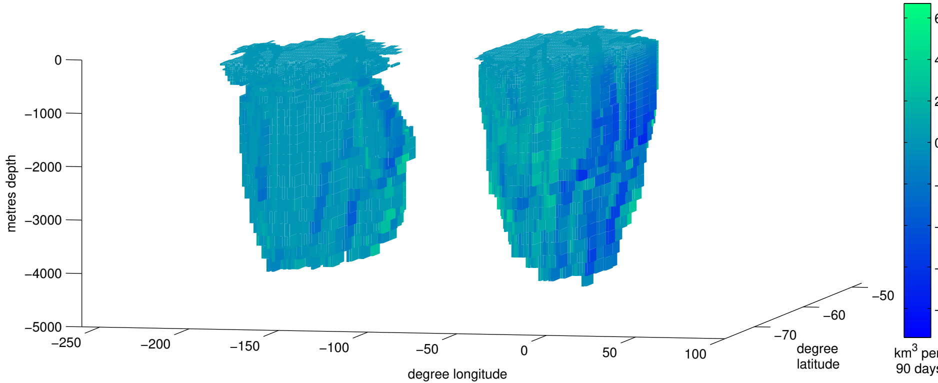
Eigenvector corresponding to large λ highlights gyres

Based on 2-month flow from ORCA025.
[F/Padberg/England/Treguier'07]

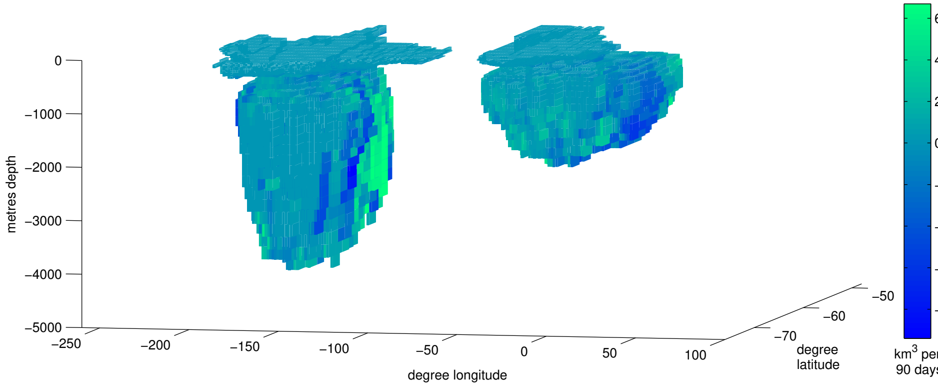


Summer location of Weddell and Ross Gyres



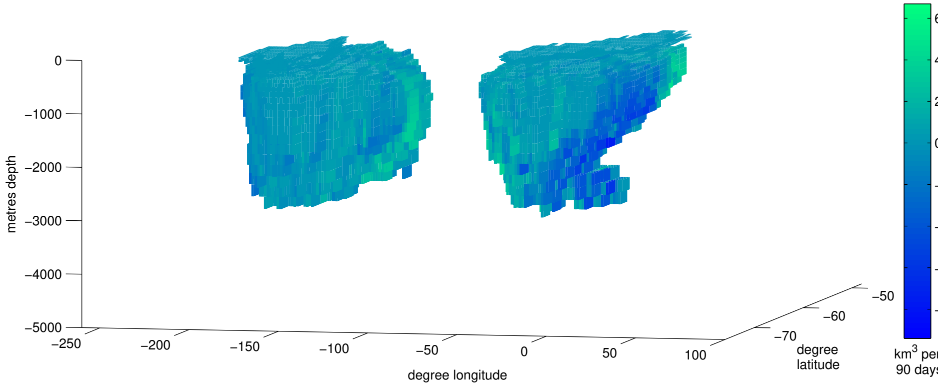
After 3 months, 92.7% of water mass retained in Weddell region, 92.4% in Ross region.
[Dellnitz/F/Horenkamp/Padberg-Gehle/Sen Gupta, '09]

Autumn location



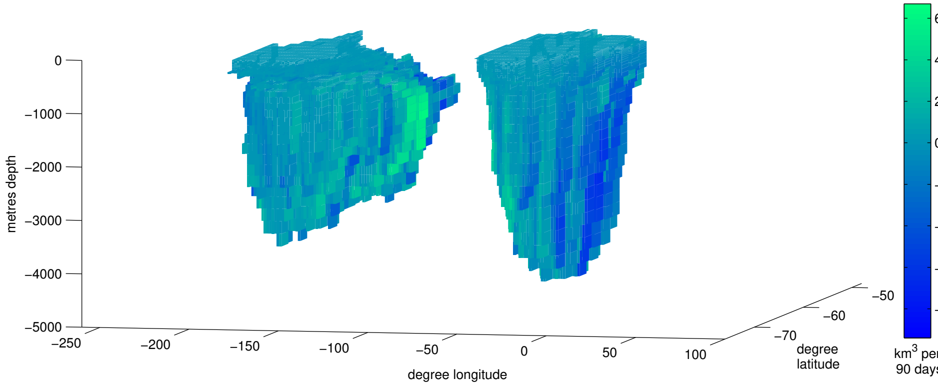
After 3 months, 91.1% of water mass retained in Weddell region, 91.8% in Ross region.

Winter location



After 3 months, 91.1% of water mass retained in Weddell region, 88.7% in Ross region.

Spring location



After 3 months, 91.9% of water mass retained in Weddell region, 90.4% in Ross region.

3D polar vortex as a coherent set (ECMWF)