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.
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].
Application 3: Gyre cores as left eigenvectors

Based on OFES (1/10°) and 2° grid cells, and the year 2001. The following leading eigenvectors, highlight the 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]).
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
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.
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 \textbf{persistently small boundary} [F’15,F/Kwok subm.,Keller/Karrasch subm.]. In particular, this is a \textbf{purely deterministic notion}.

- Uses \textit{eigenvectors of a “dynamic Laplace operator”}.
- In fact, because mixing under small diffusion occurs at the boundary, there is a \textbf{tight relationship between these two notions}. The target of persistently small boundary is also consistent with some of the work of Haller, \textit{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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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.
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 $\lambda$ highlights gyres

Based on 2-month flow from ORCA025.

[F/Padberg/England/Treguier'07]
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]
After 3 months, 91.1% of water mass retained in Weddell region, 91.8% in Ross region.
After 3 months, 91.1% of water mass retained in Weddell region, 88.7% in Ross region.
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3D polar vortex as a coherent set (ECMWF)

(a) (b) (c)

(d) (e) (f)