Coherent sets in nonautonomous dynamics

Kathrin Padberg-Gehle

Technische Universität Dresden
Institut für Wissenschaftliches Rechnen

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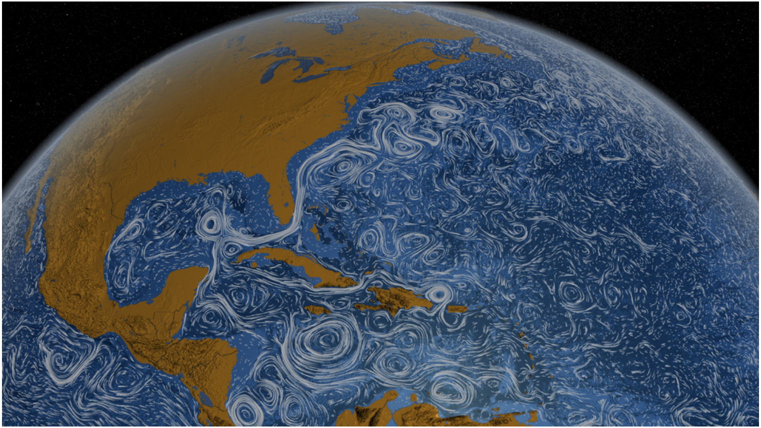
Motivation



The Perceptual Ocean.

(Movie credit: NASA/Goddard Space Flight Center, Scientific Visualization Studio)

Mathematical challenges

- How to mathematically characterize structures that remain *coherent* for an extended time span (such as ocean gyres and eddies)?
- In other words: How to define what you can physically observe?
- How to systematically, reliably, and efficiently extract these structures?
- How to quantify the mass exchange between these structures and their surroundings?
- How to enhance/mitigate/control coherence?

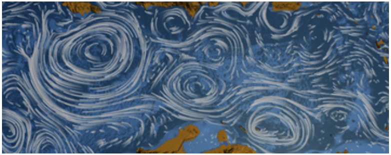
Concepts for analyzing flow structures

- **Geometric approach**: detect barriers to particle transport
  - invariant manifolds [Rom-Kedar, Wiggins, Mancho, Balasuriya, ...]
  - Lagrangian coherent structures (LCS)
    [Haller, Shadden, Lekien, Marsden, Beron-Vera,...]

  Approximate set boundaries!

- **Probabilistic approach**: detect minimally dispersive regions
  - almost-invariant sets (spatially fixed)
    [Dellnitz, Junge, Schütte, Froyland, Koltai, P., ...]
  - finite-time coherent sets (moving)
    [Froyland, Santitissadeekorn, Monahan, Bollt, Junge, P., ...]

  Approximate sets!



In this talk

Probabilistic approach

- Transfer operators and numerics
- Almost-invariant sets
- Functional analytic framework
- Finite-time coherent sets
- Clustering framework
- Examples and applications
- Conclusion and future research

Joint work with Gary Froyland, UNSW Australia

Notation

- **Discrete dynamical system**

$$T : M \to M, \quad M \subset \mathbb{R}^d \text{ compact}$$

- Here: T diffeomorphism (not formally required!),

  e.g. an autonomous flow map:

$$T(\cdot) := x(\tau; \cdot),$$

  where $x(\tau; x_0)$ solves $\dot{x} = f(x)$, $x_0 = x(0)$ for fixed flow time $\tau \in \mathbb{R}$

- A set $A \subset M$ is $T-$invariant if

$$A = T^{-1}(A).$$

- $\mathcal{M}$ space of finite signed measures on M
- Probability measure $\mu \in \mathcal{M}$ is T-invariant if

$$\mu(A) = \mu(T^{-1}(A)) \;\text{ for all }\; A \subset M.$$

Transfer operators in dynamics

- Define linear operator $\mathbf{P} : \mathcal{M} \to \mathcal{M}$

$$(\mathbf{P}\nu)(A) = \nu(T^{-1}(A)), \;\; A \subset M.$$

More relevant: $\mathbf{P} : L^1(M, m) \circlearrowleft$ with

$$\int_A \mathbf{P}f \; dm = \int_{T^{-1}(A)} f \; dm, \;\; m \text{ Lebesgue measure}$$

and for diffeomorphisms

$$\mathbf{P}f(x) = \frac{f(T^{-1}x)}{|\det DT(T^{-1}x)|}.$$

- **P** is the natural push-forward of densities under the action of T
- Invariant density corresponds to fixed point of **P**, i.e. eigenfunction to eigenvalue 1
- **Transfer operator** or **Perron-Frobenius operator**
- **P** is a Markov operator

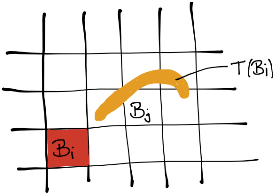
Numerical approximation of $\mathbf{P}$

- Consider $T : M \to M$
- $\{B_1, \dots, B_n\}$ partition of M
- Galerkin approximation of $\mathbf{P}$ with indicator functions on B_i, $i = 1, \dots n$, as basis functions [Ulam 1960]
- $\mathbf{P}$ represented by a sparse, stochastic matrix

$$P_{ij} = \frac{m(B_i \cap T^{-1}(B_j))}{m(B_i)} \approx \frac{\#\{k : T(x_{i,k}) \in B_j\}}{K},$$

with test points $x_{i,k}$, $k = 1, \dots, K$ uniformly distributed in B_i [Hunt 1993].

- Fixed points of P converge to invariant density of $\mathbf{P}$ as $n \to \infty$ for a very restricted class of systems [e.g. Li 1976]
- P is in general *assumed* to be a good approximation of $\mathbf{P}$



Almost-invariant sets

- μ preserved by $T : M \to M$
- $A \subset M$ is **almost-invariant** if $T(A) \approx A$, i.e.

$$\frac{\mu(A \cap T^{-1}(A))}{\mu(A)} \approx 1$$

- Application of transfer operator methods for almost-invariant sets:
  - Study eigenfunctions of transfer operator $\mathbf{P}$ / eigenvectors of P to real eigenvalues close to 1 [Dellnitz/Junge 1997/99, Deuflhard et al. 1998, Huisinga, Schmidt 2006],
  - Consider eigenfunctions of the infinitesimal generator of $\mathbf{P}$ and its discretization [Froyland/Junge/Koltai 2013]
  - Consider eigenvectors of a transition matrix R of a reversible Markov chain constructed from P [Froyland 2005; Froyland, P. 2009]
  - Consider optimal partitions of a directed graph induced by P or R [Froyland, Dellnitz 2003, Dellnitz et al. 2005]
  - Applications in physical oceanography, dynamical astronomy, fluid mixers, oil spills, epidemic spread,...

No uniform framework for deriving optimality criteria

Proposed construction [Froyland, P. 2014]

- **Task:** find nontrivial sets A, A^c
- that maximize

$$\rho(A) := \frac{\mu(A \cap T^{-1}(A))}{\mu(A)} + \frac{\mu(A^c \cap T^{-1}(A^c))}{\mu(A^c)}$$

- and are robust w.r.t. to perturbations

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- **Construction:** Use operator $\mathbf{L}$ dynamically similar to $\mathbf{P}$, with $\mathbf{L1} = \mathbf{1}$
- Functional representation of invariance condition $A \approx T(A)$:

$$\mathbf{L1}_A \approx \mathbf{1}_A \quad \text{(solution to eigenequation)}$$

- When

$$\mathbf{L} := \mathcal{D}_\epsilon \mathbf{P} \mathcal{D}_\epsilon / (\mathcal{D}_\epsilon \mathbf{P} \mathcal{D}_\epsilon \mathbf{1})$$

where $\mathcal{D}_\epsilon$ is a diffusion operator then – under mild assumptions – $\mathbf{L}$ is compact on $L^2(M, \mu)$ [Froyland 2013].

Optimization problem

Goal

Measurably partition

$$M = A \cup A^c$$

$$\text{s.t. } \mathbf{L}\mathbf{1}_A \approx \mathbf{1}_A, \quad \mathbf{L}\mathbf{1}_{A^c} \approx \mathbf{1}_{A^c} \text{ and } \mu(A) \approx \mu(A^c)$$

- **Invariance ratio:**

$$\rho(A) = \frac{\langle \mathbf{L}\mathbf{1}_A, \mathbf{1}_A \rangle_\mu}{\mu(A)} + \frac{\langle \mathbf{L}\mathbf{1}_{A^c}, \mathbf{1}_{A^c} \rangle_\mu}{\mu(A^c)} = \frac{\langle \mathbf{Q}\mathbf{1}_A, \mathbf{1}_A \rangle_\mu}{\mu(A)} + \frac{\langle \mathbf{Q}\mathbf{1}_{A^c}, \mathbf{1}_{A^c} \rangle_\mu}{\mu(A^c)}$$

  with compact, self-adjoint operator $\mathbf{Q} := (\mathbf{L} + \mathbf{L}^*)/2$, where $\mathbf{L}^*$ dual
- $\mathbf{Q}$ describes mass transport in forward and backward time

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  with compact, self-adjoint operator $\mathbf{Q} := (\mathbf{L} + \mathbf{L}^*)/2$, where $\mathbf{L}^*$ dual
- $\mathbf{Q}$ describes mass transport in forward and backward time

- Relaxed problem of constrained maximization of ρ can be shown to be

$$\max_{f \in L^2(M,\mu)} \left\{ \frac{\langle \mathbf{Q}f, f \rangle_\mu}{\langle f, f, \rangle_\mu} : \langle f, \mathbf{1} \rangle_\mu = 0 \right\} \quad (*)$$

Results

- $\mathbf{Q}$ is self-adjoint and compact, $\mathbf{Q1} = \mathbf{1}$; i.e. $u_1 = \mathbf{1}$ is eigenfunction to eigenvalue $\lambda_1 = 1$
- λ_1 is simple [Froyland 2013]

Theorem

- *Maximum in* $(*)$ *is* λ_2 *and maximizing* $f = u_2$ *[follows from min-max theorem],*
- $2 - 2\sqrt{2(1-\lambda_2)} \leq \sup_{A\subset X} \rho(A) \leq 1 + \lambda_2$

[Froyland, P. 2014]

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[Froyland, P. 2014]

- Note that $f = f^+ - f^-$ is signed - with $f^+ \approx \mathbf{1}_A$ and $f^- \approx \mathbf{1}_{A^c}$
- This suggest an extraction scheme.
- *A priori* bounds - verification of matrix based bounds [Froyland 2005, Froyland, P. 2009]
- *A posteriori* bounds also directly apply in this setting [Huisinga, Schmidt 2006]
- Influence of ϵ (e.g. spectral gaps, regularity of eigenvectors) [Froyland 2013, Froyland, P. 2014]

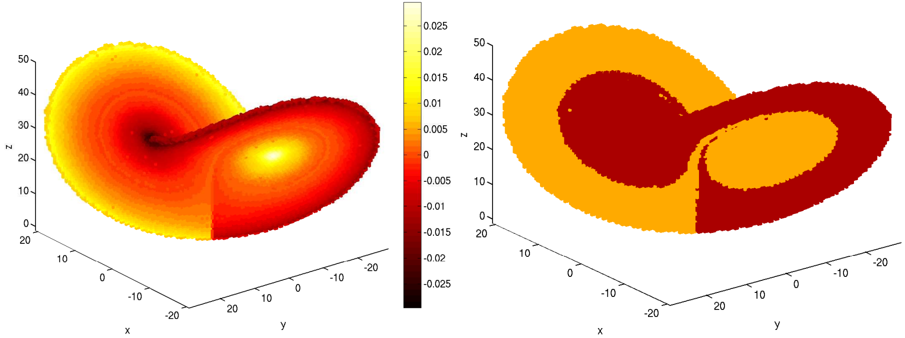
Numerical approximation of $\mathbf{L}$

- $\{B_1, \ldots, B_n\}$ partition of M
- P transition matrix obtained via Ulam's method
- By $p = pP$ we obtain $\mu(B_i) \approx p_i$.
- Approximation to $\mathbf{L}$, $\mathbf{L}^*$:

$$L_{ij} = \frac{p_i P_{ij}}{p_j}, \quad L^*_{ij} = P_{ji}$$

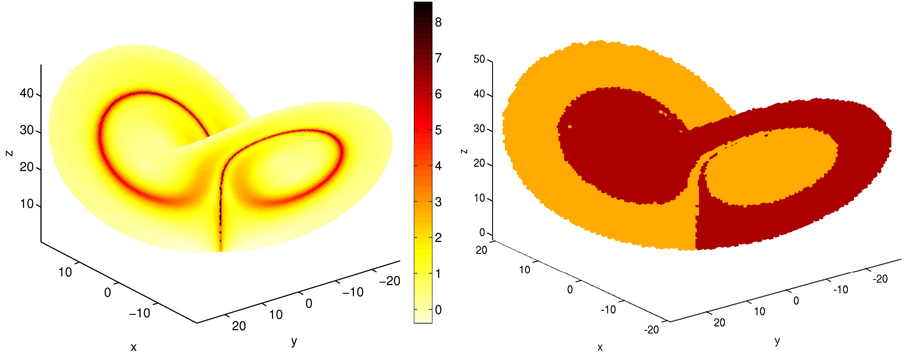
- Compute second left eigenvector of sparse $Q = (L + L^*)/2$ (e.g. by iterative schemes)
- Carry out line search to find optimal sets [Froyland, P. 2009]
- Diffusion comes for free from numerical scheme but explicit incorporation is possible
- Set-oriented numerical approach implemented in software package GAIO [Dellnitz & Junge 2001]

Example: Lorenz system



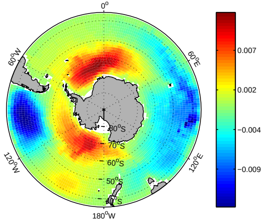
Second eigenvector of Q and almost-invariant sets in the Lorenz system for flow time $\tau = 0.4$ [Froyland, P. 2009]

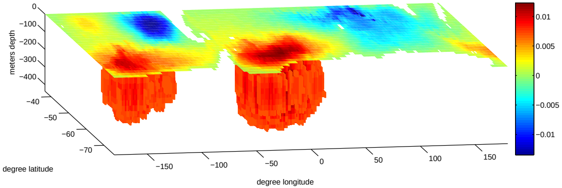
FTLE and AIS



Ridges in FTLE field bound almost-invariant sets. [Froyland, P. 2009]

Ocean structures





Major gyres in Southern Ocean extracted as almost-invariant sets ($\tau = 2$ months)

[Froyland, P., England, Treguier 2007; Dellnitz, Froyland, Horenkamp, P., Sen Gupta 2009]

Let's move: coherent sets

- **Goal:** find optimal slow mixing time-dependent structures
- Flow map $T : X \to Y$ of a nonautonomous system $\dot{x} = f(x, t)$ on $[t, t + \tau]$, $X, Y \subset M$ compact
- Probability measure μ at t (not invariant)
- **Finite-time coherent pairs:** $A_t, A_{t+\tau}$ satisfying $T(A_t) \approx A_{t+\tau}$, i.e. maximizing

$$\rho(A_t, A_{t+\tau}) = \frac{\mu(A_t \cap T^{-1}(A_{t+\tau}))}{\mu(A_t)} + \frac{\mu(A_t^c \cap T^{-1}(A_{t+\tau}^c))}{\mu(A_t^c)}$$

(plus robustness w.r.t. perturbations and mass constraints)

- Results for matrix-based setting [Froyland, Santitissadeekorn, Monahan 2010]
- Our optimization framework with compact self-adjoint operator

$$\mathbf{Q} = \mathbf{L}^* \mathbf{L}$$

applies [Froyland 2013, Froyland, P. 2014]

Numerics

- Consider $T : X \to Y$ (i.e. $Y := T(X)$)
- $\{B_1, \dots, B_m\}$ partition of X, $\{C_1, \dots, C_n\}$ partition of Y.
- **P** represented by

$$P_{ij} = \frac{m(B_i \cap T^{-1}(C_j))}{m(B_i)} \approx \frac{\#\{k : T(x_{i,k}) \in C_j\}}{K},$$

  with test points $x_{i,k}$, $k = 1, \dots, K$ uniformly distributed in B_i.
- Given a probability measure μ (not invariant!), set $p_i = \mu(B_i)$ and $q = pP$.
- Approximation to **L**, $\mathbf{L}^*$:

$$L_{ij} = \frac{p_i P_{ij}}{q_j}, \quad L^*_{ij} = P_{ji}$$

- Compute second left and right singular vectors of L and do line search to find optimal sets [Froyland et al 2010]

Transitory double gyre [Mosovsky & Meiss 2011]

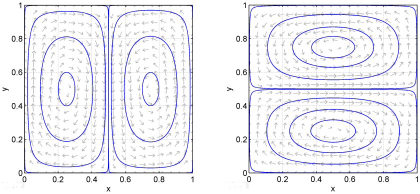
$$\dot{x} = -\frac{\partial}{\partial y}\Psi, \quad \dot{y} = \frac{\partial}{\partial x}\Psi$$

with stream function $\Psi(x, y, t) = (1 - s(t))\Psi_P + s(t)\Psi_F$ where

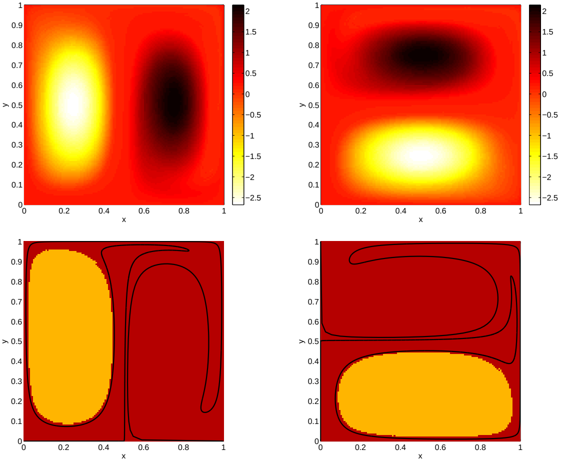
$$\Psi_P(x, y) = \sin(2\pi x)\sin(\pi y),\ \Psi_F(x, y) = \sin(\pi x)\sin(2\pi y)$$

and transition function

$$s(t) = \begin{cases} 0, & t < 0, \\ t^2(3 - 2t), & 0 \le t \le 1, \\ 1, & t > 1. \end{cases}$$

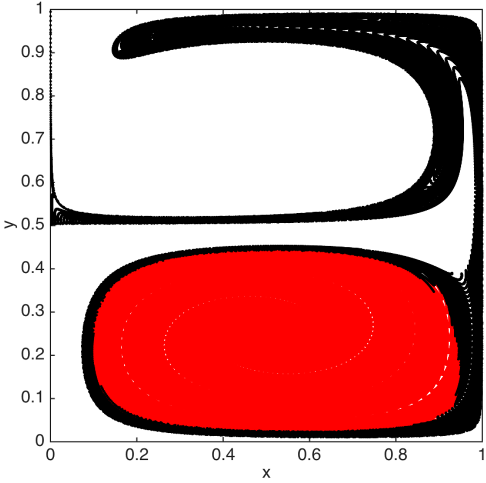


Coherent sets



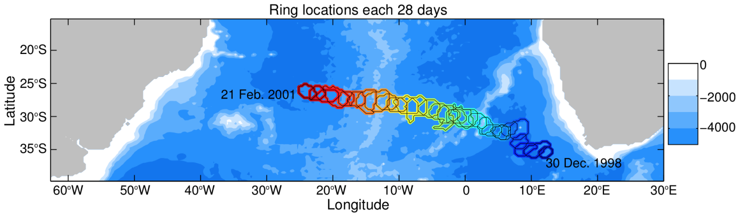
Left and right singular vectors in the transitory double gyre flow w.r.t. time span $[0, 1]$ and extracted finite-time coherent sets at $t = 0$ and $t + \tau = 1$.

Evolution of coherent sets

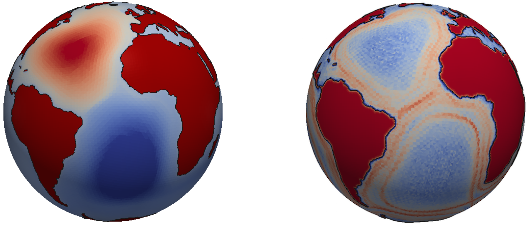


Particles evolved by the flow - red particles remain in coherent set.

Back to the ocean



Tracking of an Agulhas ring over two years. [Froyland, Horenkamp, Rossi, Sen Gupta 2015]



Coherent sets and transport barriers in the global ocean [P., Reuther, Praetorius, Voigt 2015].

Probabilistic framework for transport barriers using **finite-time entropy** in [Froyland, P. 2012]

Clustering framework

- Transfer operator-based framework is very powerful but involves considerable computational effort

- **Wish-list for new method:**

- Computationally more efficient
- Work with relatively small number of trajectories
- Respect entire trajectory not just end-points
- Deal with sparse and incomplete trajectory information
- Provide "quick and dirty" coherent sets diagnostics

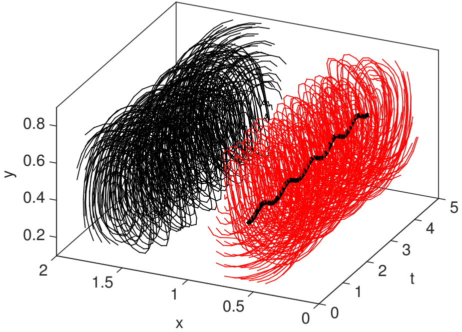
- **Our simple solution:** use geometric clustering algorithms on trajectory data [Froyland, P. 2015]

Trajectory-based coherent sets

- n trajectories given at discrete time instants:

$$x_{i,t} \in \mathbb{R}^d, i = 1, \ldots, n, t = 0, \ldots, T$$

- Extract bundles of trajectories that make up coherent sets, i.e. that minimally spread out over time



Something like that!

General clustering framework

- **Discrete dynamic metric:**

$$\mathbf{D}(x_{i,0}, x_{j,0}) = \sum_{t=0}^{T} \rho(x_{i,t}, x_{j,t})^2$$

  for $x_{i,0}$, $x_{j,0} \in \mathbb{R}^d$, $1 \leq i, j \leq n$, based on some metric ρ on $\mathbb{R}^d$ (Euclidean metric in the following)
- Gives $n(n-1)/2$ interpoint distances $\mathbf{D}(x_{i,0}, x_{j,0})$.

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- **Cluster** the initial points $x_{i,0} \in \mathbb{R}^d$ according $\mathbf{D}$

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- $x_{i,0}$ and $x_{j,0}$ are close if they stay close under time-evolution
- **Cluster** the initial points $x_{i,0} \in \mathbb{R}^d$ according $\mathbf{D}$
- Any clustering method on $\mathbb{R}^d$ could be employed at this point, e.g. k-means, fuzzy c-means, or density-based clustering approaches.

Possible simple clustering strategy

- Interpret $\{x_{i,t}\}_{0 \le t \le T}$ as a point

$$X_i = (x_{i,0}, x_{i,1}, \dots, x_{i,T}) \in \mathbb{R}^{d(T+1)}$$

- Apply **fuzzy** c**-means** [Bezdek 1981–] on the n data points in $\mathbb{R}^{d(T+1)}$
- For fixed number of clusters $K \in \mathbb{N}$ fuzzy c-means computes

- a centre $C_k \in \mathbb{R}^{d(T+1)}$ for each cluster $k = 1, \dots, K$ and
- a likelihood of membership $u_{k,i}$ of each X_i, $i = 1, \dots, n$ to each C_k.

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- **Objective:** minimise

$$\sum_{k=1}^{K}\sum_{i=1}^{n} u_{k,i}^m \|X_i - C_k\|^2 = \sum_{k=1}^{K}\sum_{i=1}^{n} u_{k,i}^m \sum_{t=0}^{T} \|x_{i,t} - c_{k,t}\|^2 \quad \text{(obj)}$$

subject to $\sum_{k=1}^{K} u_{k,i} = 1$ and $\sum_{i=1}^{n} u_{k,i} > 0$

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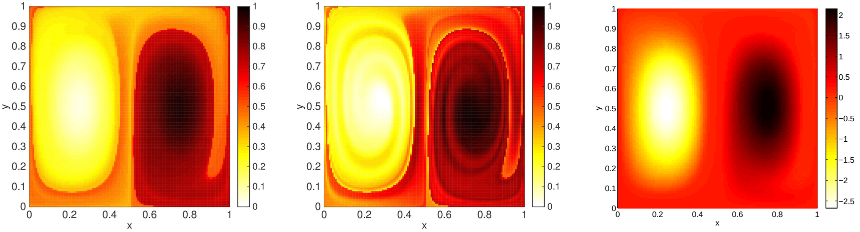
subject to $\sum_{k=1}^{K} u_{k,i} = 1$ and $\sum_{i=1}^{n} u_{k,i} > 0$

- Fuzziness exponent $m > 1$ (increasing m means softer clusters)
- **Iterative scheme**, implemented e.g. as `fcm` in MATLAB.

Coherent sets in transitory double gyre



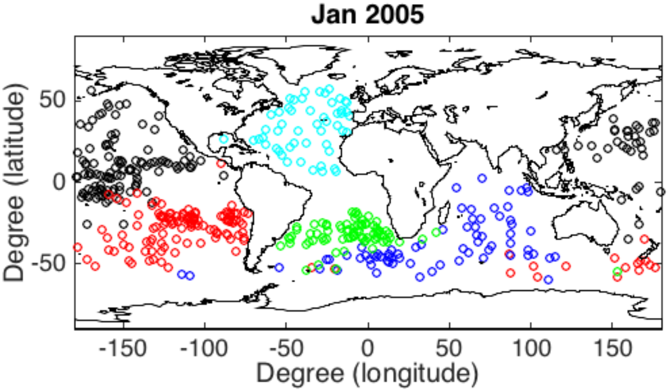
(a) (b) (c)

Approximation of coherent sets for transitory double gyre flow at $t_0 = 0$, computed on $[0, 1]$. 2^{14} initial conditions, trajectory output in 0.1 time instants. (a) Membership functions for 2-clustering using entire trajectories and for (b) 2-clustering using trajectory endpoints. (c) Second singular vector of transition matrix.

Properties and extensions

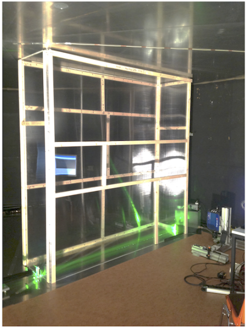
- Clustering into spheres is preferred by Euclidean norm but other distance functions could be used.
- Interpretations for continuous time and continuous space available.
- Isotropic scaling of space and time has no effect.
- **Clustering results are frame-independent.**
- Weights can be included as coefficients for $\|x_{i,t} - c_{k,t}\|^2$, which could depend on i, t, or k (e.g. discount distances far in the future).
- **Missing data can be easily handled** (restrict computations of C_k to available data per time-slice).
- Treatment of almost-invariant sets also possible.
- Normalized entropy can serve as a measure for classification uncertainty.

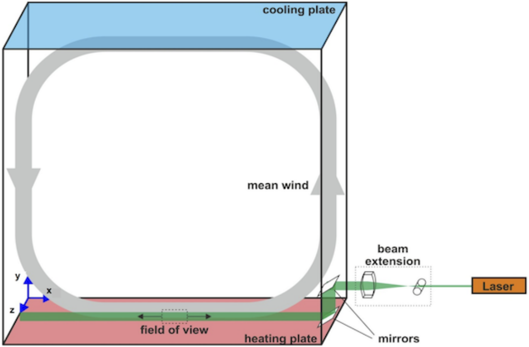
Application I: global ocean drifters



2267 drifters in 2005–2009 with minimum lifetime of one year and monthly output of positions.
Approximation of $K = 5$ clusters.

Application II: turbulent convection

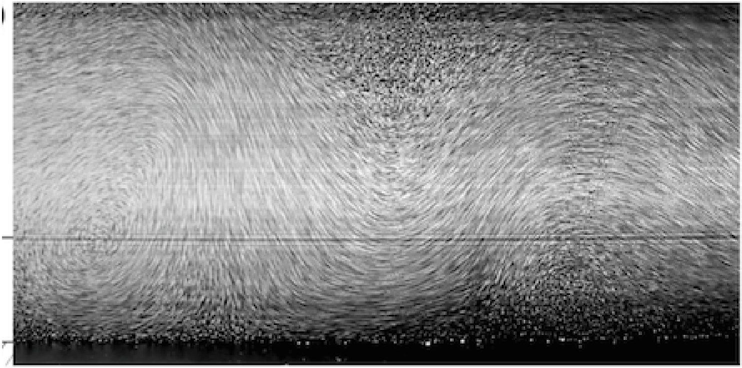




Experimental set-up in Barrel of Ilmenau, Germany.

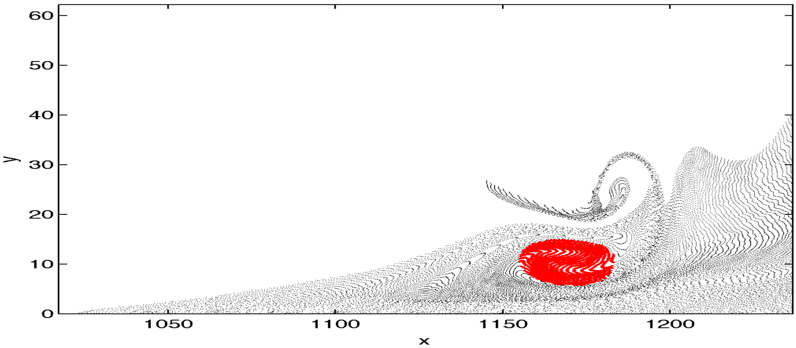
Cell dimensions: 2.5 m (H) x 2.5 m (W) x 0.65 m (D); temperature difference: 10K $T_{bot} = 35^\circ$C $T_{top} = 25^\circ$C; Rayleigh number $Ra \approx 1.5e10$

Coherent structures



Coherent plumes visible in experimental data (du Puits et al, PRL 2014)

Trajectory-based coherent sets



Coherent set in convection flow (extracted from PIV velocity data) – using only the trajectories shown.

Joint work with Ronald du Puits, Ilmenau

Conclusion and future research

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Thank you!

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