Validated Computation of Transport Barriers in Unsteady Flows

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Acknowledgments

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Outline

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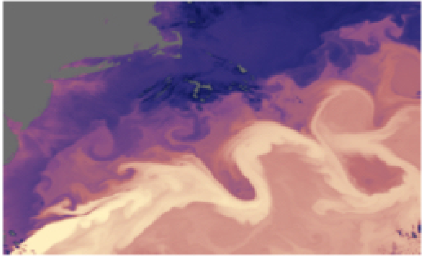
Jupiter's "big red spot"

Sea surface temperature in the gulf stream



- Trajectories in an unsteady flow often form visibly coherent sets which organize the dynamics.
- The boundaries of these sets are transport barriers which separate phase space into regions which have distinct dynamics.

Transport Barriers in Unsteady Flow

What makes detection of transport barriers hard in unsteady flows?

Transport Barriers:

- are not invariant in phase space.
- are not (un)stable manifolds of invariant sets.
- persist for finite time.
- “leak” (i.e. they allow negligible but nonzero flux).
- are not streamlines of the fixed-time vector field.

Setting and Notation

- Let $f : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ be a non-autonomous planar vector field.
- The flow generated by f, denoted by Φ_{t_0}, satisfies the initial value problem

$$\frac{d}{dt}\Phi_{t_0}(u,t) = f(u,t) \qquad u(t_0) = u_0.$$

- The spatial derivative for Φ satisfies the variational equation

$$\frac{d}{dt}D\Phi_{t_0}(u,t) = Df(u,t)D\Phi_{t_0}(u,t) \qquad D\Phi_{t_0}(u,t_0) = I.$$

- We will assume throughout that f is analytic in space and time.

Finite Time Strain and Lyapunov Exponents

- Fix $t_0, T \in \mathbb{R}$ and let $\Phi \colon \mathbb{R}^2 \to \mathbb{R}^2$ be the flow map defined by $\Phi(x, y) = \Phi_{t_0}(x, y, T)$.
- The Cauchy-Green strain tensor (CGST) is defined by

$$\Delta(x, y) = D\Phi(x, y)^* D\Phi(x, y).$$

  with real eigenvalues, $0 < \lambda_1 \leq \lambda_2$ and eigenvectors, ξ_1, ξ_2.
- The finite-time Lyapunov exponent (FTLE) is defined to be the scalar field on $\mathbb{R}^2$ given by

$$\sigma(x, y) = \frac{1}{2T} \log(||\Delta(x, y)||) = \frac{1}{2T} \log(\lambda_2(x, y)).$$

Characterizations of Transport Barriers

- Distinguished codimension-1 surfaces which organize trajectory patterns and separate regions with distinct dynamics.
- Time-varying generalizations of (un)stable manifolds.
- Maximally attracting/repelling material surfaces.

Hyperbolic Lagrangian Coherent Structures

1. (Lekien, Marsden, Ross, Shadden,...) Ridges of the finite-time Lyapunov exponent (FTLE) field.
2. (Farazmand, Haller,...) Special trajectories for the flows generated by
$$\dot{u} = \xi_1(u) \quad \text{or} \quad \dot{v} = \xi_2(v).$$
3. (Balasuriya,...) Finite time generalizations of (un)stable manifolds (Melnikov theory).

Example: Rayleigh-Benard Convection

- Hamiltonian:

$$\psi(x,y,t) = \sin(\pi(x - g(t)))\sin(\pi y)$$

  where g is a given analytic function.

- Non-autonomous vector field:

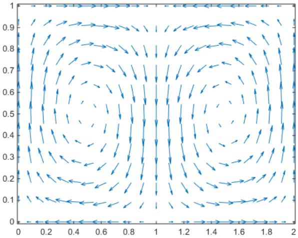
$$f(x,y,t) = \begin{pmatrix} -\psi_y \\ \psi_x \end{pmatrix} = \begin{pmatrix} -\pi\sin(\pi(x-g(t)))\cos(\pi y) \\ \pi\cos(\pi(x-g(t)))\sin(\pi y) \end{pmatrix}$$

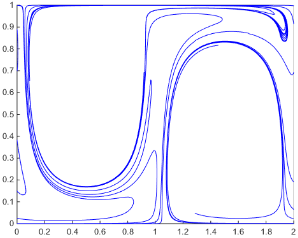
  on $[0,2]\times[0,1]$.

- Consider an analytic arc segment in $\mathbb{R}^2$ denoted by $\gamma(s)$ with $s \in [-1,1]$.

Non-Rigorous Computations

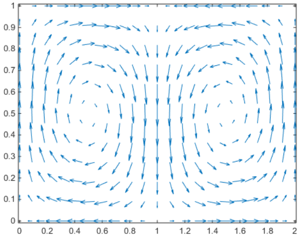
autonomous vector field

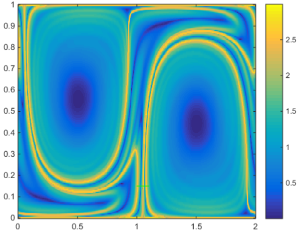




strainline LCSs (via LCStool)

forcing: $g(t) = .25\sin(3t)$





forward FTLE field

Outline

Sequence Spaces and Analytic Functions

- Fix $\nu \in \mathbb{R}^d, \tau \in \mathbb{R}$ and define the polydisc

$$\mathbb{D}_{\nu,\tau} = \{(z,t) \in \mathbb{C}^d \times \mathbb{R} \colon |t| < \tau, \ |z_j| < \nu_j \text{ for } 1 \leq j \leq d\}.$$

- Let $C^\omega(\mathbb{D}_{\nu,\tau})$ denote the set of complex valued analytic functions defined on $\mathbb{D}_{\nu,\tau}$.
- Let $\mathcal{S}_{d+1}$ denote the set of $(d+1)$-dimensional infinite multi-sequences of complex numbers equipped with the norm

$$||a||^1_{\nu,\tau} = \sum_{m=0}^{\infty} \sum_{|\alpha|=0}^{\infty} |a_{m,\alpha}| \nu^{|\alpha|} \tau^m.$$

- We will work in the Banach algebras defined by:

$$\ell^1_{\nu,\tau} = \{a \in \mathcal{S}_{d+1} \colon \ ||a||^1_{\nu,\tau} < \infty\}$$
$$\mathcal{X} = \prod \ell^1_{\nu,\tau}$$

The Taylor Transform

- If $g \in C^\omega(\mathbb{D}_{\nu,\tau})$, then its Taylor series

$$g(s,t) = \sum_{m=0}^{\infty} \sum_{|\alpha|=0}^{\infty} a_{m,\alpha} s^{|\alpha|} t^m$$

converges absolutely and uniformly on $\mathbb{D}_{\nu,\tau}$.

Definition

Let $\mathcal{T}$ denote the Taylor Transform of $g \in C^\omega(\mathbb{D}_{\nu,\tau})$ given by

$$g \stackrel{\mathcal{T}}{\longmapsto} \{a_{m,\alpha}\} = a.$$

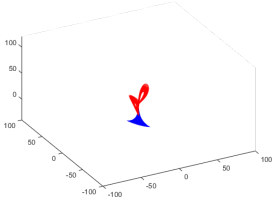
- $g \in C^\omega(\mathbb{D}_{\nu,\tau}) \implies \mathcal{T}(g) \in \ell^1_{\nu^*,\tau^*}$.
- $a \in \ell^1_{\nu,\tau} \implies \mathcal{T}^{-1}(a) \in C^\omega(\mathbb{D}_{\nu,\tau})$.

Validated Computation of Hyperbolic LCSs

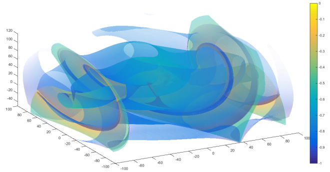
1. Given γ is an analytic surface. Characterize the following:
$$\Phi(\gamma(s),t), \quad D\Phi(\gamma(s),t), \quad \Delta(\gamma(s)), \quad \lambda_{1,2}(\gamma(s)), \quad \xi_{1,2}(\gamma(s))$$
in the product space
$$\mathcal{X} = \prod_{i=1}^{d=2+4+3+2+4+*} \ell^1_{\nu,\tau}$$
2. Define a map, $F \in C^1(\mathcal{X})$, which satisfies:
$$\gamma \text{ is an LCS} \iff F(\mathcal{T}(\gamma)) = 0.$$
3. Compute finite dimensional numerical approximations:
$$\bar{a} \approx a = \mathcal{T}(\gamma) \qquad A \approx DF(\bar{a})^{-1}$$
4. Prove (with computer assistance) the existence of a unique fixed point for $T(x) = x - AF(x)$, on some ball $B_r(\bar{a}) \subset \mathcal{X}$.
5. Evolve γ by the flow via rigorous integration.

Integration of Material Surfaces

Validated computation of $\Phi(\gamma(s), t)$ and $D\Phi(\gamma(s), t)$ amounts to rigorously integrating f and the appended variational equation with γ a given surface of initial conditions.



(a) Validated computation of the local stable manifold at the origin in the Lorenz system with $r \approx 10^{-13}$



(b) Analytic continuation of the (slow) stable manifold via rigorous integration with $r \approx 10^{-6}$

Domain Decomposition

- Under advection a typical surface undergoes rapid deformation and requires subdivision.
- Given $a = \mathcal{T}^{-1}\left(\Phi(s, t_*\right)$ with $s \in [-1, 1], t_* \in \mathbb{R}$.
- Its restriction to $[s_1, s_2] \subset [-1, 1]$ is a linear map $a \mapsto \tilde{a}$ given by:

$$\tilde{a}_n = \sum_{i=n}^{\infty} \delta^i a_i(t) \binom{i}{n} s_*^{i-n}$$

where $\delta = \frac{s_2 - s_1}{2}$ and $s_* = \frac{s_2 + s_1}{2}$

- Mapping must be computed rigorously:

$$\underbrace{\text{finite dimensions}}_{\text{interval enclosures}} + \underbrace{\text{infinite tail}}_{\text{Cauchy estimates}}$$

- (Maximum principle) Analytic error estimates improve on $(-1, 1)$.

Automatic Differentiation

- Working in $\ell^1_{\nu,\tau}$ yields straight-forward algorithms for addition, multiplication, and taking derivatives.
- More complicated operations such as $\sin, \cos, \exp, \log$ and solving algebraic equations are done using automatic differentiation.
- Main idea:

$$\text{append variables} + \text{take derivatives} + \text{solve ODE}$$

- Key feature: Analytic error estimates for operations are recovered automatically.

Example: Automatic Differentiation

Solving Algebraic Equations

Let $\nu \in \mathbb{C}$, $a \in \ell^1_{\nu,\tau}$ with $f = \mathcal{T}^{-1}(a)$ and $f(0,0) \neq 0$. Solve the equation $ax = 1_{\ell^1_{\nu,\tau}}$.

1. $g_1(t) = \frac{1}{f(0,t)}$ satisfies the initial value problem

$$\frac{dg_1}{dt} = -\frac{1}{f(0,t)^2} \cdot \frac{\partial f}{\partial t} = -g_1(t)^2 \frac{\partial f}{\partial t} \qquad g_1(0) = \frac{1}{f(0,0)}$$

2. Similarly, $g(s,t) = \frac{1}{f(s,t)}$ satisfies

$$\frac{\partial g}{\partial s_j} = -g(s,t)^2 \frac{\partial f}{\partial s} \qquad g(0,t) = \frac{1}{f(0,t)} = g_1(t)$$

3. Solving this IVP using the rigorous integrator gives the solution in the form $x = \mathcal{T}(g) = \mathcal{T}\left(\frac{1}{f}\right)$.

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Outline

Rayleigh-Benard Revisited

- Automatic differentiation:

$$u(s,t) = e^{i(\pi(x(s,t)-g(t))}$$
$$v(s,t) = e^{i\pi y(s,t)}$$

- Extended vector field:

$$\tilde{f}(x,y,u,v,t) = \begin{pmatrix} -\pi \operatorname{Im}(u) \operatorname{Re}(v) \\ \pi \operatorname{Re}(u) \operatorname{Im}(v) \\ -i\pi u(\pi \operatorname{Im}(u) \operatorname{Re}(v) + g'(t)) \\ i\pi^2 v \operatorname{Re}(u) \operatorname{Im}(v) \end{pmatrix}$$

- Jacobian:

$$Df = \begin{pmatrix} -\pi^2 \operatorname{Re}(u) \operatorname{Re}(v) & \pi^2 \operatorname{Im}(u) \operatorname{Im}(v) \\ -\pi^2 \operatorname{Im}(u) \operatorname{Im}(v) & \pi^2 \operatorname{Re}(u) \operatorname{Re}(v) \end{pmatrix}$$

Computing the CGST

- Solve the variational equation along γ:

$$\mathcal{T}\left(D\Phi(s,t)|_{t=T}\right) = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}$$

- Characterization of $\Delta(s) = D\Phi(s,T)^* D\Phi(s,T)$ in $\mathcal{X}$:

$$\begin{aligned} a_1 &= \mathcal{T}\left(\Delta_{11}\right) = c_{11} * c_{11} + c_{21} * c_{21} \\ a_2 &= \mathcal{T}\left(\Delta_{21}\right) = c_{11} * c_{12} + c_{21} * c_{22} \\ a_3 &= \mathcal{T}\left(\Delta_{22}\right) = c_{12} * c_{12} + c_{22} * c_{22} \end{aligned}$$

- $\mathcal{T}\left(\lambda_i\right)$ and $\mathcal{T}\left(\xi_i\right)$ satisfy algebraic equations:

$$\begin{aligned} x * x - (a_1 + a_3) * x + a_1 * a_3 - a_2 * a_2 &= 0_{\ell^1_{\nu,\tau}} \\ v_1 - 1_{\ell^1_{\nu,\tau}} &= 0_{\ell^1_{\nu,\tau}} \\ a_2 * v_2 + a_1 - \mathcal{T}\left(x_i\right) &= 0_{\ell^1_{\nu,\tau}} \end{aligned}$$

Outline

Finite Time Coherent Sets

- Time-varying generalizations of almost-invariant sets. Sets in phase space which minimize dispersion over a finite time interval.
- Go after coherent sets directly by measuring transport.

Transfer Operator Methods

(Froyland,Junge,Padberg-Gehle,...) Identify subsets of $\mathbb{R}^2$ whose measure is (approximately) invariant for some Φ-invariant measure.

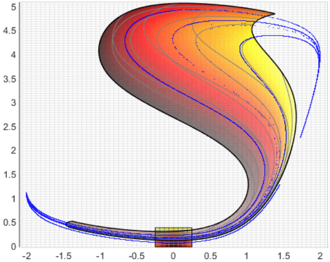
Rigorous Outer Approximation of Hybrid Maps

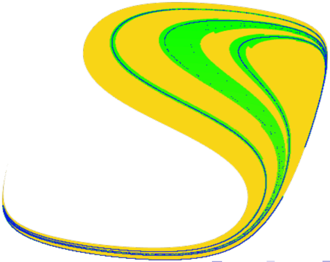
Hybrid map:

$$h(\tau, u) = g\left(u + \int_0^\tau f(\Phi(u,t))\, dt\right)$$

$$f(u) = \begin{pmatrix} u_2 - \frac{2}{3}u_1^3 - 2u_1 \\ -u_1 \end{pmatrix} \qquad g(u) = \begin{pmatrix} u_1 \\ u_2 + 2.7 \end{pmatrix}$$

Outer approximation:





Future Work

- Characterization and computation parameterized by T.
- Validating transport barriers over longer time intervals requires new validation methods.

$$\underbrace{\text{finite dimensions}}_{\text{Newton operator}} + \underbrace{\text{infinite tail}}_{\text{contraction mapping}}$$

- Validated comparison and benchmarking. Which qualities of transport barriers are detected by each diagnostic?

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Thank You!