Chaotic Mixing and Lagrangian Coordinates

Jean-Luc Thiffeault

Department of Applied Physics and Applied Mathematics

Columbia University

http://plasma.ap.columbia.edu/~jeanluc/

27 March 2001

with Allen Boozer

The Advection-diffusion Equation

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla} \phi = \frac{1}{\rho} \boldsymbol{\nabla} \cdot (\rho \, \mathbf{D} \, \boldsymbol{\nabla} \phi)$$

- $\mathbf{v}(\mathbf{x}, t)$ — Eulerian velocity field
- $\phi(\mathbf{x}, t)$ — concentration of passive scalar
- $\mathbf{D}(\mathbf{x}, t)$ — diffusivity tensor $(D/vL \ll 1)$
- $\rho(\mathbf{x}, t)$ — density

ϕ could be temperature, or the concentration of a reacting chemical, or . . .

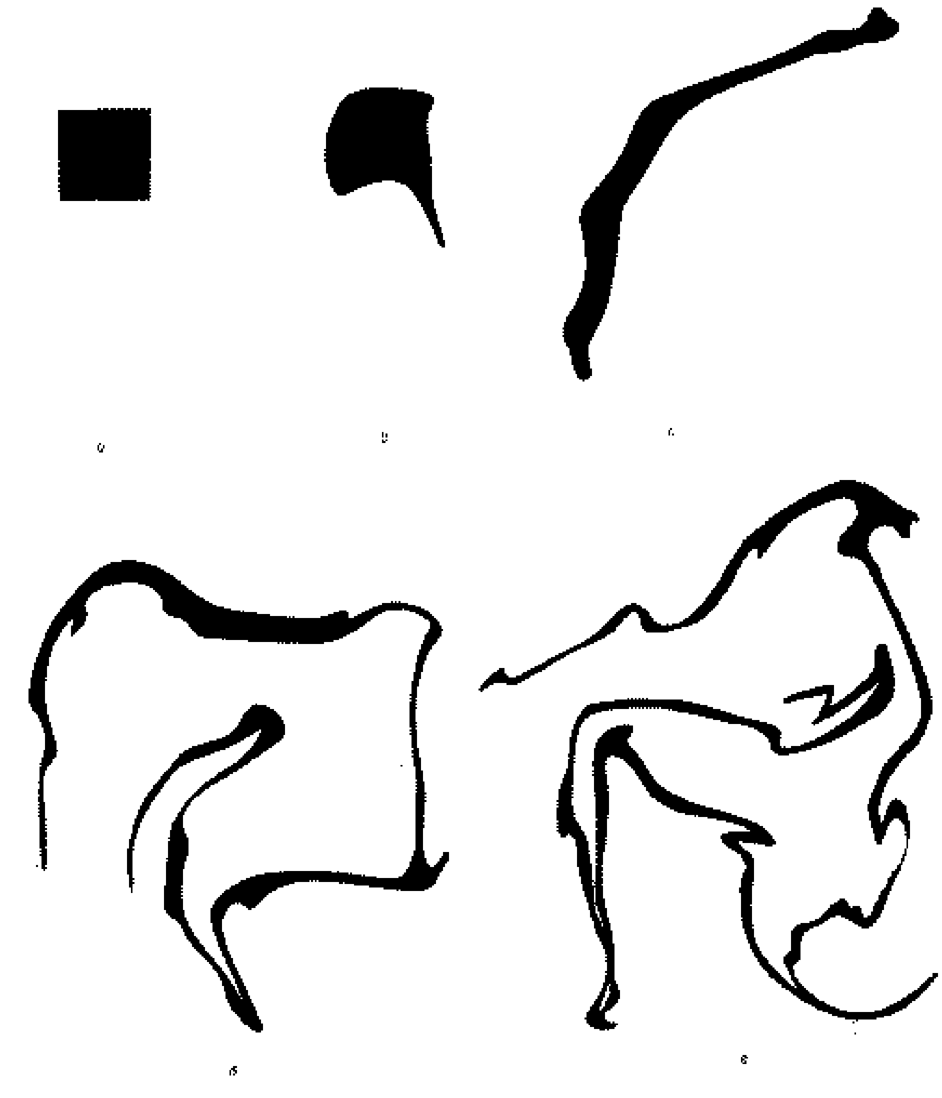
Small diffusivity is the norm rather than the exception.

Typical values of D/vL:

Core of earth	10^{-3}
Temperature in a room	10^{-10}
Solar corona	10^{-12}
Galaxy	10^{-19}

Even a tiny amount of diffusivity matters.

Chaotic Stirring



Chaotic Mixing

- Strain in the velocity field generates small scales, even for nonturbulent flows
- Huge gradients of ϕ are created
- Makes enhanced diffusion possible:
  For heat in a room, turns a diffusion time of months into minutes (exponential)
- Very difficult to simulate directly : scale separation $\sim 10^{10}$
- Lagrangian (comoving) coordinates are very convenient because the chaos gets "hidden" in the coordinate transformation.
- Differential geometry provides a novel perspective.

Overview

- In a fluid flow, Lagrangian coordinates label fluid elements. The Lagrangian frame moves and stretches with the flow.

- When the flow is chaotic, Lagrangian quantities that characterize the geometry and dynamics of the system have a well-defined asymptotic behavior: Lyapunov exponents, characteristic directions . . .

- Useful even for "short" times: finite-time Lyapunov exponents. Characteristic directions converge very quickly.

- The study of these Lagrangian quantities leads to some surprising results: they obey constraints due to the chaotic nature of the flow. The constraints tell us something about the physics.

Lagrangian Coordinates

Trajectory of a fluid element in Eulerian coordinates $\mathbf{x}$

$$\frac{d\mathbf{x}}{dt}(\mathbf{a}, t) = \mathbf{v}(\mathbf{x}(\mathbf{a}, t), t)$$

$\mathbf{a}$ are Lagrangian coordinates that label fluid elements.

$\mathbf{x}(\mathbf{a}, t = 0) = \mathbf{a}$: fluid elements are labeled by their initial position.

$\mathbf{x} = \mathbf{x}(\mathbf{a}, t)$ is thus the (smooth) transformation from Lagrangian ($\mathbf{a}$) to Eulerian ($\mathbf{x}$) coordinates.

For a chaotic flow, this transformation gets horrendously complicated as time evolves.

The Metric Tensor

The Jacobian matrix of the transformation $\mathbf{x}(\mathbf{a}, t)$ is

$$M^i{}_q \equiv \frac{\partial x^i}{\partial a^q}$$

Restrict ourselves to incompressible flows, $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$, so that $\det M = 1$.

Jacobian matrix is a precise record of how a fluid element is rotated and stretched by $\mathbf{v}$.

Interested in the stretching, not the rotation, so we construct the metric tensor

$$\boxed{g_{pq} \equiv \sum_{i=1}^{n} M^i{}_p \, M^i{}_q}$$

which contains only the information on the stretching of fluid elements.

Stretching and Contracting Directions

Metric is a symmetric, positive-definite matrix $\Longrightarrow$ can be locally diagonalized with orthogonal eigenvectors $\{\hat{\mathbf{e}}_\sigma\}$ and corresponding real, positive eigenvalues $\{\Lambda_\sigma^2\}$,

$$g_{pq} = \sum_{\sigma=1}^{n} \Lambda_\sigma^2 \, (\hat{\mathbf{e}}_\sigma)_p \, (\hat{\mathbf{e}}_\sigma)_q$$

The Λ_σ are called coefficients of expansion and are ordered such that $\Lambda_1 > \Lambda_2 > \ldots > \Lambda_n$ [assumed nondegenerate].

The Λ_σ are related to the finite-time Lyapunov exponents λ_σ by

$$\lambda_\sigma = \log \Lambda_\sigma / t$$

The incompressibility of $\mathbf{v}$ implies that $\Lambda_1 \, \Lambda_2 \cdots \Lambda_n = 1$.

The label u indicates the most unstable direction:

$$\hat{\mathbf{e}}_1 \equiv \hat{\mathbf{u}} \ , \qquad \Lambda_1 \equiv \Lambda_u$$

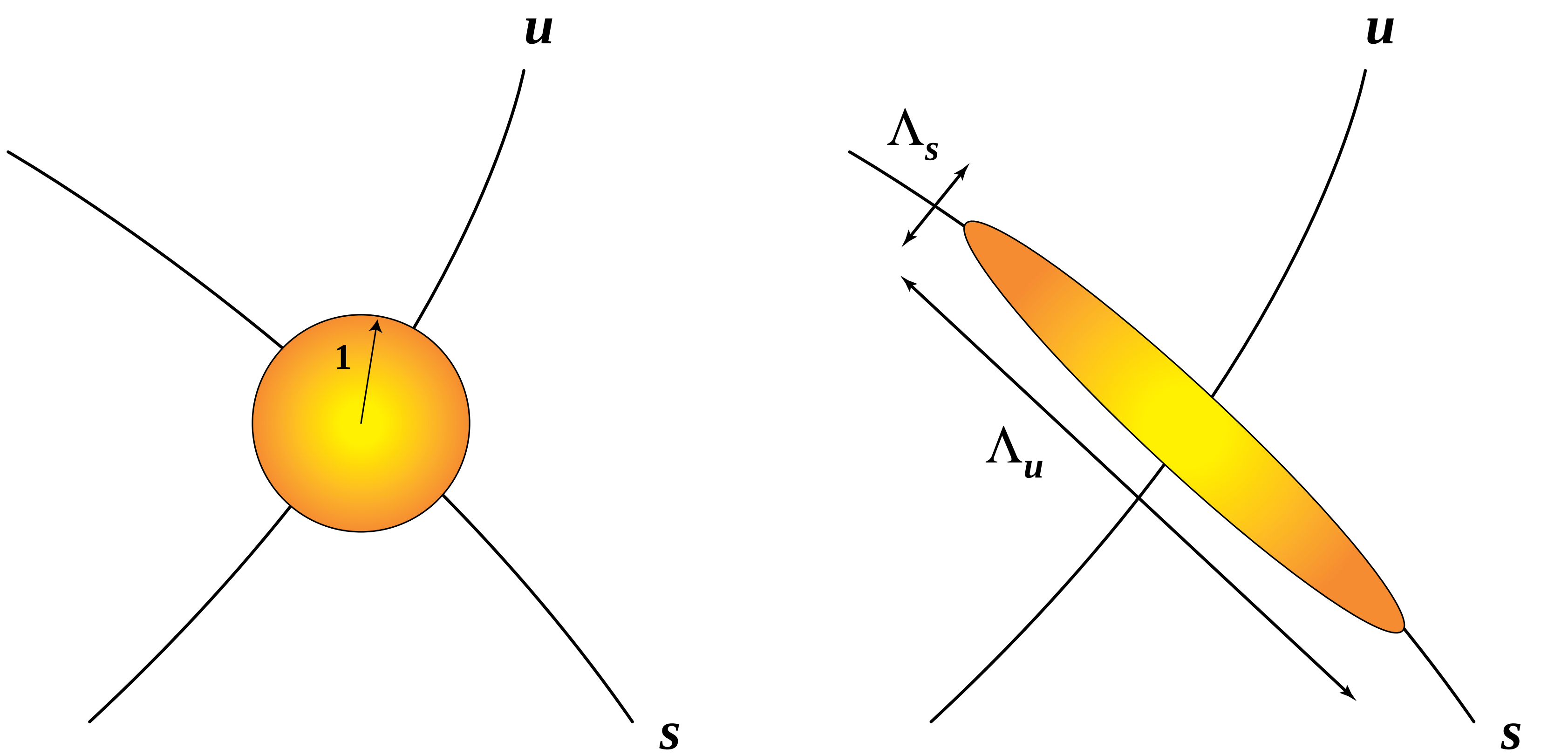
After some time, $\Lambda_u \gg 1$, growing exponentially for long times.

The label s indicates the most stable direction:

$$\hat{\mathbf{e}}_n \equiv \hat{\mathbf{s}} \ , \qquad \Lambda_n \equiv \Lambda_s$$

After some time, $\Lambda_s \ll 1$, decreasing exponentially for long times.

The eigenvalues and eigenvectors describe the deformation of a fluid element in a comoving frame:

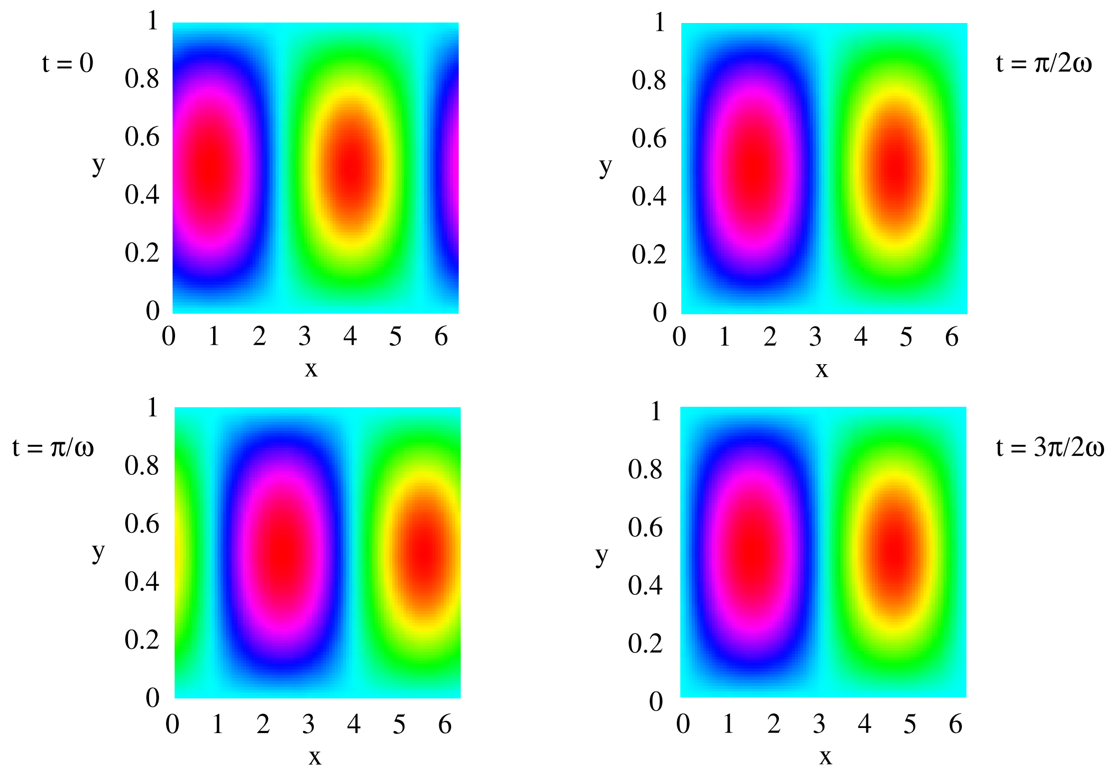


The $\hat{\mathbf{u}}$ and $\hat{\mathbf{s}}$ directions can be integrated to yield the unstable and stable manifolds.

Example: 2D Convection Rolls

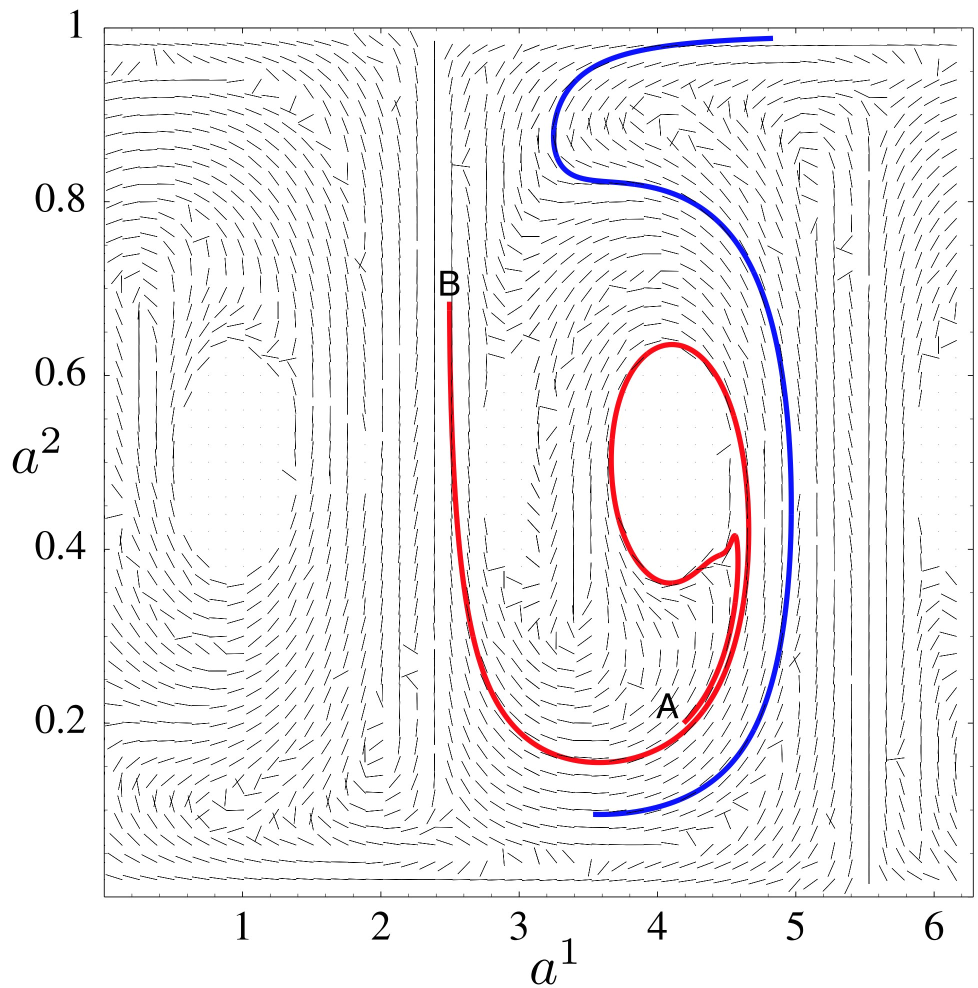
Oscillating convection rolls: $\mathbf{v} = (-\partial_y \psi, \partial_x \psi)$, with

$$\psi(\mathbf{x}, t) = Ak^{-1}(\sin kx \sin \pi y + \epsilon \cos \omega t \cos kx \cos \pi y)$$



[Movie: lyap_crolls_jet.mpeg]

- The magnitude of the Lyapunov exponents is the time-averaged straining rate encountered by a fluid element.
- More red at the beginning because some fluid elements are drawn to the hyperbolic points, where the strain is maximal.
- However, those fluid elements don't stay there long, and there is an equilibration toward blue (lowest stretching).
- Central region with low mixing, corresponding to the center of the rolls. Blue filaments extend outside the rolls.
- Study breakup of oil droplets [Solomon].



$\hat{\mathbf{s}}$ field for oscillating rolls. Two typical portions of stable manifolds in red and blue. Motion in central region is nonchaotic.

ABC Flow

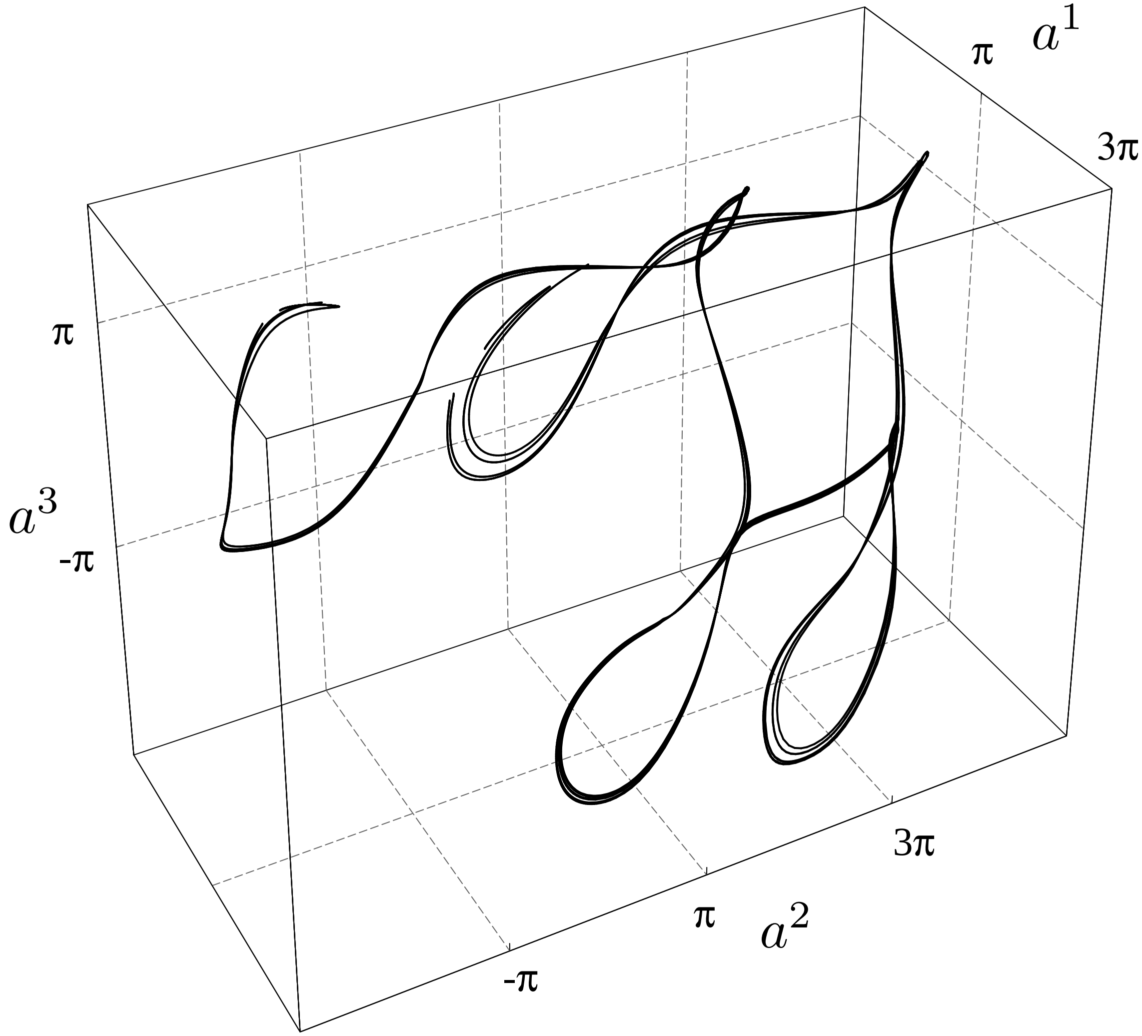
Another well-known model system is the ABC flow,

$$\mathbf{v}(\mathbf{x}) = A\,(0, \sin x_1, \cos x_1) + B\,(\cos x_2, 0, \sin x_2) + C\,(\sin x_3, \cos x_3, 0)$$

a sum of three Beltrami waves, which satisfy $\boldsymbol{\nabla} \times \mathbf{v} \propto \mathbf{v}$. It is time-independent and incompressible ($|g| = 1$).

We shall be using the parameter values $A = 5, B = C = 2$ in subsequent examples.

Here's a portion of a stable manifold $\mathbf{s}(\mathbf{a})$ for the ABC 522 flow:



Singular Value Decomposition

Cannot study the Jacobian matrix $M = \partial\mathbf{x}/\partial\mathbf{a}$ directly because it mixes vastly different scales associated with the stretching and contracting directions.

Decompose M as

$$M^i{}_q = \frac{\partial x^i}{\partial a^q} = \sum_\sigma \Lambda_\sigma \, (\hat{\mathbf{w}}_\sigma)^i \, (\hat{\mathbf{e}}_\sigma)_q$$

where $\hat{\mathbf{w}}_\sigma$ and $\hat{\mathbf{e}}_\sigma$ are orthonormal basis vectors.

Equivalent the singular value decomposition (SVD), with the Λ_σ being the singular values.

The orthonormal vectors $\{\hat{\mathbf{e}}_\sigma\}$ give the axes of stretching (strain) in Lagrangian space, and the $\{\hat{\mathbf{w}}_\sigma\}$ give the absolute orientation of a fluid element in Eulerian space.

The metric tensor in Lagrangian coordinates g_{pq} can be written

$$g_{pq} = \sum_i {M^i}_p \, {M^i}_q = \sum_{i,\sigma,\tau} (\hat{\mathbf{e}}_\sigma)_p \, \Lambda_\sigma \, (\hat{\mathbf{w}}_\sigma)^i (\hat{\mathbf{w}}_\tau)^i \, \Lambda_\tau \, \hat{\mathbf{e}}_\tau)_q$$

$$= \sum_\sigma \Lambda_\sigma^2 \, (\hat{\mathbf{e}}_\sigma)_p \, (\hat{\mathbf{e}}_\sigma)_q \ ,$$

where we used the orthonormality of $\hat{\mathbf{w}}_\sigma$.

This shows that Λ_σ and $\hat{\mathbf{e}}_\sigma$ are indeed the eigenvalues and eigenvectors of g_{pq}.

The SVD separates clearly the parts of M that are growing or shrinking exponentially in size (as determined by the coefficients of expansion Λ_σ).

Avoids the problems associated with evolving $M = \partial \mathbf{x} / \partial \mathbf{a}$ directly.

Greene and Kim (1987) derived the equations of motion for $\hat{\mathbf{w}}_\sigma$, $\hat{\mathbf{e}}_\sigma$, and Λ_σ:

$$\frac{d}{dt}\,\Lambda_\sigma = G_{\sigma\sigma}\,\Lambda_\sigma,$$

$$\hat{\mathbf{w}}_\tau \cdot \frac{d}{dt}\,\hat{\mathbf{w}}_\sigma = -\frac{G_{\tau\sigma}\Lambda_\sigma^2 + G_{\sigma\tau}\Lambda_\tau^2}{\Lambda_\tau^2 - \Lambda_\sigma^2} \qquad \tau \neq \sigma;$$

$$\hat{\mathbf{e}}_\tau \cdot \frac{d}{dt}\,\hat{\mathbf{e}}_\sigma = -\frac{\Lambda_\tau\,\Lambda_\sigma}{\Lambda_\tau^2 - \Lambda_\sigma^2}\,A_{\tau\sigma} \qquad \tau \neq \sigma;$$

where

$$G_{\tau\sigma} \equiv \sum_{i,j} (\hat{\mathbf{w}}_\tau)^i\,\frac{\partial v^i}{\partial x^j}\,(\hat{\mathbf{w}}_\sigma)^j \qquad A \equiv G + G^T.$$

Can be used to show that, in chaotic flows, the characteristic directions $\hat{\mathbf{e}}_\sigma$ converge exponentially fast to constant values.

Lagrangian Derivative of the SVD

We can take the Lagrangian derivatives of the evolution equations for the components of the SVD. We obtain the asymptotic forms

$$\begin{aligned}
\Phi_{\kappa\mu\nu} &= [(\hat{\mathbf{e}}_\kappa \cdot \boldsymbol{\nabla}_0)\hat{\mathbf{w}}_\nu] \cdot \hat{\mathbf{w}}_\mu = -\Phi_{\kappa\nu\mu} && \sim \max(\Lambda_\kappa\,,\ \Lambda_\nu/\Lambda_\mu) \\
\Psi_{\kappa\nu} &= (\hat{\mathbf{e}}_\kappa \cdot \boldsymbol{\nabla}_0)\log\Lambda_\nu && \sim \max(\Lambda_\kappa\,, 1) \\
\Theta_{\kappa\mu\nu} &= [(\hat{\mathbf{e}}_\kappa \cdot \boldsymbol{\nabla}_0)\hat{\mathbf{e}}_\nu] \cdot \hat{\mathbf{e}}_\mu = -\Theta_{\kappa\nu\mu} && \sim \max((\Lambda_\nu\,\Lambda_\kappa)/\Lambda_\mu\,, 1)
\end{aligned}$$

where $\boldsymbol{\nabla}_0 \equiv \partial/\partial\mathbf{a}$ and $\mu < \nu$.

Φ and Ψ diverge along unstable directions at a rate Λ_κ [sensitive to initial conditions], and converge along stable directions.

Θ has a more complicated behavior, but always diverges more slowly than Φ and Ψ. [Thiffeault, submitted to *Nonlinearity*.]

The Hessian

The Hessian is the quadratic form of second derivatives of $\mathbf{x}(\mathbf{a}, t)$.

Since $M = \partial\mathbf{x}/\partial\mathbf{a}$, we can write

$$\frac{\partial^2 x^i}{\partial a^p \partial a^q} = \frac{\partial M^i{}_p}{\partial a^q} = \frac{\partial M^i{}_q}{\partial a^p}\,.$$

The Hessian describes deformations of the fluid elements beyond ellipsoidal.

We define a "projected" version of the Hessian,

$$K^\kappa_{\mu\nu} \equiv \sum_{i,p,q} (\hat{\mathbf{w}}_\kappa)^i \, \frac{\partial^2 x^i}{\partial a^p \partial a^q} (\hat{\mathbf{e}}_\mu)_p \, (\hat{\mathbf{e}}_\nu)_q$$

with $K^\kappa_{\mu\nu} = K^\kappa_{\nu\mu}$.

By differentiating the SVD directly, we have

$$K^{\kappa}_{\mu\nu} = \Lambda_\kappa \, \Psi_{\mu\kappa} \, \delta_{\nu\kappa} + \Lambda_\kappa \, \Theta_{\mu\nu\kappa} + \Lambda_\nu \, \Phi_{\mu\kappa\nu} \, .$$

Using the symmetry of the Hessian, we find

$$\begin{aligned} \Lambda_\mu \, (\Theta_{\mu\mu\nu} + \Psi_{\nu\mu}) &= \Lambda_\nu \, \Phi_{\mu\mu\nu}, && \mu \neq \nu, \\ \Lambda_\kappa \, (\Theta_{\mu\nu\kappa} - \Theta_{\nu\mu\kappa}) &= \Lambda_\nu \, \Phi_{\mu\nu\kappa} - \Lambda_\mu \, \Phi_{\nu\mu\kappa}, && \mu, \nu, \kappa \text{ differ.} \end{aligned}$$

These relations allow us to solve for the Φ in terms of the Θ and Ψ. However, in a chaotic system this inversion is highly singular, and so is not very useful.

Constraints

The relations can be used in other ways. Since we are not interested in the Φ's [Eulerian], we substitute their asymptotic form and rewrite the relations as

$$\Theta_{\mu\mu\nu} + \Psi_{\nu\mu} \sim \max\left(\Lambda_\nu, \frac{\Lambda_\nu^2}{\Lambda_\mu^2}\right), \qquad \mu < \nu, \tag{1}$$

$$\Theta_{\mu\nu\kappa} - \Theta_{\nu\mu\kappa} \sim \max\left(\frac{\Lambda_\mu\,\Lambda_\nu}{\Lambda_\kappa}, \frac{\Lambda_\mu^2}{\Lambda_\kappa^2}\right), \qquad \kappa < \mu < \nu. \tag{2}$$

When Λ_ν corresponds to a contracting direction, (1) goes to zero asymptotically.

When $(\Lambda_\mu\,\Lambda_\nu)/\Lambda_\kappa \to 0$, (2) goes to zero asymptotically.

These are constraints on the asymptotic form of the Ψ's and Θ's.

Constraint, Type I

The first type of constraint implies that in any chaotic flow

$$\boxed{\nabla_0 \cdot \hat{\mathbf{s}} - \hat{\mathbf{s}} \cdot \nabla_0 \log \Lambda_s \longrightarrow 0,}$$

where s denotes a contracting direction and ∇_0 denotes a gradient with respect to Lagrangian coordinates.

[Tang & Boozer 1996, Thiffeault & Boozer 2001]

In Lagrangian coordinates, the advection-diffusion equation is

$$\frac{\partial \phi}{\partial t} = \sum_{p,q} D \, \frac{\partial}{\partial a^p} \left[g^{pq} \, \frac{\partial \phi}{\partial a^q} \right]$$

where $g^{pq} = (g^{-1})^{pq}$. Assuming $\Lambda_s \ll 1$, can approximate by

$$\frac{\partial \phi}{\partial t} = \sum_{p,q} D \, \frac{\partial}{\partial a^p} \left[\Lambda_s^{-2} \, \hat{s}^p \, \hat{s}^q \, \frac{\partial \phi}{\partial a^q} \right]$$

Define:

$$\tilde{\mathbf{s}} \equiv \Lambda_s^{-1} \, \hat{\mathbf{s}},$$

$$\frac{\partial \phi}{\partial t} = \sum_{p,q} D \, \frac{\partial}{\partial a^p} \left[\tilde{s}^p \, \tilde{s}^q \, \frac{\partial \phi}{\partial a^q} \right]$$

Still not a 1–D diffusion equation . . .

But the constraint derived before can be written

$$\boldsymbol{\nabla}_0 \cdot \tilde{\mathbf{s}} = 0$$

so that finally

$$\frac{\partial \phi}{\partial t} = \sum_{p,q} \widetilde{D}(t)\, \tilde{s}^p \, \frac{\partial}{\partial a^p} \left[\tilde{s}^q \, \frac{\partial \phi}{\partial a^q} \right]$$

or

$$\boxed{\frac{\partial \phi}{\partial t} = \widetilde{D}(t)\, \frac{\partial^2 \phi}{\partial s^2}} \qquad \text{where} \quad \frac{\partial}{\partial s} \equiv \tilde{\mathbf{s}} \cdot \boldsymbol{\nabla}_0$$

This is a bona-fide one-dimensional diffusion equation with a time-dependent diffusion coefficient!

Raises the possibility of solving the advection-diffusion equation in the small diffusivity limit (the difficult one).

Constraint, Type II

Another type of constraint we obtain is that for any chaotic flow (specializing to 3D)

$$\hat{\mathbf{u}} \cdot \boldsymbol{\nabla}_0 \times \hat{\mathbf{u}} \longrightarrow 0.$$

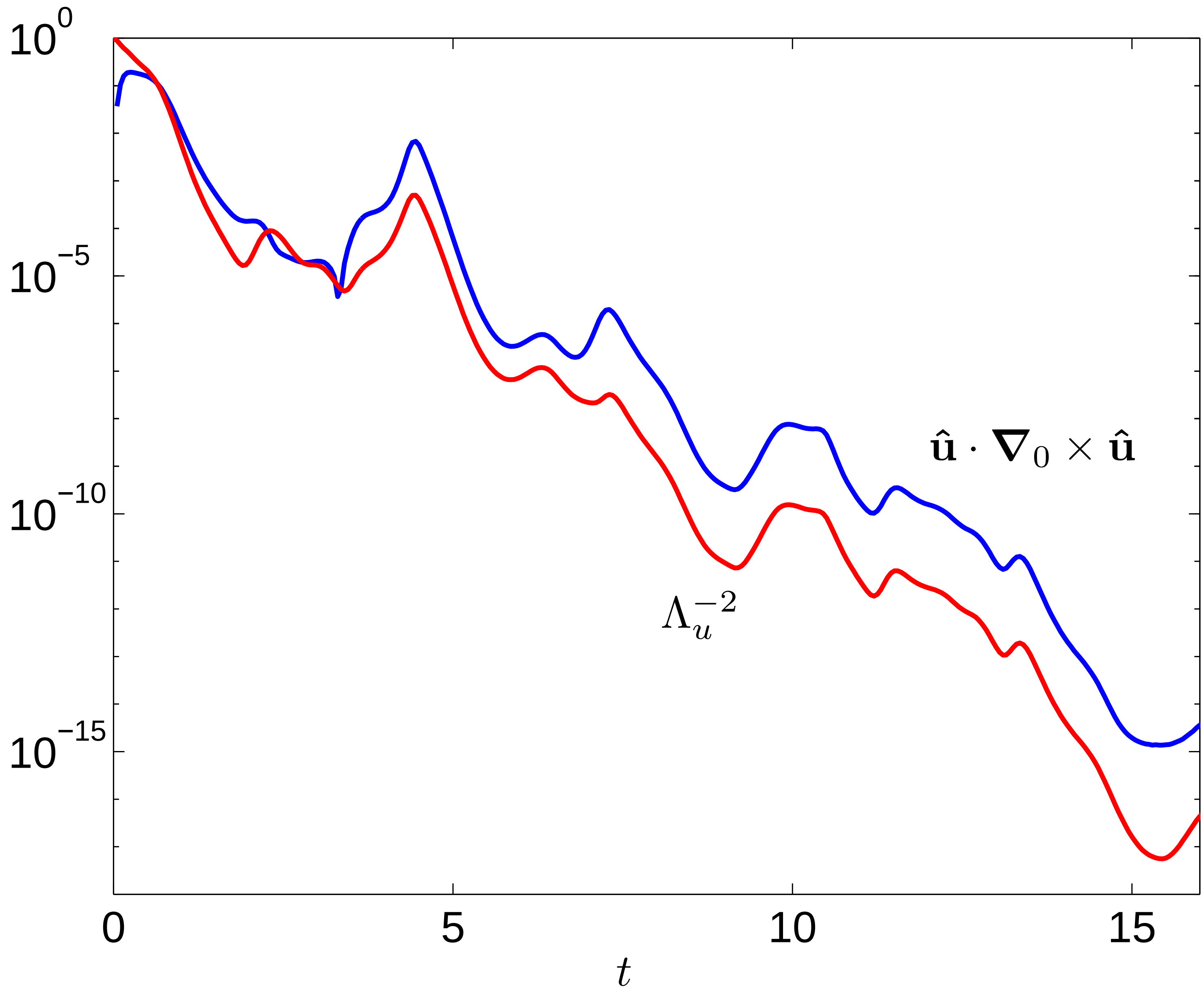
This implies that locally we can write

$$\hat{\mathbf{u}} = \frac{\boldsymbol{\nabla}_0 \varphi}{\|\boldsymbol{\nabla}_0 \varphi\|}$$

for some scalar φ.

This constraint was also derived using curvature arguments by Thiffeault and Boozer (Chaos, 2001).

The global consequences of this constraint have yet to be investigated. (Alignment of material lines)



10^{0}
10^{-5}
10^{-10}
10^{-15}
0
5
10
15
t
$\hat{\mathbf{u}} \cdot \boldsymbol{\nabla}_0 \times \hat{\mathbf{u}}$
Λ_u^{-2}

Constraints for the Dynamo

Let $\mu_0\, j^u$ be the projection of $\mu_0\,\mathbf{j} = \boldsymbol{\nabla}_0 \times \mathbf{B}$ in Lagrangian coordinates along the unstable direction $\hat{\mathbf{u}}$:

$$\mu_0\, j^u = \Lambda_u^2\, b^u\, \hat{\mathbf{u}} \cdot \boldsymbol{\nabla}_0 \times \hat{\mathbf{u}} + \mathrm{O}(1).$$

If not for the constraint $\hat{\mathbf{u}} \cdot \boldsymbol{\nabla}_0 \times \hat{\mathbf{u}} \sim \Lambda_u^{-2} \rightarrow 0$, j^u would go as Λ_u^2. After taking the constraint into account, we find

$$j_{\|}^2 = \frac{(\mathbf{j} \cdot \mathbf{B})^2}{\mathbf{B}^2} \sim \Lambda_u^2, \qquad j^2 \sim \Lambda_u^4$$

so that $j_\perp \gg j_\|$. The opposite would be true without the constraint. This is the case in any “generic” chaotic flow.

Hence, the magnetic field is perpendicular to the current in the case of ideal evolution.

Summary

- In the small diffusivity limit, the advection-diffusion equation cannot be solved directly because of scale separation.
- Lagrangian coordinates are a powerful tool for studying chaotic flows, because inessential information can be discarded.
- The asymptotic behavior of the Lagrangian derivatives can be obtained by differentiating the SVD method directly.
- These derivatives are not all independent and must obey constraints due to the exponential behavior in chaotic flows. The constraints have consequences in physical problems.
- For example, one type of constraint helps reduce the advection-diffusion equation to 1 dimension. A second type tells us that the induced current $\mathbf{j}$ is perpendicular to $\mathbf{B}$ for the kinematic dynamo. Much remains to be done ...