Chaotic Mixing and Lagrangian Coordinates

Jean-Luc Thiffeault

Department of Applied Physics and Applied Mathematics
Columbia University

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

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The Advection-diffusion Equation

\[ \frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = \frac{1}{\rho} \nabla \cdot (\rho \mathbf{D} \nabla \phi) \]

- \( \mathbf{v}(\mathbf{x}, t) \) — 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

\( \phi \) could be temperature, or the concentration of a reacting chemical, or...
Small diffusivity is the **norm** rather than the exception.

Typical values of $D/\nu L$:

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<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>Core of earth</td>
<td>$10^{-3}$</td>
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<tr>
<td>Temperature in a room</td>
<td>$10^{-10}$</td>
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<tr>
<td>Solar corona</td>
<td>$10^{-12}$</td>
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<tr>
<td>Galaxy</td>
<td>$10^{-19}$</td>
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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 $\phi$ 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, which leads to a one-dimensional diffusion equation in Lagrangian coordinates.
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, $\nabla \cdot \mathbf{v} = 0$, 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

$$ g_{pq} \equiv \sum_{i=1}^{n} M_{i p} M_{i q} $$

which contains only the information on the stretching of fluid elements.
Stretching and Contracting Directions

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

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

The \( \Lambda_\sigma \) are called coefficients of expansion and are ordered such that \( \Lambda_1 > \Lambda_2 > \ldots > \Lambda_n \) [assumed nondegenerate].

The \( \Lambda_\sigma \) are related to the finite-time Lyapunov exponents \( \lambda_\sigma \) 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:

\[ \hat{e}_1 \equiv \hat{u} , \quad \Lambda_1 \equiv \Lambda_u \]

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

The label $s$ indicates the most stable direction:

\[ \hat{e}_n \equiv \hat{s} , \quad \Lambda_n \equiv \Lambda_s \]

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 $\hat{u}$ and $\hat{s}$ 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
\[
\psi(x, t) = Ak^{-1}(\sin kx \sin \pi y + \epsilon \cos \omega t \cos kx \cos \pi y)
\]
The magnitude of the Lyapunov exponents is the \textit{time-averaged straining rate} encountered by a fluid element.

More \textcolor{red}{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 \textcolor{blue}{blue} (lowest stretching).

Central region with low mixing, corresponding to the center of the rolls. \textcolor{blue}{Blue} filaments extend outside the rolls.

Study breakup of \textit{oil droplets} [Solomon].
S field for oscillating rolls. Two typical portions of stable manifolds in red and blue. Motion in central region is nonchaotic.
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 \( \nabla \times \mathbf{v} \propto \mathbf{v} \). 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 $s(a)$ for the $ABC$ 522 flow:
Advection–Diffusion: Lagrangian Picture

In Lagrangian coordinates, the advection-diffusion equation is

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

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

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

Define: $\hat{s} \equiv \Lambda_s^{-1} \hat{s}$,

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

Not quite a 1–D diffusion equation...
It was shown that arbitrary chaotic flows satisfy several differential constraints, one of which can be written

\[
\sum_p \left( \frac{\partial}{\partial a_p} \mathcal{S}^p - \mathcal{S}^p \frac{\partial}{\partial a_p} \log \Lambda_s \right) \rightarrow 0,
\]

where \(s\) denotes any contracting direction.

In terms of \(\mathcal{S}\), can write the constraint as

\[
\sum_p \frac{\partial}{\partial a_p} \mathcal{S}^p = 0.
\]

Using this constraint in our advection-diffusion equation, we find

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

or

\[ \frac{\partial \phi}{\partial t} \bigg|_a = \tilde{D}(t) \frac{\partial^2 \phi}{\partial s^2} \quad \text{where} \quad \frac{\partial}{\partial s} \equiv \sum_p a^p \frac{\partial}{\partial a^q} \]

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).

[Submitted to Physical Review Letters]
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.

• 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.