The Geometry of Mixing

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March 2000

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Overview

Kinematic transport processes are described by equations such as the advection-diffusion equation

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

where the Eulerian velocity field $\mathbf{v}(\boldsymbol{x}, t)$ is some prescribed time-dependent flow. The quantity ϕ represents the concentration of some passive scalar, and D is the diffusion coefficient.

When the Lagrangian trajectories are chaotic, the diffusion is enhanced greatly due to the exponential stretching of fluid elements. This is known as chaotic mixing.

Lagrangian Coordinates

The trajectory of a fluid element in Eulerian coordinates $\boldsymbol{x}$ satisfies

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

where $\boldsymbol{\xi}$ are Lagrangian coordinates that label fluid elements. The usual choice is to take as initial condition $\boldsymbol{x}(\boldsymbol{\xi}, t = 0) = \boldsymbol{\xi}$, which says that fluid elements are labeled by their initial position.

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

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

Lyapunov Exponents

The rate of exponential separation of neighbouring Lagrangian trajectories is measured by Lyapunov exponents

$$\lambda_\infty = \lim_{t\to\infty} \frac{1}{t} \ln \|(T_{\boldsymbol{x}}\mathbf{v})\hat{\mathbf{u}}_0\|,$$

where $T_{\boldsymbol{x}}\mathbf{v}$ is the tangent map of the velocity field (the matrix $\partial\mathbf{v}/\partial\boldsymbol{x}$) and $\hat{\mathbf{u}}_0$ is some constant vector.

Lyapunov exponents converge very slowly. So, for practical purposes we are always dealing with finite-time Lyapunov exponents.

The Idea

- The coordinate transformation $\boldsymbol{x}(\boldsymbol{\xi}, t)$ is best studied using the tools of differential geometry.
- For instance: the Riemann curvature tensor is a quantity which is invariant under coordinate transformations. In "normal" space, the Riemann tensor vanishes. Therefore, it must also vanish in Lagrangian coordinates.
- Enforcing the vanishing of the Riemann tensor allows us to derive constraints on the spatial dependence of finite-time Lyapunov exponents and their associated characteristic directions.
- Can be tied to the local efficiency of mixing in a flow.

The Metric Tensor

The metric tensor in Lagrangian coordinates is defined by

$$g_{ij}(\boldsymbol{\xi}, t) \equiv \sum_{\ell} \frac{\partial x^\ell}{\partial \xi^i} \frac{\partial x^\ell}{\partial \xi^j}.$$

(g_{ij} is the flat metric δ_{ij} transformed to Lagrangian coordinates.)

g is a symmetric positive-definite matrix that tells us the distance between two infinitesimally separated points in Lagrangian space

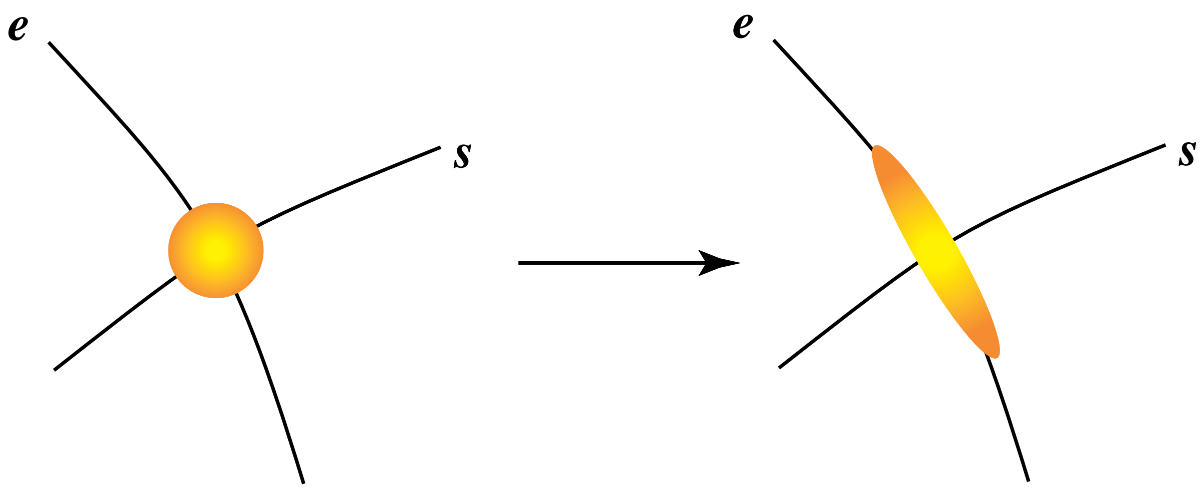
$$ds^2 = d\boldsymbol{x} \cdot d\boldsymbol{x} = g_{ij}\, d\xi^i d\xi^j \,.$$

The eigenvalues $\Lambda_\mu(\boldsymbol{\xi}, t)$ of g are thus related to the finite-time Lyapunov exponents by

$$\lambda_\mu(\boldsymbol{\xi}, t) = \ln \Lambda_\mu(\boldsymbol{\xi}, t) / 2\, t$$

Stable and Unstable Directions

At a fixed coordinate $\boldsymbol{\xi}$, there are directions $\hat{\mathbf{e}}$ and $\hat{\mathbf{s}}$ associated with the largest and smallest Lyapunov exponent, respectively:

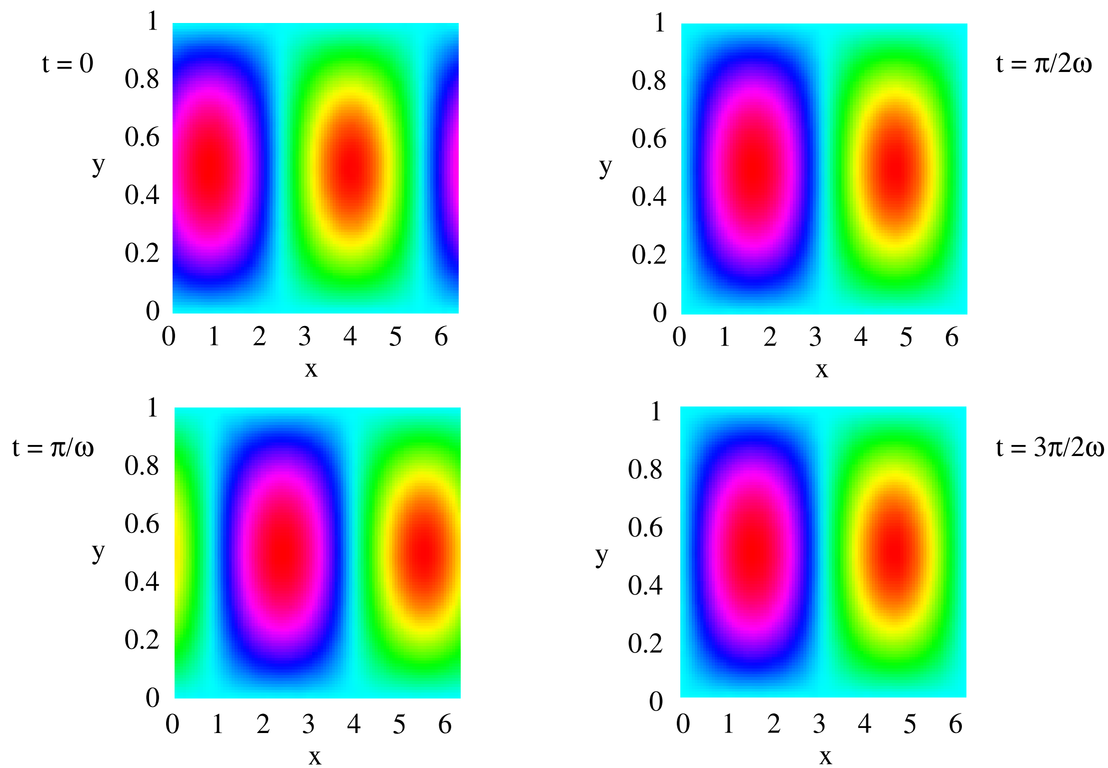


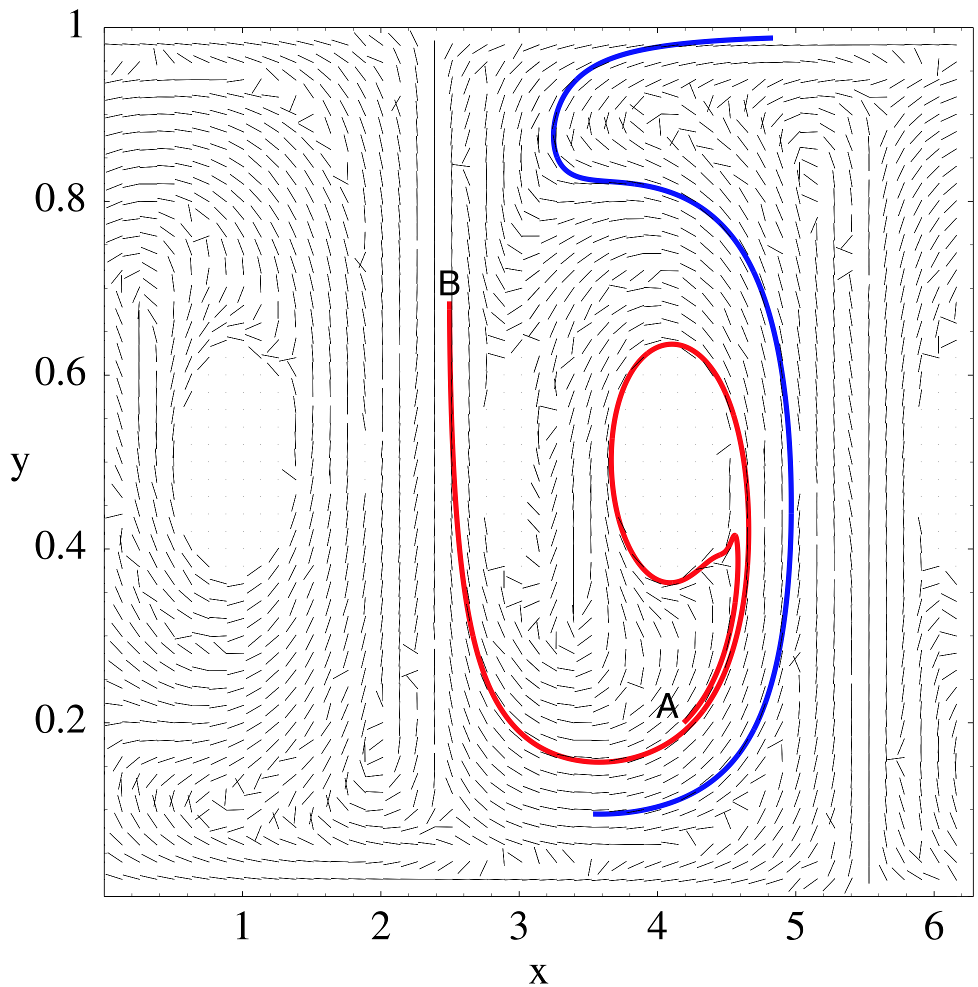
The characteristic directions $\hat{\mathbf{e}}(\boldsymbol{\xi}, t)$ and $\hat{\mathbf{s}}(\boldsymbol{\xi}, t)$ converge exponentially to their asymptotic values $\hat{\mathbf{e}}_\infty(\boldsymbol{\xi})$ and $\hat{\mathbf{s}}_\infty(\boldsymbol{\xi})$, whereas Lyapunov exponents $\lambda_\mu(\boldsymbol{\xi}, t)$ converge logarithmically to λ_μ^∞.

Model System

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

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





$\hat{\mathbf{s}}_\infty$ field for oscillating rolls with $A = k = \epsilon = \omega = 1$, with two typical portions of the stable manifold in red and blue.

The Advection-diffusion Equation

Under the coordinate change to Lagrangian variables the diffusion term becomes

$$\nabla \cdot (D \nabla \phi) = \frac{\partial}{\partial x^i} \left(D \delta^{ij} \frac{\partial \phi}{\partial x^j} \right) = \frac{\partial}{\partial \xi^i} \left(D g^{ij} \frac{\partial \phi}{\partial \xi^j} \right).$$

In Lagrangian coordinates the diffusivity becomes $D g^{ij}$: it is no longer isotropic.

The advection-diffusion equation is thus just the diffusion equation,

$$\boxed{\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial \xi^i} \left(D g^{ij} \frac{\partial \phi}{\partial \xi^j} \right),}$$

because by construction the advection term drops out.

Diffusion along $\hat{\mathbf{s}}_\infty$ and $\hat{\mathbf{e}}_\infty$

The metric g_{ij} can be written in diagonal form as

$$g_{ij} = \Lambda_e \, \hat{\mathbf{e}} \, \hat{\mathbf{e}} + \Lambda_m \, \hat{\mathbf{m}} \, \hat{\mathbf{m}} + \Lambda_s \, \hat{\mathbf{s}} \, \hat{\mathbf{s}}$$

where $\Lambda_\mu = \exp(2\lambda_\mu t)$. The inverse g^{ij} is

$$g^{ij} = \Lambda_e^{-1} \, \hat{\mathbf{e}} \, \hat{\mathbf{e}} + \Lambda_m^{-1} \, \hat{\mathbf{m}} \, \hat{\mathbf{m}} + \Lambda_s^{-1} \, \hat{\mathbf{s}} \, \hat{\mathbf{s}}$$

The diffusion coefficients along the $\hat{\mathbf{s}}$ and $\hat{\mathbf{e}}$ directions are

$$D^{ss} = s_i (D g^{ij}) s_j = D \exp(-2\lambda_s \, t),$$

$$D^{ee} = e_i (D g^{ij}) e_j = D \exp(-2\lambda_e \, t).$$

For a chaotic flow, D^{ee} goes to zero exponentially quickly, while D^{ss} grows exponentially.

Hence, essentially all the diffusion occurs along the $\hat{\mathbf{s}}$-line.

Riemannian Curvature

Differential geometry tells us that if a metric describes a flat space, then its Riemann curvature tensor

$$R^m{}_{ijk} \equiv \Gamma^m_{ji,k} - \Gamma^m_{ki,j} + \Gamma^m_{ks}\,\Gamma^s_{ji} - \Gamma^m_{js}\,\Gamma^s_{ki},$$

must vanish in every coordinate system.

The Christoffel symbols Γ contain derivatives of the metric,

$$\Gamma^i_{jk} \equiv \tfrac{1}{2} g^{i\ell}\left(g_{\ell j,k} + g_{\ell k,j} - g_{jk,\ell}\right)$$

In three dimensions, the Riemann tensor has six independent components, equivalent to the Ricci tensor $R_{ik} \equiv R^j{}_{ijk}$.

In two dimensions, the Riemann tensor has one independent component, equivalent the Ricci scalar $R \equiv g^{ik}\,R_{ik}$.

Two-dimensional Case

In two dimensions, the Ricci scalar written in terms of the characteristic directions $\hat{\mathbf{w}}^{(\mu)} = (\hat{\mathbf{e}}, \hat{\mathbf{s}})$ is

$$R = \sum_{\mu=1}^{2} \frac{1}{\sqrt{|g|}} \nabla_0 \cdot \left(\Lambda_\mu^{-1/2} \, \hat{\mathbf{w}}^{(\mu)} \, \nabla_0 \cdot \left(\sqrt{|g|} \, \Lambda_\mu^{-1/2} \, \hat{\mathbf{w}}^{(\mu)} \right) \right)$$

Notice that the Lyapunov exponent enter as $\Lambda_\mu^{-1/2} = \exp(-\lambda_\mu \, t)$.

The 0 subscript on ∇ denotes derivatives with respect to the Lagrangian coordinates, $\boldsymbol{\xi}$.

A Nonchaotic Example

As a simple demonstration, let us take the flow $\mathbf{v}(x_1, x_2) = (0, f(x_1))$. The Lagrangian trajectories are

$$x_1 = \xi_1$$
$$x_2 = \xi_2 + t\, f(\xi_1)$$

The metric tensor is then

$$g_{ij} = \sum_\ell \frac{\partial x^\ell}{\partial \xi^i} \frac{\partial x^\ell}{\partial \xi^j} = \begin{pmatrix} 1 + t^2\, f'(\xi_1)^2 & t\, f'(\xi_1) \\ t\, f'(\xi_1) & 1 \end{pmatrix}$$

The eigenvalues and eigenvectors of g are then easily derived. Direct insertion into the formula for the 2D curvature confirms, after a tedious calculation, that it does indeed vanish identically.

The Chaotic Case

Assume the Lagrangian trajectories are chaotic (which in 2D requires a time-dependent $\mathbf{v}$). The Ricci scalar is the sum of two terms:

$$\frac{1}{\sqrt{|g|}}\,\nabla_0\cdot\left(\mathrm{e}^{-\lambda_e\,t}\,\hat{\mathbf{e}}\,\nabla_0\cdot\left(\sqrt{|g|}\,\mathrm{e}^{-\lambda_e\,t}\,\hat{\mathbf{e}}\right)\right)\sim\exp(-2|\lambda_e|\,t)$$

$$\frac{1}{\sqrt{|g|}}\,\nabla_0\cdot\left(\mathrm{e}^{-\lambda_s\,t}\,\hat{\mathbf{s}}\,\nabla_0\cdot\left(\sqrt{|g|}\,\mathrm{e}^{-\lambda_s\,t}\,\hat{\mathbf{s}}\right)\right)\sim\exp(+2|\lambda_s|\,t)$$

These terms cannot balance each other unless

$$\frac{1}{\sqrt{|g|}}\,\nabla_0\cdot\left(\mathrm{e}^{-\tilde{\lambda}_s}\,\hat{\mathbf{s}}\,\nabla_0\cdot\left(\sqrt{|g|}\,\mathrm{e}^{-\tilde{\lambda}_s}\,\hat{\mathbf{s}}\right)\right)\sim\exp(-2|\lambda_s^\infty|\,t)\longrightarrow 0$$

where $\tilde{\lambda}_s(\boldsymbol{\xi},t)=\lambda_s(\boldsymbol{\xi},t)-\lambda_s^\infty$.

The form assumed for the diagonalized metric is too general: the characteristic directions and exponents are related to each other.

Now let

$$K \equiv \frac{1}{\sqrt{|g|}} \nabla_0 \cdot \left(\sqrt{|g|}\, \mathrm{e}^{-\tilde{\lambda}_s} \,\hat{\mathbf{s}} \right)$$

Then the constraint can be written

$$(\mathrm{e}^{-\tilde{\lambda}_s} \,\hat{\mathbf{s}} \cdot \nabla) K = \frac{dK}{d\tau} = -K^2$$

K will decrease without bound on an $\hat{\mathbf{s}}$-line with a value dependent on the choice of parameter τ, unless $K = 0$. Hence:

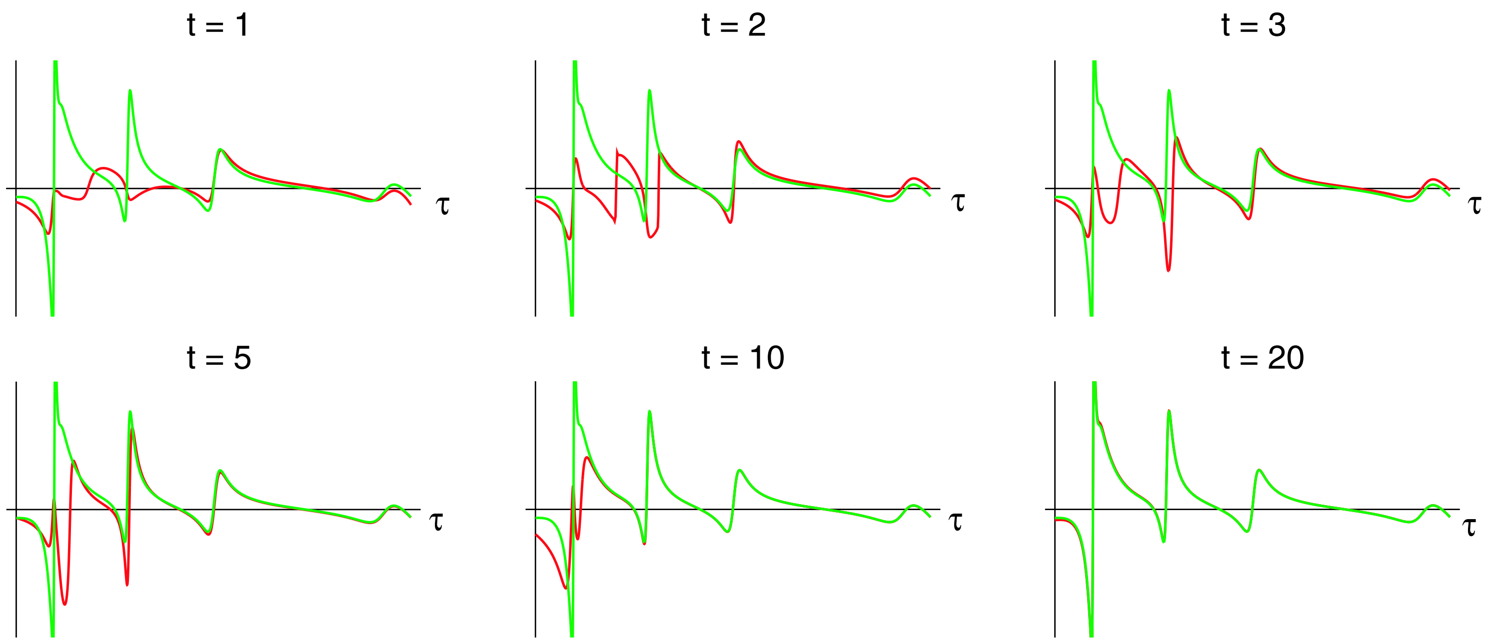
$$\frac{1}{\sqrt{|g|}} \nabla_0 \cdot \left(\sqrt{|g|}\, \mathrm{e}^{-\tilde{\lambda}_s} \,\hat{\mathbf{s}} \right) \longrightarrow 0$$

or

$$\boxed{\frac{1}{\sqrt{|g|}} \nabla_0 \cdot \left(\sqrt{|g|}\, \hat{\mathbf{s}} \right) - \hat{\mathbf{s}} \cdot \nabla_0 \lambda_s \, t \longrightarrow 0}$$

Convergence on the $\hat{\mathbf{s}}_\infty$-line

$\nabla_0 \cdot \hat{\mathbf{s}}_\infty - (\hat{\mathbf{s}}_\infty \cdot \nabla_0)\lambda_s\, t$ evaluated on an $\hat{\mathbf{s}}_\infty$-line.



τ is the distance along the red $\hat{\mathbf{s}}_\infty$-line on page 9.

Green: $\quad -\nabla_0 \cdot \hat{\mathbf{s}}_\infty$

Red: $\quad (\hat{\mathbf{s}}_\infty \cdot \nabla_0)\lambda\, t.$

The Three-dimensional Case

In a coordinate system aligned with the characteristic directions $\hat{\mathbf{w}}_\mu \equiv (\hat{\mathbf{e}}, \hat{\mathbf{m}}, \hat{\mathbf{s}})$, a typical diagonal element of the Ricci tensor is

$$R_{ee} = \frac{1}{\sqrt{|g|}} \nabla_0 \cdot \left[\sqrt{|g|} \left(\Lambda_{(e)}^{-1} \hat{\mathbf{e}} \left(H^{(sm)} - H^{(ms)} \right) \right) \right]$$
$$- \frac{1}{\sqrt{|g|}} \nabla_0 \cdot \left[\sqrt{|g|} \left(\Lambda_{(m)}^{-1} \hat{\mathbf{m}} H^{(se)} + \boxed{\Lambda_{(s)}^{-1} \hat{\mathbf{s}} H^{(me)}} \right) \right]$$
$$+ 2\Lambda_{(e)}^{-1} H^{(ms)} H^{(sm)} + \frac{1}{2|g|} \left[\left(\Lambda_{(m)} H^{(mm)} - \Lambda_{(s)} H^{(ss)} \right)^2 - \Lambda_{(e)}^2 {H^{(ee)}}^2 \right]$$

where the characteristic helicities are defined as

$$H^{(\mu\nu)} \equiv \Lambda_{(\nu)}^{-1/2} \hat{\mathbf{w}}^{(\mu)} \cdot \nabla_0 \times (\Lambda_{(\nu)}^{1/2} \hat{\mathbf{w}}^{(\nu)})$$

and $|g| \equiv \det g$.

If we seek to balance the terms that grow exponentially in the Ricci tensor, we find that

$$H^{(em)} \longrightarrow 0 \qquad \text{and} \qquad H^{(me)} \longrightarrow 0$$

This is equivalent to

$$\hat{\mathbf{e}} \cdot \nabla_0 \times \hat{\mathbf{m}} - \hat{\mathbf{s}} \cdot \nabla \lambda_m \, t \longrightarrow 0$$
$$\hat{\mathbf{m}} \cdot \nabla_0 \times \hat{\mathbf{e}} + \hat{\mathbf{s}} \cdot \nabla \lambda_e \, t \longrightarrow 0$$

Taking the difference of these two constraints yields

$$\boxed{\frac{1}{\sqrt{|g|}} \nabla_0 \cdot \left(\sqrt{|g|} \, \hat{\mathbf{s}} \right) - \hat{\mathbf{s}} \cdot \nabla_0 \lambda_s \, t \longrightarrow 0,}$$

the same constraint as in two dimensions. This was observed numerically for incompressible flows in 3D by Tang and Boozer (1999). The two constraints involving the helicities are new.

ABC Flow

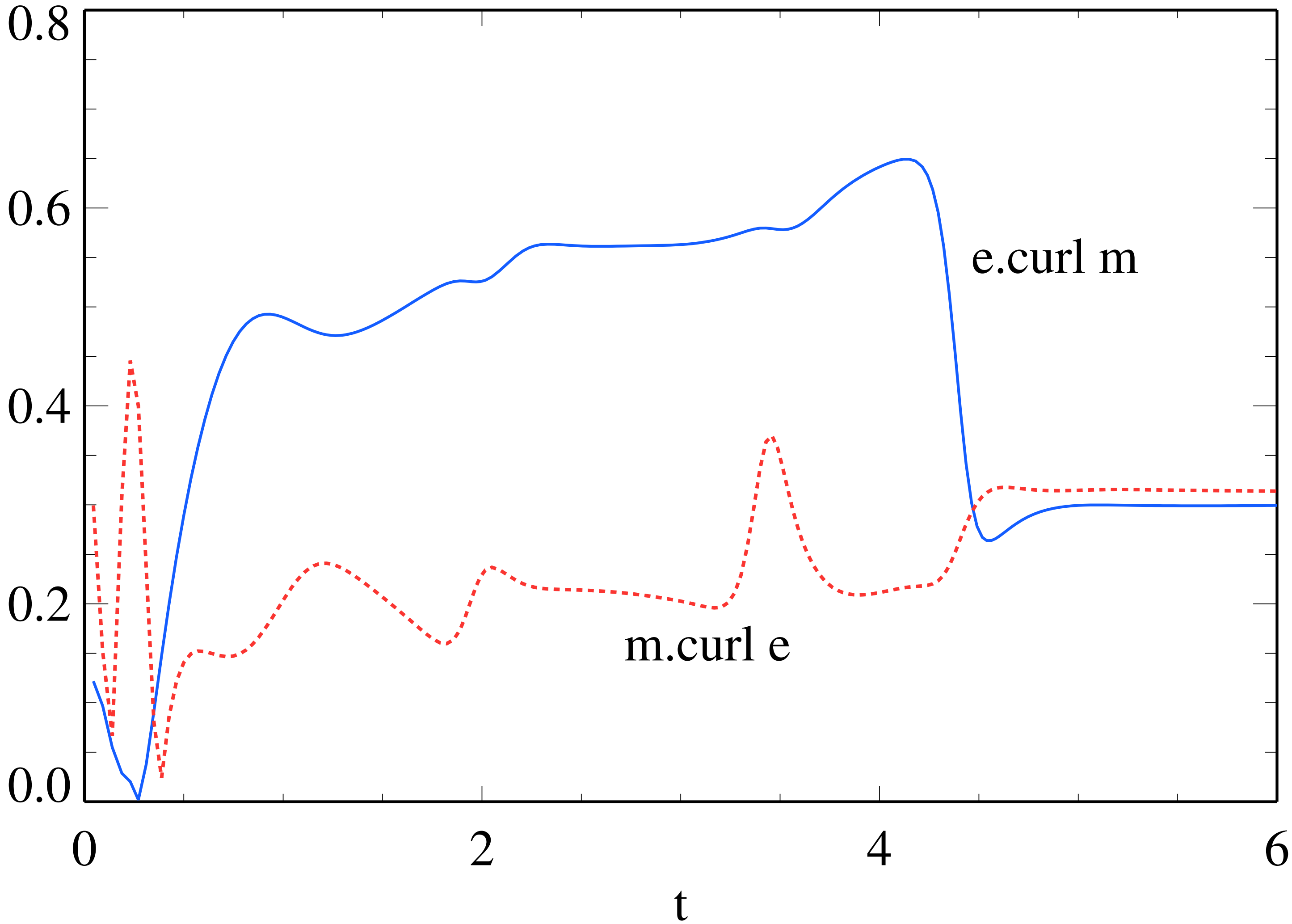
To exhibit the convergence of these quantities, we use the ABC flow,

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

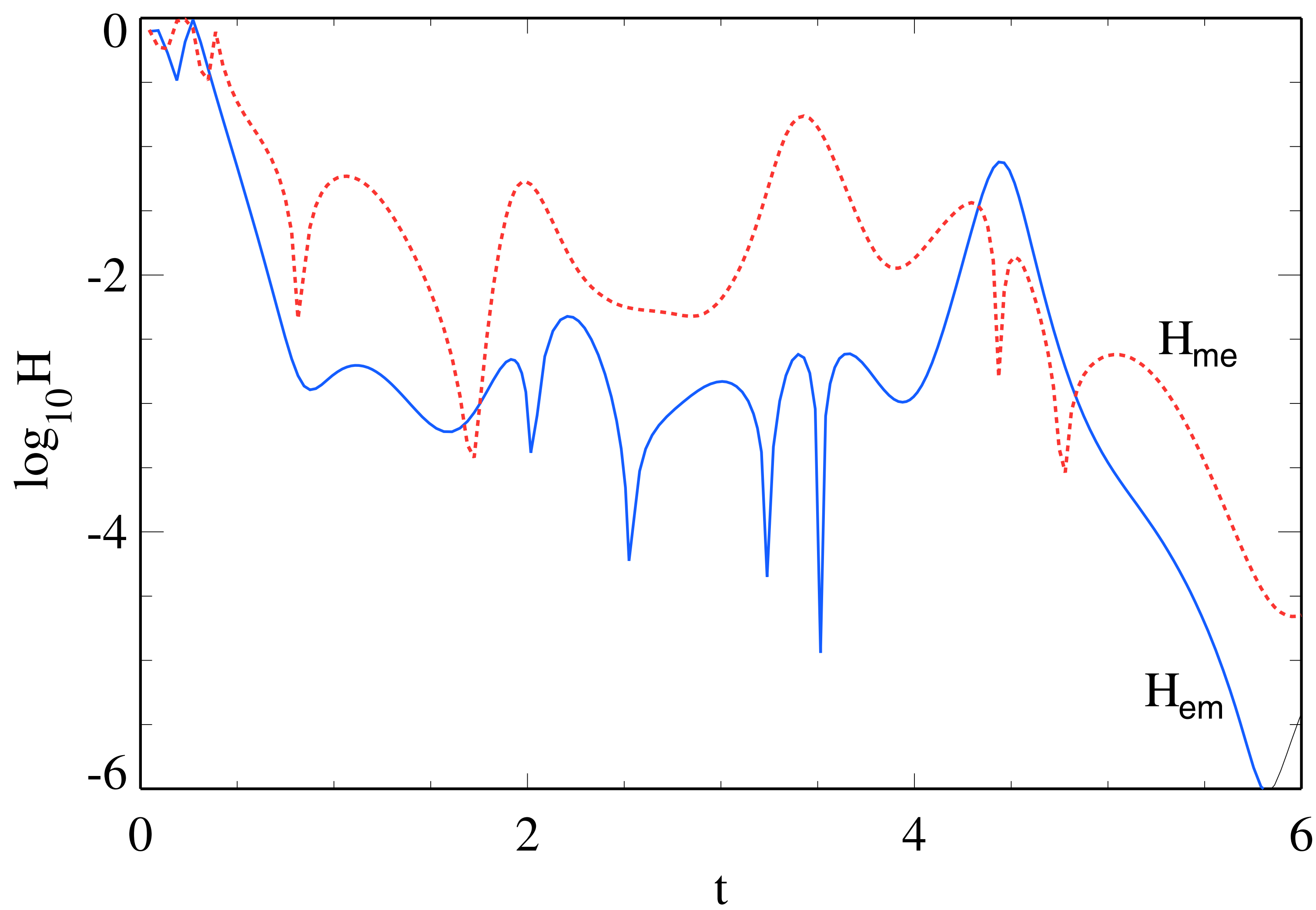
a sum of three Beltrami waves that satisfy $\nabla \times \mathbf{v} \propto \mathbf{v}$. It is time-independent and incompressible ($|g| = 1$).

This flow is well-studied in the context of dynamo theory. We shall be using the habitual parameter values of $A = B = C = 1$ in subsequent examples.

ABC Flow, $A = B = C = 1$



ABC Flow, $A = B = C = 1$



More Constraints...

The story is not quite complete: the "balance of curvature" also requires that

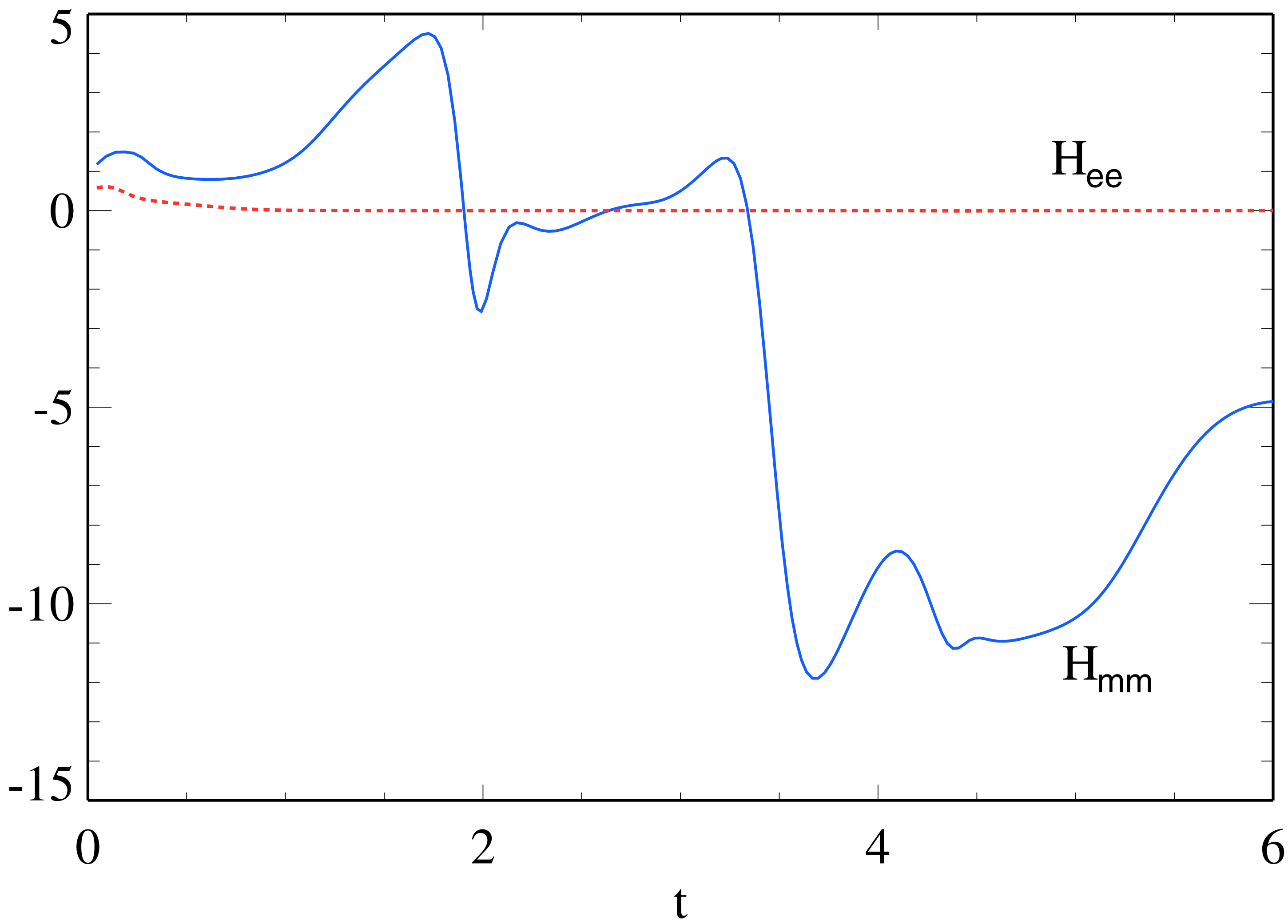
$$\Lambda_e \, H^{(ee)} \sim \Lambda_m \, H^{(mm)}$$

or

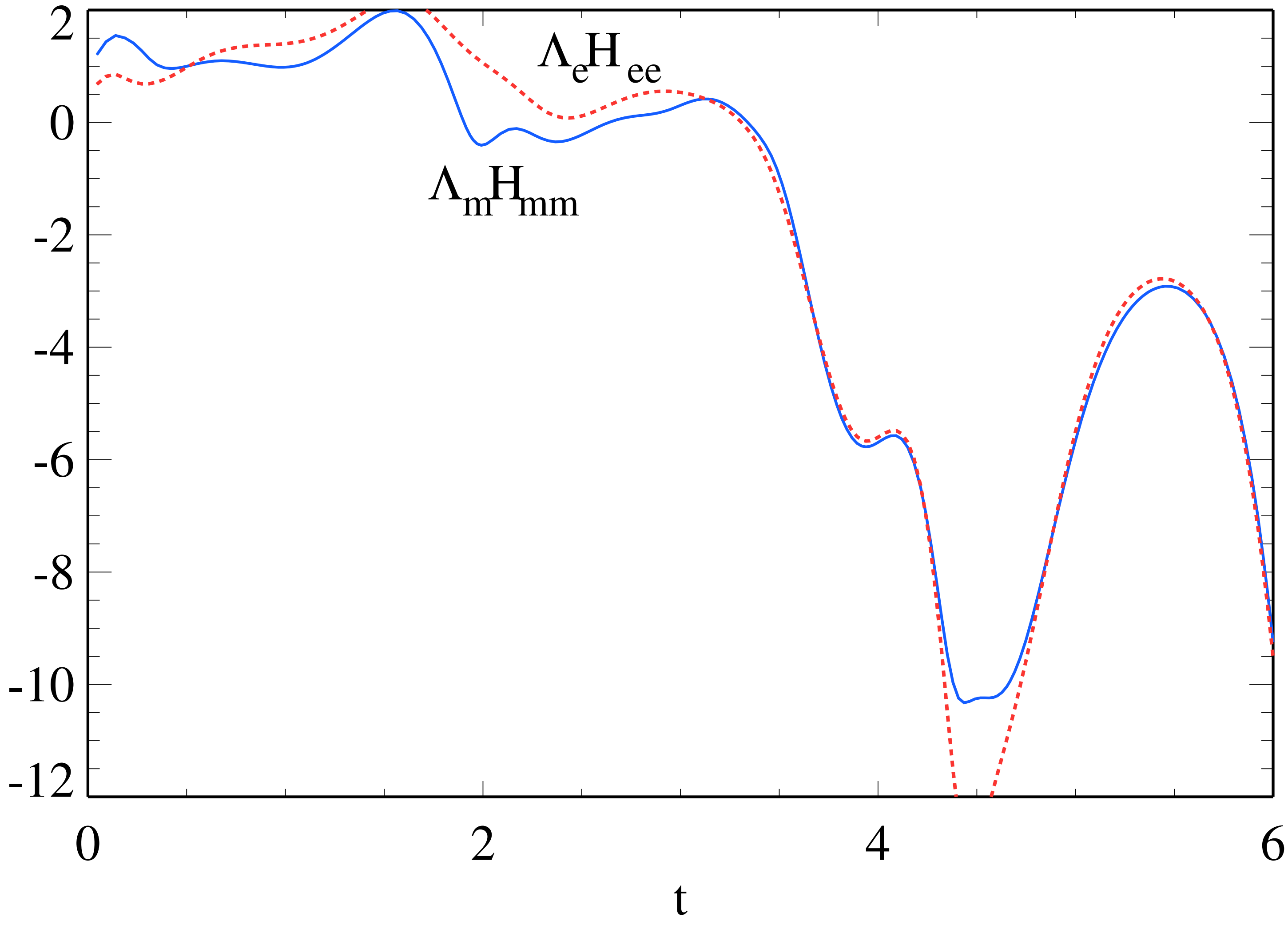
$$\Lambda_e \, (\hat{\mathbf{e}} \cdot \nabla_0 \times \hat{\mathbf{e}}) \sim \Lambda_m \, (\hat{\mathbf{m}} \cdot \nabla_0 \times \hat{\mathbf{m}})$$

This constraint is slightly different in nature than the previous ones, since it involves no λ derivatives.

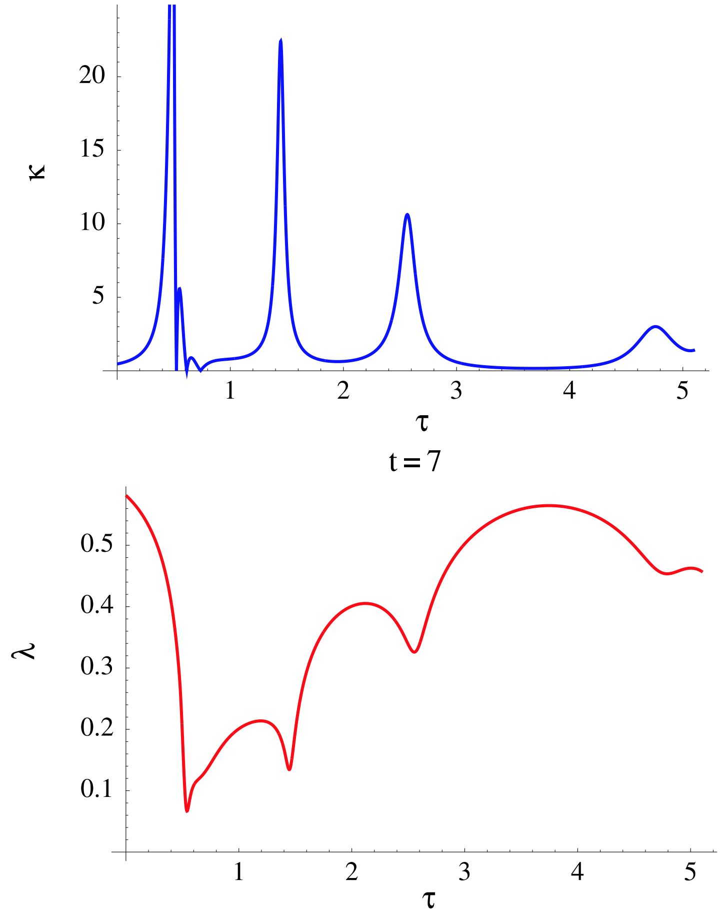
ABC Flow, $A = B = C = 1$



ABC Flow, $A = B = C = 1$



Curvature and Lyapunov Exponents



Finite-time Lyapunov exponent $\lambda_s(\xi(\tau), t)$ has local minima near high-curvature $\kappa \equiv (\hat{\mathbf{s}} \cdot \nabla_0)\hat{\mathbf{s}}$ regions of $\hat{\mathbf{s}}$-line.

Conclusions

- Diffusion occurs overwhelmingly along the stable direction.
- Relationships between characteristic directions and exponents. These work best in highly chaotic flows.
- Sharp bends in the $\hat{\mathbf{s}}$ line lead to locally small finite-time Lyapunov exponents (diffusion is hindered).
- Verified constraints directly on oscillating-rolls flow in 2D and ABC flow in 3D.
- Seek applications to characterize mixing properties in 2D and 3D fluids, and to the dynamo problem in plasmas.