

Nonuniform mixing

Jean-Luc Thiffeault

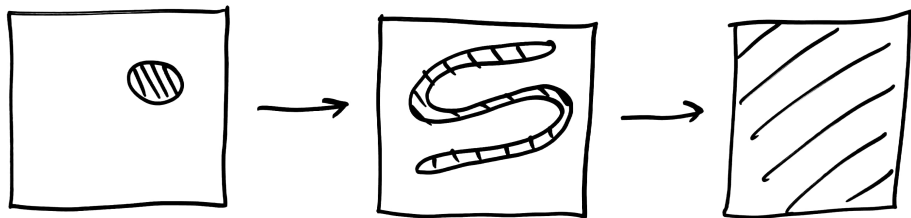
Department of Mathematics
University of Wisconsin – Madison

Ref.: *Physical Review Fluids* **6**(9), 090501, 2021

Closing Meeting of the Priority Programme on
Turbulent Superstructures
Seeheim, Germany
2 May 2023



The usual scenario in mixing is that we want to homogenize some initial distribution of **particles** or **dye**.



This will happen naturally via **molecular diffusion**, but is greatly accelerated by stirring.

See for instance Welander (1955); Young (1999); J-LT (2012); Doering & Nobili (2020).

The **advection-diffusion equation** governs the evolution of a passive scalar concentration $\theta(\mathbf{x}, t)$:

$$\partial_t \theta + \mathbf{u} \cdot \nabla \theta = D \nabla^2 \theta, \quad \nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega$$

where $\mathbf{u}(\mathbf{x}, t)$ is a divergence-free **velocity field**, and D is the **diffusivity**.

We typically use **no-flux boundary conditions**

$$\mathbf{F}[\theta] \cdot \hat{\mathbf{n}} := (\mathbf{u} \theta - D \nabla \theta) \cdot \hat{\mathbf{n}} = 0 \quad \text{on } \partial \Omega \text{ (boundary).}$$

The integral $\int_{\Omega} \theta \, dV$ is conserved:

$$\frac{d}{dt} \int_{\Omega} \theta \, dV = - \int_{\Omega} \nabla \cdot \mathbf{F}[\theta] \, dV = - \int_{\partial \Omega} \mathbf{F}[\theta] \cdot \hat{\mathbf{n}} \, dS = 0.$$



How do we know that the concentration will **eventually mix**? A few integration by parts and use of boundary conditions give

$$\frac{d}{dt} \int_{\Omega} \theta^2 dV = -2D \int_{\Omega} |\nabla\theta|^2 dV \leq 0.$$

The decay of **variance** (L^2 norm) is monotonic: it can never increase. It can only stop decreasing if θ is **uniform in space** ($\nabla\theta \equiv 0$).

This bound underpins the usefulness of variance as a measure of mixing.

It is also useful in rigorous math as an *a priori* estimate that must be satisfied if strong solutions exist.

In oceanography, $D|\nabla\theta|^2$ is said to measure **variance destruction**.

What if the velocity field is **compressible**? Then the **fluid density** $\rho(\mathbf{x}, t) > 0$ is solved for along with the concentration:

$$\partial_t \rho + \nabla \cdot (\mathbf{u} \rho) = 0, \quad \partial_t (\rho \theta) + \nabla \cdot (\mathbf{u} \rho \theta) = D \nabla^2 \theta.$$

Notice that $\theta = \text{const.}$ is still a solution, so the ultimate steady state remains uniform.

The concentration variance equation

$$\frac{d}{dt} \int_{\Omega} \rho \theta^2 dV = -2D \int_{\Omega} |\nabla \theta|^2 dV \leq 0,$$

again assuming no-flux boundary conditions on θ .

The variance will **decay to zero over time**, implying that $\theta(\mathbf{x}, t)$ reaches the uniform mixed state.

In that sense compressible mixing is also an instance of a uniform mixing scenario.



The **relaxation to a uniform state** requires this uniform state to be a steady solution of the advection–diffusion equation.

This is not always the case!

Consider again:

$$\partial_t \theta + \nabla \cdot \mathbf{F}[\theta] = 0, \quad \mathbf{F}[\theta] = \mathbf{u} \theta - D \nabla \theta, \quad \text{in } \Omega$$

with

$$\mathbf{F}[\theta] \cdot \hat{\mathbf{n}} = 0 \quad \text{on } \partial\Omega.$$

But now we **assume neither $\nabla \cdot \mathbf{u} = 0$ nor $\mathbf{u} \cdot \hat{\mathbf{n}} = 0$ on $\partial\Omega$** , the latter of which was a hidden assumption so far.



If we insert $\theta(\mathbf{x}, t) = \theta_0 = \text{const.}$ into our equation, we get

$$\theta_0 \nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega$$

and for the boundary conditions

$$\mathbf{F}[\theta_0] \cdot \hat{\mathbf{n}} = \theta_0 \mathbf{u} \cdot \hat{\mathbf{n}} = 0 \quad \text{on } \partial\Omega.$$

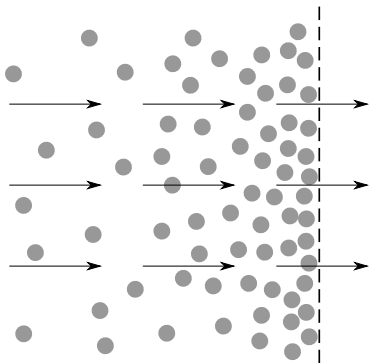
We thus see the necessity of **both** $\nabla \cdot \mathbf{u} = 0$ and $\mathbf{u} \cdot \hat{\mathbf{n}} = 0$ for the existence of a uniform steady state.

If either condition is violated, then the steady state is **nonuniform**. In fact it may not be steady at all.

Example: Particle filter



The simplest example of a nonuniform steady state is a **filter**: $\mathbf{u} \cdot \hat{\mathbf{n}} \neq 0$ at the boundary, since fluid can cross the boundary, but the **particles cannot**.



The equilibrium state is then **nonuniform**: particles tend to accumulate at suction regions on the boundary.

Example: Particle filter (cont'd)



A simple one-dimensional model for a filter has domain $\Omega = [0, L]$ and velocity $\mathbf{u} = U \hat{\mathbf{x}}$:

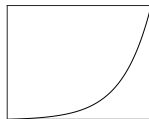
$$\partial_t \theta + U \partial_x \theta - D \partial_x^2 \theta = 0, \quad 0 < x < L$$

with no-flux boundary conditions at 0 and L :

$$U\theta - D \partial_x \theta = 0, \quad x = 0, L.$$

Here $\nabla \cdot \mathbf{u} = 0$ but $\mathbf{u} \cdot \hat{\mathbf{x}}|_{\partial\Omega} = U \neq 0$. The steady state is

$$\varphi(x) \sim e^{Ux/D}.$$



The flow pushes particles against the boundary at $x = L$ (for $U > 0$), creating a **boundary layer** of thickness D/U .



The equation for a **surfactant concentration** $\theta(\mathbf{x}, t)$ evaluated at a free surface is (Aris, 1989; Stone, 1990)

$$\partial_t \theta + \nabla_s \cdot (\mathbf{u}_s \theta) = D \nabla_s^2 \theta - \theta (\nabla_s \cdot \hat{\mathbf{n}}_s) \mathbf{u} \cdot \hat{\mathbf{n}}_s$$

The surface velocity \mathbf{u}_s is **not generally divergence-free**. Surfactants can collect at 'downwelling' regions, in a similar manner to **drifters in the ocean**.



In a popular model for 2D swimmers, the probability density $p(\mathbf{x}, \phi, t)$ obeys a Fokker–Planck (or Smoluchowski) equation

$$\partial_t p + (\mathbf{u} + U\hat{\mathbf{q}}) \cdot \nabla p = D \nabla^2 p + D_{\text{rot}} \partial_\phi^2 p$$

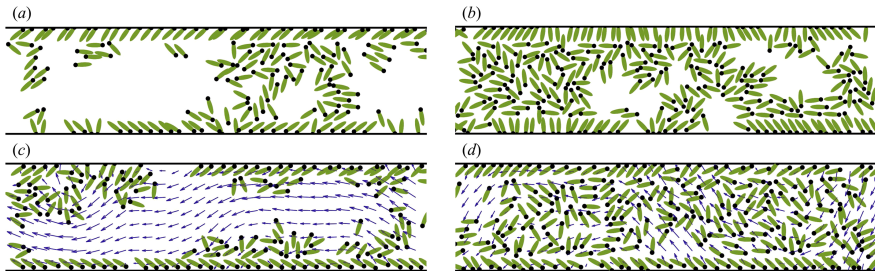
with direction of swimming $\hat{\mathbf{q}} = (\cos \phi, \sin \phi)$ and rotational diffusion D_{rot} .

The fluid velocity $\mathbf{u}(\mathbf{x}, t)$ obeys $\mathbf{u} \cdot \hat{\mathbf{n}} = 0$ at boundaries, but the **swimming velocity $U\hat{\mathbf{q}}$ does not**: a particle may keep pushing against a boundary even after it makes contact. (It is prevented from entering the wall by the no-flux boundary condition on p .)

Example: Microswimmers (cont'd)



Hence, the steady solution is not uniform: swimmers tend to accumulate near boundaries, in a manner similar to the filter example [Lee (2013); Ezhilan & Saintillan (2015); Chen & J-LT (2021)].



[Wioland *et al.* (2016)].

Example: Evaporation and precipitation



Concentration $\theta(t, z)$ of a passive scalar (e.g., salt) confined to **time-varying domain** $\Omega(t) = [0, h(t)]$:

$$\begin{aligned}\partial_t \theta - D_0 \partial_z^2 \theta &= 0, & z \in (0, h(t)), \\ \partial_z \theta &= 0, & z = 0, \\ \dot{h} \theta + D_0 \partial_z \theta &= 0, & z = h(t).\end{aligned}$$



No scalar flux at either the top or bottom.

Models rain and evaporation on the surface of a body of water, with $\dot{h} < 0$ corresponding to **evaporation**, and $\dot{h} > 0$ corresponding to **rain**.

[Part of ongoing work with Albion Lawrence and Raf Ferrari, though Raf probably doesn't know about it.]



Since time-dependent boundaries are tricky to deal with, we rescale the variables as

$$Z = z/h(t), \quad \psi(t, Z) = h \theta(t, hZ)$$

and obtain the advection-diffusion equation

$$\begin{aligned} \partial_t \psi + \partial_Z (W \psi) - D \partial_Z^2 \psi &= 0, & Z \in (0, 1), \\ \partial_Z \psi &= 0, & Z = 0, \\ W \psi - D \partial_Z \psi &= 0, & Z = 1, \end{aligned}$$

with time-dependent velocity and diffusion:

$$W(t, Z) = -Z \dot{h}(t)/h(t), \quad D(t) = D_0/h^2(t).$$

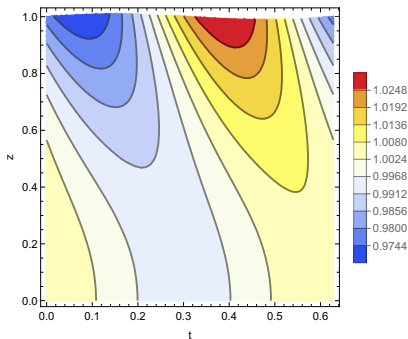
There is an 'apparent velocity' due to the moving surface. The velocity does not vanish at the top surface, so $\mathbf{u} \cdot \hat{\mathbf{n}} \neq 0$.

Example: Evaporation and precipitation (cont'd)

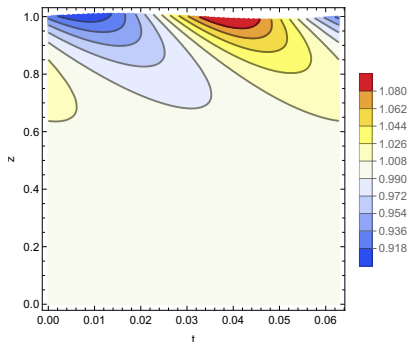


There is no steady solution to this problem. Rather, for periodic $h(t) = h_0 + H \sin(\omega t)$ all solutions converges to a **periodic limit** $\varphi(z, t)$.

$$\omega h_0^2 / D = 10$$



$$\omega h_0^2 / D = 100$$



$$\varepsilon = H/h_0 = 0.01$$

So what's the big deal? It still makes sense to define concentration variance as

$$\int_{\Omega} |\theta - \varphi|^2 dV$$

where φ is the ultimate state (not necessarily uniform or steady).

With $\nabla \cdot \mathbf{u} \neq 0$ and $\mathbf{u} \cdot \hat{\mathbf{n}} \neq 0$ on the boundary, the evolution of variance is

$$\frac{d}{dt} \int_{\Omega} |\theta - \varphi|^2 dV = \boxed{\int_{\Omega} \mathbf{u} \cdot \nabla (\theta - \varphi)^2 dV} - 2D \int_{\Omega} |\nabla (\theta - \varphi)|^2 dV.$$

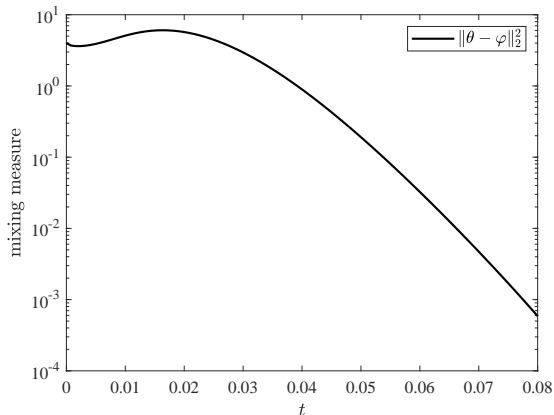
Note the boundary term on the right is not sign-definite. Hence variance no longer has to decrease monotonically. It can exhibit transient growth.

Of course variance must ultimately decay, which we know from other considerations. But the above equation does not show that, and suggests that variance can be poorly-behaved if used as a measure of mixing.

Relaxation to equilibrium: Example



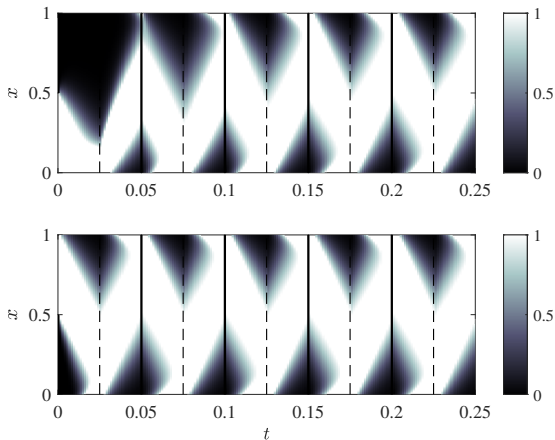
In practice the variance can transiently increase, for instance in our uniform flow example:



Relaxation to periodic solution: Example

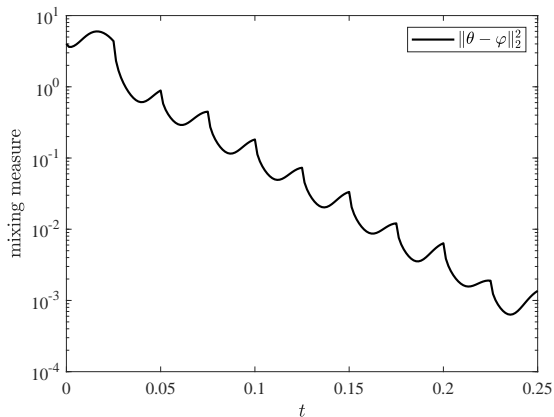


We periodically reverse the direction of the flow ('breathing').



Two different initial conditions converge to the same periodic solution $\varphi(\mathbf{x}, t)$.

Relaxation to periodic solution: Convergence

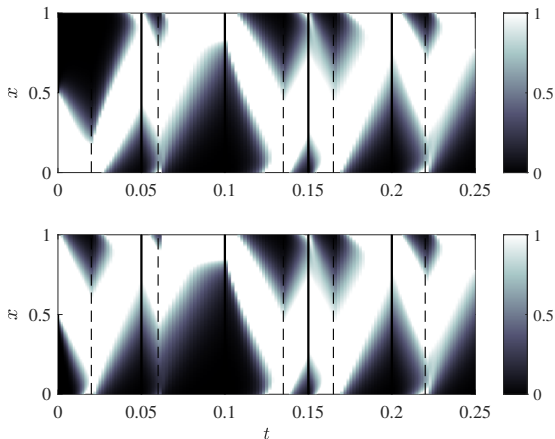


Notice that variance (solid line) shows significant oscillations. Fitting a decay rate to this, or trying to optimize, is more challenging than it needs to be.

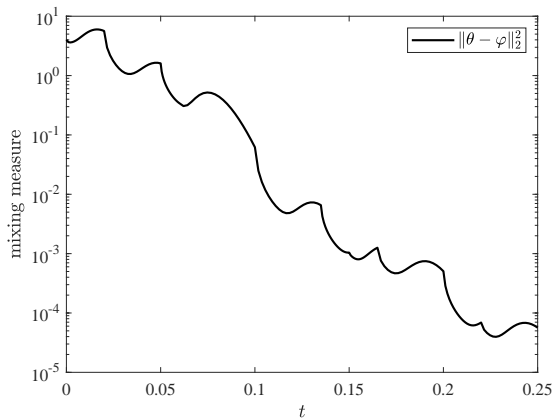
Relaxation to aperiodic solution: Example



We reverse the direction of the flow at random times.



Two different initial conditions converge to the same **aperiodic** solution $\varphi(\mathbf{x}, t)$.



Again nonmonotonic.

To summarize so far:

- When either $\nabla \cdot \mathbf{u} \neq 0$ or $\mathbf{u} \cdot \hat{\mathbf{n}} \neq 0$, the ultimate state φ is **not uniform**.
- The ultimate state can be **steady, periodic, or aperiodic**, depending on the time dependence of $\mathbf{u}(\mathbf{x}, t)$ and $D(\mathbf{x}, t)$.
- The **mixing rate** should be defined as the rate of convergence of any initial condition to $\varphi(\mathbf{x}, t)$.
- Alternatively, we can define the mixing rate as the rate of convergence of **any two initial conditions** to each other.
- However, the L^2 norm (variance) is not monotonically decreasing, which is undesirable.
- Can we improve this by using **a different mixing measure**?

Entropy and f -divergence



An alternative measure of mixing in the nonuniform case is the f -divergence (Österreicher & Vajda, 2003; Liese & Vajda, 2006):

$$H_f[p_1, p_2] := \int_{\Omega} p_2 f(p_1/p_2) dV.$$

Here $p_1, p_2 \geq 0$ are two normalized probability densities, and f is a convex function with $f(1) = 0$, $f'' > 0$.

For example we can choose

$$f(u) = u \log u$$

which gives the Kullback–Leibler divergence or relative entropy.

[Note: opposite sign of physics convention.]

H_f measures the ‘distance’ (divergence) between p_1 and p_2 . Not in general symmetric, so not a metric!

Time-evolution of f -divergence



Take p_1 and p_2 to satisfy the same advection-diffusion problem:

$$\partial_t p_i = -\nabla \cdot \mathbf{F}[p_i], \quad \mathbf{F}[p_i] = \mathbf{u} p_i - \mathbb{D} \cdot \nabla p_i$$

with $\mathbf{F}[p_i] \cdot \hat{\mathbf{n}} = 0$ on $\partial\Omega$.

$$\begin{aligned} \dot{H}_f[p_1, p_2] &= \frac{d}{dt} \int_{\Omega} p_2 f(p_1/p_2) dV \\ &= \int_{\Omega} (\partial_t p_2 f(p_1/p_2) + p_2 f'(p_1/p_2) (\partial_t p_1/p_2 - p_1 \partial_t p_2/p_2^2)) dV \\ &= - \int_{\Omega} \left(\nabla \cdot \mathbf{F}[p_2] f(p_1/p_2) \right. \\ &\quad \left. + f'(p_1/p_2) (\nabla \cdot \mathbf{F}[p_1] - (p_1/p_2) \nabla \cdot \mathbf{F}[p_2]) \right) dV. \end{aligned}$$

We integrate by parts, and two terms containing $f'(p_1/p_2) \mathbf{F}[p_2] \cdot \nabla(p_1/p_2)$ cancel.



We are left with

$$\begin{aligned}\dot{H}_f[p_1, p_2] &= \text{BT}[p_1, p_2] \\ &+ \int_{\Omega} p_2^{-1} f''(p_1/p_2) \nabla(p_1/p_2) \cdot (p_2 \mathbf{F}[p_1] - p_1 \mathbf{F}[p_2]) \, dV\end{aligned}$$

The **boundary terms** vanish when $\mathbf{F}[p_i] \cdot \hat{\mathbf{n}} = 0$ on $\partial\Omega$.

Crucially:

$$\begin{aligned}p_2 \mathbf{F}[p_1] - p_1 \mathbf{F}[p_2] &= p_2(\mathbf{u} p_1 - \mathbb{D} \cdot \nabla p_1) - p_1(\mathbf{u} p_2 - \mathbb{D} \cdot \nabla p_2) \\ &= -p_2 \mathbb{D} \cdot \nabla p_1 + p_1 \mathbb{D} \cdot \nabla p_2 \\ &= -p_2^2 \mathbb{D} \cdot \nabla(p_1/p_2).\end{aligned}$$

We finally obtain the time-evolution

$$\frac{d}{dt} H_f[p_1, p_2] = - \int_{\Omega} p_2 f''(p_1/p_2) \nabla(p_1/p_2) \cdot \mathbb{D} \cdot \nabla(p_1/p_2) dV \leq 0$$

for general no-flux boundary conditions, that is, even if $\mathbf{u} \cdot \hat{\mathbf{n}} \neq 0$. The relaxation of f -divergence is thus **always monotonic**.

This is essentially an *H-theorem* from statistical physics. The novelty here is that in those applications the boundary conditions are often not at the forefront, since quantities such as momentum vanish at infinity. In the fluid-dynamical context it is **precisely the no-flux boundary conditions** that give this monotonic evolution of H_f .

Choice of $f(u)$



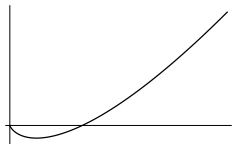
The convex function f is so far arbitrary:

$$H_f[p_1, p_2] = \int_{\Omega} p_2 f(p_1/p_2) dV.$$

There are many good choices, with different trade-offs.

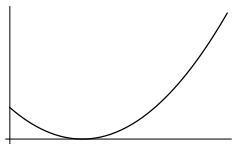
Relative entropy: $f(u) = u \log u$:

$$H_{\text{KL}}[p_1, p_2] := \int_{\Omega} p_1 \log(p_1/p_2) dV.$$



Chi-square divergence: $f(u) = (1 - u)^2$:

$$H_{\chi}[p_1, p_2] := \int_{\Omega} \frac{(p_1 - p_2)^2}{p_2} dV.$$

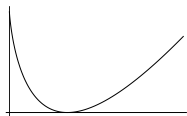


Almost like concentration variance, but not quite!

Jensen–Shannon divergence:

$$f(u) = \frac{1}{2}u \log u - \frac{1}{2}(1+u) \log\left[\frac{1}{2}(1+u)\right]$$

$$\begin{aligned} H_{\text{JS}}(p_1, p_2) &= \frac{1}{2}\{H_{\text{KL}}(p_1, p_{12}) + H_{\text{KL}}(p_2, p_{12})\} \\ &= \frac{1}{2} \int_{\Omega} \{p_1 \log(p_1/p_{12}) + p_2 \log(p_2/p_{12})\} dV \end{aligned}$$

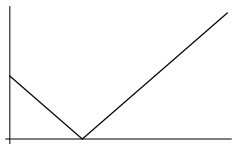


where $p_{12} := \frac{1}{2}(p_1 + p_2)$. $\sqrt{H_{\text{JS}}}$ is a metric, and it is bounded:

$$H_{\text{JS}}(p_1, p_2) \leq \frac{1}{2}(\log 2) \|p_1 - p_2\|_1 \leq \log 2.$$

Total variation distance: $f(u) = \frac{1}{2}|1 - u|$:

$$H_{\text{TV}}[p_1, p_2] = \frac{1}{2} \int_{\Omega} |p_1 - p_2| dV \leq 1.$$



This is just the L^1 norm!

The L^1 norm ($f(u) = |1 - u|$)

$$\int_{\Omega} |p_1 - p_2| dV = \int_{\Omega} |\theta| dV, \quad \theta := p_1 - p_2$$

is an f -divergence, **unlike L^2** .

However, the time-evolution from earlier requires f' and f'' , which are not defined at 0.

We can derive a formula customized for L^1 :

$$\frac{d}{dt} \int_{\Omega} |\theta| dV = -2 \int_{\{\theta=0\}} \nabla \theta \cdot \mathbb{D} \cdot \nabla \theta \frac{dS}{|\nabla \theta|} = -2 \int_{\{\theta=0\}} \mathbf{F}[\theta] \cdot d\mathbf{S} \leq 0$$

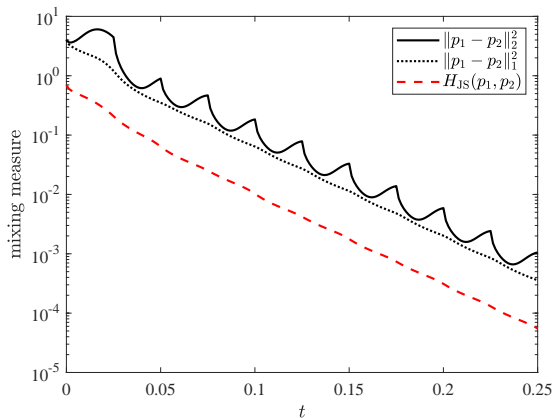
where the integral on the right is taken over the **zero level set** of $\theta(\cdot, t)$.

This suggests that L^1 is **a more reliable measure of mixing than variance** for nonuniform mixing.

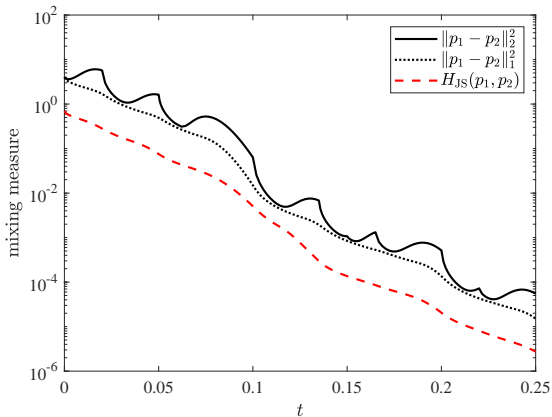
Relaxation of f -divergence: Periodic example



Return to the earlier periodic flow example: the dashed red line is the f -divergence H_{JS} . Notice how nice and monotonic it is compared to variance (solid).



Also true in the aperiodic case:





For the f -divergence, we require the passive scalar p to be a normalized probability distribution.

We can generalize the formalism to a **number density** $n(\mathbf{x}, t)$:

$$\partial_t n + \nabla \cdot \mathbf{F}(n) = Q(\mathbf{x}, t; n), \quad \mathbf{x} \in \Omega.$$

The number of particles

$$N(t) = \int_{\Omega} n(\mathbf{x}, t) dV$$

can change in time:

$$\dot{N} = \int_{\Omega} Q dV.$$



We can't take the source-sink Q to be general, since we need to **maintain** $n(\mathbf{x}, t) \geq 0$. A common, sensible form is

$$Q(\mathbf{x}, t; n) = S(\mathbf{x}, t) - K(\mathbf{x}, t) n, \quad S \geq 0, K \geq 0.$$

With this choice of source-sink, we make the obvious generalization

$$H_f[n_1, n_2] = \int_{\Omega} n_2 f(n_1/n_2) dV$$

which is no longer strictly-speaking an f -divergence. We make the further trivial restriction that $f \geq 0$.

We find after a similar process as earlier:

$$\begin{aligned} \dot{H}_f[n_1, n_2] = & - \int_{\Omega} n_2 f''(n_1/n_2) \nabla(n_1/n_2) \cdot \mathbb{D} \cdot \nabla(n_1/n_2) dV \\ & - \int_{\Omega} (K n_2 f(n_1/n_2) + S g_f(n_1/n_2)) dV \leq 0 \quad (*) \end{aligned}$$

where

$$g_f(u) := (u - 1)f'(u) - f(u) \geq 0, \quad g_f(1) = 0. \quad (**)$$

The inequality in (*) follows from the positivity of n_i , the strict convexity of f ($f'' > 0$), the positive-definiteness of \mathbb{D} , the nonnegativity of f , K , S , and the inequality in (**).

The right-hand side of (*) vanishes if and only if $n_1 = n_2$.

- Mixing is usually regarded as the **relaxation to a uniform state**.
- The **concentration variance** (L^2 norm) is often taken as a **convenient measure**, since it relaxes **monotonically** to a uniform state.
- However, in some cases the ultimate state is **not uniform**.
- For example: **suction boundary conditions**, or divergent flows.
- In those nonuniform cases **variance is less reliable** as a mixing measure, since it can exhibit oscillations: **it is not constrained to decay monotonically**.
- Better measures of mixing in the nonuniform case are the entropy-like quantities called **f -divergences**, including the **L^1 norm**.
- Since we usually don't know the ultimate state $\varphi(\mathbf{x}, t)$, it is preferable to look for **convergence of two different initial conditions** [see atmospheric tracers in Haynes & Shuckburgh (2000)].
- See J-LT (2021). *Physical Review Fluids*, **6** (9), 090501.

- Aref, H., Blake, J. R., Budišić, M., Cardoso, S. S., Cartwright, J. H., Clercx, H. J., El Omari, K., Feudel, U., Golestanian, R., Gouillart, E., van Heijst, G. F., Krasnopolskaya, T. S., Le Guer, Y., MacKay, R. S., Meleshko, V. V., Metcalfe, G., Mezić, I., de Moura, A. P., Piro, O., Speetjens, M. F. M., Sturman, R., J-LT, & Tuval, I. (2017). *Reviews of Modern Physics*, **89** (2), 025007.
- Aris, R. (1989). *Vectors, Tensors, and the Basic Equations of Fluid Mechanics*. New York: Dover.
- Chen, H. & J-LT (2021). *Journal of Fluid Mechanics*, **916**, A15.
- Doering, C. R. & Nobili, C. (2020). *Lectures on Stirring, Mixing and Transport* pp. 8–34. : De Gruyter Open Poland.
- Ezhilan, B. & Saintillan, D. (2015). *Journal of Fluid Mechanics*, , **777**, 482–522.
- Haynes, P. & Shuckburgh, E. (2000). *Journal of Geophysical Research: Atmospheres*, , **105** (D18), 22777–22794.
- Lee, C. F. (2013). *New Journal of Physics*, , **15**, 055007.
- Liese, F. & Vajda, I. (2006). *IEEE Transactions on Information Theory*, , **52** (10), 4394–4412.
- Österreicher, F. & Vajda, I. (2003). *Annals of the Institute of Statistical Mathematics*, , **55** (3), 639–653.
- Risken, H. (1996). *The Fokker–Planck Equation: Methods of Solution and Applications*. Berlin: Springer, second edition.



- Stone, H. A. (1990). *Physics of Fluids A*, **2** (1), 111–112.
- J-LT (2008). In: *Transport and Mixing in Geophysical Flows*, (Weiss, J. B. & Provenzale, A., eds) volume 744 of *Lecture Notes in Physics* pp. 3–35, Berlin: Springer.
- J-LT (2012). *Nonlinearity*, **25** (2), R1–R44.
- J-LT (2021). *Physical Review Fluids*, **6** (9), 090501.
- Welander, P. (1955). *Tellus*, **7** (2), 141–156.
- Wioland, H., Lushi, E., & Goldstein, R. E. (2016). *New Journal of Physics*, **18**, 081001.
- Young, W. R. (1999). In: *Proceedings of the 1999 Summer Program in Geophysical Fluid Dynamics*, (J-LT & Pasquero, C., eds) , Woods Hole, MA: Woods Hole Oceanographic Institution. <http://gfd.whoi.edu/proceedings/1999/PDFvol1999.html>.