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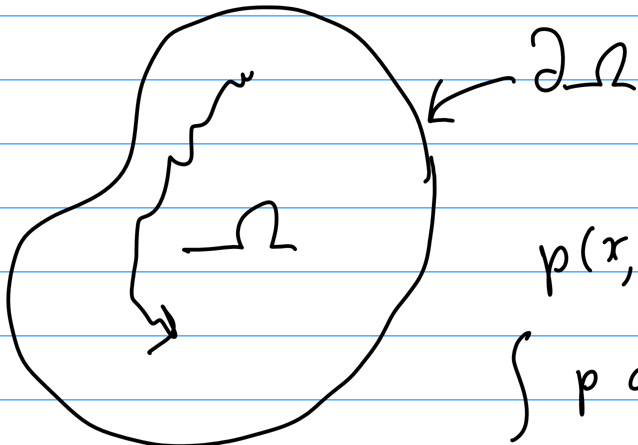
Aspen 6/5/21

Mixing sucks:

How to mix with compressibility & suction

Today: pedagogical, basic. Mathematical angle (reassuring?)



Non-interaction particles in closed domain Ω

$p(x,t)$ = probability density

x is a vector

$$\int_\Omega p\, dV = 1, \quad p > 0$$

Goal: quantify mixing, show that it mixes

Governing eq'n is advection-diffusion: $u(x,t)$, $D(x,t)$ tensor

$$\boxed{\partial_t p + \nabla\cdot f = 0}, \quad \boxed{f[p] = up - D\cdot\nabla p}$$

probability flux

Conservation: $\dfrac{d}{dt}\displaystyle\int_\Omega p\, dV = -\int_{\partial\Omega} f\cdot n\, dS$ $\quad n$ = outward unit normal

Suggests: to conserve total probability, take no-flux boundary condition:

(BC) $$\boxed{f\cdot n = 0 \quad \text{on } \partial\Omega}$$

(Could also assume periodicity, or nonlocal BC.)

No assumptions on $u(x,t)$, $D(x,t)$ so far.

Now assume $\nabla \cdot u = 0$ and $u \cdot n = 0$ on $\partial\Omega$.

Special solution: $\varphi(x) = \dfrac{1}{|\Omega|} \leftarrow$ volume of Ω

"uniform density", constant in space and time.

EVEN FOR $u(x,t)$!!!

How do we approach this steady solution?

Let $\theta = p - \dfrac{1}{|\Omega|}$. Then $\displaystyle\int_\Omega \theta \, dV = 0, \quad \frac{d}{dt}\int_\Omega \theta \, dV = 0.$

Variance: $\displaystyle\int_\Omega \theta^2 \, dV$

$$\frac{d}{dt}\int_\Omega \theta^2 \, dV = 2\int_\Omega \theta \, \partial_t \theta \, dV = -2\int_\Omega \theta \, \nabla\cdot \overbrace{(u\theta - D\cdot\nabla\theta)}^{f[\theta]} \, dV$$

$$= -2\int_{\partial\Omega} \theta \, \underbrace{f[\theta]\cdot n}_{0} \, dS + 2\int_\Omega \nabla\theta \cdot (u\theta - D\nabla\theta) \, dV$$

$$= \int_\Omega u\cdot\nabla\theta^2 \, dV - 2\int_\Omega \nabla\theta\cdot D\cdot\nabla\theta \, dV$$

$\nabla\cdot u = 0$

$$= \int_\Omega \nabla\cdot(u\theta^2) \, dV - (\;''\;)$$

$$= \int_{\partial\Omega} \theta^2 \underbrace{u\cdot n}_{0} \, dS - (\;''\;)$$

Conclude: $$\frac{d}{dt}\int_\Omega \theta^2\,dV = -2\int_\Omega \nabla\theta\cdot D\cdot\nabla\theta\,dV$$

Note: We used both $\nabla\cdot u = 0$ (incompressible)
and $u\cdot n = 0$ (no suction)

What can we deduce? Assume $D(x,t)$ gives a uniformly elliptic operator:

For all v, $\dfrac{v\cdot D\cdot v}{\|v\|^2} \geq \sigma > 0$ $\quad$ σ independent of x and t ("uniform")

Then $$\frac{d}{dt}\int_\Omega \theta^2\,dV \leq -2\sigma\int_\Omega |\nabla\theta|^2\,dV$$
$$\leq -2\sigma\lambda\int_\Omega \theta^2\,dV$$

$\boxed{\text{Poincaré inequality}}$

Here $\lambda > 0$ is the smallest nonzero eigenvalue of $-\nabla^2$. (Depends on domain shape Ω.)

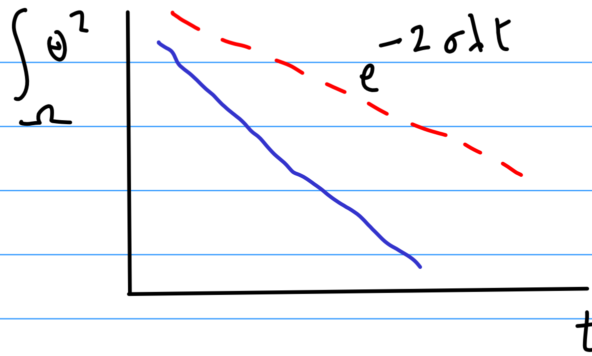
Gronwall's lemma then tells us that

$$\int_\Omega \theta^2\,dV \leq \left(\int_\Omega \theta_0^2\,dV\right)\exp\left(-2\sigma\lambda t\right)$$

Hence $\displaystyle\int_\Omega \theta^2\,dV \to 0$, so $\theta \to 0$: $\quad p \to \dfrac{1}{|\Omega|}$

p gets homogenized ("mixed").

The rate $\sigma\lambda$ is usually a vast underestimate, because of stirring.



What about when $\nabla\cdot u \neq 0$, or $u\cdot n\big|_{\partial\Omega} \neq 0$?

In both cases, $p = \text{const}$ is not a steady solution!

Assume $u = u(x)$ (steady flow)

Steady sol'n: $\nabla\cdot(u\varphi - D\,\nabla\varphi) = 0$

If we insert $\varphi = \text{const}$, we get $\nabla\cdot u = 0$, so necessary.

But even if $\nabla\cdot u = 0$, we have to satisfy $f\cdot n = 0$ on $\partial\Omega$

$$f[\varphi]\cdot n = (u\varphi - D\underbrace{\nabla\varphi)\cdot n}_{0} = \varphi\,(u\cdot n) \quad \text{on } \partial\Omega$$

So we also need $u\cdot n = 0$ on boundary.

In any case, can solve $\nabla\cdot(u\varphi - D\,\nabla\varphi) = 0$

with $\int_\Omega \varphi\, dV = 1$, $\varphi > 0$ (unique for connected Ω)

$\varphi(x)$ is called the invariant density.

(Note that it only exists for $u(x)$ autonomous)

Can we still use variance to prove approach to φ?

$$\theta = p - \varphi, \qquad \int_\Omega \theta \, dV = 0$$

$$\frac{d}{dt}\int_\Omega \theta^2 dV = \underbrace{\int_\Omega u \cdot \nabla\theta^2 \, dV}_{\text{this doesn't vanish!}} - 2\int_\Omega \nabla\theta \cdot D \cdot \nabla\theta \, dV$$

NOT SIGN DEFINITE!

Variance is not (necessarily) decreasing. Could cook up initial conditions that are such that variance increases.

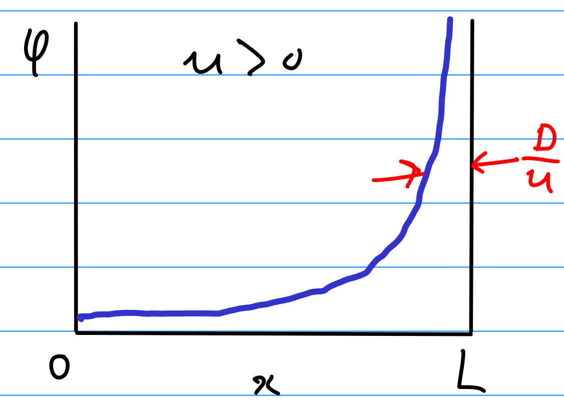
Variance will eventually decrease to zero, but this doesn't show it.

example: $$\partial_t p + u\,\partial_x p = D\,\partial_x^2 p, \qquad 0 < x < L$$

$$u p - D\,\partial_x p = 0, \qquad x = 0, L$$ FILTER

Steady state: $u\varphi - D\varphi' = 0$

$$\varphi(x) = \frac{u}{D}\,\frac{e^{ux/D}}{e^{uL/D} - 1}$$



The rate of approach to equilibrium is

$$p = \varphi + (\cdots)\exp(-\gamma t)$$

$$\gamma = \underbrace{\frac{\pi^2 D}{L^2}}_{\text{diffusion alone}} + \frac{u^2}{4D}$$

"stirring", sort of. Very fast!

Is there a measure we can use other than variance?

Relative entropy, or Kullback-Leibler divergence.

$$\boxed{\psi(p_1, p_2) = \int_\Omega p_1 \log(p_1/p_2)\, dV}$$

as opposed to "metric", since not symmetric.

where $p_i > 0$, $\displaystyle\int_\Omega p_i\, dV = 1$.

Note: physics uses $-\psi$

Not obvious that $\psi \geq 0$! Use $\log x \leq x - 1$, $x > 0$

$$-\psi(p_1, p_2) = \int_\Omega p_1 \log(p_2/p_1)\, dV$$

$$\leq \int_\Omega p_1\left(\frac{p_2}{p_1} - 1\right) dV$$

$$= \int_\Omega p_2\, dV - \int_\Omega p_1\, dV = 1 - 1 = 0!$$

$\psi(p_1, p_2) = 0$ iff $p_1 = p_2$.

Now assume $\partial_t p_i + \nabla \cdot f[p_i] = 0$, $f[p_i] \cdot n = 0$ on $\partial\Omega$

(So, p_1 and p_2 are any two solutions.)

Then we can show (longish, surprising calculation)

$$\frac{d}{dt}\psi(p_1,p_2) = -\int_\Omega p_1 \nabla \log(p_1/p_2) \cdot D \cdot \nabla \log(p_1/p_2)\, dV$$

$$\leq -\sigma \int_\Omega p_1 \left|\nabla \log(p_1/p_2)\right|^2 dV$$

$\therefore \psi$ decreases until $p_1 = p_2$. "H-theorem" for entropy.

(Can get a rate bound using log-Sobolev inequality.)

$\Rightarrow$ ANY 2 INITIAL CONDITIONS CONVERGE TO THE SAME THING

That is, they converge to $\varphi(x)$. (Set $p_2 = \varphi(x)$ above)

The ψ formula above holds for

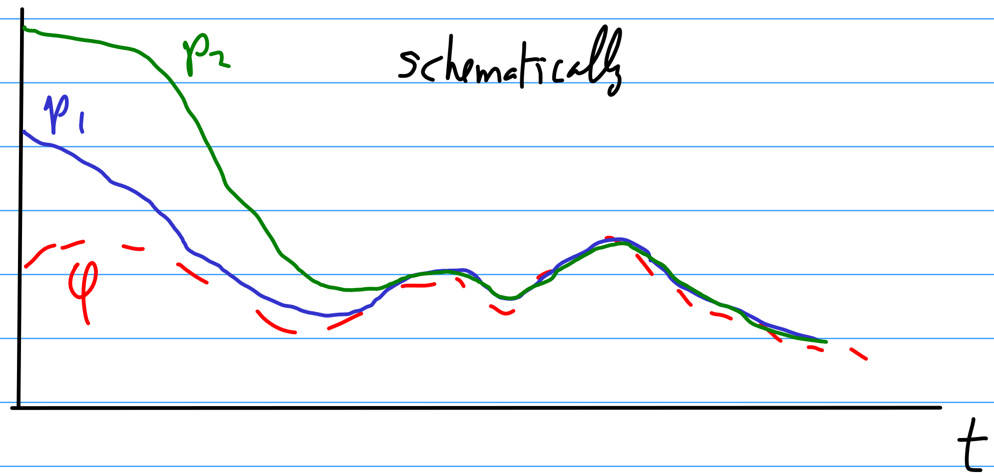
(i) $\nabla \cdot u \neq 0$

(ii) $u \cdot n \neq 0$ on $\partial\Omega$

(iii) $u = u(x,t)$ (non-autonomous)

For case (iii), p does not converge to $\varphi(x)$, but to $\varphi(x,t)$.

$\varphi(x,t)$ is a kind of "invariant density"



However, we don't necessarily want to compute $\varphi(x,t)$ ahead of time.

Instead, to quantify mixing, just follow any two initial conditions $p_1(x,0)$ and $p_2(x,0)$.