Stability Estimates for Advection-Diffusion Equations with Rough Vector Fields

Víctor Navarro-Fernández

Institut für Analysis und Numerik,
Westfälische Wilhelms–Universität Münster

Max–Planck–Institute for Mathematics in the Sciences, Leipzig
October 12, 2022

Outline

Introduction: the Advection-Diffusion Equation

The Advection-Diffusion Equation

Consider the transport of a passive scalar $\theta : (0, T) \times \mathbb{R}^d \to \mathbb{R}$ by the action of a vector field $u : (0, T) \times \mathbb{R}^d \to \mathbb{R}^d$ and in presence of diffusion $\kappa > 0$.

$$\begin{cases} \partial_t \theta + u \cdot \nabla \theta = \kappa \Delta \theta & \text{in } (0, T) \times \mathbb{R}^d, \\ \theta(0, \cdot) = \theta^0 & \text{in } \mathbb{R}^d. \end{cases} \tag{AD}$$

Figure: Action of an alternating shear flow

The Advection-Diffusion Equation

A different framework: one could instead follow the trajectories of a single particle, that are given by the flow map $\phi : (0, T) \times \mathbb{R}^d \to \mathbb{R}^d$ as follows,

$$\begin{cases} d\phi_t = u_t \circ \phi_t dt + \sqrt{2\kappa} dB_t, \\ \phi_0 = \mathtt{id}, \end{cases} \tag{SDE}$$

where $(B_t)_{t\geq 0}$ is a standard Brownian motion in $\mathbb{R}^d$ defined on a filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t\geq 0}, \mathbb{P})$.

- The solutions to (AD) and (SDE) are related through the Feynman-Kac formula

$$\theta(t, \cdot) = \mathbb{E}[(\phi_t)_\# \theta^0].$$

$$\kappa = 0 \quad \Rightarrow \quad \text{(SDE) is a deterministic ODE}$$

The DiPerna-Lions Setting

We are interested in Sobolev vector fields, i.e. let

- $u \in L^1(W^{1,p})$ for some $p \in (1, \infty]$,
- $(\nabla \cdot u)^- \in L^1(L^\infty)$.

Theorem [DiPerna, Lions (1989) & Le Bris, Lions (2008)]

1. If $\kappa = 0$, let $\theta^0 \in L^q$ with $1/p + 1/q \geq 1$. Then there exists a unique distributional solution to (AD)
$$\theta \in L^\infty(L^q).$$
2. If $\kappa > 0$, let $p = 2$ and $\theta^0 \in L^2 \cap L^\infty$. Then there exists a unique distributional solution to (AD)
$$\theta \in L^\infty(L^2 \cap L^\infty) \cap L^2(\dot{H}^1).$$

Uniqueness of Distributional Solutions

What happens out of DiPerna-Lions?

- Modena, Székelihidi (2018) & Modena, Sattig (2020).
  Let $u \in L^1(L^p) \cap L^1(W^{1,r})$, $\theta^0 \in L^q$ with $1/p + 1/q \leq 1$,

$$\frac{1}{r} + \frac{1}{q} > 1 + \frac{1}{d} \quad \Rightarrow \quad \theta \in L^\infty(L^q) \quad \textbf{nonunique}.$$

- Ladyzhenskaya (1967), Prodi (1959) & Serrin (1962).
  Let $u \in L^r(L^p)$, $\theta^0 \in L^q$ with $1/p + 1/q \leq 1$,

$$\frac{2}{r} + \frac{d}{p} \leq 1, \quad \text{with} \quad \begin{cases} r \in [2,\infty) \text{ and } p \in (d,\infty] & \text{if } d \geq 2, \\ r \in [2,4] \text{ and } p \in [2,\infty] & \text{if } d = 1. \end{cases}$$

$$\Rightarrow \quad \theta \in L^\infty(L^q) \quad \textbf{unique}.$$

$\kappa > 0 \Rightarrow$ some control over the gradient of θ

We are interested in the DiPerna-Lions setting for the vector field in (AD). For the construction of the distance we want $\nabla\theta$ to be controlled in $L^1(L^1)$. Consider initial data with **finite entropy**, i.e.

$$\int_{\mathbb{R}^d} \theta^0 \log \theta^0 dx < \infty.$$

then

$$\iint_{(0,T)\times\mathbb{R}^d} |\nabla\theta| dxdt \lesssim \sqrt{\frac{T}{\kappa}}.$$

How to achieve finite entropy?

- *Bounded domain*: $\theta^0 \in L^q$, $q > 1$.
- *Unbounded domain*: $\theta^0 \in L^1 \cap L^q$, $q > 1$ and finite first moments,

$$\int_{\mathbb{R}^d} |x||\theta^0(x)|dx < \infty.$$

Optimal Transport Distances

- Let $\mu, \nu \in L^1_+$ be nonnegative densities.
- Let $\Pi(\mu, \nu)$ be the set of all transport plans between μ and ν.
- Let $c : [0, \infty) \to [0, \infty)$ be a nondecreasing *cost function*.

The optimal transport problem consists of finding the transport plan that minimizes the total cost of transportation from one configuration to another,

$$\mathcal{D}_c(\mu, \nu) = \inf_{\pi \in \Pi(\mu,\nu)} \iint_{\mathbb{R}^d \times \mathbb{R}^d} c(|x - y|) d\pi(x, y).$$

$c(z)$ is a distance $\Rightarrow \mathcal{D}_c$ metrizes **weak convergence** of measures.
$c(z)$ is concave $\Rightarrow$ the OT problem admits a dual formulation,

$$\mathcal{D}_c(\mu, \nu) = \sup_{|\xi(x) - \xi(y)| \le c(|x-y|)} \int_{\mathbb{R}^d} \xi d(\mu - \nu).$$

- μ and ν can be negative/not-signed if $\mu(\mathbb{R}^d) = \nu(\mathbb{R}^d)$.

Logarithmic OT Distances

The distance that we consider is given by the cost function

$$c(z) = \log\left(\frac{z}{\delta} + 1\right) \quad \text{with} \quad \delta > 0.$$

The Kantorovich potentials from the dual formulation $\xi \in \dot{W}^{1,\infty}$ satisfy

$$\|\nabla \xi\|_{L^\infty} \leq \frac{1}{\delta}.$$

Why should we consider such logarithmic cost?

1. It already appears for estimates at the level of the flow ($\kappa = 0$)

$$\log\left(\frac{|\phi^1 - \phi^2|}{\delta} + 1\right) \lesssim \|\nabla u_1\|_{L^1(L^\infty)} + 1, \quad \delta = \|u_1 - u_2\|_{L^1(L^\infty)}.$$

2. If $\mu_n \rightharpoonup \mu$, then $\mathcal{D}_\delta(\mu_n, \mu)$ already has the rate of convergence incorporated in δ.

Stability for Distributional Solutions

Stability for Distributional Solutions in $\mathbb{R}^d$

Goal: Measure the distance between two distributional solutions to (AD) given by two different vector fields, diffusion coefficients and initial data.

- $u \in L^1(W^{1,p})$, $(\nabla \cdot u)^- \in L^1(L^\infty)$,
- $\theta^0 \in L^1 \cap L^q$ and finite first moments.

Theorem 1 [NF, Schlichting, Seis (2021)]

Let $\theta_1, \theta_2 \in L^\infty(L^q) \cap L^1(W^{1,1})$ be the unique solutions to (AD) defined by $(u_1, \kappa_1, \theta_1^0)$ and $(u_2, \kappa_2, \theta_2^0)$ respectively. Then the following stability estimate holds,

$$\sup_{t \in (0,T)} \mathcal{D}_\delta(\theta_1, \theta_2)(t) \lesssim 1 + \mathcal{D}_\delta(\theta_1^0, \theta_2^0) + \frac{\|u_1 - u_2\|_{L^1(L^p)}}{\delta} + \frac{|\kappa_1 - \kappa_2|}{\delta},$$

for every $\delta > 0$.

Outline of the Proof

Let ξ_t be the optimal Kantorovich potential at time $t \in (0, T)$, then

$$
\begin{aligned}
\frac{d}{dt}\mathcal{D}_\delta(\theta_1, \theta_2) = &\int_{\mathbb{R}^d} \nabla \xi_t \cdot (u_1\theta_1 - u_2\theta_2) dx \\
&+ (\kappa_1 - \kappa_2) \int_{\mathbb{R}^d} \nabla \xi_t \cdot \nabla \theta_2 dx \\
&+ \kappa_1 \int_{\mathbb{R}^d} \xi_t (\Delta\theta_1 - \Delta\theta_2) dx \\
= \ & \mathrm{I}(t) + \mathrm{II}(t) + \mathrm{III}(t).
\end{aligned}
$$

We can bound these terms by

$$
\mathrm{I}(t) \lesssim \|\nabla u(t)\|_{L^p} + \frac{\|u_1(t) - u_2(t)\|_{L^p}}{\delta},
$$

$$
\mathrm{II}(t) \leq \frac{|\kappa_1 - \kappa_2|}{\delta} \|\nabla \theta_2(t)\|_{L^1}, \quad \mathrm{III}(t) \leq 0.
$$

The Zero-Diffusivity Limit

Consider two solutions to (AD) with $u_1 = u_2$ and $\theta_1^0 = \theta_2^0$,

$$\sup_{t\in(0,T)} \mathcal{D}_\delta(\theta_1,\theta_2)(t) \lesssim 1 + \frac{|\kappa_1 - \kappa_2| \|\nabla\theta_2\|_{L^1(L^1)}}{\delta}.$$

- Seis (2018).
  If we consider the vanishing diffusion limit $\kappa \to 0$ the rate of convergence is not the same. Let $\kappa_2 = 0$, then

$$\mathcal{D}_\delta(\theta_1,\theta_2)(t) \lesssim \|\nabla u\|_{L^1(L^p)} + \frac{\sqrt{t\kappa_1}}{\delta}$$

- Ciampa, Crippa, Spirito (2021).
  The vanishing viscosity limit $\nu \to 0$ for Navier-Stokes in the vorticity formulation has similar estimates for convergence in strong norms,

$$\sup_{t\in(0,T)} \|\omega^\nu(t) - \omega(t)\|_{L^p} \lesssim 1 + \frac{1}{|\log\nu|}.$$

Optimality of the Estimate

$$\sup_{t\in(0,T)} \mathcal{D}_\delta(\theta_1,\theta_2)(t) \lesssim 1 + \mathcal{D}_\delta(\theta_1^0,\theta_2^0) + \frac{\|u_1-u_2\|_{L^1(L^p)}}{\delta} + \frac{|\kappa_1-\kappa_2|}{\delta}.$$

Rate of convergence: smallest $\delta = \delta_n$ for which the RHS is finite,

$$\mathcal{D}_{\delta_n}(\theta^0,\theta_n^0) \sim 1, \quad \|u-u_n\|_{L^1(L^p)} \sim \delta_n, \quad |\kappa-\kappa_n| \sim \delta_n.$$

1. **Initial data**. The rate is optimal for weak convergence, e.g. a finite volume discretization.
2. **Vector field**. If $\kappa = 0$, the rate is optimal. If $\kappa > 0$,
   - DiPerna-Lions: strong convergence. Rates?
   - Ladyzhenskaya-Prodi-Serrin: strong convergence and rates.
3. **Diffusivity constant**. The rate is the best known so far. Optimal?

$$\frac{t|\kappa_1-\kappa_2|}{\sqrt{\kappa_1}+\sqrt{\kappa_2}} \lesssim W_1(\theta_1,\theta_2)(t), \quad \theta_1,\theta_2 \text{ heat kernels.}$$

Other Regularity Settings

Can we derive similar estimates for other regularity settings?

- Let u be such that $\nabla u = K * \omega$ where $\omega \in L^1(L^1)$ and K is a singular integral kernel $\rightsquigarrow$ *Navier-Stokes in 2D*.
- Let $\theta^0 \in L^1 \cap L^\infty$ with $\int_{\mathbb{R}^d} \theta^0 dx = 0$ but not identically zero.

In this setting there exists distributional solutions to (AD) $\theta \in L^\infty(L^1 \cap L^\infty)$ and the following stability estimate holds: $\forall \varepsilon > 0$, $\exists C_\varepsilon > 0$ such that

$$\sup_{t\in(0,T)} \mathcal{D}_\delta(\theta, 0)(t) \lesssim \mathcal{D}_\delta(\theta^0, 0) + \varepsilon \left(1 + \log \frac{\|u\|_{L^{p,\infty}}}{\varepsilon\delta}\right) + C_\varepsilon,$$

for all $\delta > 0$.

- Crippa, Nobili, Seis, Spirito (2017).
  Solutions to (AD) with $\kappa = 0$ in this regularity setting are unique.
- NF, Schlichting, Seis (2022).
  Solutions to (AD) with $\kappa > 0$ in this regularity setting are unique.

Stability for the Implicit Finite Volume Scheme

The Implicit Finite Volume Scheme

Goal: Derive an error estimate for the convergence of a finite volume approximation to the distributional solution of (AD).

$$\begin{cases} \partial_t \theta + u \cdot \nabla \theta = \kappa \Delta \theta & \text{in } (0,T) \times D, \\ (\kappa \nabla \theta - u) \cdot n = 0 & \text{in } (0,T) \times \partial D. \end{cases}$$

Diffusion process on a bounded domain with no-flow boundary conditions:

PDE	$\leftrightarrow$	SDE
Laplacian operator	$\leftrightarrow$	Reflecting Brownian Motion

$$d\phi_t = u_t \circ \phi_t dt + \sqrt{2\kappa} dB_t - n \circ \phi_t dL_t,$$

with $(L_t)_{t \geq 0}$ such that

$$L_0 = 0, \quad \int_0^t dL_s \leq t, \quad \int_0^t \chi_{\{\phi_s \notin \partial D\}} dL_s = 0.$$

Unstructured Meshes

Consider a tessellation of $D \subset \mathbb{R}^d$ with closed, polygonal, convex cells K. Let h be the size of the mesh,

$$h = \max_K \operatorname{diam} K.$$

The admissible tessellations verify,

- ∂D is $C^{1,1}$, i.e. the uniform exterior ball condition holds;
- trace and Poincaré inequalities hold,

$$\begin{aligned} \|f\|_{L^1(\partial K)} &\lesssim \|\nabla f\|_{L^1(K)} + h^{-1}\|f\|_{L^1(K)}, \\ \|f - {\textstyle⨍_K} f dx\|_{L^1(K)} &\lesssim h\|\nabla f\|_{L^1(K)}, \end{aligned}$$

  for every cell K and $f \in W^{1,1}(K) \cap C(\overline{K})$.

Unstructured Meshes

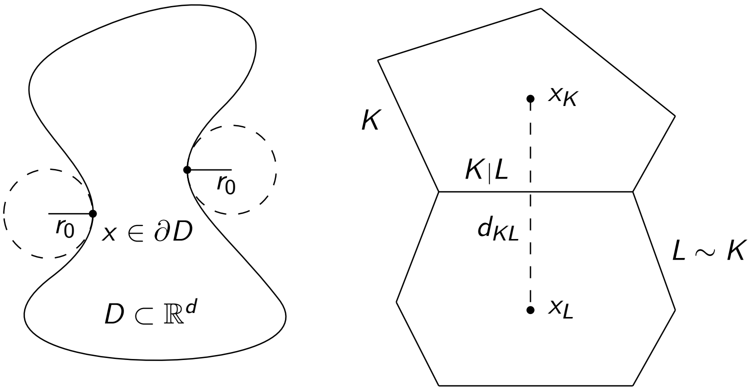

Figure: The exterior ball condition and an example of control cells.

The Implicit Finite Volume Scheme

Let $\tau > 0$ be the time step.

- Initial datum averaged on every cell $\theta_K^0 = \fint_K \theta^0 dx$.
- Discrete normal velocity from control cell K to neighboring L,

$$u_{KL}^n = \int_{n\tau}^{(n+1)\tau} \int_{K|L} u \cdot n_{KL} dH^{d-1} dt.$$

Then the finite volume scheme is given by

$$\frac{\theta_K^{n+1} - \theta_K^n}{\tau} + \sum_{L \sim K} \frac{|K|L|}{|K|} \left(u_{KL}^{n+} \theta_K^{n+1} - u_{KL}^{n-} \theta_L^{n+1} + \kappa \frac{\theta_K^{n+1} - \theta_L^{n+1}}{d_{KL}} \right) = 0.$$

The approximate solution $\theta_{\tau h}$ is defined by

$$\theta_{\tau h}(t, x) = \theta_K^n \quad \text{a.e. } (t, x) \in [n\tau, (n+1)\tau) \times K. \tag{FV}$$

Stability for the Implicit Finite Volume Scheme

We study the converegence of the approximate solution towards the distributional solution on the DiPerna-Lions setting:

- $u \in L^1(W^{1,p})$ with $p \in (1, \infty]$, $(\nabla \cdot u)^- \in L^1(L^\infty)$;
- $\theta^0 \in L^q$ with $q \in (1, \infty]$ and $1/p + 1/q \leq 1$.

In addition we assume: $u \in L^\infty((0, T) \times D)$.

Theorem 2 [NF, Schlichting (2022)]

Let (u, θ^0) be as defined before. Let $\theta \in L^\infty(L^q) \cap L^1(W^{1,1})$ be the unique distributional solutions to (AD) and $\theta_{\tau h}$ the unique approximate solution given by (FV). Then, for $\tau > 0$ small enough, it holds

$$\sup_{t \in (0,T)} \mathcal{D}_\delta(\theta, \theta_{\tau h})(t) \lesssim 1 + \frac{h}{\delta} + \frac{\sqrt{\tau T}\|u\|_\infty}{\delta} + \frac{\sqrt{\tau \kappa}}{\delta},$$

for every $\delta > 0$.

Outline of the Proof

To derive the error estimate between θ and $\theta_{\tau h}$ we split the different contributions to the errors as follows.

- Let $m \in \mathbb{N}$ and $t \in [m\tau, (m+1)\tau)$.
- Let θ^h be the solution to (AD) with the discretized initial datum.
- Let θ^τ be the solution to (AD) with a temporary averaged vector field

$$u^\tau(t, \cdot) = \fint_{n\tau}^{(n+1)\tau} u(t, \cdot) dt \quad \text{for a.e. } t \in [(n\tau, (n+1)\tau).$$

- Let $\theta^{\tau h}$ be the solution to (AD) with discrete initial datum and time-discrete vector field.

$$\begin{aligned} \mathcal{D}_\delta(\theta, \theta_{\tau h})(t) \leq \mathcal{D}_\delta(\theta(t), \theta(m\tau)) &+ \mathcal{D}_\delta(\theta, \theta^h)(m\tau) \\ &+ \mathcal{D}_\delta(\theta^h, \theta^{\tau h})(m\tau) + \mathcal{D}_\delta(\theta^{\tau h}, \theta_{\tau h})(m\tau). \end{aligned}$$

Outline of the Proof

Error due to the discretization of the data.

1. Discretization of the time domain.
   Choose $t \in [m\tau, (m+1)\tau)$, then
   $$\mathcal{D}_\delta(\theta(t), \theta(m\tau)) \lesssim \frac{\tau\|u\|_\infty}{\delta}.$$
2. Discretization of the initial datum.
   Let θ^h be the solution to (AD) with the discrete initial datum, then
   $$\mathcal{D}_\delta(\theta, \theta^h)(t) \lesssim 1 + \frac{h}{\delta}.$$
3. Time discretization of the vector field.
   Let θ^τ be the solution to (AD) with a time.discrete vector field, then
   $$\mathcal{D}_\delta(\theta^h, \theta^{\tau h})(m\tau) \lesssim 1 + \frac{\sqrt{\tau\kappa}}{\delta} + \frac{\tau(\|u\|_\infty + 1)}{\delta}.$$

Outline of the Proof

Error due to the discretization of the scheme.
Consider the piecewise linear approximation to the solution of (FV)

$$\hat{\theta}_{\tau h}(t,x) = \frac{t-n\tau}{\tau}\theta_K^{n+1} + \frac{(n+1)\tau - t}{\tau}\theta_K^n$$

for a.e. $(t,x) \in [nt,(n+1)t) \times K$.

- $\hat{\theta}_{\tau h}(n\tau,\cdot) = \theta_{\tau h}(n\tau,\cdot)$ for every $n \Rightarrow$ no extra error.
- $\hat{\theta}_{\tau h}(t,\cdot)$ is weakly differentiable: $\partial_t\hat{\theta}_{\tau h} = \tau^{-1}(\theta_K^{n+1} - \theta_K^n)$.

Then,

$$\begin{aligned}\frac{d}{dt}\mathcal{D}_\delta(\theta^{\tau h},\hat{\theta}_{\tau h}) = \int_D \nabla\xi\cdot u^\tau\theta^{\tau h}dx + \kappa\int_D \xi\Delta\theta^{\tau h} \\ - \frac{1}{\tau}\sum_K\int_K \xi(\theta_K^{n+1} - \theta_K^n)dx.\end{aligned}$$

Outline of the Proof

Integrate from $n\tau$ to $(n+1)\tau$,

$$\mathcal{D}_\delta(\theta^{\tau h}, \theta_{\tau h})((n+1)\tau) - \mathcal{D}_\delta(\theta^{\tau h}, \theta_{\tau h})(n\tau) = A_n + D_n,$$

- A_n rearrangement of the advective terms,
- D_n rearrangement of the diffusive terms.

Since $\theta^{\tau h}$ and $\theta_{\tau h}$ have the same initial datum

$$\mathcal{D}_\delta(\theta^{\tau h}, \theta_{\tau h})(m\tau) = \sum_{n=0}^{m}(A_n + D_n),$$

and then we obtain

$$\sum_{n=0}^{m} A_n \lesssim 1 + \frac{h}{\delta} + \frac{\sqrt{\tau T}\|u\|_\infty}{\delta}, \quad \sum_{n=0}^{m} D_n \leq 0.$$

Numerical Diffusion and Optimality

- Guo, Stynes (1997) & Droniou (2002).
  The classical rate of convergence for the finite volume scheme with smooth vector fields is h.
- Schlichting, Seis (2018).
  For the case $\kappa = 0$ with rough vector fields (DiPerna-Lions) the rate of convergence is $\sqrt{h}$.

How do we improve the rate of convergence?

Weak BV estimates

$$\kappa = 0 \quad \leftrightarrow \quad \tau \sum_n \sum_K \sum_{L \sim K} |K_| L| |\theta_K^{n+1} - \theta_L^{n+1}| \lesssim \frac{1}{\sqrt{h}}$$

$$\kappa > 0 \quad \leftrightarrow \quad \tau \sum_n \sum_K \sum_{L \sim K} |K_| L| |\theta_K^{n+1} - \theta_L^{n+1}| \lesssim 1$$

Numerical Diffusion and Optimality

$$\sup_{t\in(0,T)} \mathcal{D}_\delta(\theta,\theta_{\tau h})(t) \lesssim 1 + \frac{h+\sqrt{\tau}+\sqrt{\kappa}}{\delta}$$

The discretization of $D \subset \mathbb{R}^d$ generates numerical diffusion that heuristically corresponds to a second diffusion with coefficient $h > 0$,

$$\partial_t\theta + u\cdot\nabla\theta = (\kappa + h)\Delta\theta.$$

- If $\kappa > 0$, then $\kappa + h \to \kappa$
  Theorem 1 $\Rightarrow$ order of convergence h.
- If $\kappa = 0$, then $h \to 0$ corresponds to the zero-diffusivity limit
  Seis (2017) $\Rightarrow$ order of convergence $\sqrt{h}$.

(Some) References

1. G. Crippa and C. De Lellis. Estimates and regularity results for the DiPerna-Lions flow. *J. Reine Angew. Math. 616 (2008), 15–46.*
2. R. J. DiPerna and P.-L. Lions. Ordinary differential equations, transport theory and Sobolev spaces. *Invent. Math. 98, 3 (1989), 511–547.*
3. C. Le Bris and P.-L. Lions. Existence and uniqueness of solutions to Fokker-Planck type equations with irregular coefficients. *Comm. Partial Differential Equations 33, 7-9 (2008), 1272–1317.*
4. V. Navarro-Fernández and A. Schlichting. Error estimates for a finite volume scheme for advection-diffusion equations with rough coefficients. *Preprint arXiv:2201.10411 (2022).*
5. V. Navarro-Fernández, A. Schlichting and C. Seis. Optimal stability estimates and a new uniqueness result for advection-diffusion equations. *Pure and Applied Analysis, to appear (2022).*
6. A. Schlichting and C. Seis. Analysis of the implicit upwind finite volume scheme with rough coefficients. *Numer. Math. 139, 1 (2018), 155–186.*
7. C. Seis. A quantitative theory for the continuity equation. *Ann. Inst. H. Poincaré Anal. Non Linéaire 34, 7 (2017), 1837–1850.*