From fluctuations in conservative systems, to large deviations, to PDEs with irregular coefficients

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joint work with Ben Fehrman [Invent. Math. 2023+] and Daniel Heydecker [arxiv]

Aim:

- From a statistical physics perspective: How do partial differential equations (PDEs) arise? What do they describe?
- When they are insufficient, which mathematical structures go beyond?
- Generally: How to correct for fluctuations around PDEs?

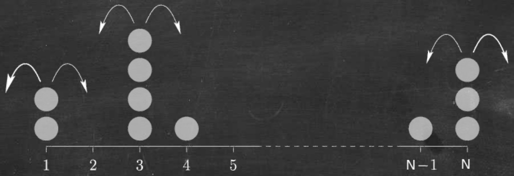
Here: Toy model: Zero range process and (nonlinear) diffusion equations

From particles to PDEs

"Microscopic world": Interacting atoms. Newtonian dynamics yield a high dimensional differential equation.

Stochastic particle systems as simplified mathematical models. An example:

The zero range process



State space $\mathbb{M}_N := \mathbb{N}_0^{\mathbb{T}_N}$, i.e. configurations $\eta : \mathbb{T}_N \to \mathbb{N}_0$: System in state η if container k contains $\eta(k)$ particles.

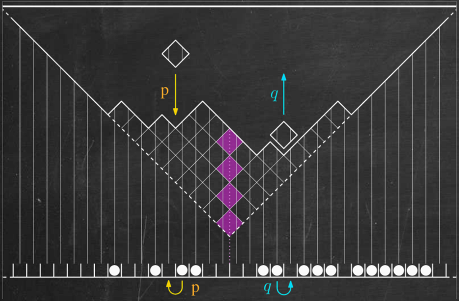
Local jump rate function $g : \mathbb{N}_0 \to \mathbb{R}_0^+$, here $g(n) = n^\alpha$, $\alpha \geq 1$.

Zero mean transition probability $p(k, l)$, that is,

$$p(k, l) = p(k - l), \quad \sum_k kp(k) = 0.$$

Markov jump process η: $\eta(k, t) = \text{number of particles in box } k \text{ at time } t$.

For the “totally asymmetric simple exclusion process” (TASEP) this looks like this



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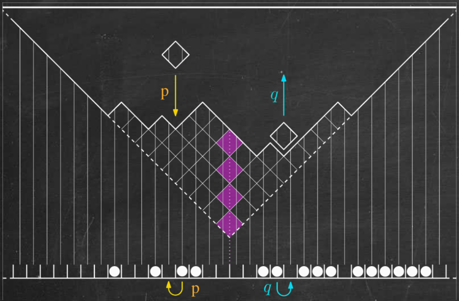
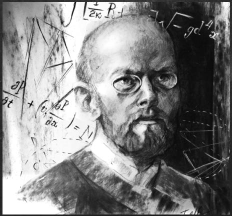


Hilbert's Sixth Problem: "[...] Boltzmann's work on the principles of mechanics suggests the problem of developing mathematically the limiting processes, there merely indicated, which lead from the atomistic view to the laws of motion of continua."



- Empirical density field:

$$\mu^N(x,t) := \frac{1}{N}\sum_k \delta_{\frac{k}{N}}(x)\eta(k,tN^2) : [0,T]\times\Omega \to \mathcal{P}(\mathbb{T}_N).$$

- [Hydrodynamic limit - Ferrari, Presutti, Vares; 1987]

$$\mu^N(t) \rightharpoonup^* \bar{\rho}(t)\,dx$$

with $\bar{\rho} : [0,T]\times\mathbb{T}_N \to \mathbb{R}$ a solution to

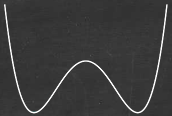
$$\partial_t\bar{\rho} = \partial_{xx}\Phi(\bar{\rho})$$

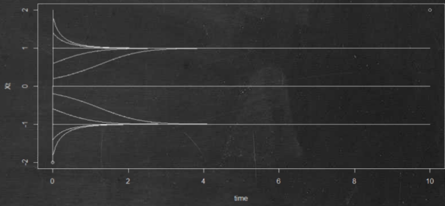
with Φ the mean local jump rate $\Phi(\rho) = \mathbb{E}_{\nu_\rho}[g(\eta(0))]$.

- This corresponds to a law of large numbers.
- Loss of information:
  - Fluctuations, rare events / large deviations?
  - Model / Approximation error: $\mu^N = \bar{\rho} + O(N^{-\frac{1}{2}})$

Typical/mean behavior:

$$\dot{\mu}(t) = -\nabla V(\mu(t))$$

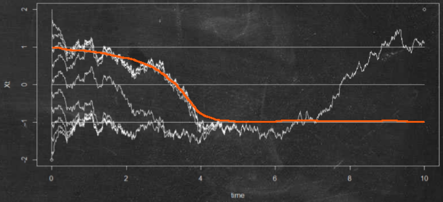




$$V(\mu) = |\mu|^4 - |\mu|^2$$

Fluctuations make a difference on long time-scales

$$\dot{\mu}^N(t) = -\nabla V(\mu^N(t)) + N^{-\frac{1}{2}}\dot{W}(t)$$



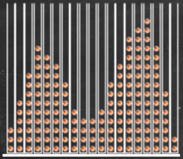
Importance: Tipping points, climate dynamics, failure of mechanical devices, ...

Three extensions:

- Fluctuating Hydrodynamics / Stochastic PDEs
- Rare events / large deviations
- Gradient flow structure

Fluctuating Hydrodynamics / Stochastic PDEs?

Microscopic scale: Particles

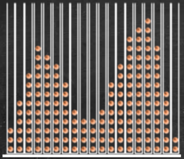


Gridsize = $\frac{1}{N}$

Macroscopic scale: PDEs

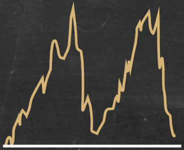
Mean dynamics

Microscopic scale: Particles



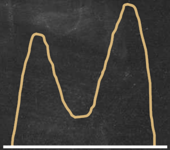
Gridsize = $\frac{1}{N}$

Mesoscopic scale: Conservative SPDEs



Fluctuation correction

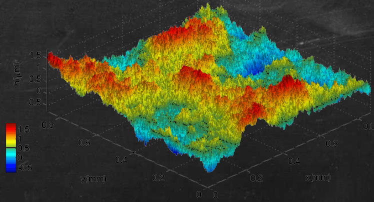
Macroscopic scale: PDEs



Mean dynamics

Ansatz: Conservative SPDEs

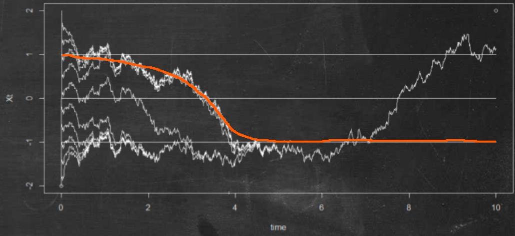
$$\partial_t \rho^N = \partial_{xx}\Phi(\rho^N) + N^{-\frac{1}{2}}\partial_x\left(\Phi^{\frac{1}{2}}(\rho^N)\xi^N\right),$$



with ξ^N noise, spatially correlated with decorrelation length $\frac{1}{N}$, and white in time,

Rare events/ Large deviations:

$$\dot{\mu}^N(t) = -\nabla V(\mu^N(t)) + N^{-\frac{1}{2}}\dot{W}(t)$$



Probability to observe a fluctuation ρ

$$\mathbb{P}[\mu^N \approx \rho] = e^{-N\,I(\rho)} \quad N \text{ large},$$

with $I(\rho) = \inf\{\int_0^T g^2\,ds : \dot{\rho}(s) = -\nabla V(\rho(s)) + g(s)\}$.

Note: ρ is a solution iff $I(\rho) = 0$.

Rare events / large deviations?

$$\mathbb{P}[\mu^N \approx \rho] = e^{-N\, I(\rho)} \quad N \text{ large}$$

Zero range process

$$I(\rho) = \inf \left\{ \int_0^T \int_{\mathbb{T}^d} |g|^2 dxds : \ g \in L^2_{t,x}, \ \underbrace{\partial_t \rho = \Delta \rho^\alpha + \nabla \cdot (\rho^{\alpha/2} g)}_{\text{"skeleton equation"}} \right\}.$$

Theorem ([Large deviation principle, Benois, Kipnis, Landim; 1995])

We have

$$e^{-N\, \overline{I_{|A}}(\rho)} \lesssim \mathbb{P}[\mu^N \approx \rho] \lesssim e^{-N\, I(\rho)}$$

where A is the set of nice fluctuations ρ that are solution to

$$\partial_t \rho = \Delta \rho^\alpha + \nabla \cdot (\rho^{\alpha/2} g)$$

for some $\underline{g \in C^{1,3}_{t,x}}$. Problem: $I = \overline{I_{|A}}$?

This is a frequently observed problem: E.g. Fluctuations around Boltzmann equation [Rezakhanlou 1998], [Bodineau, Gallagher, Saint-Raymond, Simonella 2020].
Counter-example for Boltzmann [Heydecker; 2021].

Recall

$$I(\rho) = \inf \left\{ \int_0^T \int_{\mathbb{T}^d} |g|^2 dxds : \; g \in L^2_{t,x}, \underbrace{\partial_t \rho = \Delta \rho^\alpha + \nabla \cdot (\rho^{\alpha/2} g)}_{\text{"skeleton equation"}} \right\}.$$

Problem:

$$I = \overline{I_{|A}} = \sup\{ \phi(\rho) \,|\, \phi : X \to \mathbb{R} \,\text{is l.s.c. and}\, \phi \leq I_{|A} \}?$$

Existence of a "recovery sequence"? Consider fluctuation ρ so that $I(\rho) < \infty$. That means, for some $g \in L^2_{t,x}$,

$$\partial_t \rho = \Delta \rho^\alpha + \nabla \cdot (\rho^{\alpha/2} g).$$

Need to find sequence of nice fluctuations $\rho^\varepsilon \in A$ so that $\rho^\varepsilon \to \rho$ and $I(\rho^\varepsilon) \to I(\rho)$. That is, find $g^\varepsilon \in C^{1,3}([0,T] \times \mathbb{T})$ so that $\|g^\varepsilon\|_{L^2_{t,x}} \to \|g\|_{L^2_{t,x}}$ and

$$\partial_t \rho^\varepsilon = \Delta (\rho^\varepsilon)^\alpha + \nabla \cdot ((\rho^\varepsilon)^{\alpha/2} g^\varepsilon)$$

satisfies $\rho^\varepsilon \to \rho$.

Difficult problem: Open problem since [Benois, Kipnis, Landim; 1995].

Skeleton equation

$$\partial_t \rho = \Delta \rho^\alpha + \nabla \cdot (\rho^{\alpha/2} \underbrace{g}_{\in L^2_{t,x}}).$$

How difficult is the well-posedness?

Literature: [DiPerna, Lions; Invent. Math. 1989], [Le Bris, Lions; 2008], [Karlsen, Risebro; 2003], [Barbu, Röckner; 2021], roughly speaking

$$\partial_t \rho = \Delta \Phi(\rho) + \nabla \cdot (\Psi(\rho) g)$$

for $g \in W^{1,1}_{loc,x}$, $\operatorname{div} g \in L^\infty$, Ψ locally Lipschitz.

Scaling and energy-criticality: Let ρ be a solution. Set $\tilde{\rho}(t,x) = \lambda\rho(\tau t, \eta x)$ and compute

$$\partial_t \tilde{\rho} = \frac{\tau}{\lambda^{\alpha-1}\eta^2}\Delta\tilde{\rho}^{\alpha} + \nabla\cdot(\underbrace{\frac{\tau}{\lambda^{n-1}\eta}g(\tau t, \eta x)}_{=:\tilde{g}(t,x)}\tilde{\rho}^{\alpha/2})).$$

Choose $\frac{\tau}{\lambda^{\alpha-1}\eta^2} = 1$ and aim to "zoom in", i.e. to consider $\lambda, \tau, \eta \to 0$.

Preserving initial mass in energy space $L^r(\mathbb{R}^d_x)$: $\lambda = \eta^{\frac{d}{r}}$.

We get

$$\|\tilde{g}\|_{L^q_t L^p_x} = \eta^{\frac{d}{r}(\alpha-\alpha/2) - \frac{\frac{d}{r}(\alpha-1)+2}{q} + 1 - \frac{d}{p}}\|g\|_{L^q_t L^p_x}.$$

Need the exponent to be non-negative, otherwise the skeleton equation is super-critical (convection dominated).

Optimizing in r yields $r = 1$ and we get

$$1 + \frac{\alpha}{2} \geq \frac{\alpha+1}{q} + \frac{1}{p},$$

i.e. $p = q = 2$ is critical for $g \in L^q(\mathbb{R}_{+,t}; L^p(\mathbb{R}^d_x; \mathbb{R}^d_x))$.

Ingredients of the proof: Nonlinear "DiPerna-Lions" theory [DiPerna, Lions; Invent. Math. 1989], and merge with kinetic solution theory [Lions, Perthame, Tadmor; JAMS, 1994].

Theorem (Fehrman, G.; Invent. Math. 2023)

Let $g \in L^2_{t,x}$, ρ_0 non-negative and $\int \rho_0 \log(\rho_0) dx < \infty$. There is a unique weak solution to

$$\partial_t \rho = \Delta \rho^\alpha + \nabla \cdot (\rho^{\alpha/2} g).$$

The map $g \mapsto \rho$, $L^2_{t,x} \to L^1_{t,x}$, is weak-strong continuous.In particular,

$$\overline{I_{|A}} = \begin{cases} \inf\left\{ \|g\|^2_{L^2_{t,x}} : \partial_t \rho = \Delta \rho^\alpha + \nabla \cdot (\rho^{\alpha/2} g) \right\} & \text{if } \rho^{\alpha/2} \in L^2_t \dot{H}^1_x \\ +\infty & \text{otherwise.} \end{cases}$$

Gradient flow structure for the porous medium equation

$$\partial_t \rho = \Delta \rho^\alpha = -\nabla_{\mathcal{M}} E(\rho) = -M(\rho)\frac{DE}{D\rho}(\rho),$$

where $M(\rho)$ corresponds to the inverse Riemannian tensor, and E is some energy/entropy.

Gradient flows for the porous medium equation:

- Brezis ['71]: $\mathcal{M} = H^{-1}$, $M(\rho) = -\Delta$, $E(\rho) = \int \rho^{\alpha+1}$.
- Otto ['01]: $\mathcal{M} = \mathcal{P}(\mathbb{T}^d)$, $M(\rho) = -\nabla \cdot (\rho \nabla \cdot)$, $E(\rho) = \int \rho^\alpha$ pressure,
$$\partial_t \rho = \nabla \cdot (\rho \nabla \rho^{\alpha-1}).$$
- "Thermodynamic metric": $\mathcal{M} = \mathcal{P}(\mathbb{T}^d)$, $M(\rho) = -\nabla \cdot (\rho^\alpha \nabla \cdot)$, $E(\rho) = \mathcal{H}(\rho)$ Boltzmann entropy,
$$\partial_t \rho = \nabla \cdot (\rho^\alpha \nabla \log(\rho)).$$

The large deviations principle selects one of these gradient flow pictures.

Note: Skeleton equation & fluctuation-dissipation

$$\begin{aligned}\partial_t \rho &= \Delta \rho^\alpha + \nabla \cdot (\rho^{\alpha/2} g)\\ &= \nabla \cdot (\rho^\alpha \nabla \log(\rho)) + \underbrace{\nabla \cdot (\rho^{\alpha/2}}_{=(\nabla \cdot (\rho^\alpha \nabla \cdot))^{\frac{1}{2}}} g).\end{aligned}$$

If we are able to write $\Delta\rho^\alpha = -\nabla_{\mathcal{M}} E(\rho)$ then we have informally *De Giorgi's Energy-Dissipation Principle*[1]

$$I(\rho) = E(\rho(T)) - E(\rho(0)) + \underbrace{\frac{1}{2}\int_0^T \|\partial_t \rho\|^2_{\dot{H}^{-1}_{\rho^\alpha}}}_{=\text{Length of } \rho \text{ in } \mathcal{M}} + \frac{1}{2}\int_0^T \|\Delta\rho^\alpha\|^2_{\dot{H}^{-1}_{\rho^\alpha}}. \qquad (\star)$$

Theorem (Entropy dissipation equality, G., Heydecker, 2023)

Let $\rho \in D$, $\mathcal{H}(\rho_0) < \infty$. Then $(\star)$ is satisfied with E the Boltzmann entropy. In the special case, where ρ is a solution to the PME, we have the energy equality

$$0 = E(\rho(T)) - E(\rho(0)) + \int_0^T \|\Delta\rho^\alpha(s)\|^2_{\dot{H}^{-1}_{\rho^\alpha}}\, ds.$$

References

B. Fehrman and B. Gess.
Non-equilibrium large deviations and parabolic-hyperbolic PDE with irregular drift.

B. Gess and D. Heydecker.
A Rescaled Zero-Range Process for the Porous Medium Equation: Hydrodynamic Limit, Large Deviations and Gradient Flow.

[1] e.g. [Sandier-Serfaty, CPAM, '04]