Breakdown of the mean-field description for interacting systems: Phase transitions, metastability and coarsening

Workshop on "New Perspectives in Nonlocal and Nonlinear PDEs" — Anacapri

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Institute for Applied Analysis

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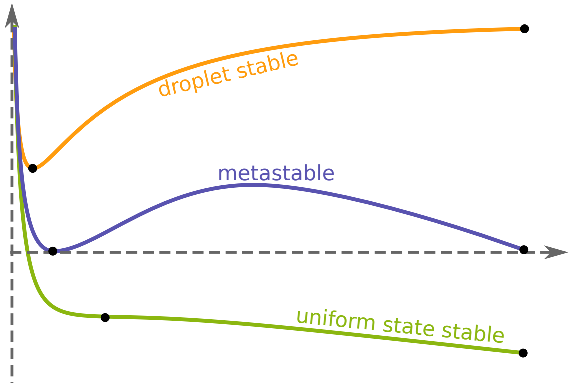
Phase transitions in the McKean–Vlasov model

[Carrillo-Gvalani-Paviliotis-S. '20]



The McKean–Vlasov equation – Derivation

- Overdamped Langevin equation defined on $\mathbb{T}_L^d \simeq [0, L)^d$

$$\mathrm{d}X_t^i = -\frac{\gamma}{N} \sum_{j=1, j\neq i}^{N} \nabla W(X^i - X^j)dt + \sqrt{2}\,\mathrm{d}B_t^i \qquad , i = 1, \dots, N$$

- $\gamma \in [0, \infty)$ interaction strength (bifurcation parameter)
- The mean-field limit $N \to \infty$ is governed by the McKean–Vlasov equation

$$\partial_t \varrho = \Delta \varrho + \gamma \nabla \cdot (\varrho \nabla W \star \varrho) \qquad \text{in } \mathbb{T}_L^d \times (0, T]$$

- properties encoded in interaction potential $W : \mathbb{T}_L^d \to \mathbb{R}$ (coordinate-wise even)

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Some applications: Models for finite N or mean-field limit include

- Molecular dynamic (Lennard–Jones, Van-der-Waals)
- Collective motion of agents (attractive-repulsive)
- Opinions of individuals (Hegselmann–Krause)
- Liquid crystals / nanorods (anisotropic, Onsager, Maier–Saupe)
- Nonlinear synchronizing oscillators (Kuramoto)
- Chemotaxis models (Patlak–Keller–Segel)

Example: Nonlinear synchronization of oscillators

The Kuramoto model: $W(x) = -\cos x$ and $L = 2\pi$

$\gamma < \gamma_c$, no phase locking

$\gamma > \gamma_c$, phase locking

Example: 2d Gaussian attractive interaction potential

$$W(x) = -\frac{1}{\ell} e^{-\frac{|x|^2}{2\ell^2}}$$

with $\ell = \frac{\pi}{2}$, $L = 10$, $\gamma = \sqrt{2L} > \gamma_c$.

Transition points and types of phase transitions

Free energy functional (Lyapunov property, gradient flow)

$$\mathcal{F}_\gamma(\varrho) = \int_{\mathbb{T}_L^d} \varrho \log \varrho \,\mathrm{d}x + \frac{\gamma}{2} \iint_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y)\varrho(x)\varrho(y)\,\mathrm{d}x\,\mathrm{d}y \ .$$

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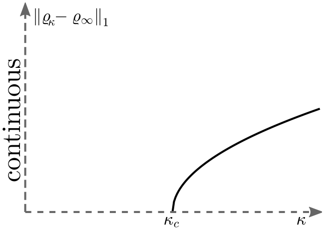
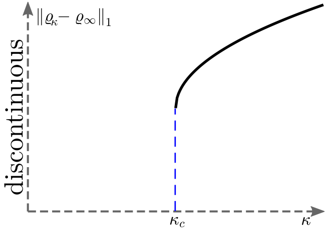
Definition: Let $\varrho_\infty \equiv L^{-d}$. γ_c is transition point, if:

- For $\gamma \le \gamma_c$ is ϱ_∞ global minimizer of $\mathcal{F}_\gamma$ and unique for $\gamma < \gamma_c$
- For $\gamma > \gamma_c$ exists another global minimizer ϱ_γ





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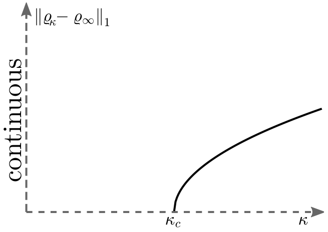
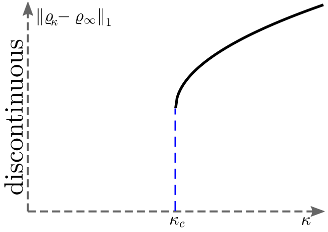


Results and Goals:

- Bifurcation analysis and local stability around $\varrho_\infty \equiv L^{-d}$
- Classification for continuous and discontinuous transitions
- Understanding of the free energy landscape
- Dynamical properties related to nucleation and coarsening



Characterization of phase transition

Theorem [Carrillo-Gvalani-Pavliotis-S. '20]

Let $\widetilde{W} : \mathbb{N}^d \to \mathbb{R}$ denote the (real) Fourier modes of W.

- If there is only one dominant unstable mode k^*: For $\alpha > 0$ small enough holds

$$\alpha \widetilde{W}(k^*) \le \widetilde{W}(k) \qquad \text{for all } k \neq k^* : \widetilde{W}(k) < 0 \, ,$$

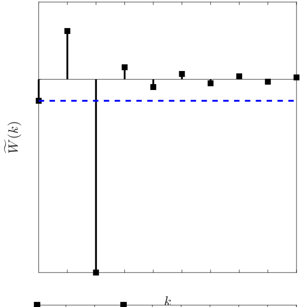
  then the transition point γ_c is continuous.

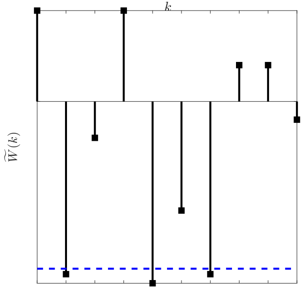
- If there exist (near)-dominant resonating modes k^a, k^b, k^c: That is for δ small enough exist

$$k^a, k^b, k^c \in \left\{ k' \in \mathbb{N}^d : \widetilde{W}(k') \le \min_{k \in \mathbb{N}^d} \widetilde{W}(k) + \delta \right\} \quad \text{with } k^a = k^b + k^c ,$$

  then the transition point γ_c is discontinuous.

$\Rightarrow$ local attractive potentials lead to discontinuous phase transitions





Basic properties of transition points

Summary of critical points:

- γ_c transition point (defined before)
- γ_* bifurcation point (Hessian of $\mathcal{F}$ becomes non-definite)
- $\gamma_\sharp$ point of linear stability of ρ_∞, i.e., $\gamma_\sharp = -\frac{L^{\frac{d}{2}}}{\beta \min_k \widetilde{W}(k)/\Theta(k)}$.

  If $k_\sharp = \arg\min \widetilde{W}(k)$ is unique, then $\gamma_\sharp = \gamma_*$ is a bifurcation point (Crandall-Rabinowitz)

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Results from [Gates & Penrose 1970] and [Chayes & Panferov '10]

- $\mathscr{F}_\gamma$ has a transition point γ_c iff $W \notin \mathbb{H}_s$, that is $\widetilde{W}(k)$ negative for some k
- $\min \mathscr{F}_\gamma$ is non-increasing as a function of γ
- If for some γ' : ϱ_∞ is no longer the unique minimiser,
  then $\forall \gamma > \gamma'$: ϱ_∞ is no longer a unique minimizer
- If γ_c is continuous, then $\gamma_c = \gamma_\sharp$

Conclusion:

- To proof a discontinuous transition: Show ϱ_∞ is no longer global minimizer at $\gamma_\sharp$.
- To proof a continuous transition:
  If $\gamma_* = \gamma_\sharp$, sufficient to show that ϱ_∞ at $\gamma_\sharp$ is the unique global minimizer.

Argument for resonating dominant modes ($\delta = 0$)

Let $\varepsilon > 0$ be sufficiently small such that $\varrho = \varrho_\infty\left(1 + \varepsilon \sum_{k\in K^\delta} w_k\right) \in \mathcal{P}^+(\mathbb{T}^d)$.

Entropy and energy of Ansatz:

$$\beta^{-1} S(\varrho) = \beta^{-1}\left(S(\varrho_\infty) + \frac{|K^\delta|}{2}\varrho_\infty \varepsilon^2 - \frac{\varrho_\infty}{3}\int \varepsilon^3 \Bigg(\sum_{k\in K^\delta} w_k\Bigg)^3 + O(\varepsilon^4)\right)$$

$$\frac{\gamma_\sharp}{2}\mathcal{E}(\varrho,\varrho) = \frac{\gamma_\sharp}{2}\mathcal{E}(\varrho_\infty,\varrho_\infty) + \frac{\gamma_\sharp \varepsilon^2 |K^\delta| \varrho_\infty^2}{2} \min_{k\in\mathbb{N}^d} \frac{\widetilde{W}(k)}{\Theta(k)} L^{d/2}$$

Combining both estimates, recalling $\gamma_\sharp = -\frac{L^{\frac{d}{2}}}{\beta \min_k \widetilde{W}(k)/\Theta(k)}$, yields

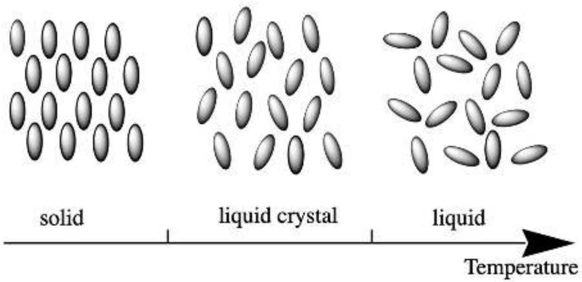
$$\mathscr{F}_{\gamma_\sharp}(\varrho) - \mathscr{F}_{\gamma_\sharp}(\varrho_\infty) \le -\frac{\varepsilon^3 \varrho_\infty}{3\beta}\int \Bigg(\sum_{k\in K^\delta} w_k\Bigg)^3 + O(\varepsilon^4).$$

The resonance condition $k^a = k^b + k^c$ ensures that

$$\int \Bigg(\sum_{k\in K^{\delta*}} w_k\Bigg)^3 > 0\ .$$

Phase transitions on high dimensional spheres

[Shalova-S. arXiv:2412.14813]



https://advlabs.aapt.org/wiki/Physics_of_Liquid_Crystals

Generalization to spheres

What changes if $\mathbb{T}_L^d$ is replaced by compact Riemannian manifold $\mathcal{M}^d$?

General case: $\mathcal{M}^d$

- thermodynamic formulation of stationary points is coordinate free:

  Stationary McKean-Vlasov equation: $\gamma^{-1}\Delta\rho + \nabla\cdot(\rho\nabla W * \rho) = 0$

  Zero of Gibbs Map $F : \mathcal{P}_{ac}(\mathcal{M}) \times \mathbb{R}_+ \to \mathcal{P}_{ac}(\mathcal{M})$: $F(\rho,\gamma) = \rho - \frac{1}{Z(\gamma,\rho)} e^{-\gamma W * \rho}$

  Critical point for free energy functional $\mathcal{F} : \mathcal{P}_{ac}^+(\mathcal{M}) \to \mathbb{R}$ with

  $$\mathcal{F}(\mu) := \gamma^{-1}\int \log\mu \,\mathrm{d}\mu + \frac{1}{2}\int_{\mathcal{M}\times\mathcal{M}} W(x,y)d\mu(x)d\mu(y)$$

- Ricci curvature enters condition on convextiy and uniqueness of stationary points [Sturm '05]

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Model case: $\mathbb{S}^{n-1}$

- Use spherical harmonics ONS
- translational symmetry on $\mathbb{T}^d$ replaced by spherical symmetry on $\mathbb{S}^{n-1}$ (zonal spherical harmonics)
- local bifurcation analysis via Crandall-Rabinowitz
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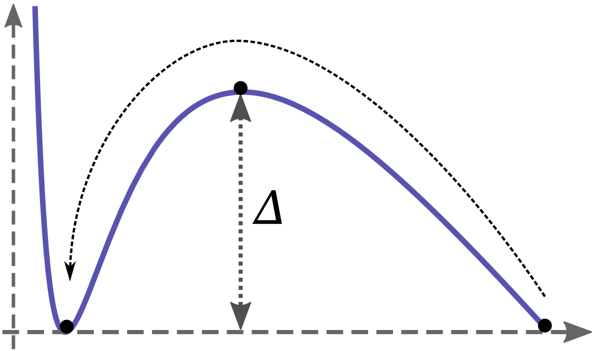
Link to condensation in noisy transformer models (LLM)
$\Rightarrow$ Phd thesis [**Shalova**]

A mountain pass theorem

[Gvalani-S. '20]



Noise-induced transitions in $\mathbb{R}^d$

Start form deterministic gradient flow in $\mathbb{R}^d$

$$\dot{x}(t) = -\nabla F(x) \quad \text{with} \quad x(0) = x_0 \in \mathbb{R}^d$$

- F has two global minima $m_1, m_2 \in \mathbb{R}^d$.

Describe the particle transition from m_1 to m_2 under the influence of noise.

Modelproblem: Add Brownian motion

$$dX_t = -\nabla F(X_t)\,\mathrm{d}t + \sqrt{2\sigma} dB_t\,,$$

Question: Given $X(0) = m_1$, what is the probability that in some finite time $T > 0$, we have that $X(T) = m_2$ in the regime $\sigma \ll 1$?

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Theorem (Freidlin–Wentzell)

The family of processes $\{X_t^\sigma\} \in C([0,T];\mathbb{R}^2)$ satisfy a LDP with good rate function $I : C([0,T];\mathbb{R}^d) \to \mathbb{R} \cup \{+\infty\}$

$$I(x(\cdot)) = \frac{1}{4} \int_0^T |\dot{x}(t) + \nabla F(x(t))|^2 \,\mathrm{d}t.$$

and it holds

$$\mathbb{P}(X_t^\sigma \in \Gamma) \approx \exp\left(-\sigma^{-1} \inf_{x \in \Gamma} I(x(\cdot))\right) \qquad \sigma \ll 1,$$

for any $\Gamma \subset C([0,T];\mathbb{R}^d)$.

Noise-induced transitions in $\mathbb{R}^d$

For $x \in \Gamma = \{f \in C^1([0,T];\mathbb{R}^d) : x(0) = m_1, x(T) = m_2\}$ let $T^* = \arg\max_{t\in[0,T]}(F(x(t)) - F(x(0)))$:

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$$= \frac{1}{4}\int_0^{T^*} |\dot{x}(t) - \nabla F(x(t))|^2 \,\mathrm{d}t + \int_0^{T^*} \dot{x}(t)\cdot\nabla F(x(t))\,\mathrm{d}t + \frac{1}{4}\int_{T^*}^{T} |\dot{x}(t) + \nabla F(x(t))|^2 \,\mathrm{d}t$$

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&\geq F(x(T^*)) - F(x(0)) \geq \inf_{x(\cdot)\in\Gamma}(F(x(T^*)) - F(x(0))) =: c - F(x(0))\,,
\end{aligned}$$

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Classical mountain pass theorem.
c a *critical value* of F, that is $\exists s \in \mathbb{R}^d : \nabla F(s) = 0, F(s) = c$.

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Freidlin-Wentzell:

$$\Rightarrow \qquad \mathrm{P}(X_t^\sigma \in \Gamma) \lesssim \exp(-\sigma^{-1}\Delta F) \qquad \text{where} \quad \Delta F = F(s) - F(m_1).$$

LDP for McKean-Vlasov interaction particle system

- Apply argument to the McKean–Vlasov N-particle system for $N \gg 1$

$$\mathrm{d}X_t^i = -\frac{\gamma}{N} \sum_{j=1, j\neq i}^{N} \nabla W(X^i - X^j)dt + \sqrt{2}\,\mathrm{d}B_t^i, \qquad i = 1, \dots, N$$

- [Dawson-Gärtner 1987] proved LDP with rate function for $\mu \in \mathrm{AC}^2([0,T], \mathcal{P}_2(\mathbb{T}_L^d))$ given by

$$I_\gamma(\mu(\cdot)) := \frac{1}{4} \int_0^T \|\partial_t \mu_t - \nabla \cdot (\mu_t \nabla(\log \mu_t + \gamma W \star \mu_t))\|_{-1,\mu_t}^2 \,\mathrm{d}t$$

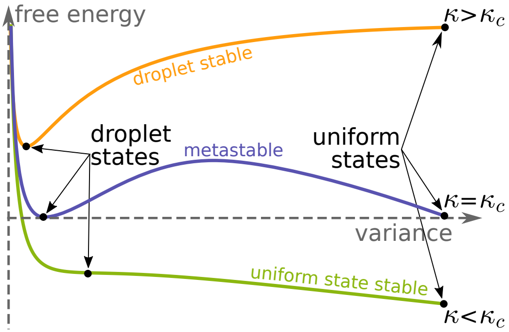
- McKean-Vlasov is GF w.r.t. W_2: Associated quasipotential to LDP is $\mathcal{F}_\gamma$!

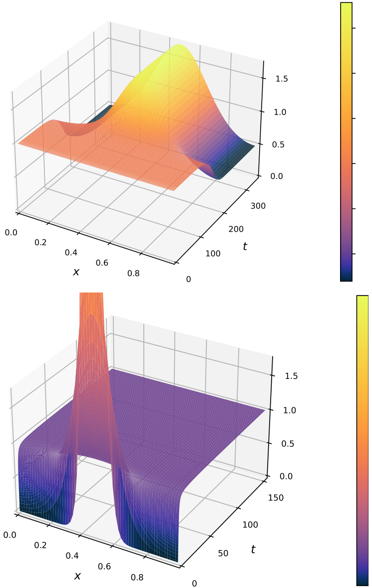
$$\mathbb{P}(\text{transition: } \varrho_\infty \to \varrho_{\gamma_c}) \simeq \exp\Big(-N \inf\{I_\gamma(\mu(\cdot)) : \mu(0) = \varrho_\infty, \mu(T) = \varrho_{\gamma_c}\}\Big)$$

$$\leq \exp\left(-N \inf_\mu \left\{ \sup_{T^* \in [0,T]} (\mathcal{F}_\gamma(\mu(T^*)) - \mathcal{F}_\gamma(\mu(0))) : \mu(0) = \varrho_\infty, \mu(T) = \varrho_{\gamma_c} \right\}\right).$$

Discontinuous phase transitions and metastability

- N-particle system is metastable at disc. phase transition
- By [Dawson-Gärtner 1989] need to understand free energy





- Missing ingredient: mountain pass theorem for $\mathcal{F}_\gamma$
  Difficulties:
  - $(\mathcal{P}(\mathbb{T}_L^d), W_2)$ only metric space
  - $\mathcal{F}_\gamma$ only lower semicontinuous

A mountain pass theorem

Theorem [Gvalani-S. '20]

If $\mathcal{F}_{\gamma_c}$ has two distinct minimizers $\varrho_\infty \equiv 1/L^d$ and $\varrho_{\gamma_c} \in \mathcal{P}(\mathbb{T}^d_L)$, then there exists $\varrho^* \in \mathcal{P}(\mathbb{T}^d_L)$ distinct from ϱ_∞ and ϱ_{γ_c} such that $|\partial \mathcal{F}_{\gamma_c}|(\varrho^*) = 0$.

Moreover: $\mathcal{F}_{\gamma_c}(\varrho^*) = c$ with $c = \inf_{\gamma \in \Gamma} \max_{t \in [0,Ts]} \mathcal{F}(\mu(t))$,

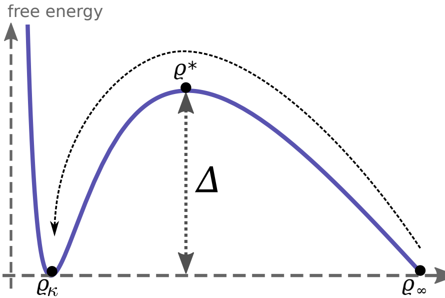
where $\Gamma = \{C([0,T];\mathcal{P}(\mathbb{T}^d_L)) : \mu(0) = \varrho_\infty, \mu(T) = \varrho_{\gamma_c}\}$.

Corollary (Arrhenius law)

The empirical McKean-Vlasov process $\varrho^{(N)}$ satisfies

$$\mathbb{P}\left[\varrho^N(T) \in \overline{B}^{W_2}_\varepsilon(\varrho_{\gamma_c}), \varrho^{(N)}(0) = \varrho_0^{(N)}\right] \lesssim e^{-N\Delta}$$

for N sufficiently large with $\mathbb{E}(W_2(\varrho_0^{(N)}, \varrho_\infty)) \to 0$ and $\Delta := \mathcal{F}_{\gamma_c}(\varrho^*) - \mathcal{F}_{\gamma_c}(\varrho_\infty)$ with ϱ^* the mountain pass point.



Coarsening close to a discontinuous phase transition

[Gerber-Gvalani-Pavliotis-S. '25 WIP]

Locally interacting particle system on 1-dim torus

Let $\ell > 0$ interaction range and $\gamma > 0$ interaction strength.
Consider a locally attractive interaction potential $w : \mathbb{R} \to \mathbb{R}$ and define

$$W(x) := \gamma \ell w\left(\frac{x}{\ell}\right) \mathrm{d}y \qquad \text{for } |x| < \frac{1}{2}$$

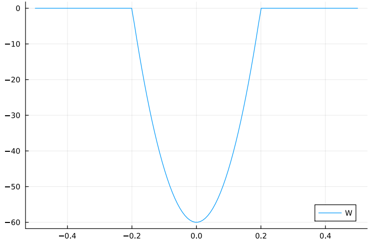
and extend $W_{\gamma,\ell}$ 1-periodically to $\mathbb{R}$.
For $i = 1, \dots, N$, consider

$$\mathrm{d}X_t^i = -\frac{1}{N} \sum_{j=1}^{N} \nabla W_{\gamma,\ell}\left(X_t^i - X_t^j\right) \mathrm{d}t + \sqrt{2}\, \mathrm{d}B_t^i$$

on the periodic domain $\mathbb{T} = \mathbb{R}/\mathbb{Z} \cong [0,1]$.

Main example: $w(x) = \frac{1}{2}\chi_{|x|\le 1}\left(|x|^2 - 1\right)$

Interested in the regime: $\gamma \gg 1$ **and** $\ell \ll 1$



Locally attractive: $w : \mathbb{R} \to (-\infty, 0]$

- is even
- has compact support
- has a global minimum at $x = 0$ with $w(0) < 0$, $w''(0) < 0$.

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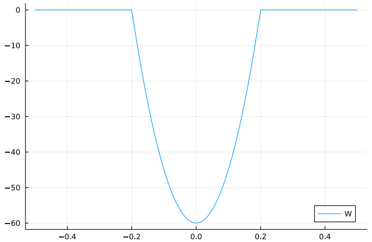
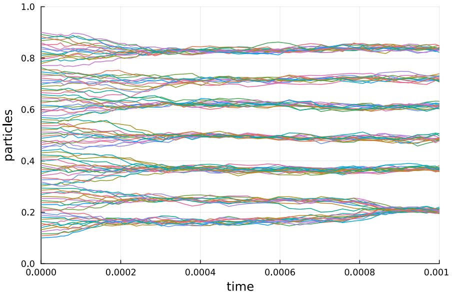
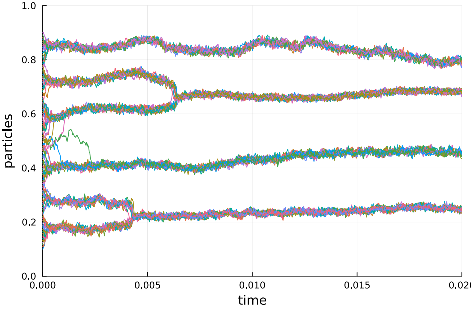


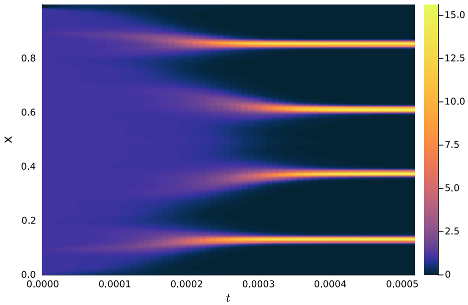


Motivation

Both particle model and mean-field PDE $\partial_t \rho = \Delta \rho + \nabla \cdot \big((\nabla W_{\gamma,\ell} * \rho)\rho \big)$ show **initial clustering**



clusters move and behave like
coalescing Brownian motions



clusters cannot move.

How can we explain this? Does coarsening appear for the PDE?

Initial clustering

Initial clustering

Heuristics by [Garnier, Papanicolaou, and Yang 2017]: Linearize the **mean-field PDE**

$$\partial_t \rho = \Delta \rho + \nabla \cdot \big((\nabla W_{\gamma,\ell} * \rho)\rho \big) \qquad \text{on } [0,1]$$

around uniform state $\rho_\infty \equiv 1$:

$$\rho \approx \rho_\infty + \rho_1(t,x) \qquad \Rightarrow \qquad \partial_t \rho_1(t,x) = \partial_x^2 \rho_1(t,x) + \partial_x(\rho_\infty W'_{\gamma,\ell} * \rho_1(t,x)).$$

Fourier modes $\hat{\rho}_1(t,k) := \int_0^1 \rho_1(t,x) e^{-ikx} \, \mathrm{d}x$ where $k \in 2\pi\mathbb{Z}$ satisfy

$$\partial_t \hat{\rho}_1(t,k) = \left(i\rho_\infty k \int_{[0,L]} W'_{\gamma,\ell}(x) e^{-ikx} \, \mathrm{d}x - k^2 \right) \hat{\rho}_1(t,k).$$

Growth rates

$$\psi(k) := \mathrm{Re} \left(\rho_\infty k \int_{[0,L]} W'_{\gamma,\ell}(x) e^{-ikx} \, \mathrm{d}x - k^2 \right) = -k^2 \left(\frac{1}{L} \widehat{W}_{\gamma,\ell}(k) + 1 \right)$$

are maximized for some

$$k_{\max} := \arg\max_{k \in 2\pi\mathbb{Z}} \psi(k).$$

Linear stability

universität ulm

For the linearized PDE

$$\rho \approx \rho_\infty + \rho_1(t,x) \qquad \Rightarrow \qquad \partial_t \rho_1(t,x) = \partial_x^2 \rho_1(t,x) + \partial_x(\rho_\infty W'_{\gamma,\ell} * \rho_1(t,x)), \qquad \text{(LinPDE)}$$

Fourier modes have the growth rates $\psi(k) = -k^2 \left(\frac{1}{L} \widehat{W}_{\gamma,\ell}(k) + 1 \right)$ where

$$\widehat{W}_{\gamma,\ell}(k) = \int_0^L W_{\gamma,\ell}(x) \cos(kx) \,\mathrm{d}x$$

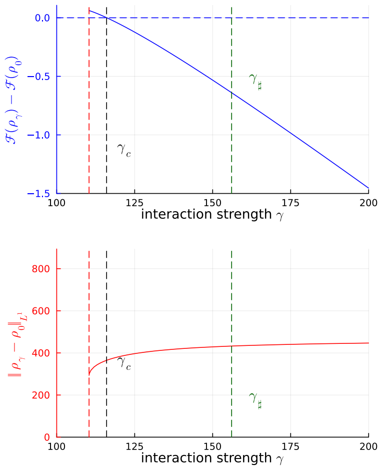
Thus, (LinPDE) is stable if and only if

$$\psi(k_{\max}) < 0 \qquad \Leftrightarrow \qquad \gamma < \gamma_\sharp := -\frac{L}{\min_{k \in \mathcal{K} \setminus \{0\}} \widehat{W}_{\gamma=1,\ell}(k)} > 0,$$

If $\gamma < \gamma_\sharp$: Convergence to uniform state ρ_∞ for (LinPDE)
If $\gamma > \gamma_\sharp$: (LinPDE) is unstable and initial clustering occurs with

$$n_{\text{clusters}} := \frac{k_{\max}}{2\pi} \text{ clusters} \quad \left(= 0.44 \frac{L}{\ell} \text{ for Hegselmann-Krause}\right).$$

Bifurcation diagram



Trivial branch $\rho_\infty \equiv 1$ and single-cluster branch ρ_γ.

Theorem ([Carrillo et al. 2020], [GS21])

Assume that $w\colon \mathbb{R} \to \mathbb{R}$ has compact support and that $\int_{\mathbb{R}} w(x)\,\mathrm{d}x < 0$. Then for sufficiently small $\ell > 0$, the potential $W_{\gamma,\ell}$ has a discontinuous transition point $\gamma_c < \gamma_\sharp$.

Free energy:

$$\mathcal{F}_{\gamma,\ell}(\rho) = \int_{[0,1]} \rho \log \rho + \frac{1}{2} \iint_{[0,1]^2} W_{\gamma,\ell}(x-y)\rho(x)\rho(y).$$

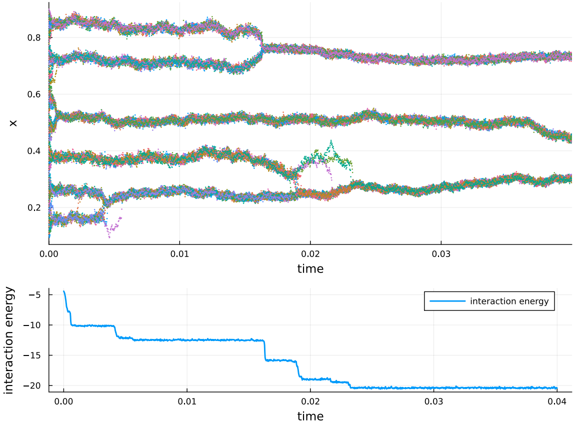
Coarsening after initial clustering

Coarsening in the particle model by merging

Assume $0 < \ell \ll 1$ and $\gamma \gg 1$.
After initial clustering, the cluster centers $X^{(1)}, \ldots, X^{(K)}$ move like Brownian particles

$$X_t^{(j)} = X_{\tau_0}^{(j)} + \frac{\sqrt{2}}{\sqrt{N m^{(j)}}} W_t^{(j)},$$

where initially the masses $m(j)$ of the clusters are given by $m(j) = \frac{1}{n_{\text{clusters}}}$.

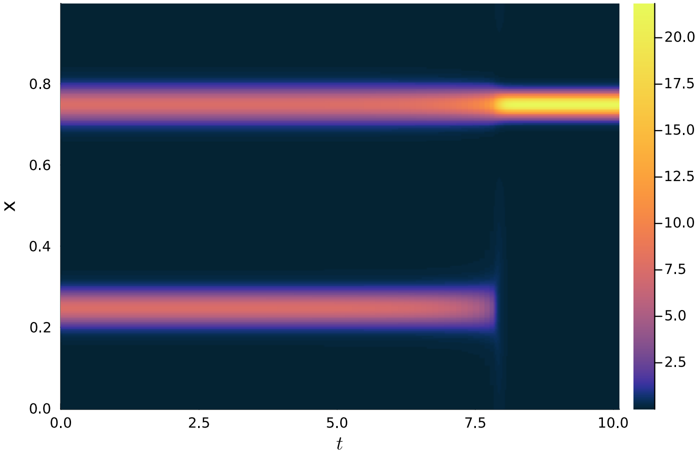


Coalesence: Two clusters j and k come close and merge to a cluster with mass $m^{(j)} + m^{(k)}$. The process continues until all clusters have merged into one cluster.

$\Rightarrow$ **System of coalescing heavy Brownian particles.**

Coarsening in the PDE by mass transfer

Starting two clusters with masses $m^{(1)} = 0.49$ and $m^{(2)} = 0.51$ at distance 0.5, we observe



Dynamical metastability by means of mass transfer in the PDE

Introducing mass transfer

Joint model for positions and masses of clusters

At time t, there are $K(t)$ clusters with centers $X_t^{(1)}, \dots, X_t^{(K(t))}$, and masses $m_t^{(1)}, \dots, m_t^{(K(t))}$.

$$X_t^{(j)} = X_{\tau_0}^{(j)} + \frac{\sqrt{2}}{\sqrt{N m^{(j)}}} W_t^{(j)} \qquad \text{for } j = 1, \dots, K(t)$$

$$\frac{\mathrm{d}}{\mathrm{d}t} m^{(j)} = \phi_{j-1}^{(r)} m^{(j-1)} + \phi_{j+1}^{(l)} m^{(j+1)} - \left(\phi_j^{(r)} + \phi_j^{(l)}\right) m^{(j)} \quad \text{for } j = 1, \dots, K(t),$$

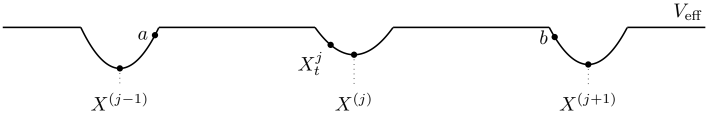
Rates $\phi_j^{(r/l)}$ are the hitting times to leave towards the right/left cluster Eyring-Kramers law

$$\phi^{(r/l)}(m, x_l, x, x_r) = \frac{1}{\left|x_{r/l} - x\right|_{\mathrm{dir}}} \sqrt{\frac{2\pi\ell}{\gamma w''(0) m}} \; \exp(-\gamma \ell \Delta m)\,.$$

where $\Delta = \sup w - \inf w$ (potential barrier)

Derivation of the joint model

Consider particle X_t^i in cluster j.



Particle X_t^i moves in the effective potential

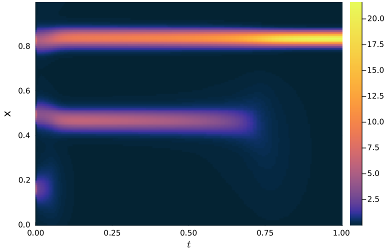
$$V_{\text{eff}}(x) = \left(W_{\gamma,\ell} \star \mu_t^N\right)(x) \approx \sum_{k=1}^{K(t)} \gamma \ell m^{(k)} w\left(\frac{x - X^{(k)}}{\ell}\right),$$

that is $\mathrm{d}X_t^i = -V'_{\text{eff}}(X_t^i)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}B_t^i$
$\Rightarrow$ Use potential theory to calculate hitting rates a before b and vice versa.

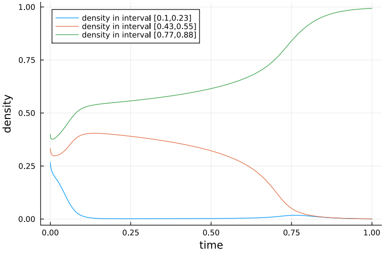
Qualitative comparison of PDE-mass and ODE-masses

Consider three equidistant clusters with masses $\frac{4}{15}$, $\frac{5}{15}$ and $\frac{6}{15}$

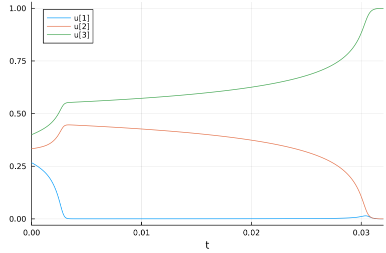
PDE simulation



Cluster masses PDE
(mass in subintervals)



Cluster masses ODE
(no parameter fitting)



Boundary conditions for the proposed model

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is subject to the boundary conditions:

- **Cluster merging:** If two clusters with centers $X^{(j)}$ and $X^{(k)}$ meet, they merge into a single cluster of mass $m^{(j)} + m^{(k)}$
- **Dissolution below critical mass m_{crit}:** If the mass $m^{(j)}$ of a cluster becomes smaller than the critical mass m_{crit}, cluster is removed from the system

Why is there minimal mass m_{crit} for a cluster to be stable?

- Particles in cluster of mass $m \in (0, 1)$ perform Ornstein-Uhlenbeck motion with variance $\sigma^2 = \frac{\ell}{\gamma w''(0) m}$.
- Interaction potential has finite interaction range of order ℓ.
- Therefore, cluster is stable only if $\sigma \gg \ell$, that is

$$m > m_{\text{crit}} \asymp \frac{1}{\gamma \ell w''(0)}.$$

Timescales

Joint model for positions and masses of clusters

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Coalescence timescale:

$$t_{\text{coalesence}} \asymp N.$$

Mass transfer timescale / Metastability timescale:

t_{metastab} is of the order $e^{\gamma \ell \Delta}$, where $\Delta = \sup w - \inf w$.

Outlook: A structure-preserving scheme for the SPDE

Need to reintroduce noise to the McKean-Vlasov model: Dean-Kawasaki equation

$$\partial_t \rho_t = \nabla \cdot \left(\nabla \rho + \rho \nabla W * \rho + N^{-1/2} \sqrt{\rho}\, \xi_t \right)$$

with $(\xi_t)_{t \geq 0}$ space-time white noise.

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- or **trivial**: Martingale solutions on empirical measures with N atoms are equivalent to the N particle system
- In general: Suitable finite dimensional approximations are closer to the particle system than the mean-field limit [Cornalba, Fischer, '21+]

Question: Is there a fluctuating Scharfetter-Gummel scheme?

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Stochastic two-point flux approximation between volume-cell K and L at distance $h > 0$: Solve for given $\beta > 0$, $q, \xi \in \mathbb{R}$ the boundary value problem $a, b > 0$ in $\rho : [0, h] \to \mathbb{R}$ and $j \in R$

$$j = -\beta^{-1} \partial_x \rho + \rho q + \sqrt{\rho} \xi, \qquad \rho(0) = a \quad \text{and} \quad \rho(h) = b.$$

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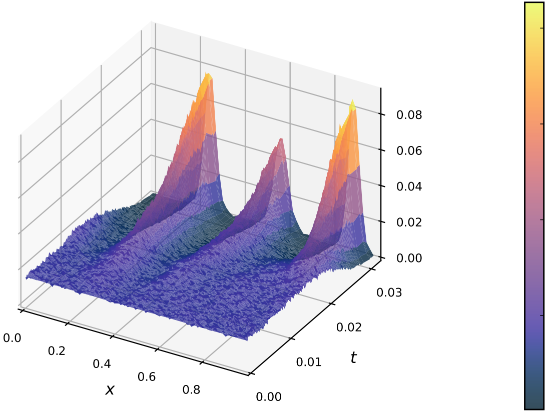
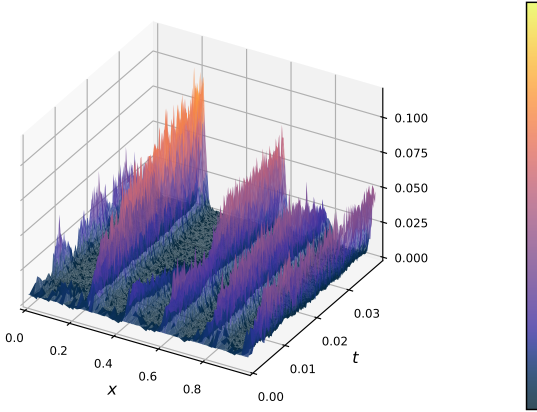
Solution is an implicit integral equation:
$\Rightarrow$ Together with time-implicit Euler, get a positivity preserving scheme!

Outlook: Numerical results

Scheme captures initial clustering regime:



Clusters merge thanks to local diffusion:



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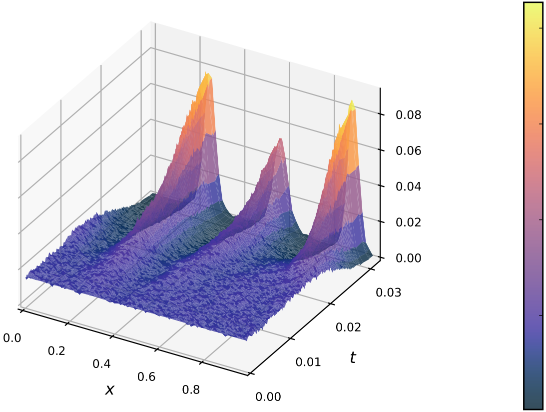

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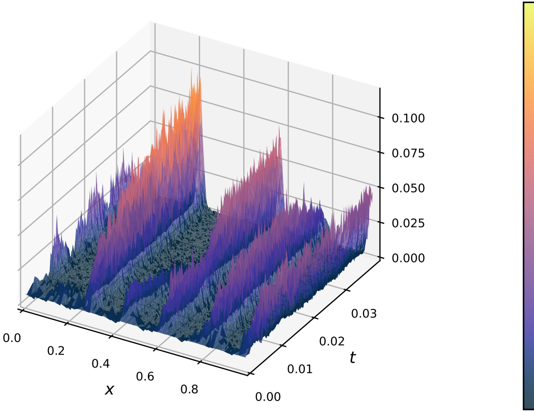

Thank you for your attention!