

Alignment of self-propelled particles : from microscopic to hydrodynamic kinetic models.

Amic Frouvelle – CEREMADE – Université Paris Dauphine
Mathematical Methods for the Study of Self-organization in the
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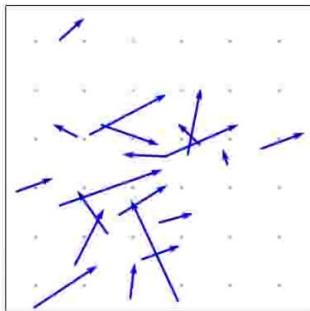
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First example: Cucker–Smale Model

N particles, at positions $x_i \in \mathbb{R}^d$, aligning their velocities $v_i \in \mathbb{R}^d$.

$$\frac{dx_i}{dt} = v_i,$$

$$\frac{dv_i}{dt} = \frac{1}{N} \sum_{j=1}^N K(|x_j - x_i|)(v_j - v_i).$$

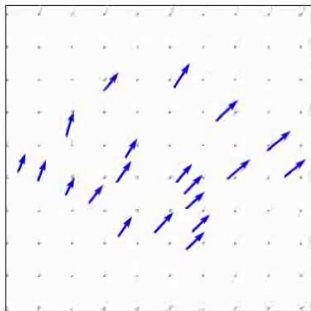


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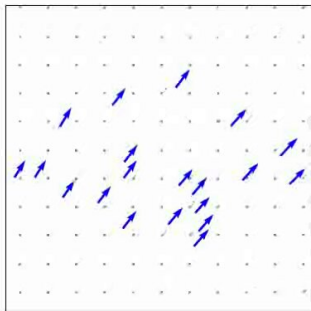


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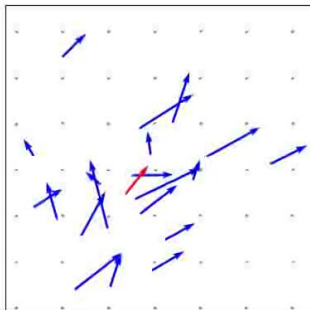


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Theorem : Cucker-Smale 2007 [CS07, HL09]

Flocking if $\int_0^{+\infty} K(r)dr = \infty$.

For any initial condition, there exists $C, \lambda, M > 0$ and $v_\infty \in \mathbb{R}^d$ such that $|v_i(t) - v_\infty| \leq Ce^{-\lambda t}$ and $|x_i(t) - x_j(t)| \leq M$ (for all i, j and $t \in \mathbb{R}$).

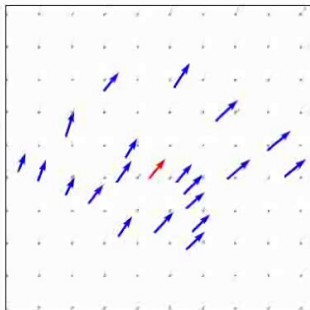


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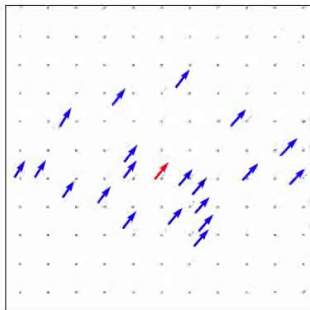


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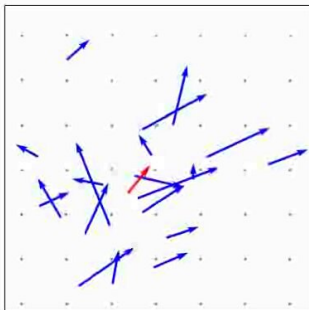


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Exercise : a strong observation kernel is needed

For 2 particles, with $x_1 = x_2 = 0$ initially, prove that there exists some “observation kernel” $K > 0$ such that $|x_1(t) - x_2(t)| \rightarrow +\infty$.

Idea : reverse engineering (start by given trajectories $x_1(t)$ and $x_2(t)$ and find K).

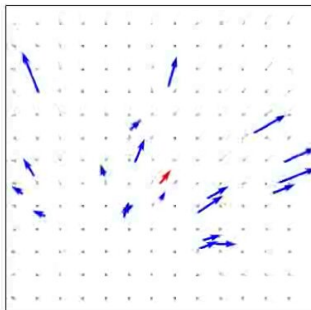


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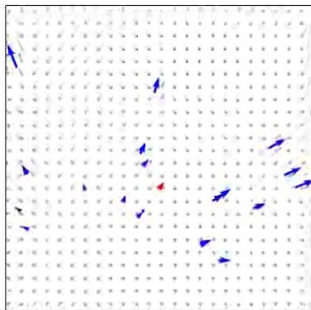


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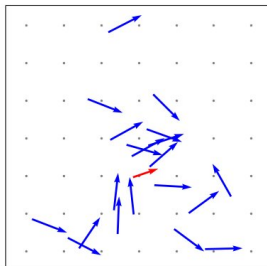
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Second example: aligning self-propelled particles (2D)

N particles, at positions $x_i \in \mathbb{R}^2$, with speed 1 and angle $\theta_i \in \mathbb{R}$.

$$\frac{dx_i}{dt} = \begin{pmatrix} \cos \theta_i \\ \sin \theta_i \end{pmatrix} = \tau(\theta_i), \quad \frac{d\theta_i}{dt} = \frac{1}{N} \sum_{j=1}^N K(x_j - x_i) \sin(\theta_j - \theta_i).$$



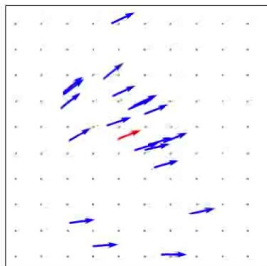
Exercise : well-posed ODE in \mathbb{R}^{3N}

This is an ODE of the form $\frac{dZ}{dt} = B(Z)$. If K is bounded and Lipschitz, then B is globally Lipschitz and Cauchy-Lipschitz theorem applies.

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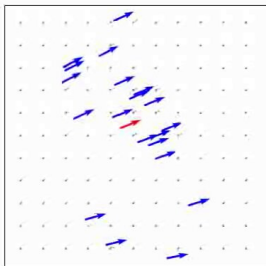
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Empirical measure, indistinguishable particles

Definition : Empirical measure $\mu_t^N = \frac{1}{N} \sum_{i=1}^N \delta_{x_i} \otimes \delta_{\theta_i}$

$$\forall \varphi \in C^b(\mathbb{R}^2 \times \mathbb{R}), \langle \varphi \rangle_{\mu_t^N} = \int_{\mathbb{R}^2 \times \mathbb{R}} \varphi \, d\mu_t^N = \frac{1}{N} \sum_{i=1}^N \varphi(x_i(t), \theta_i(t))$$

Exchangeability : μ_t^N invariant under label permutations, all the particles $z_i = (x_i, \theta_i)$ follow the (non-autonomous) flow

$$\begin{cases} \frac{dx}{dt} = \tau(\theta) \\ \frac{d\theta}{dt} = b[\mu_t^N](x, \theta), \end{cases}$$

where we have set $b[f](x, \theta) = \int_{\mathbb{R}^2 \times \mathbb{R}} K(x' - x) \sin(\theta' - \theta) df(x', \theta')$.

Exercise : close equation for μ_t^N !

Prove that μ_t^N is a weak solution of the following kinetic equation :

$$\partial_t \mu_t^N + \tau(\theta) \cdot \nabla_x \mu_t^N + \partial_\theta (b[\mu_t^N] \mu_t^N) = 0.$$

Useful notation : $\mathcal{J}_f = \int_{\mathbb{R}} \tau(\theta) df(\theta)$, and $\mathcal{J}_f^K = K * \mathcal{J}_f$. We then get $b[f](x, \theta) = \partial_{\theta}(\tau(\theta) \cdot \mathcal{J}_f^K)$.

Theorem : global well-posedness

If K is bounded and Lipschitz, then the Vlasov equation

$$\partial_t f + \tau(\theta) \cdot \nabla_x f + \partial_{\theta}(\partial_{\theta}(\tau(\theta) \cdot \mathcal{J}_f^K) f) = 0$$

is well-posed in $C([0, T], \mathcal{P}_1(\mathbb{R}^2 \times \mathbb{R}))$.

Ref.: H. Spohn, "Large scale dynamics of interacting particles" [Spo91].

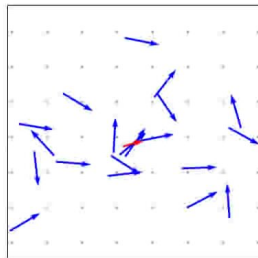
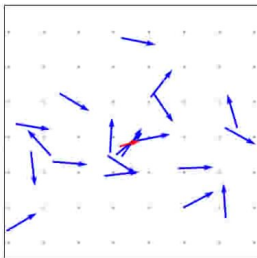
- Solve the linear (nonautonomous) equation $\partial_t f + \tau(\theta) \cdot \nabla_x f + \partial_{\theta}(\partial_{\theta}(\tau(\theta) \cdot J(x, t)) f) = 0$ by characteristics : $f = \Phi(J)$.
- Fixed point in $C([0, T], \mathcal{P}_1(\mathbb{R}^2 \times \mathbb{R}))$ of $f \mapsto \Phi(\mathcal{J}_f^K)$. Links between the Lipschitz character of K and contraction in Wasserstein distance.

Third example: same thing, with noise !

System of stochastic differential equations (SDE).

$$dx_i = \begin{pmatrix} \cos \theta_i(t) \\ \sin \theta_i(t) \end{pmatrix} dt,$$

$$d\theta_i = \frac{1}{N} \sum_{j=1}^N K(|x_j - x_i|) \sin(\theta_j - \theta_i) dt + \sqrt{2\sigma} dB_t^i.$$

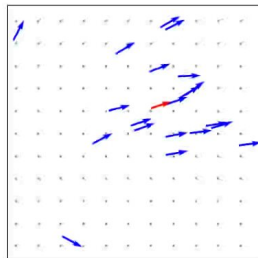
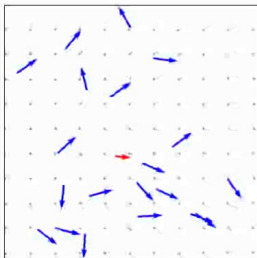


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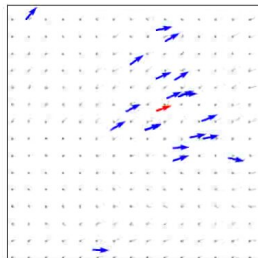
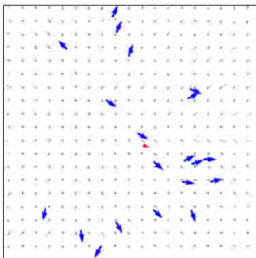


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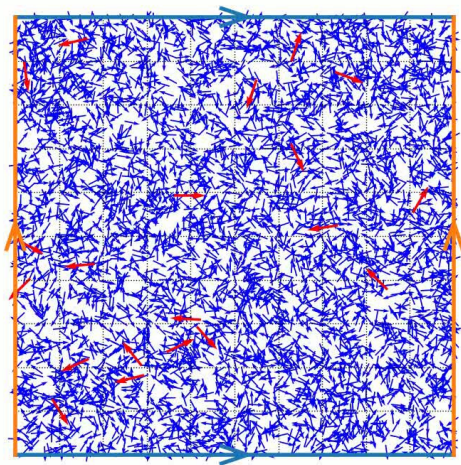
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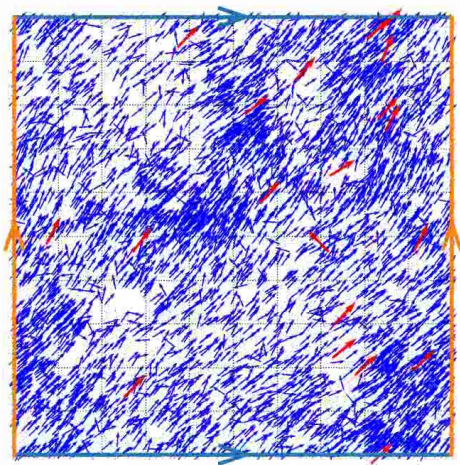
Artificial confinement

If $x \mapsto K(|x|)$ is periodic (think with small compact support + periodic extension), then everything works in $C([0, T], \mathcal{P}(\mathbb{R}^2/\Gamma \times \mathbb{R}/2\pi\mathbb{Z}))$.



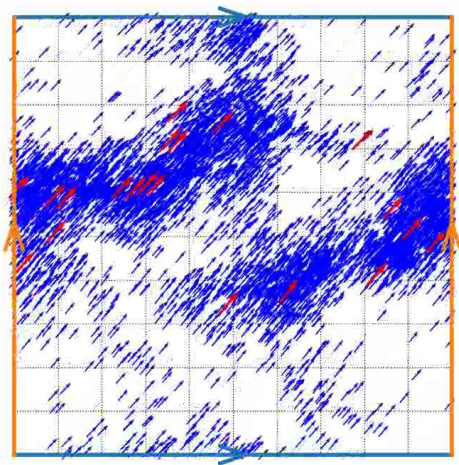
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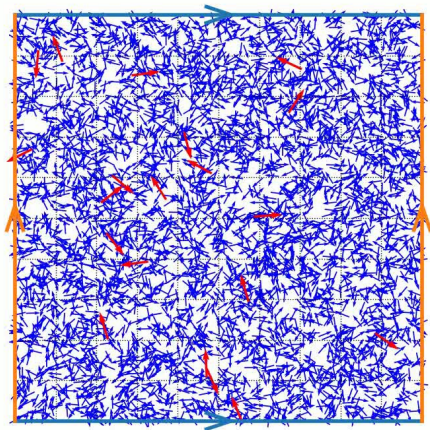
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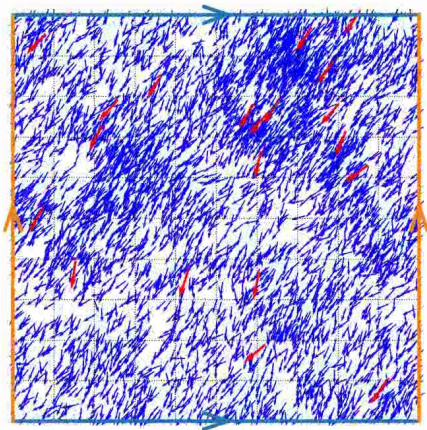
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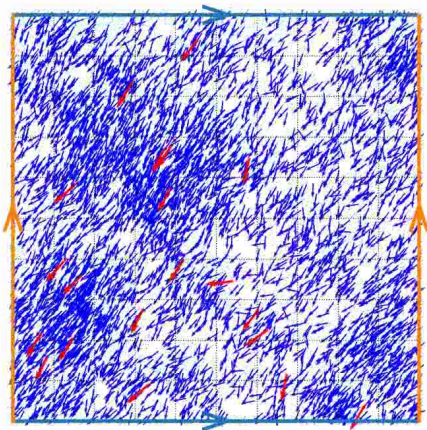
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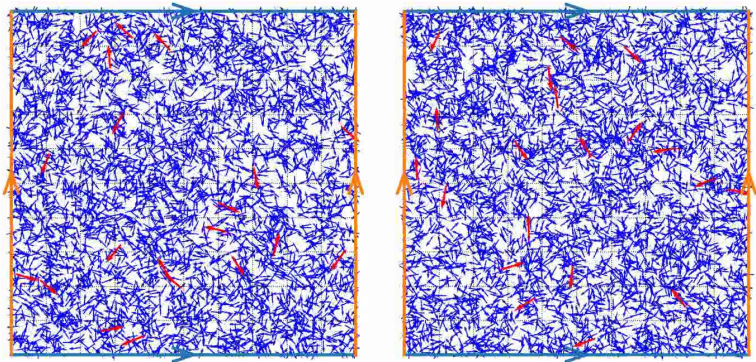


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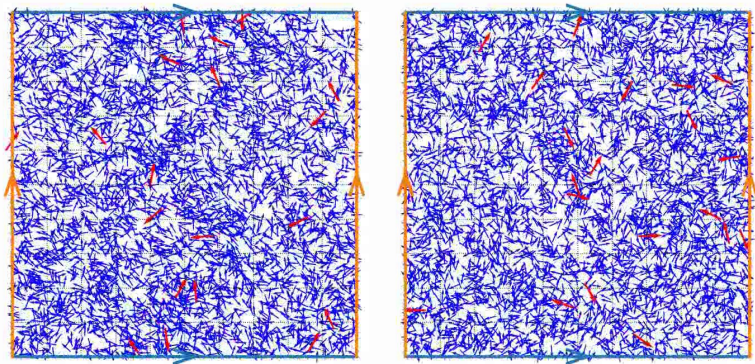


Now μ_t^N is a probabilistic object (realisations of the brownian motions).
How to get a kinetic equation for that ?

\rightsquigarrow Law of large numbers. . . $\langle \varphi \rangle_{\mu_t^N} = \frac{1}{N} \sum_{i=1}^N \varphi(x_i(t), \theta_i(t)) \xrightarrow{?} \langle \varphi \rangle_{\mu_t}$.

Main ref.: A.-S. Sznitman, "Topics in propagation of chaos" [Szn91].

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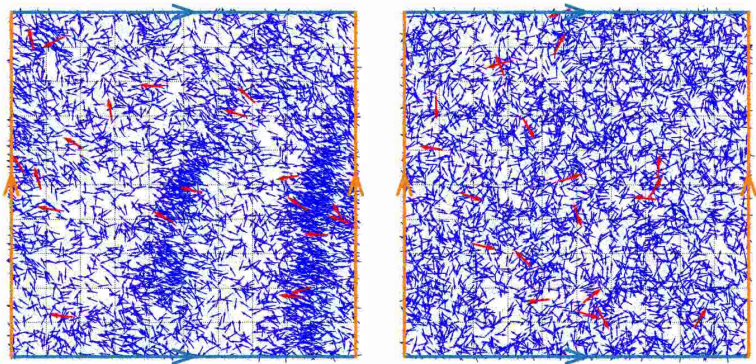


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Existence theory for SDEs

Rewrite the system in integral formulation, and with $b[\mu_t^N]$ (exchangeability).

$$x_i(t) = x_i^0 + \int_0^t \tau(\theta_i(s)) ds,$$

$$\theta_i(t) = \theta_i^0 + \int_0^t b[\mu_s^N](x_i(s), \theta_i(s)) ds + \sqrt{2\sigma} B_t^i.$$

If K is bounded and Lipschitz : fixed point argument as in Cauchy-Lipschitz theory. Pathwise global existence and uniqueness of solutions.

Law of the $3N$ -dimensional process (linear), Ito formula

Probability density $f^N(x_1, \theta_1, \dots)$ of finding particles around (x_i, θ_i) :

$$\partial_t f^N + \sum_{i=1}^N [\tau(\theta_i) \cdot \nabla_{x_i} f^N + \partial_{\theta_i} (b[\mu^N](x_i, \theta_i) f^N)] = \sigma \sum_{i=1}^N \partial_{\theta_i}^2 f^N,$$

where $b[\mu^N](x, \theta) = \frac{1}{N} \sum_{j=1}^N K(x_j - x) \sin(\theta_j - \theta)$.

Exercise : equation of the first marginal

If $f^{N,1}(x, \theta) = \int f^N(x, \theta, x_2, \theta_2 \dots) dx_2 d\theta_2 \dots dx_n d\theta_n$
and $f^{N,2}(x, \theta, x', \theta') = \dots$, then

$$\partial_t f^{N,1} + \tau(\theta) \cdot \nabla_x f^{N,1} + \frac{N-1}{N} \partial_\theta (b[f^{N,2}(x, \theta, \cdot, \cdot)](x, \theta)) = \sigma \partial_{\theta\theta}^2 f^{N,1}.$$

If $f^{N,1} \rightarrow f$ and $f^{N,2} \rightarrow f \otimes f$ (asymptotic indep. of two particles), then

$$\partial_t f + \tau(\theta) \cdot \nabla_x f + \partial_\theta (b[f]f) = \sigma \partial_{\theta\theta}^2 f.$$

This is very formal, but we recover the (nonlinear) Vlasov equation with a diffusion. Can we rigorously derive this equation ?

Notice that it can be written (since $b[f] = \partial_\theta (\mathcal{J}_f^K \cdot \tau(\theta))$) as

$$\partial_t f + \tau(\theta) \cdot \nabla_x f = \sigma \partial_\theta \left(e^{\frac{1}{\sigma} \mathcal{J}_f^K \cdot \tau(\theta)} \partial_\theta \left(\frac{f}{e^{\frac{1}{\sigma} \mathcal{J}_f^K \cdot \tau(\theta)}} \right) \right).$$

The nonlinear coupling processes

We look at processes which are the natural limits of (x_i, θ_i) as $N \rightarrow \infty$.

Theorem [Szn91]

There exist a unique solution, pathwise and in law, to

$$\begin{aligned}\bar{x}(t) &= x^0 + \int_0^t \tau(\bar{\theta}(s)) ds, \\ \bar{\theta}(t) &= \theta^0 + \int_0^t b[\bar{\mu}_s](\bar{x}(s), \bar{\theta}(s)) ds + \sqrt{2\sigma} B_t,\end{aligned}$$

where $\bar{\mu}_t$ is the law of the process $\bar{x}(t), \bar{\theta}(t) : \mathbb{E}[\varphi(\bar{x}(t), \bar{\theta}(t))] = \langle \varphi \rangle_{\bar{\mu}_t}$.

- No more index i , no more N , only one particle interacting with its own law.
- Fixed point problem for the law $\bar{\mu}_t$.
- PDE satisfied by $\bar{\mu}_t$? by Itô formula, we get

$$\partial_t \bar{\mu}_t + \tau(\theta) \cdot \nabla_x \bar{\mu}_t + \partial_\theta (b[\bar{\mu}_t] \bar{\mu}_t) = \sigma \partial_{\theta\theta}^2 \bar{\mu}_t.$$

Distance between processes

We therefore introduce $(\bar{x}_i, \bar{\theta}_i)$, the nonlinear coupling processes associated to the same initial conditions x_i^0, θ_i^0 and Brownian motion B_t^i . Their law is always $\bar{\mu}_t$ (if the initial condition are iid), and they are independent. They satisfy

$$x_i - \bar{x}_i(t) = \int_0^t [\tau(\theta_i) - \tau(\bar{\theta}_i)](s) ds,$$

$$\theta_i - \bar{\theta}_i(t) = \int_0^t (b[\mu_s^N](x_i(s), \theta_i(s)) - b[\bar{\mu}_s](\bar{x}_i(s), \bar{\theta}_i(s))) ds,$$

For convenience : $z_t^i = (x_i(t), \theta_i(t))$, $\bar{z}_t^i = (\bar{x}_i(t), \bar{\theta}_i(t))$, and the new empirical distribution $\bar{\mu}_t^N = \frac{1}{N} \sum_{i=1}^N \delta_{\bar{z}_t^i}$. We obtain

$$\begin{aligned} |\theta_i - \bar{\theta}_i(t)| &\leq \int_0^t |b[\mu_s^N](z_s^i) - b[\mu_s^N](\bar{z}_s^i)| ds \quad (\text{use } b[f](\cdot) \text{ Lipschitz}) \\ &+ \int_0^t |b[\mu_s^N](\bar{z}_s^i) - b[\bar{\mu}_s^N](\bar{z}_s^i)| ds \quad (\text{use } b[\cdot](z) \text{ Lipschitz}) \\ &+ \int_0^t |b[\bar{\mu}_s^N](\bar{z}_s^i) - b[\mu_s](\bar{z}_s^i)| ds \quad (\text{LLN for indep. processes}). \end{aligned}$$

Distance between processes (continued)

We obtain, after using exchangeability and taking expectation

$$\mathbb{E}[|z_t^1 - \bar{z}_t^1|] \leq C \int_0^t \mathbb{E}[|z_s^1 - \bar{z}_s^1|] ds + \int_0^t \mathbb{E}[|b[\bar{\mu}_s^N](\bar{z}_s^1) - b[\mu_s](\bar{z}_s^1)|] ds.$$

Recall: $b[\bar{\mu}_s^N](\bar{z}_s^1) = \frac{1}{N} \sum_{i=1}^N \beta(\bar{z}_s^i, \bar{z}_s^1)$ and $b[\mu_s](\bar{z}_s^1) = \int \beta(z, \bar{z}_s^1) d\mu_s(z)$, with $\beta(z, z') = K(x - x') \sin(\theta - \theta')$, so β is bounded and Lipschitz.

Therefore $\mathbb{E}[|b[\bar{\mu}_s^N](\bar{z}_s^1) - b[\mu_s](\bar{z}_s^1)|] = \mathbb{E}\left[\left|\frac{1}{N} \sum_{i=1}^N Y_i\right|\right]$, where the random variables $Y_i = \beta(\bar{z}_s^i, \bar{z}_s^1) - \int \beta(z, \bar{z}_s^1) d\mu_s(z)$ are centered, bounded, pairwise independent. We get $\mathbb{E}\left[\left|\frac{1}{N} \sum_{i=1}^N Y_i\right|\right]^2 \leq \frac{1}{N^2} \mathbb{E}\left[\left(\sum_{i=1}^N Y_i\right)^2\right] \leq \frac{C}{N}$.

Final estimation (with Gronwall)

$$\sup_{t \in [0, T]} W_1(f^{N,1}(t), \bar{\mu}_t) \leq \sup_{t \in [0, T]} \mathbb{E}[|z_t^1 - \bar{z}_t^1|] \leq \frac{e^{CT}}{\sqrt{N}}.$$

Remarks, to go beyond

- More details in [Szn91] : convergence of the empirical measure, case of non independent initial conditions, but “chaotic”.
- No propagation of chaos uniformly in time : $\frac{e^{CT}}{\sqrt{N}}$ is small only if $T \ll \ln N$.
- Can be adapted to non binary collisions, when $b[\mu^N]$ is not linear in μ^N , but only Lipschitz, and when σ also depends on μ^N [Oel84].
- Same model in higher dimensions (on the sphere) : [BCC12]

Unit speed particles $(X_i, V_i) \in \mathbb{R}^d \times \mathbb{S}^{d-1}$

$$dX_i = V_i dt, dV_i = \frac{1}{N} \sum_{j=1}^N K(X_i - X_j) P_{V_i^\perp} V_j + \sqrt{2\sigma} P_{V_i^\perp} \circ dB_t^i.$$

Careful : orthogonal projection to keep unit speed + Stratonovich formulation for diffusion on the sphere. Limit law, density $f(t, x, v)$:

$$\begin{cases} \partial_t f + v \cdot \nabla_x f + \nabla_v \cdot (\nabla_v (\mathcal{J}_f^K \cdot v) f) = \sigma \Delta_v f \\ \mathcal{J}_f^K = \int_{\mathbb{R}^d \times \mathbb{S}^{d-1}} K(x - y) v f(t, y, v) dy dv. \end{cases}$$

Careful : divergence and gradient on the sphere, Laplace-Beltrami.

Space-homogeneous model

No space, or $K = 1$: only equations on angles (f is 2π -periodic now).

$$\begin{cases} \partial_t f + \partial_\theta(\partial_\theta(\mathcal{J}_f \cdot \tau(\theta))f) = \sigma \partial_{\theta\theta} f \\ \mathcal{J}_f = \frac{1}{2\pi} \int_{-\pi}^{\pi} \tau(\theta) f(t, \theta) d\theta. \end{cases}$$

Fokker-Planck factorized formulations :

$$\partial_t f = \sigma \partial_\theta \left(e^{\frac{1}{\sigma} \mathcal{J}_f \cdot \tau(\theta)} \partial_\theta \left(e^{-\frac{1}{\sigma} \mathcal{J}_f \cdot \tau(\theta)} f \right) \right) = \sigma \partial_\theta \left(M_{\mathcal{J}_f} \partial_\theta \left(\frac{f}{M_{\mathcal{J}_f}} \right) \right),$$

with von-Mises distribution

$$M_J(\theta) = \frac{e^{\frac{1}{\sigma} J \cdot \tau(\theta)}}{\mathcal{Z}(J)}, \quad \mathcal{Z}(J) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{\frac{|J|}{\sigma} \cos \theta} d\theta.$$

Useful : $\partial_t f = \sigma \partial_\theta (\partial_\theta (\ln f - \frac{1}{\sigma} \mathcal{J}_f \cdot \tau(\theta)) f)$.

Dissipation of free energy $\mathcal{F}(f) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f \ln f d\theta - \frac{1}{2\sigma} \|\mathcal{J}_f\|^2$

$$\frac{d}{dt} \mathcal{F}(f) = -\frac{\sigma}{2\pi} \int_{-\pi}^{\pi} |\partial_\theta (\ln f - \frac{1}{\sigma} \mathcal{J}_f \cdot \tau(\theta))|^2 f d\theta := -\sigma \mathcal{D}[f].$$

Homogeneous steady-states

Equivalent conditions for steady states of FP equation

- $\mathcal{D}[f] = 0$.
- $f = M_J$ where $\mathcal{J}_{M_J} = \langle \tau \rangle_{M_J} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \tau(\theta) M_J(\theta) d\theta = J$.
- $f = M_J$ where J is a critical point of $V(J) = \frac{1}{2\sigma} \|J\|^2 - \ln \mathcal{Z}(J)$.
- f is a critical point of \mathcal{F} under unit mass constraint.
- $f = M_J$ where J is a critical point of $W(J) = \mathcal{F}[M_J]$.
- $f = M_{\kappa\Omega}$ for $\Omega \in \mathbb{S}^1$ and $\kappa = c(\kappa)$ for $c(\kappa) = \frac{\frac{1}{2\pi} \int_{-\pi}^{\pi} \cos \theta e^{\frac{\kappa}{\sigma} \cos \theta} d\theta}{\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{\frac{\kappa}{\sigma} \cos \theta} d\theta}$.

$\frac{\kappa}{c(\kappa)} \nearrow +\infty$ as $\kappa \rightarrow +\infty$, and $\searrow 2\sigma$ as $\kappa \rightarrow 0$.

Families of equilibria : threshold of phase transition

- Case $\sigma \geq \frac{1}{2}$. Only solution : $\kappa = 0$. Isotropic equilibrium (global minimizer of \mathcal{F} , 0 is global min for W and V).
- Case $\sigma < \frac{1}{2}$. Either isotropic (saddle for \mathcal{F} , local max for W , V), or unique solution $\kappa(\sigma) > 0$: family of von-Mises distributions (global min of \mathcal{F} , same for W , V). Close to Diracs if σ small.

Relative entropy and Fisher information.

$$\mathcal{H}(f|g) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f \ln \left(\frac{f}{g} \right) d\theta, \quad \mathcal{I}(f|g) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f \left| \partial_{\theta} \ln \left(\frac{f}{g} \right) \right|^2 d\theta.$$

Free energy / relative entropy identities :

- $\mathcal{F}[f] - \mathcal{F}[f_{\text{eq}}] = \mathcal{H}(f|M_{\mathcal{J}_f}) + V(\mathcal{J}_f) - V(\mathcal{J}_{\text{eq}}),$
- $\mathcal{H}(f|f_{\text{eq}}) = \mathcal{F}[f] - \mathcal{F}[f_{\text{eq}}] + \frac{1}{2\sigma} \|\mathcal{J}_{\text{eq}} - \mathcal{J}_f\|^2,$
- $\mathcal{D}[f] = \mathcal{I}(f|M_{\mathcal{J}_f}).$

Csiszár-Kullback-Pinsker and log-Sobolev inequalities

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} |f(\theta) - g(\theta)| d\theta \leq \sqrt{2 \mathcal{H}(f|g)}.$$

There exists $\lambda > 0$ such that for all $\|J\| \leq 1$ and proba f on \mathbb{S}^1 we have

$$\mathcal{H}(f|M_J) \leq \frac{1}{2\lambda} \mathcal{I}(f|M_J).$$

Exponential convergence to a stable steady-state

Coercivity properties of V : there exists $C > 0$ such for J close the set \mathcal{V}_∞ of minimizers, there exists $J_\infty \in \mathcal{V}_\infty$ such that (using CKP):

$$\frac{1}{C} \|J - J_\infty\|^2 \leq |V(J) - V(J_\infty)| \leq C \|\nabla V(J)\|^2 = \frac{C}{\sigma} \|\mathcal{J}_{M_J} - J\|^2$$

For $J = \mathcal{J}_f$, using CKP: $|V(J) - V_\infty| \leq \frac{2C}{\sigma} \mathcal{H}(f|M_{\mathcal{J}_f})$.

Therefore by the free energy / relative entropy identities and LSI :

$$0 \leq \mathcal{F}[f] - \mathcal{F}_\infty \leq (1 + \frac{2C}{\sigma}) \mathcal{H}(f|M_{\mathcal{J}_f}) \leq \tilde{C} \mathcal{D}[f].$$

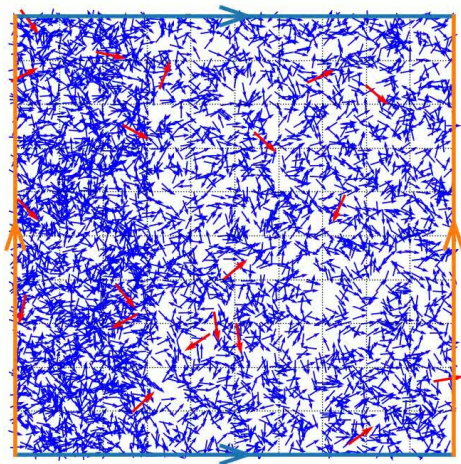
Gronwall : exponential decay of free energy, controlled by $\mathcal{H}(f|f_{eq,0})$ thanks to the identities. Stability: \mathcal{J}_f stays close to \mathcal{V}_∞ (coercivity + identities). Then $\frac{d}{dt} \mathcal{J}_f$ exponentially controlled (CKB + identities).

Theorem (see also [FL12]): exponential stability

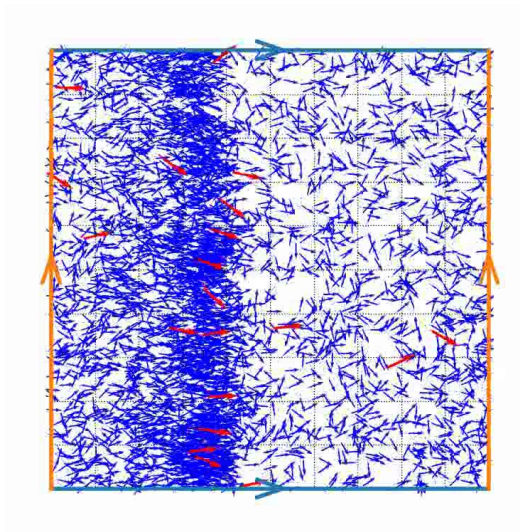
Let \mathcal{E}_∞ be the family of stable equilibria (in the sense of free energy), then there exists $\delta, \lambda, C > 0$ such that if $\mathcal{H}(f_0|f_{eq,0}) < \delta$ for $f_{eq,0} \in \mathcal{E}_\infty$, then there exists $f_\infty \in \mathcal{E}_\infty$ such that

$$\forall t \geq 0, \mathcal{H}(f(t, \cdot)|f_\infty) \leq C e^{-2\lambda t} \mathcal{H}(f_0|f_{eq,0}).$$

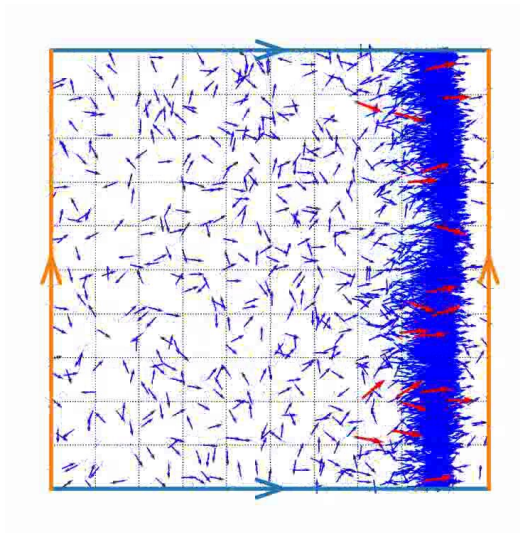
Movie time : the travelling bands (the phase transition picture for the inhomogeneous model is hard !)



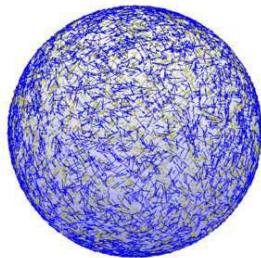
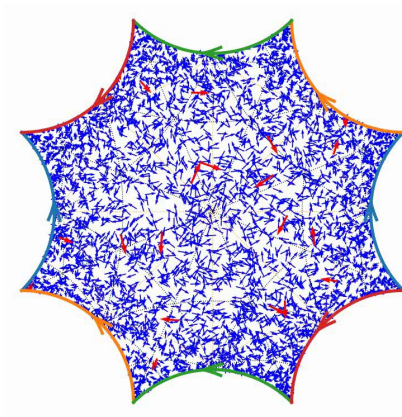
Movie time : the travelling bands (the phase transition picture for the inhomogeneous model is hard !)



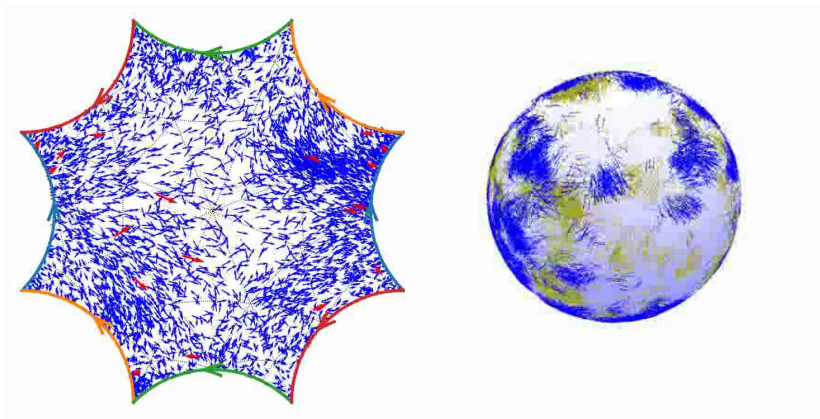
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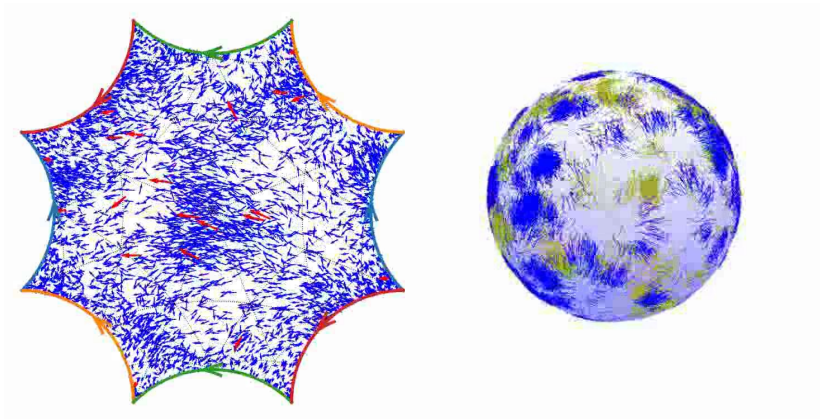
More geometries, more movies (in progress, with S. Motsch and A. Diez) !



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