Macroscopic limits of a system of self-propelled particles with phase transition

Amic Frouvelle

Archimedes Center for Modeling, Analysis & Computation (ACMAC)
University of Crete, Heraklion, Crete, Greece

Joint work with Jian-Guo Liu (Duke University)
and Pierre Degond (Institut de Mathématiques de Toulouse, France)

Emergent behaviour in multi-particle systems with non-local interactions
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Modeling alignment interaction of self-propelled particles

- Vicsek *et al.* (1995).
  Alignment only, constant speed, discrete in time (interval Δt), synchronous reorientation.

  $$\begin{array}{c}\text{New}\\ \text{direction}\end{array} = \begin{array}{c}\text{Mean direction of neighboring}\\ \text{particles at previous step}\end{array} + \text{Noise}$$

  Simulations: phase transition phenomenon, emergence of coherent structures.
- Degond-Motsch (2008).
  Time-continuous version: relaxation (with constant rate ν) towards the local mean direction.
  Hydrodynamic limit without phase transition phenomenon.
- Model presented here: making ν proportional to the local mean momentum.

Outline

1. Time-continuous Vicsek model with phase transition
   - Presentation of the model
   - Kinetic model – Hydrodynamic scaling
   - The phase transition
2. Formal derivation of macroscopic models
   - Ordered phase, hydrodynamic model
   - Disordered phase, diffusion

Individual dynamics

Particles at positions: $X_1, \dots, X_N$ in $\mathbb{R}^n$.
Orientations $\omega_1, \dots, \omega_N$ in $\mathbb{S}$ (unit sphere).

$$\begin{cases} \mathrm{d}X_k = \omega_k \mathrm{d}t \\ \mathrm{d}\omega_k = \nu(\mathrm{Id} - \omega_k \otimes \omega_k)\,\bar\omega_k \mathrm{d}t + \sqrt{2d}(\mathrm{Id} - \omega_k \otimes \omega_k) \circ \mathrm{d}B_t^k \end{cases}$$

Target direction:

$$\bar\omega_k = \frac{J_k}{|J_k|}, \quad J_k = \frac{1}{N}\sum_{j=1}^{N} K(|X_j - X_k|)\,\omega_j.$$

Setting $\nu = |J_k|\,\nu_0$, no more singularity (binary interactions):

$$\begin{cases} \mathrm{d}X_k = \omega_k \mathrm{d}t \\ \mathrm{d}\omega_k = \nu_0(\mathrm{Id} - \omega_k \otimes \omega_k)\,J_k \mathrm{d}t + \sqrt{2d}(\mathrm{Id} - \omega_k \otimes \omega_k) \circ \mathrm{d}B_t^k \end{cases}$$

Kinetic description

Theorem (F. Bolley, J. A. Cañizo, J. A. Carrillo, 2012)

Probability density function $f(x,\omega,t)$, as $N \to \infty$:

$$\partial_t f + \omega \cdot \nabla_x f + \nu_0 \nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega)\mathcal{J}_f\, f) = d\Delta_\omega f$$

$$\mathcal{J}_f(x,\omega,t) = \int_{y\in\mathbb{R}^n,\, \upsilon\in\mathbb{S}} K(|y-x|)\, \upsilon\, f(y,\upsilon,t)\,\mathrm{d}y\,\mathrm{d}\upsilon\,.$$

Tool : coupling process + estimations.

$$\begin{cases} \mathrm{d}\bar{X}_k = \bar{\omega}_k \mathrm{d}t \\ \mathrm{d}\bar{\omega}_k = \nu_0(\mathrm{Id} - \bar{\omega}_k \otimes \bar{\omega}_k)\,\mathcal{J}_{f_t^N}\,\mathrm{d}t + \sqrt{2d}(\mathrm{Id} - \bar{\omega}_k \otimes \bar{\omega}_k) \circ \mathrm{d}B_t^k \\ f_t^N = \mathrm{law}(\bar{X}_1, \bar{\omega}_1) = \mathrm{law}(\bar{X}_k, \bar{\omega}_k) \end{cases}$$

Hydrodynamic scaling

Scaling, with $\varepsilon \ll 1$ (and $K_0 = \int_{\mathbb{R}^n} K(x)\mathrm{d}x$):

$$f^\varepsilon(x,\omega,t) = \nu_0 K_0 f(\tfrac{1}{d\varepsilon}x, \omega, \tfrac{1}{d\varepsilon}t).$$

Mean-field reduced and rescaled equation:

$$\varepsilon(\partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon) = Q(f^\varepsilon) + O(\varepsilon^2),$$

with an effect of localization in space:

$$Q(f) = -\nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega) J_f\, f) + \Delta_\omega f,$$

$$J_f(x,t) = \int_{\mathbb{S}} f(x,\omega,t)\,\omega\,\mathrm{d}\omega.$$

Since $(\mathrm{Id} - \omega \otimes \omega) J = \nabla_\omega (J \cdot \omega)$, we get

$$Q(f) = \nabla_\omega \cdot (e^{\omega \cdot J_f} \nabla_\omega (e^{-\omega \cdot J_f} f)).$$

Local equilibria

Definitions: Fisher–von Mises distribution

$$M_{\kappa\Omega}(\omega) = \frac{e^{\kappa\,\omega\cdot\Omega}}{\int_{\mathbb{S}} e^{\kappa\,\upsilon\cdot\Omega}\,\mathrm{d}\upsilon}.$$

Orientation $\Omega \in \mathbb{S}$, concentration $\kappa \geqslant 0$.

Order parameter: $c(\kappa) = |J_{M_{\kappa\Omega}}| = \dfrac{\int_0^\pi \cos\theta\, e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}$.

For $J_f = \kappa_f\Omega_f$, we can write Q under the form:

$$Q(f) = \nabla_\omega \cdot \left[M_{\kappa_f\Omega_f}\nabla_\omega\left(\frac{f}{M_{\kappa_f\Omega_f}}\right)\right].$$

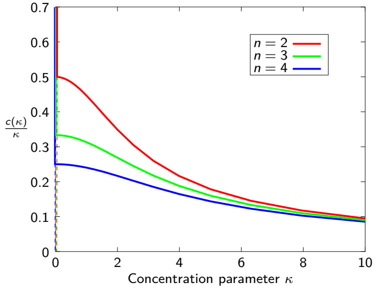
Local equilibria: $f_{eq} = \rho M_{\kappa\Omega}$, for some $\Omega \in \mathbb{S}$.

Compatibility condition: $\kappa = \kappa_{f_{eq}} = |J_{f_{eq}}| = \rho|J_{\kappa\Omega}| = \rho c(\kappa)$.

Solutions to the compatibility condition $\rho c(\kappa) = \kappa$

Proposition

The function $\kappa \mapsto \frac{c(\kappa)}{\kappa}$ is decreasing, its limit is $\frac{1}{n}$ when $\kappa \to 0$.



- $\rho \leqslant n$, only one solution: $\kappa = 0$. Uniform equilibrium.
- $\rho > n$, uniform equilibrium for $\kappa = 0$.
  Unique solution $\kappa(\rho) > 0$.
  Manifold of equilibria:

$$\{\rho M_{\kappa(\rho)\Omega}, \Omega \in \mathbb{S}\}.$$

Homogeneous case: convergence to the equilibrium

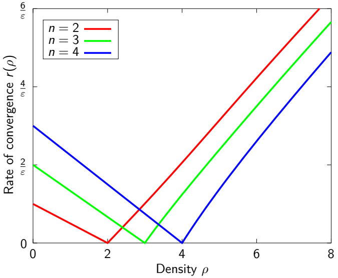
Spatial homogeneous case: the equation becomes

$$\varepsilon\partial_t f = -\nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega) J_f\, f) + \Delta_\omega f,$$

also called Smoluchowski equation (with dipolar potential).

Theorem (AF, J.-G. Liu)

- If $\rho_{f_0} < n$, exponential convergence to the uniform distribution $f \to \rho_{f_0}$.
- If $\rho_{f_0} > n$ and $J_{f_0} \neq 0$, there exists $\Omega_\infty \in \mathbb{S}$ such that f converges exponentially to $\rho_{f_0} M_{\kappa(\rho)\Omega_\infty}$.



Ideas of the proofs, tools used

- Decay of the free energy $\mathcal{F}(f) = \int_{\mathbb{S}} f \ln f - \frac{1}{2}|J_f|^2$
- Instantaneous regularity, compactness $\Rightarrow$ LaSalle Principle
- Use of the spherical harmonics to derive a new conservation relation:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|f-1\|^2_{\widetilde{H}^{-\frac{n-1}{2}}} = -\tau\|f-1\|^2_{\widetilde{H}^{-\frac{n-3}{2}}} + \frac{1}{(n-2)!}|J[f]|^2,$$

  viewed as the dissipation of a "new entropy" when $\rho < n$
- Expansion of $\mathcal{F}$ and its dissipation term around a "moving equilibrium" $M_{\kappa\Omega(t)}$ when $\rho > n$:

$$f = (1 + \alpha\,\omega\cdot\Omega(t) + g)M_{\kappa(\tau)\Omega(t)},$$

  with exponential decay of α and g, which then gives the convergence of $\Omega(t)$ to Ω_∞.

Outline

Region where $\rho^\varepsilon(x,t) - n \gg \varepsilon$

Starting point: when $\varepsilon \to 0$, f^ε converges (formally) to $\rho M_{\kappa(\rho)\Omega}$.
Equation on ρ: conservation of mass (integration of the kinetic equation against a constant).

$$\partial_t \rho^\varepsilon + \nabla_x \cdot \mathcal{J}^\varepsilon = 0$$

In the limit $\varepsilon \to 0$, we get

$$\partial_t \rho + \nabla_x \cdot (\rho c(\kappa(\rho))\Omega) = 0$$

Evolution of Ω? No more conservation relation…

$$\int_{\mathbb{S}} Q(f^\varepsilon)\,\psi(\omega)\mathrm{d}\omega \neq 0 \text{ in general } (\psi \text{ non constant}).$$

Idea: integrate against $\psi_{\rho^\varepsilon,\Omega^\varepsilon}(\omega)$ instead.

Generalized collisional invariants

Linearized operator: $Q(f) = L_{\kappa(\rho_f)\Omega_f}(f)$, with

$$L_{\kappa\Omega}(f) = -\Delta_\omega f + \kappa \nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega)\Omega f) = -\nabla_\omega \cdot \left[M_{\kappa\Omega} \nabla_\omega \left(\frac{f}{M_{\kappa\Omega}} \right) \right],$$

Definition: GCIs associated to κ and Ω

$$\mathcal{C}_{\kappa\Omega} = \left\{ \psi \middle| \int_{\omega\in\mathbb{S}} L_{\kappa\Omega}(f)\, \psi \,\mathrm{d}\omega = 0, \forall f \text{ such that } J_f \parallel \Omega \right\}.$$

In particular, for any generalized collisional invariant $\psi \in \mathcal{C}_{\kappa\Omega}$:

$$\forall f \text{ such that } \Omega_f = \Omega \text{ and } \kappa(\rho_f) = \kappa, \int_{\omega\in\mathbb{S}} Q(f)\, \psi \,\mathrm{d}\omega = 0.$$

Proposition

$$\psi \in \mathcal{C}_{\kappa\Omega} \Leftrightarrow \psi = Cte + h_\kappa(\omega \cdot \Omega)\, A \cdot \omega, A \in \mathbb{R}^n, A \perp \Omega.$$

The macroscopic model

$$A\cdot\int_{\omega\in\mathbb{S}} Q(f^\varepsilon)\, h_{\kappa_{f^\varepsilon}}(\omega\cdot\Omega_{f^\varepsilon})\,\omega\,\mathrm{d}\omega = 0 \text{ for all } A\in\mathbb{R}^n \text{ s.t. } A\cdot\Omega_{f^\varepsilon}=0$$

Equivalently, defining $\vec{\psi}_{\kappa,\Omega} = h_{\kappa\Omega}(\omega\cdot\Omega)(\mathrm{Id}-\Omega\otimes\Omega)\omega$, we get

$$\int_{\omega\in\mathbb{S}} Q(f^\varepsilon)\vec{\psi}_{\kappa_{f^\varepsilon},\Omega_{f^\varepsilon}}\mathrm{d}\omega = 0$$

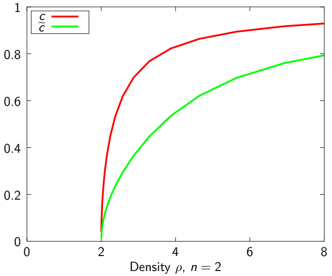
Theorem (P. Degond, AF, J.-G. Liu)

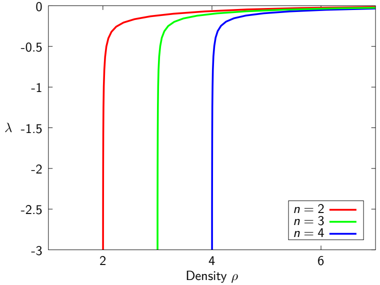
When $\varepsilon\to 0$, the (formal) limit of f^ε is $f^0=\rho(x,t)M_{\kappa(\rho)\Omega(x,t)}$ and the functions ρ,Ω satisfy the system

$$\begin{cases}\partial_t\rho+\nabla_x\cdot(\rho\, c\,\Omega)=0,\\ \rho\,(\partial_t\Omega+\widetilde{c}(\Omega\cdot\nabla_x)\Omega)+\lambda\,(\mathrm{Id}-\Omega\otimes\Omega)\nabla_x\rho=0,\end{cases}$$

with $\widetilde{c}=\langle\cos\theta\rangle_{\widetilde{M}_\kappa}$, and $\lambda=\frac{\rho-n-\kappa\widetilde{c}}{\kappa(\rho-n-\kappa c)}$.

Study of the coefficients





$$c = \begin{cases} \frac{n+2}{n\sqrt{n+2}}\sqrt{\rho - n} + O(\rho - n), \\ 1 - \frac{n-1}{2}\rho^{-1} + \frac{(n-1)(n+1)}{8}\rho^{-2} + O(\rho^{-3}), \end{cases} \qquad \widetilde{c} = \begin{cases} \frac{2n-1}{2n\sqrt{n+2}}\sqrt{\rho - n} + O(\rho - n), \\ 1 - \frac{n+1}{2}\rho^{-1} - \frac{(n+1)(3n+1)}{24}\rho^{-2} + O(\rho^{-3}), \end{cases}$$

$$\lambda = \begin{cases} \frac{-1}{4\sqrt{n+2}}\frac{1}{\sqrt{\rho - n}} + O(1), \\ -\frac{n+1}{6}\rho^{-2} + O(\rho^{-3}). \end{cases}$$ $\Rightarrow$ Loss of hyperbolicity.

Region where $n - \rho^\varepsilon(x,t) \gg \varepsilon$

Chapman–Enskog expansion.

Theorem (P. Degond, AF, J.-G. Liu)

When $\varepsilon \to 0$, a first order correction is (formally) given by

$$f^\varepsilon(x,\omega,t) = \rho^\varepsilon(x,t) - \varepsilon \, \frac{n\,\omega \cdot \nabla_x \rho^\varepsilon(x,t)}{(n-1)(n-\rho^\varepsilon(x,t))},$$

And the density $\rho^\varepsilon(x,t)$ satisfies the following (nonlinear) diffusion equation:

$$\partial_t \rho^\varepsilon = \frac{\varepsilon}{n-1} \nabla_x \cdot \left(\frac{1}{n-\rho^\varepsilon} \nabla_x \rho^\varepsilon \right).$$

Perspectives

- Take a more general function of $|J|$ for the relaxation rate. Allows to overcome the problem of the lack of hyperbolicity (work in progress with J.-G. Liu and Pierre Degond).
- More precise numerical study: comparison of the particular model and its macroscopic limits (work in progress with S. Motsch).
- Understanding the "boundary region" where $\rho^\varepsilon(x,t) - n = O(\varepsilon)$? How to connect the two models?