

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)

Duke University, January 2012

Goal: macroscopic description of some animal societies



- Local interactions without leader
- Emergence of macroscopic structures

Images  Benson Kua (flickr) and 

Modeling of interacting self-propelled particles

- Vicsek *et al.* (1995).
Discrete in time (interval Δt), alignment only, synchronous reorientation.

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

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).

$$\begin{cases} dX_k = \omega_k dt \\ d\omega_k = \nu(\text{Id} - \omega_k \otimes \omega_k) \bar{\omega}_k dt + \sqrt{2d}(\text{Id} - \omega_k \otimes \omega_k) \circ dB_t^k \end{cases}$$

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):

$$\begin{cases} dX_k = \omega_k dt \\ d\omega_k = \nu_0(\text{Id} - \omega_k \otimes \omega_k) J_k dt + \sqrt{2d}(\text{Id} - \omega_k \otimes \omega_k) \circ dB_t^k \end{cases}$$

Kinetic description

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

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

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

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

Tool : coupling process + estimations.

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

Hydrodynamic scaling

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

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

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**:

$$Q(f) = -\nabla_\omega \cdot ((\text{Id} - \omega \otimes \omega)J_f f) + \Delta_\omega f,$$
$$J_f(x, t) = \int_{\mathbb{S}} f(x, \omega, t) \omega \, d\omega.$$

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

$$M_{\kappa\Omega}(\omega) = \frac{e^{\kappa\omega\cdot\Omega}}{\int_{\mathbb{S}} e^{\kappa v\cdot\Omega} dv}.$$

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

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

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

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

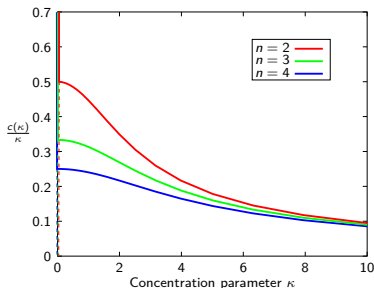
Local equilibria: $f_{eq} = \rho M_{\kappa\Omega}$, for some $\Omega \in \mathbb{S}$.

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 $\kappa \rightarrow 0$.



- $\rho \leq n$, 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

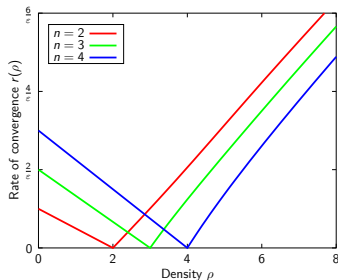
Spatial homogeneous case: the equation becomes

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

also called Smoluchowski equation (with dipolar potential).

Theorem (AF, J.-G. Liu)

- If $\rho_{f_0} < n$, exponential convergence to the uniform distribution $f \rightarrow \rho_{f_0}$.
- 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:

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

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

- 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

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

Starting point: when $\varepsilon \rightarrow 0$, 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 $\varepsilon \rightarrow 0$, we get

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

Evolution of Ω ? No more conservation relation...

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

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

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

Definition: GCIs associated to κ and Ω

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

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

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

Proposition

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

The macroscopic model

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

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

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

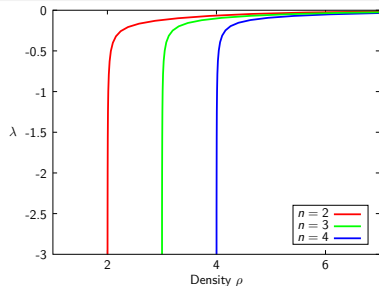
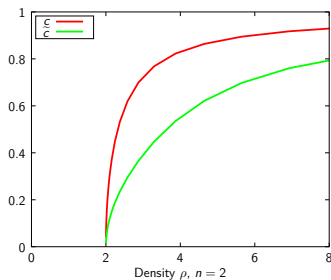
Theorem (P. Degond, AF, J.-G. Liu)

When $\varepsilon \rightarrow 0$, 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

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

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

Study of the coefficients



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

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

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

\Rightarrow Loss of hyperbolicity.

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

Chapman–Enskog expansion.

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

When $\varepsilon \rightarrow 0$, 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?