

A model of alignment interaction for oriented particles with phase transition

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Goal: macroscopic description of some animal societies



- Local interactions without leader
- Emergence of macroscopic structures

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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 Homogeneous case: Doi equation with dipolar potential
 - General results
 - Convergence to equilibrium

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 (Bolley, Cañizo, Carrillo, 2011)

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

$$\begin{aligned} \partial_t f + \omega \cdot \nabla_x f + \nu_0 \nabla_\omega \cdot ((\text{Id} - \omega \otimes \omega) \mathcal{J}_f f) &= d \Delta_\omega f \\ \mathcal{J}_f(x, \omega, t) &= \int_{y \in \mathbb{R}^n, v \in \mathbb{S}} K(|y - x|) v f(y, v, t) dy dv. \end{aligned}$$

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 $\kappa \geq 0$.

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

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

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

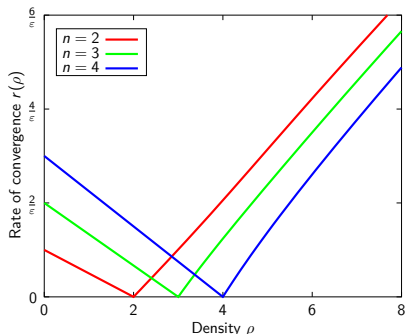
Local equilibria: $f_{eq} = \rho M_{\kappa\Omega}$, for some $\Omega \in \mathbb{S}$.

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

Solutions to the compatibility condition, equilibria

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 (“stable”).
- $\rho > n$, uniform equilibrium (“unstable”) for $\kappa = 0$. Unique solution $\kappa(\rho) > 0$. Manifold of equilibria (“stable”): $\rho M_{\kappa(\rho)}\Omega$, $\Omega \in \mathbb{S}$.

Formal derivation of macroscopic models

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

- Region where $\rho^\varepsilon(x, t) - n \gg \varepsilon$: hydrodynamic model.
As $\varepsilon \rightarrow 0$, the limit of f^ε is $f^0 = \rho(x, t)M_{\kappa(\rho)\Omega(x,t)}$ (formally),
and the functions ρ, Ω satisfy the system:

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

- Region where $\rho^\varepsilon(x, t) - n \gg \varepsilon$: diffusion model.
First order correction in ε for ρ^ε :

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

Stochastic model and its mean-field limit

Orientations ω_k only.

$$\begin{cases} d\omega_k = (\text{Id} - \omega_k \otimes \omega_k) J_k dt + \sqrt{2\tau} (\text{Id} - \omega_k \otimes \omega_k) \circ dB_t^k, \\ J_k = \frac{1}{N} \sum_{j=1}^N \omega_j. \end{cases}$$

Limit as $N \rightarrow \infty$ (Bolley-Cañizo-Carrillo):

$$\partial_t f = -\nabla_\omega \cdot ((\text{Id} - \omega \otimes \omega) J[f] f) + \tau \Delta_\omega f, \text{ with } J[f] = \int_{\mathbb{S}} \omega f d\omega.$$

Doi equation:

$$\begin{cases} \partial_t f = \nabla \cdot (f \nabla \Psi) + \tau \Delta f, \\ \Psi(\omega) = \int_{\mathbb{S}} K(\omega, \bar{\omega}) f(\bar{\omega}) d\bar{\omega} \quad (= -J[f] \cdot \omega). \end{cases}$$

Here $K = -\omega \cdot \bar{\omega}$ (dipolar potential).

Polymers: $|\omega \times \bar{\omega}|$ (Onsager) or $-(\omega \cdot \bar{\omega})^2$ (Maier-Saupe).

Existence, uniqueness, regularity, positivity, bounds

Theorem (AF, J.-G. Liu, 2011)

For an initial probability measure $f_0 \in H^s(\mathbb{S})$, (for an arbitrary s):

- Existence and uniqueness of a weak solution f .
- Global solution, in $C^\infty(\mathbb{R}_+^* \times \mathbb{S})$, and $f > 0$ for $t > 0$.
- Instantaneous regularity estimates and uniform bounds:

$$\|f(t)\|_{H^{s+m}}^2 \leq C \left(1 + \frac{1}{t^m}\right) \|f_0\|_{H^s}^2.$$

Tool: spherical harmonics decomposition.

Nonlinearity: finite number of coefficients.

Onsager free energy

Free energy (non convex): $\mathcal{F}(f) = \tau \int_{\mathbb{S}} f \ln f - \frac{1}{2} |J[f]|^2$.

Dissipation term: $\mathcal{D}(f) = \int_{\mathbb{S}} f |\nabla_{\omega}(\tau \ln f - \omega \cdot J[f])|^2 \geq 0$.

$$\frac{d}{dt} \mathcal{F} + \mathcal{D} = 0.$$

The free energy $\mathcal{F}(f)$ is decreasing towards \mathcal{F}_{∞} .

LaSalle's principle

Limit set: $\mathcal{E}_{\infty} = \{f \in C^{\infty}(\mathbb{S}) \mid \mathcal{D}(f) = 0 \text{ and } \mathcal{F}(f) = \mathcal{F}_{\infty}\}$.

$$\lim_{t \rightarrow \infty} \inf_{g \in \mathcal{E}_{\infty}} \|f(t) - g\|_{H^s} = 0.$$

Equilibria

Equivalent conditions:
$$\begin{cases} \mathcal{D}(f) = 0 \text{ (no dissipation)} \\ Q(f) = 0 \text{ (stationary solution)} \\ f \text{ critical point of } \mathcal{F} \\ \tau \ln f - J[f] \cdot \omega = Cte \end{cases}$$

Amounts to $f = M_{\kappa\Omega}$, with the compatibility condition $\tau\kappa = c(\kappa)$.

Proposition

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

- $\tau \geq \frac{1}{n}$. Only one solution: $\kappa = 0$.
Uniform equilibrium (unique minimizer of \mathcal{F}).
- $\tau < \frac{1}{n}$: uniform equilibrium for $\kappa = 0$, not minimizing \mathcal{F} .
Only positive solution: $\kappa(\tau)$.
Manifold of equilibria: $M_{\kappa(\tau)\Omega}$, $\Omega \in \mathbb{S}$.

Additional conservation relation

Conformal Laplacian: $\tilde{\Delta}_{n-1} Y_\ell = \ell(\ell + 1) \dots (\ell + n - 2) Y_\ell$, for a spherical harmonic Y_ℓ of degree ℓ .

Proposition

For $g \in H^{\frac{n+1}{2}}(\mathbb{S})$ with mean zero, $\int_{\mathbb{S}} \nabla g \tilde{\Delta}_{n-1} g = 0$.

Norms $\|g\|_{\tilde{H}^{-\frac{n-1}{2}}}^2 = \int_{\mathbb{S}} g \tilde{\Delta}_{n-1}^{-1} g$, $\|g\|_{\tilde{H}^{-\frac{n-3}{2}}}^2 = \int_{\mathbb{S}} \Delta g \tilde{\Delta}_{n-1}^{-1} g$:

Conservation relation

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

For $\tau > \frac{1}{n}$, it is an “entropy” dissipation!

Global exponential convergence with rate $(n-1)(\tau - \frac{1}{n})$ towards uniform equilibrium (in any H^s).

Case $\tau < \frac{1}{n}$: the “moving” Fisher–von Mises distribution

- “ODE” for $J[f(t)]$: $J[f_0] \neq 0 \Rightarrow J[f(t)] \neq 0$ for all t .

We define $\Omega(t) = \frac{J[f(t)]}{|J[f(t)]|}$.

- Expansion around the “moving equilibrium” $M_{\kappa(\tau)\Omega(t)}$:

$$f = (1 + h)M_{\kappa(\tau)\Omega(t)},$$

Notation $\langle \cdot \rangle_{M_{\kappa\Omega}}$ for the mean against this measure.

- Unique decomposition of the form

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

with $\langle g \rangle_{M_{\kappa\Omega}} = 0$ and $\langle g\omega \rangle_{M_{\kappa\Omega}} = 0$.

By LaSalle’s principle an unstability of the uniform distribution: h , α and g converge to 0.

Exponential convergence to a fixed equilibrium

- Poincaré inequality:

$$\langle |\nabla h|^2 \rangle_{M_{\kappa\Omega}} \geq \Lambda_{\kappa} \langle (h - \langle h \rangle_{M_{\kappa\Omega}})^2 \rangle_{M_{\kappa\Omega}}$$

Expansion of $\mathcal{D}(f)$ and $\mathcal{F}(f) - \mathcal{F}_{\infty}$, in α^2 and $\langle g^2 \rangle_{M_{\kappa\Omega}}$, with $\|h\|_{\infty}$ small: exponential decay of $\|f - M_{\kappa\Omega}(t)\|$ with rate r for all $r < r_{\infty}(\tau) = (c(\kappa)^2 + n\tau - 1)\Lambda_{\kappa}$.

- Dynamics of $\Omega(t)$:

$$\frac{d\Omega}{dt} = -(\text{Id} - \Omega \otimes \Omega) \langle g \omega \cdot \Omega \omega \rangle_{M_{\kappa\Omega}}$$

So we get $\left| \frac{d\Omega}{dt} \right| \leq C \sqrt{\langle g^2 \rangle_{M_{\kappa\Omega}}} \leq \tilde{C} e^{-rt}$: exponential convergence of Ω to some $\Omega_{\infty} \in \mathbb{S}$.

- Interpolation + uniform bounds: exponential convergence to $M_{\kappa\Omega_{\infty}}$ in any H^s .

Special cases

- Critical case $\tau = \frac{1}{n}$.

Same type of method, with the decomposition

$$f = 1 + \alpha \cos \theta + \frac{1}{2} \alpha^2 (\cos^2 \theta - \frac{1}{n}) + \frac{1}{6} \alpha^3 (\cos^3 \theta - \frac{3}{n+2} \cos \theta) + g,$$

with $\alpha = n \langle f \cos \theta \rangle$ and $\cos \theta = \omega \cdot \Omega$.

Expansion of $\mathcal{D}(f)$ in terms of $\langle g^2 \rangle$ and α^6 , and of $\mathcal{F}(f)$ in terms of $\langle g^2 \rangle$ and α^4 : algebraic convergence in $\frac{1}{\sqrt{t}}$ towards the uniform distribution.

- Case of no noise: $\tau = 0$.

The norm of $|J[f]|$ increases and the $H^{-\frac{n-1}{2}}$ norm of f explodes...