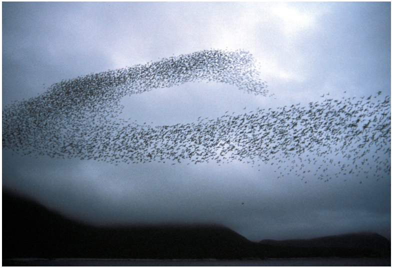
A model of alignment interaction for oriented particles with phase transition

Amic Frouvelle

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

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

Goal: macroscopic description of some animal societies



- Local interactions without leader
- Emergence of macroscopic structures

Modeling of interacting self-propelled particles

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

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

  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.

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 (Bolley, Cañizo, Carrillo, 2011)

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.

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

Homogeneous version: stochastic model, mean-field limit

Orientations ω_k only.

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

Limit as $N \to \infty$: probability density function f satisfying

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

Doi equation:

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

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:

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

Tool: spherical harmonics decomposition.
Nonlinearity: finite number of coefficients.

Fisher–von Mises distribution

Definition

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

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

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

Doi equation can be written:

$$\partial_t f = Q(f) = \tau\,\nabla_\omega \cdot \Big(e^{\frac{1}{\tau}\omega\cdot J[f]}\nabla_\omega(e^{-\frac{1}{\tau}\omega\cdot J[f]}\,f)\Big).$$

For $\frac{1}{\tau}J[f] = \kappa_f\Omega_f$, we can write Q under the form:

$$Q(f) = \tau\,\nabla_\omega \cdot \Big[M_{\kappa_f\Omega_f}\nabla_\omega\Big(\frac{f}{M_{\kappa_f\Omega_f}}\Big)\Big].$$

Onsager free energy

Doi equation rewritten:

$$\partial_t f = \nabla_\omega \cdot \left(f \nabla_\omega (\tau \ln f - \omega \cdot J[f]) \right).$$

Free energy (non convex): $\mathcal{F}(f) = \tau \int_{\mathbb{S}} f \ln f - \frac{1}{2}|J[f]|^2$.
Dissipation term: $\mathcal{D}(f) = \int_{\mathbb{S}} f |\nabla_\omega (\tau \ln f - \omega \cdot J[f])|^2 \geqslant 0$.

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

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

LaSalle's principle

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

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

Equilibria

Equivalent conditions:

$$\begin{cases} \mathcal{D}(f) = 0 \text{ (no dissipation)} \\ Q(f) = 0 \text{ (stationary solution)} \\ f \text{ critical point of } \mathcal{F} \text{ (under the constraint } \int_{\mathbb{S}} f = 1) \\ \tau \ln f - J[f] \cdot \omega \text{ is constant.} \end{cases}$$

Amounts to $f = M_{\kappa\Omega}$, with $\kappa\Omega = \frac{1}{\tau} J[f]$.
In this case $\kappa = \kappa_f = \frac{1}{\tau}|J[f]| = \frac{1}{\tau}|J[M_{\kappa\Omega}]| = \frac{c(\kappa)}{\tau}$.

Compatibility condition

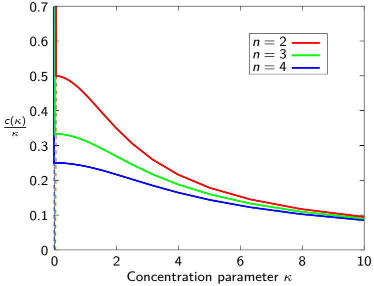
The von Mises distribution $f = M_{\kappa\Omega}$ is an equilibrium if and only if the concentration parameter κ satisfies

$$\tau\kappa = c(\kappa).$$

Solutions to the compatibility equation

Proposition

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



- $\tau \geqslant \frac{1}{n}$. Unique 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: decay when $\tau > 1/n$

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

Proposition

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

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

Conservation relation

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

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 $\tau < 1/n$: initial condition gives the ω-limit set

- Integrating Doi equation against ω: "ODE" for $J[f(t)]$:

$$\frac{\mathrm{d}}{\mathrm{d}t}J[f] = -\tau(n-1)J[f] + \left(\int_{\mathbb{S}} (\mathrm{Id} - \omega \otimes \omega)\, f \,\mathrm{d}\omega\right) J[f].$$

First order linear ODE of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}J[f] = M(t)J[f].$$

So $J[f_0] \neq 0 \Rightarrow J[f(t)] \neq 0$ for all t, we define $\Omega(t) = \frac{J[f(t)]}{|J[f(t)]|}$.

- Unstability of the uniform distribution:

$$f \to 1 \Rightarrow M(t) \to (n-1)(\tfrac{1}{n} - \tau)\mathrm{Id}.$$

Unless $J[f_0] = 0$ (heat equation), the norm of $J[f]$ explodes...

The "moving" Fisher–von Mises distribution

- 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 "orthogonal" decomposition of the form

$$h = \alpha\left[\omega \cdot \Omega(t) - c(\kappa(\tau))\right] + g.$$

with $\langle g\rangle_{M_{\kappa\Omega}} = 0$ and $\langle g\omega\rangle_{M_{\kappa\Omega}} = 0$.
By LaSalle's principle + unstability of the uniform distribution: h, α and g converge to 0.

Exponential convergence to a fixed equilibrium

- Poincaré inequality:

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

  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 $\Omega(t)$:

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

  So we get $\left|\frac{\mathrm{d}\Omega}{\mathrm{d}t}\right| \leqslant C\sqrt{\langle g^2\rangle_{M_{\kappa\Omega}}} \leqslant \widetilde{C}e^{-rt}$: 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: $\tau = 0$.

Some results for the dynamical system of N particles, but harder at the kinetic level.
The norm of $|J[f]|$ increases and the $H^{-\frac{n-1}{2}}$ norm of f explodes...

Back to the inhomogeneous case

Hydrodynamic scaling (+ reduction to $\nu = d = 1$) with an effect of localization in space.

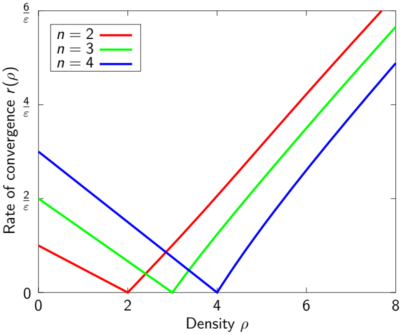
$$\varepsilon(\partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon) = Q(f^\varepsilon) + O(\varepsilon^2).$$

Same equilibria, with the compatibility condition $\kappa = \rho c(\kappa)$: threshold for $\rho = \int_{\mathbb{S}} f \,\mathrm{d}\omega$ at $\rho = n$.

"Stable" equilibria:

- $\rho \leqslant n$: uniform distribution.
- $\rho > n$: manifold of equilibria:

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



Formal derivation of macroscopic models

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

- Region where $\rho^\varepsilon(x,t) - n \gg \varepsilon$: hydrodynamic model.
  As $\varepsilon \to 0$, 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:

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

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

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