Hydrodynamics of self–organization for self–propelled particles

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Workshop “Waves and imaging in complex media”
Heraklion

Joint work with Jian-Guo Liu (Duke University)
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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 $\Delta t$), alignment only, synchronous reorientation.

  New direction = Mean direction of neighboring particles at previous step + Noise
Modeling of interacting self-propelled particles

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- Simulations (Chaté et al. PRE 08): phase transition phenomenon, emergence of coherent structures.
Modeling of interacting self-propelled particles

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- Simulations (Chaté et al. PRE 08): phase transition phenomenon, emergence of coherent structures.

- Degond-Motsch (2008). Time-continuous version: relaxation (with constant rate $\nu$) towards the local mean direction.
Original discrete model
\[ \Delta t = 0,07 \]

Time-continuous version
\[ \nu = 15 \]
Outline

1. Time-continuous variants of the Vicsek model
2. The macroscopic model
3. The phase transition
Time-continuous variants of the Vicsek model

1. Presentation of the model
2. Kinetic model – Hydrodynamic scaling

The macroscopic model

The phase transition
Individual dynamics

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

\[
\begin{aligned}
\frac{dX_k}{dt} &= \omega_k \\
\frac{d\omega_k}{dt} &= \nu P_{\omega_k^\perp}(\bar{\omega}_k - \omega_k)
\end{aligned}
\]
Individual dynamics

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

\[
\begin{align*}
\frac{dX_k}{dt} &= \omega_k \\
\frac{d\omega_k}{dt} &= \nu P_{\omega_k} \bar{\omega}_k \\
&= \nu \nabla_\omega (\omega \cdot \bar{\omega}_k) |_{\omega=\omega_k}
\end{align*}
\]
Individual dynamics

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

\[
\begin{align*}
\text{d}X_k &= \omega_k \text{d}t \\
\text{d}\omega_k &= \nu P_{\omega_k} \bar{\omega}_k \text{d}t + \sqrt{2} dP_{\omega_k} \circ dB^k_t
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Individual dynamics

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\[
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\frac{dX_k}{dt} &= \omega_k dt \\
\frac{d\omega_k}{dt} &= \nu P_{\omega_k} \bar{\omega}_k dt + \sqrt{2d} P_{\omega_k} \circ dB_t^k
\end{aligned}
\]

Target direction :

\[
\bar{\omega}_k = \frac{J_k}{|J_k|}, \quad J_k = \frac{1}{N} \sum_{j=1}^{N} K(|X_j - X_k|) \omega_j.
\]
Individual dynamics

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

\[
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\]

Degond, Motsch (2008): **Formal** derivation of a mean-field kinetic equation and its hydrodynamic limit. Removing the singularity: $\nu$ function of $|J_k|$. 
Kinetic description

Theorem (Bolley, Cañizo, Carrillo, 2011: case \( \nu \) linear in \( |J| \))

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

\[
\partial_t f + \omega \cdot \nabla_x f + \nu(|J_f|) \nabla \omega \cdot (P_{\omega \perp} \bar{\omega}_f f) = d\Delta_\omega f
\]

\[
J_f(x, t) = \int_{y \in \mathbb{R}^n, \nu \in S} K(|y - x|) \nu f(y, \nu, t) \, dy \, d\nu, \quad \bar{\omega}_f = \frac{J_f}{|J_f|}.
\]
Theorem (Bolley, Cañizo, Carrillo, 2011: case \( \nu \) linear in \(|J|\))

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

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\]

Tool : coupling process + estimations.

\[
\begin{align*}
\text{d}\bar{X}_k &= \bar{\omega}_k \, \text{d}t \\
\text{d}\bar{\omega}_k &= \nu(|J_{f_t}^N|) P_{\omega_k} \bar{\omega}_{f_t} \, \text{d}t + \sqrt{2d} P_{\omega_k} \circ \text{d}B^k_t \\
f_t^N &= \text{law}(\bar{X}_1, \bar{\omega}_1) = \text{law}(\bar{X}_k, \bar{\omega}_k)
\end{align*}
\]
Hydrodynamic scaling

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

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

Mean-field reduced and rescaled equation:

\[
\varepsilon \left( \partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon \right) = Q(f^\varepsilon) + O(\varepsilon^2),
\]

with an effect of localization in space (here \( \kappa = \frac{\nu}{d} \)):

\[
Q(f) = -\kappa(|J_f|) \nabla \omega \cdot (P_{\omega \perp \Omega_f} f) + \Delta \omega f,
\]

\[
J_f(x, t) = \int_{\mathbb{S}} f(x, \omega, t) \, \omega \, d\omega, \quad \Omega_f = \frac{J_f}{|J_f|}.
\]
Hydrodynamic scaling

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$$Q(f) = -\kappa(|J_f|) \nabla_\omega \cdot (P_{\omega \perp \Omega_f} f) + \Delta_\omega f,$$

$$J_f(x, t) = \int_S f(x, \omega, t) \omega d\omega, \quad \Omega_f = \frac{J_f}{|J_f|}.$$

Since $P_{\omega \perp \Omega} = \nabla_\omega (\Omega \cdot \omega)$, we get

$$Q(f) = \nabla_\omega \cdot (e^{\kappa \omega \cdot \Omega_f} \nabla_\omega (e^{-\kappa \omega \cdot \Omega_f} f)).$$
Local equilibria

Definitions: Fisher–von Mises distribution

\[ M_{\kappa \Omega}(\omega) = \frac{e^{\kappa \omega \cdot \Omega}}{\int_{\mathbb{S}} e^{\kappa \nu \cdot \Omega} d\nu} \cdot \]

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

Order parameter: \( c(\kappa) = |J_{M_{\kappa \Omega}}| = \frac{\int_{0}^{\pi} \cos \theta e^{\kappa \cos \theta \sin^{n-2} \theta} d\theta}{\int_{0}^{\pi} e^{\kappa \cos \theta \sin^{n-2} \theta} d\theta} \).
Local equilibria

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For \( \kappa_f = \kappa(|J_f|) \), 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

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For \( \kappa_f = \kappa(|J_f|) \), we can write \( Q \) under the form:

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

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

1 Time-continuous variants of the Vicsek model

2 The macroscopic model
   • Derivation of the model
   • Numerical simulations

3 The phase transition
Collisional invariants

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

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

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

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

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Evolution of $\Omega$? No more conservation relation... 

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

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Evolution of $\Omega$? No more conservation relation... 

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

Idea: integrate against $\psi_{\Omega^\varepsilon}(\omega)$ instead.
Generalized collisional invariants

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

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

Definition: GCIs associated to $\kappa$ and $\Omega$

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

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

$$\forall f \text{ such that } \Omega_f = \Omega, \int_{\omega \in S} Q(f) \psi \, d\omega = 0.$$
Generalized collisional invariants

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Definition: GCIs associated to $\kappa$ and $\Omega$

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

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

Proposition

$$\psi \in C_{\kappa \Omega} \Leftrightarrow \psi = Cte + h_\kappa(\omega \cdot \Omega) A \cdot \omega, A \in \mathbb{R}^n, A \perp \Omega.$$
The macroscopic model

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

Equivalently, defining \( \bar{\psi}_{\kappa,\Omega} = h_\kappa(\omega \cdot \Omega) P_{\Omega \perp} \omega \), we get

\[ \int_{\omega \in S} Q(f^\varepsilon) \bar{\psi}_{\kappa,\Omega_{f^\varepsilon}} \, d\omega = 0 \]

Theorem

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

\[
\begin{align*}
\partial_t \rho + \nabla_x \cdot (\rho \, c(\kappa) \, \Omega) &= 0, \\
\rho \, (\partial_t \Omega + \tilde{c}(\Omega \cdot \nabla_x) \Omega) + \lambda \, P_{\Omega \perp} \nabla_x \rho &= 0,
\end{align*}
\]

with \( \tilde{c} = \langle \cos \theta \rangle M_{\kappa} \), and \( \lambda = \frac{1}{\kappa} \).
Splitting method

Main idea: geometric constraint ($|\Omega| = 1$) replaced by a relaxation operator:

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

$$\rho(\partial_t \Omega + \tilde{c}(\Omega \cdot \nabla_x)\Omega) + \lambda P_{\Omega \perp} \nabla_x \rho = 0.$$
Splitting method

Main idea: geometric constraint ($|\Omega| = 1$) replaced by a relaxation operator:

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

$$\partial_t (\rho \Omega) + \tilde{c} \nabla_x \cdot (\rho \Omega \otimes \Omega) + \lambda \nabla_x \rho = \frac{\rho}{\eta} (1 - |\Omega|^2) \Omega.$$

In the limit $\eta \to 0$, we recover the original macroscopic model.
Splitting method

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In the limit $\eta \to 0$, we recover the original macroscopic model.

Numerically, two steps (splitting): first, solve the conservative part, and then the relaxation part.
In one direction, the system is written:

\[
\begin{align*}
\partial_t \rho + c \partial_x (\rho \cos \theta) &= 0 \\
\partial_t \theta + \tilde{c} \cos \theta \partial_x \theta - \lambda \frac{\sin \theta}{\rho} \partial_x \rho &= 0.
\end{align*}
\]
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\[
\begin{align*}
\partial_t \rho + c \partial_x (\rho \cos \theta) &= 0 \\
\partial_t \theta + \tilde{c} \cos \theta \partial_x \theta - \lambda \frac{\sin \theta}{\rho} \partial_x \rho &= 0.
\end{align*}
\]  

(1)

Multiplying (1) by \(1/\sin \theta\) and integrating in \(\theta\): conservative formulation of the model. Solved by a conservative method.
The numerical schemes agree with each other on \textit{rarefaction waves} (smooth solutions)
However, the numerical schemes disagree when the solution is a shock wave (non-smooth solutions)
Simulations 2

However, the numerical schemes disagree when the solution is a shock wave (non-smooth solutions)

Correct solution? Do we have it?
However, the numerical schemes disagree when the solution is a shock wave (non-smooth solutions).

Correct solution ? Do we have it ?

⇒ Back to the microscopic model...
Since there is no theoretical solution to test our numerical simulations, we use the microscopic model as a benchmark:
Since there is no theoretical solution to test our numerical simulations, we use the microscopic model as a benchmark:

\[
\frac{d\mathbf{x}_k^\varepsilon}{dt} = \omega_k^\varepsilon,
\]

\[
\frac{d\omega_k^\varepsilon}{\varepsilon} = \frac{1}{\varepsilon} P(\omega_k^\varepsilon) \perp (\bar{\omega}_k^\varepsilon \, dt + \sqrt{2d} \, dB_t),
\]

with

\[
\bar{\omega}_k^\varepsilon = \frac{J_k^\varepsilon}{|J_k^\varepsilon|}, \quad J_k^\varepsilon = \sum_{j, |x_j^\varepsilon - x_k^\varepsilon| \leq \varepsilon R} \omega_j^\varepsilon.
\]
Initial condition: Riemann problem.

Figure: Density $\rho$: Micro (left) and Macro (right)
Cross section of the distribution in the $x$-direction:

![Graph showing cross section of distribution](image)

**Figure:** macro. equation (line) and micro. equation (dot) at time $t = 2$. 
Cross section of the distribution in the $x$-direction:

![Graph showing the cross section of the distribution in the x-direction.](image)

**Figure:** macro. equation (line) and micro. equation (dot) at time $t = 4$. 
We compare the solutions of the macroscopic model with the particles for the shock-wave solution:
We compare the solutions of the macroscopic model with the particles for the shock-wave solution:

The splitting method has the “correct speed”.

\[ \rho, \cos \theta \]
Contact discontinuity

For an initial condition given as a contact discontinuity, a weak solution is given by a traveling wave. Numerically, another type of solution:
Contact discontinuity

For an initial condition given as a contact discontinuity, a weak solution is given by a traveling wave. Numerically, another type of solution:

All these simulations: Motsch, Navoret, SIAM MMS 2011.
Sommaire

1 Time-continuous variants of the Vicsek model

2 The macroscopic model

3 The phase transition
   - Phase transition at the level of equilibria
   - Ordered phase, hydrodynamic model
   - Disordered phase, diffusion
Numerical observation

Case $\nu$ constant: Order parameter $\varphi = c(\kappa) = \frac{|J|}{\rho}$ is also constant...
Numerical observation

Case $\nu$ constant: Order parameter $\varphi = c(\kappa) = \frac{|J|}{\rho}$ is also constant...

If $\nu$ is an increasing function of $|J|$: positive feedback (the more the particles are ordered, the faster they align).
Example presented here: $\nu = |J|$. 
Numerical observation

Case \( \nu \) constant: Order parameter \( \varphi = c(\kappa) = \frac{|J|}{\rho} \) is also constant...

If \( \nu \) is an increasing function of \( |J| \): positive feedback (the more the particles are ordered, the faster they align).

Example presented here: \( \nu = |J| \).

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

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

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

- $\rho \leq n$, only one solution: $\kappa = 0$. Uniform equilibrium.
- $\rho > n$, uniform equilibrium for $\kappa = 0$. Unique solution $\kappa(\rho) > 0$. Manifold of equilibria:
  $$\{\rho M_{\kappa(\rho)} \Omega, \, \Omega \in S\}.$$
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 \( S \) (with dipolar potential).

**Theorem (AF, J.-G. Liu, 2012)**

- If \( \rho < n \), exponential convergence to the uniform distribution \( f \to \rho f_0 \).
- If \( \rho > n \) and \( J f_0 \neq 0 \), there exists \( \Omega_\infty \in S \) 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 $\mathcal{F}(f) = \int_S f \ln f - \frac{1}{2} |J_f|^2$
Ideas of the proofs, tools used

- Decay of the free energy $\mathcal{F}(f) = \int_S f \ln f - \frac{1}{2} |J_f|^2$
- Instantaneous regularity, compactness $\Rightarrow$ LaSalle Principle
Ideas of the proofs, tools used

- Decay of the free energy $\mathcal{F}(f) = \int_{S} f \ln f - \frac{1}{2} |J_f|^2$
- 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 $\rho < n$
Ideas of the proofs, tools used

- Decay of the free energy $\mathcal{F}(f) = \int_S f \ln f - \frac{1}{2} |J_f|^2$
- Instantaneous regularity, compactness $\Rightarrow$ LaSalle Principle
- Use of the spherical harmonics to derive a new conservation relation:
  \[
  \frac{1}{2} \frac{d}{dt} \| f - 1 \|^2_{\widetilde{H} - \frac{n-1}{2}} = -\tau \| f - 1 \|^2_{\widetilde{H} - \frac{n-3}{2}} + \frac{1}{(n-2)!} |J[f]|^2,
  \]
  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 $\alpha$ and $g$, which then gives the convergence of $\Omega(t)$ to $\Omega_\infty$. 
Subcritical case
\[ \nu = 1.9 \]

Supercritical case
\[ \nu = 2.3 \]
Region where $n - \rho^\varepsilon(x, t) \gg \varepsilon$

Adaptation of the concept of generalized collisional invariants.

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

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

\[
\begin{aligned}
\partial_t \rho + \nabla_x \cdot (\rho \ c \ \Omega) &= 0, \\
\rho \left( \partial_t \Omega + \tilde{c} (\Omega \cdot \nabla_x \Omega) \right) + \lambda \left( \text{Id} - \Omega \otimes \Omega \right) \nabla_x \rho &= 0,
\end{aligned}
\]

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

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

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

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

\( \Rightarrow \) 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:

$$\partial_t \rho^\varepsilon = \frac{\varepsilon}{n - 1} \nabla_x \cdot \left( \frac{1}{n - \rho^\varepsilon} \nabla_x \rho^\varepsilon \right).$$
Region where $n - \rho^\varepsilon(x, t) \gg \varepsilon$

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**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:

$$\partial_t \rho^\varepsilon = \frac{\varepsilon}{n - 1} \nabla_x \cdot \left( \frac{1}{n - \rho^\varepsilon} \nabla_x \rho^\varepsilon \right).$$
A more general function of $|J|$ for the relaxation rate allows to overcome the problem of the lack of hyperbolicity (with J.-G. Liu and P. Degond).

Taking in account non-locality in the scaling: viscous term in the orientation equation.

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?
Thanks!