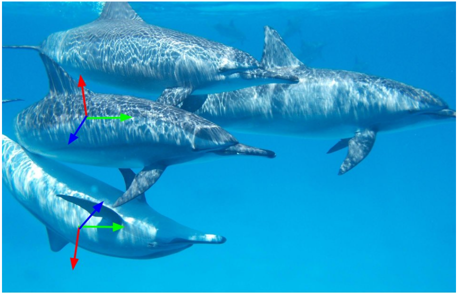
Body-attitude alignment : link with rodlike polymers, quaternions and phase transition

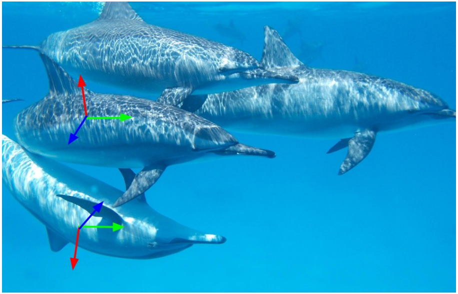
Amic Frouvelle – CEREMADE – Université Paris Dauphine

[i$\mathbb{N}\delta$AM] Workshop : Recent Advances in Kinetic Equations and Applications
Rome, November 11$^{\text{th}}$
From collaborations with Pierre Degond (London), Antoine Diez (London), Sara Merino-Aceituno (Vienna), Ariane Trescases (Toulouse)
[DFMA17, DFMAT18, DFMAT19, DDFMA19]

Motivation



Motivation

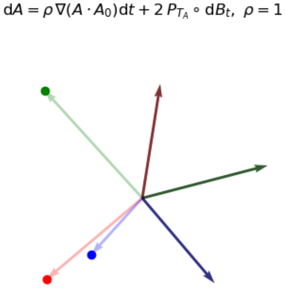


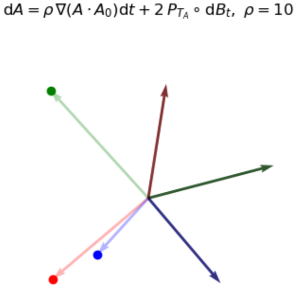
Self-propelled particles aligning their body orientation [DFMA17]

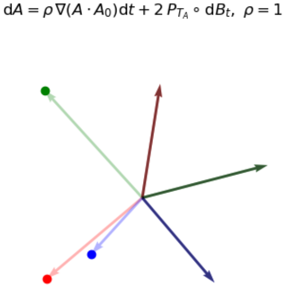
Positions $X_k \in \mathbb{R}^3$, orientations $A_k \in SO_3(\mathbb{R})$.

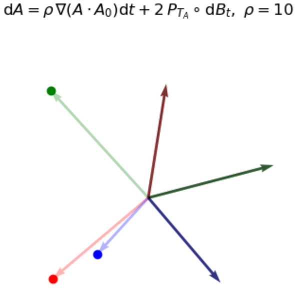
$$\begin{cases} \mathrm{d}X_k = A_k e_1 \mathrm{d}t \\ \mathrm{d}A_k = -\sum_{j\sim k} \nu_{j,k} \nabla_A \left(\frac{1}{2}\|A_k - A_j\|^2\right)\mathrm{d}t + 2\sqrt{\tau} P_{T_{A_k}} \circ \mathrm{d}B_{t,k} \end{cases}$$

Individual mechanisms : noise and alignment





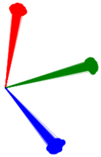




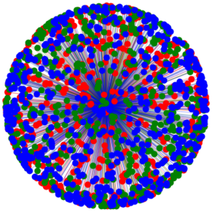
Interacting particles (orientations only, mean-field, strength $\frac{\rho}{N}$)

$$\begin{cases} dA_k = \nabla_{A_k}(A_k \cdot J)dt + 2P_{T_{A_k}} \circ dB_{t,k} \\ J = \rho\langle A\rangle = \frac{\rho}{N}\sum_k A_k \end{cases}$$

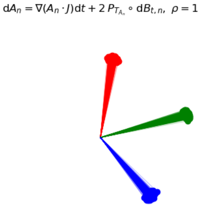
$\mathrm{d}A_n = \nabla(A_n \cdot J)\mathrm{d}t + 2\,P_{T_{A_n}} \circ \mathrm{d}B_{t,n},\ \ \rho = 1$

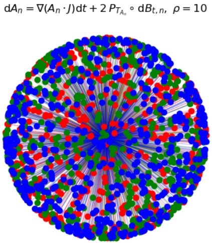


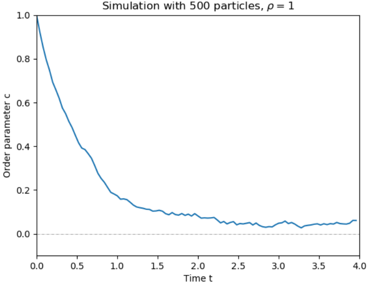
$\mathrm{d}A_n = \nabla(A_n \cdot J)\mathrm{d}t + 2\,P_{T_{A_n}} \circ \mathrm{d}B_{t,n},\ \ \rho = 10$

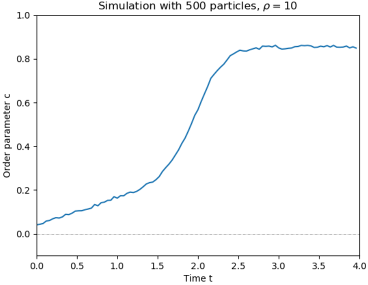


How to measure alignment ? $c = \sqrt{\frac{1}{3}\mathrm{Tr}(\langle A\rangle\langle A\rangle^T)} = \frac{\sqrt{2}}{\sqrt{3}\rho}\|J\|$

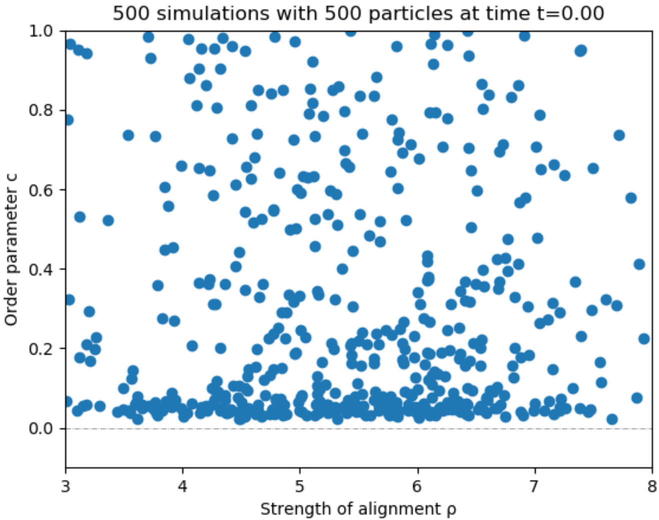








Numerical evidence of a first order phase transition



Equilibria of the space-homogeneous kinetic equation

Aggregation-Diffusion on $SO_3(\mathbb{R})$ for $f(t,A)$

$$\begin{cases}\partial_t f + \nabla_A \cdot [\nabla_A (A \cdot J_f) f] = \Delta_A f \\ \rho = \int_{SO_3(\mathbb{R})} f(A) \mathrm{d}A \text{ (constant !)}, \; J_f = \rho \langle A \rangle = \int_{SO_3(\mathbb{R})} A\, f(A) \mathrm{d}A \end{cases}$$

Equilibria of the space-homogeneous kinetic equation

Aggregation-Diffusion on $SO_3(\mathbb{R})$ for $f(t, A)$

$$\begin{cases}\partial_t f + \nabla_A \cdot [\nabla_A (A \cdot J_f) f] = \Delta_A f \\ \rho = \int_{SO_3(\mathbb{R})} f(A) \mathrm{d}A \text{ (constant !)}, \; J_f = \rho \langle A \rangle = \int_{SO_3(\mathbb{R})} A\, f(A) \mathrm{d}A \end{cases}$$

"von Mises" associated to $J \in M_3(\mathbb{R})$: $M_J(A) = \frac{1}{\mathcal{Z}(J)} exp(J \cdot A)$.

Fokker-Planck formulation : $\partial_t f = \nabla_A \left[M_{J_f} \nabla_A \cdot \left(\frac{f}{M_{J_f}} \right) \right]$.

Equilibria of the space-homogeneous kinetic equation

Aggregation-Diffusion on $SO_3(\mathbb{R})$ for $f(t,A)$

$$\begin{cases}\partial_t f + \nabla_A \cdot [\nabla_A(A\cdot J_f) f] = \Delta_A f \\ \rho = \int_{SO_3(\mathbb{R})} f(A)\mathrm{d}A \text{ (constant !)},\ J_f = \rho\langle A\rangle = \int_{SO_3(\mathbb{R})} A\, f(A)\mathrm{d}A\end{cases}$$

"von Mises" associated to $J \in M_3(\mathbb{R})$: $M_J(A) = \frac{1}{\mathcal{Z}(J)} exp(J\cdot A)$.

Fokker-Planck formulation : $\partial_t f = \nabla_A \left[M_{J_f} \nabla_A \cdot (\frac{f}{M_{J_f}})\right]$.

Compatibility equation on $M_3(\mathbb{R})$ (9-dimensional ?)

Equilibria are functions of the form $f = \rho M_J$ such that

$$J = \rho\langle A\rangle_{M_J} \quad (= \rho \int_{SO_3(\mathbb{R})} A\, M_J(A)\,\mathrm{d}A = \rho J_{M_J})$$

Equilibria of the space-homogeneous kinetic equation

Aggregation-Diffusion on $SO_3(\mathbb{R})$ for $f(t, A)$

$$\begin{cases}\partial_t f + \nabla_A \cdot [\nabla_A (A \cdot J_f) f] = \Delta_A f \\ \rho = \int_{SO_3(\mathbb{R})} f(A)\mathrm{d}A \text{ (constant !)}, \; J_f = \rho\langle A\rangle = \int_{SO_3(\mathbb{R})} A\, f(A)\mathrm{d}A\end{cases}$$

"von Mises" associated to $J \in M_3(\mathbb{R})$: $M_J(A) = \frac{1}{\mathcal{Z}(J)} exp(J \cdot A)$.

Fokker-Planck formulation : $\partial_t f = \nabla_A \left[M_{J_f} \nabla_A \cdot (\frac{f}{M_{J_f}}) \right]$.

Compatibility equation on $M_3(\mathbb{R})$ (9-dimensional ?)

Equilibria are functions of the form $f = \rho M_J$ such that

$$J = \rho \langle A \rangle_{M_J} \quad \left(= \rho \int_{SO_3(\mathbb{R})} A\, M_J(A)\, \mathrm{d}A = \rho J_{M_J}\right)$$

Actually 3d : $\langle A \rangle_{M_{PJQ}} = P \langle A \rangle_{M_J} Q$ for $P, Q \in SO_3(\mathbb{R})$.

Link with quaternions and rodlike polymers

Doi-Onsager theory with Maier-Saupe potential

Density $f(t,q)$, $q \in \mathbb{S}_2/\{\pm 1\}$: try to maximise $(\widetilde{q}\cdot q)^2$.

$$\begin{cases} \partial_t f + \nabla_q \cdot [\nabla_q (q \cdot Q_f q))] = \Delta_q f \\ \rho = \int_{\mathbb{S}_2/\{\pm 1\}} f(q)\mathrm{d}q, \quad Q_f = \int_{\mathbb{S}_2/\{\pm 1\}} (q \otimes q - \frac{1}{3}\mathrm{Id}) f(q)\mathrm{d}q \end{cases}$$

Link with quaternions and rodlike polymers

Doi-Onsager theory with Maier-Saupe potential

Density $f(t,q)$, $q \in \mathbb{S}_2/\{\pm 1\}$: try to maximise $(\tilde{q}\cdot q)^2$.

$$\begin{cases}\partial_t f + \nabla_q \cdot [\nabla_q (q \cdot Q_f q))] = \Delta_q f \\ \rho = \int_{\mathbb{S}_2/\{\pm 1\}} f(q)\mathrm{d}q, \quad Q_f = \int_{\mathbb{S}_2/\{\pm 1\}} (q\otimes q - \frac{1}{3}\mathrm{Id}) f(q)\mathrm{d}q\end{cases}$$

An isometry and isomorphism

Unit quaternion $\mapsto$ Rotation matrix.

Matrix in $M_3(\mathbb{R})$ $\mapsto$Symmetric, trace-free matrix in $\mathcal{S}_4^0(\mathbb{R})$.

Link with quaternions and rodlike polymers

Doi-Onsager theory with Maier-Saupe potential

Density $f(t,q)$, $q \in \mathbb{S}_2/\{\pm 1\}$: try to maximise $(\widetilde{q}\cdot q)^2$.

$$\begin{cases} \partial_t f + \nabla_q \cdot [\nabla_q (q\cdot Q_f q))] = \Delta_q f \\ \rho = \int_{\mathbb{S}_2/\{\pm 1\}} f(q)\mathrm{d}q, \quad Q_f = \int_{\mathbb{S}_2/\{\pm 1\}} (q\otimes q - \frac{1}{3}\mathrm{Id}) f(q)\mathrm{d}q \end{cases}$$

An isometry and isomorphism

Unit quaternion $\mapsto$ Rotation matrix.
Matrix in $M_3(\mathbb{R}) \mapsto$Symmetric, trace-free matrix in $\mathcal{S}_4^0(\mathbb{R})$.

"Polymers" in $\mathbb{R}^4$: equivalence of models [DFMAT18].

Link with quaternions and rodlike polymers

Doi-Onsager theory with Maier-Saupe potential

Density $f(t, q)$, $q \in \mathbb{S}_2/\{\pm 1\}$: try to maximise $(\tilde{q} \cdot q)^2$.

$$\begin{cases} \partial_t f + \nabla_q \cdot [\nabla_q (q \cdot Q_f q))] = \Delta_q f \\ \rho = \int_{\mathbb{S}_2/\{\pm 1\}} f(q) \mathrm{d}q, \quad Q_f = \int_{\mathbb{S}_2/\{\pm 1\}} (q \otimes q - \frac{1}{3} \mathrm{Id}) f(q) \mathrm{d}q \end{cases}$$

An isometry and isomorphism

Unit quaternion $\mapsto$ Rotation matrix.
Matrix in $M_3(\mathbb{R})$ $\mapsto$Symmetric, trace-free matrix in $\mathcal{S}_4^0(\mathbb{R})$.

"Polymers" in $\mathbb{R}^4$: equivalence of models [DFMAT18].
Higher dimensional polymers : theorem of Wang and Hoffmann [WH08].

Dynamical study : BGK instead of Fokker-Planck

The special singular value decomposition [DDFMA19].

Bibliography

P. Degond, A. Diez, A. Frouvelle, and S. Merino-Aceituno.
Phase transitions and macroscopic limits in a BGK model of body-attitude coordination.
preprint, 2019.

P. Degond, A. Frouvelle, and S. Merino-Aceituno.
A new flocking model through body attitude coordination.
Math. Models Methods Appl. Sci., 27(06):1005–1049, 2017.

P. Degond, A. Frouvelle, S. Merino-Aceituno, and A. Trescases.
Quaternions in collective dynamics.
Multiscale Mod. Simul., 16(1):28–77, 2018.

P. Degond, A. Frouvelle, S. Merino-Aceituno, and A. Trescases.
Alignment of self-propelled rigid bodies : from particle systems to macroscopic equations.
In G. Giacomin, S. Olla, E. Saada, H. Spohn, and Stoltz G., editors, *Stochastic Dynamics Out of Equilibrium. IHPStochDyn 2017*, volume 282 of *Springer proceedings in mathematics and statistics*, pages 28–66. Springer, 2019.

H. Wang and P. J. Hoffman.
A unified view on the rotational symmetry of equilibria of nematic polymers, dipolar nematic polymers and polymers in higher dimensional space.
Commun. Math. Sci., 6(4):949–974, 2008.