

Rigid body alignment: phase transition, link with suspensions of rodlike polymers and quaternions.

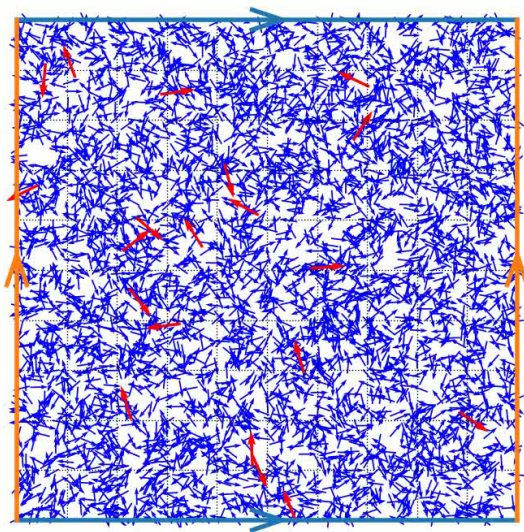
Amic Frouvelle – CEREMADE (Université Paris Dauphine) & LMA
(Université de Poitiers)

France-Korea IRL webinar in PDE
Somewhere online, October 29th, 2021

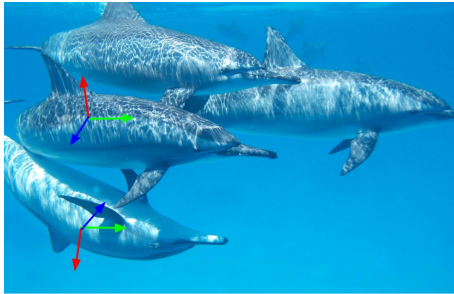
From collaborations with Pierre Degond (Toulouse), Antoine Diez (London), Sara Merino-Aceituno (Vienna), Ariane Trescases (Toulouse) [DFMA17, DFMAT18, DFMAT19, DDFMA20]

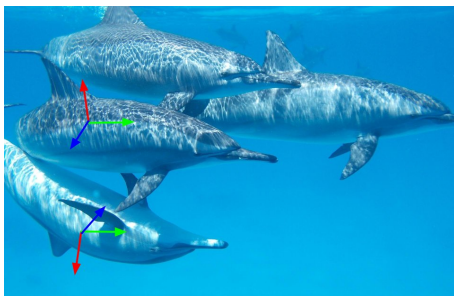
Motivation: “active matter”

Vicsek model (1995): self-propulsion, alignment, angular noise.



Motivation

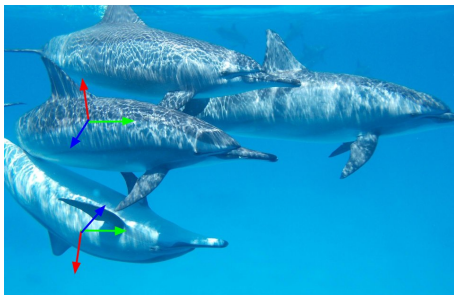




Self-propelled particles aligning their body orientation [DFMA17]

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

$$\begin{cases} dX_k = A_k e_1 dt \\ dA_k = - \sum_{j \sim k} \nu_{j,k} \nabla_A (\frac{1}{2} \|A_k - A_j\|^2) dt + 2\sqrt{\tau} P_{T_{A_k}} \circ dB_{t,k} \end{cases}$$



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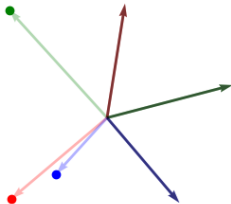
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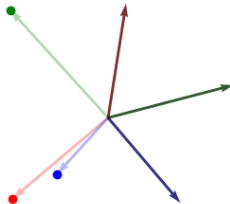
In this talk: spatially homogeneous model.

Individual mechanisms: noise and alignment

$$dA = \rho \nabla(A \cdot A_0) dt + 2 P_{T_A} \circ dB_t, \quad \rho = 1$$



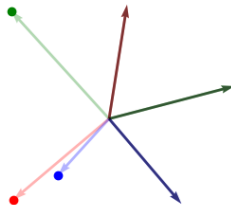
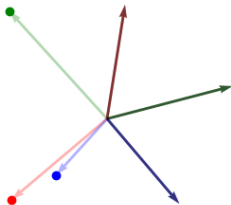
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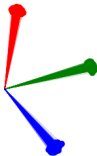


Interacting particles (orientations only, mean-field, strength $\frac{\rho}{N}$)

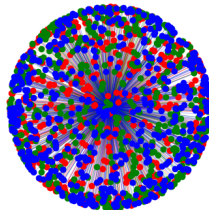
$$\begin{cases} dA_k = \nabla_{A_k}(A_k \cdot J) dt + 2 P_{T_{A_k}} \circ dB_{t,k} \\ J = \rho \langle A \rangle = \frac{\rho}{N} \sum_k A_k \end{cases}$$

How to measure alignment ?

$$dA_n = \nabla(A_n \cdot j) dt + 2 P_{T_{A_n}} \circ dB_{t,n}, \quad \rho = 1$$

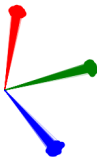


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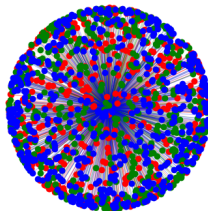


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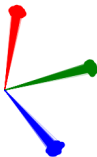


$$\text{Variance: } \langle \|A\|^2 \rangle - \|\langle A \rangle\|^2 = \frac{3}{2} - \left(\frac{\|J\|}{\rho} \right)^2 \in [0, \frac{3}{2}].$$

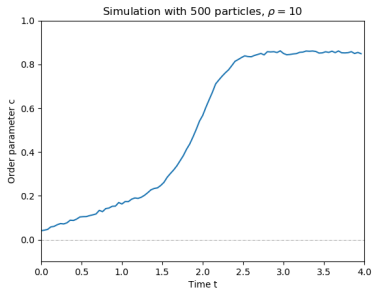
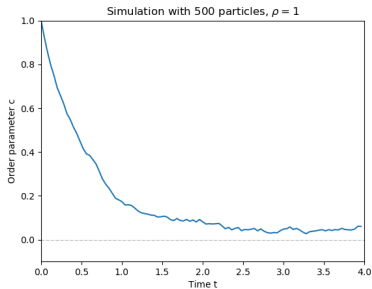
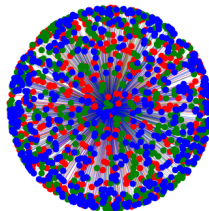
Therefore $c = \sqrt{\frac{2}{3} \text{Tr}(\langle A \rangle \langle A \rangle^T)} = \frac{\sqrt{2}}{\sqrt{3}\rho} \|J\|$ is an order parameter: $c \in [0, 1]$,
 concentration $\Leftrightarrow c \approx 1$, disorder (uniform) $\Rightarrow c = 0$.

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

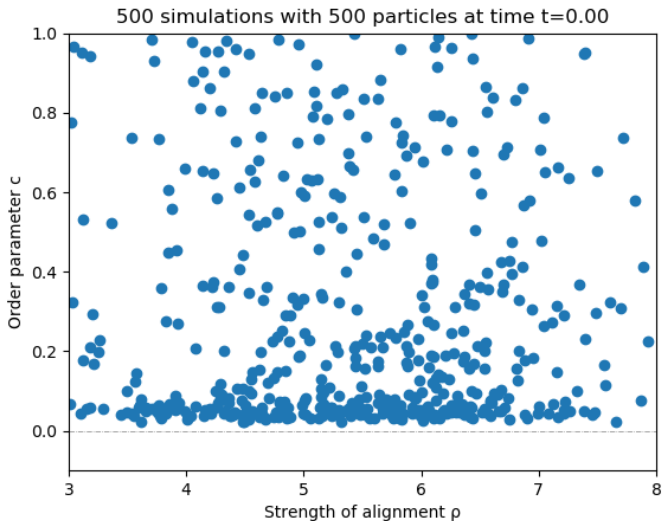
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Numerical evidence of a first order phase transition



Mean-field limit: propagation of chaos

Given $J(t) \in M_3(\mathbb{R})$, the law μ of $dA = \nabla_A(A \cdot J)dt + 2P_{T_A} \circ dB_t$ satisfies the Fokker–Planck equation:

$$\partial_t \mu + \nabla_A \cdot [\nabla_A(A \cdot J)\mu] = \Delta_A \mu.$$

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If now $J = \frac{\rho}{N} \sum_k A_k$, no more independence, but when $N \rightarrow +\infty$, we recover asymptotic independence: propagation of chaos [Szn91].

Aggregation-diffusion on $SO_3(\mathbb{R})$ in the mean-field limit

If $f^N = \frac{\rho}{N} \sum_k \delta_{A_k}$, where (A_k) is the solution of the coupled SDE system, then for fixed $T > 0$, $f^N \rightharpoonup f$ on $[0, T]$, where

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

Equilibria of the space-homogeneous kinetic equation

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

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

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

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

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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 $(\tilde{q} \cdot q)^2$.

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An isometry and an isomorphism ($\mathbb{R}^3$: purely imaginary quaternions)

$$\Phi(q) : \mathbf{u} \in \mathbb{R}^3 \mapsto q \mathbf{u} q^* \in \mathbb{R}^3$$

Unit quaternion $\mapsto$ rotation matrix.

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

$$\frac{1}{2} J \cdot \Phi(q) = q \cdot \phi(J) q, \quad \phi(\Phi(q)) = q \otimes q - \frac{1}{4} I_4$$

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

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“Polymers” in $\mathbb{R}^d$, Wang and Hoffmann [WH08]: only 2 eigenvalues for the solutions of the compatibility equation.

Solutions of the compatibility equation

The special singular value decomposition (SSVD) [DDFMA20]:
if $J \in M_3(\mathbb{R})$, there exists (a unique) $D = \text{diag}(d_1, d_2, d_3)$
and $P, Q \in SO_3(\mathbb{R})$ (non unique) such that

$$d_1 \geq d_2 \geq |d_3| \quad \text{and} \quad J = PDQ.$$

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Solutions to $J = \rho \langle A \rangle_{M_J}$:

- the matrix $J = 0$,
- matrices of the form $J = \alpha \Lambda$, with $\Lambda \in SO_3(\mathbb{R})$ and $\alpha = \rho c_1(\alpha)$,
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Stability ?

A simplified model

$$\begin{cases} \partial_t f = \rho M_{J_f} - f \\ \rho = \int_{SO_3(\mathbb{R})} f(A) dA \quad \text{and} \quad J_f = \int_{SO_3(\mathbb{R})} A f(A) dA. \end{cases}$$

Same compatibility condition: $J = \rho \langle A \rangle_{M_{J_f}}$.

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$$\frac{d}{dt} J_f = \rho \langle A \rangle_{M_{J_f}} - J_f.$$

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Reduction and "conservation"

If PD_0Q is the SSVD of J_0 , then $J_{f(t)} = PD(t)Q$, with the same ODE on D (in $\mathbb{R}^3$).

$$\frac{d}{dt} D = \rho \langle A \rangle_{M_D} - D.$$

The equation is a gradient flow

We set $V(J) = \frac{1}{2}|J|^2 - \rho \ln \mathcal{Z}(J)$, where $\mathcal{Z}(J) = \int_{SO_3(\mathbb{R})} e^{J \cdot A} dA$. Then

$$\frac{d}{dt} J_f = -\nabla V(J_f) \quad (\text{or } \frac{d}{dt} D = -\nabla V(D)).$$

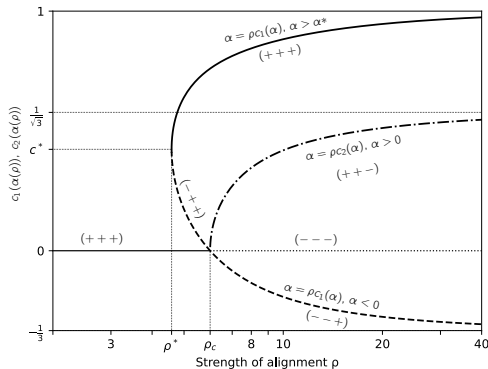
Gradient flow and long time behavior, BGK [DDFMA20]

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Bonus: we know the signature of the Hessian of V (restricted to diagonal matrices) !



Same free energy: $\frac{d}{dt}\mathcal{F}[f] = -\mathcal{D}[f]$ (FP) or $\frac{d}{dt}\mathcal{F}[f] = -\tilde{\mathcal{D}}[f]$ (BGK).

$$\mathcal{F}[f] = \int_{SO_3(\mathbb{R})} f(A) \ln f(A) dA - \frac{1}{2} \|J_f\|^2,$$

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We then set $W(J) = \mathcal{F}[\rho M_J]$ and we get

$$\nabla W(J) = 0 \Leftrightarrow \nabla V(J) = 0 \Leftrightarrow J \text{ solution of the compatibility equation.}$$

Furthermore, the critical points have the same signature! We manage to deduce stability in the sense of free energy (tool: Lassalle's principle for FP, the solution converges towards a family of equilibria).

Exponential convergence towards stable equilibria

Relative entropy and Fisher information.

$$\mathcal{H}(f|g) = \int_{SO_3(\mathbb{R})} f \ln \left(\frac{f}{g} \right) dA, \quad \mathcal{I}(f|g) = \int_{SO_3(\mathbb{R})} f \left\| \nabla \ln \left(\frac{f}{g} \right) \right\|^2 dA.$$

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Theorem [Fro21]: exponential stability

If $\mathcal{E}_\infty$ is one of the two families of stable equilibria (in the sense of free energy), then there exists $\delta > 0$, $\tilde{\lambda} > 0$, and $C > 0$ such that if there exists $f_{\text{eq},0} \in \mathcal{E}_\infty$ with $\mathcal{H}(f_0|f_{\text{eq},0}) < \delta$, then there exists $f_\infty \in \mathcal{E}_\infty$ such that

$$\forall t \geq 0, \mathcal{H}(f(t, \cdot)|f_\infty) \leq C e^{-2\tilde{\lambda}t} \mathcal{H}(f_0|f_{\text{eq},0}).$$

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Tools: log-Sobolev and Csiszár–Kullback–Pinsker inequalities on $SO_3(\mathbb{R})$ to get a Gronwall estimate of $\mathcal{H}(f|\rho M_{J_f})$. Then control of the displacement of J_f .



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