# Rigid body alignment: phase transition and links with quaternions and rodlike polymer suspensions.

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

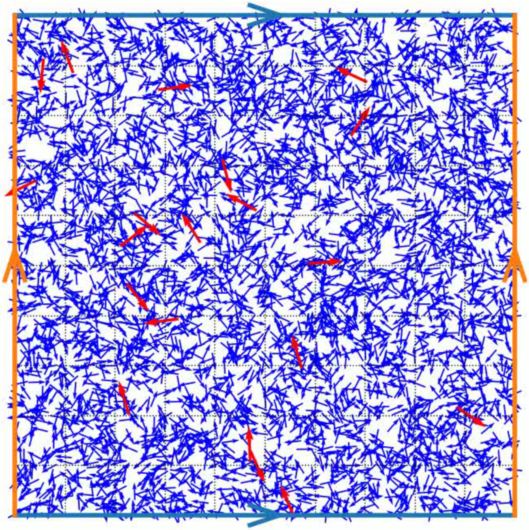
IML Summer School: Multi-scale modeling for pattern formation in biological systems

Somewhere online, July 23rd, 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.



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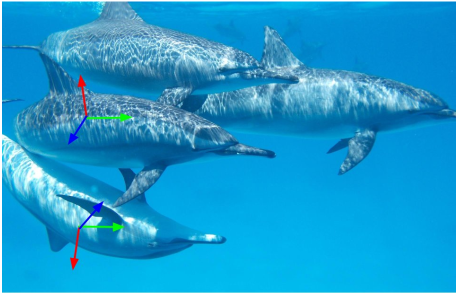

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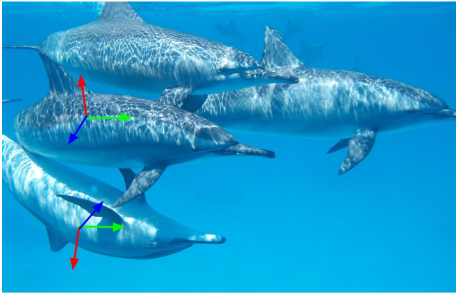

## Self-propelled particles aligning their body orientation [DFMA17]

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

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

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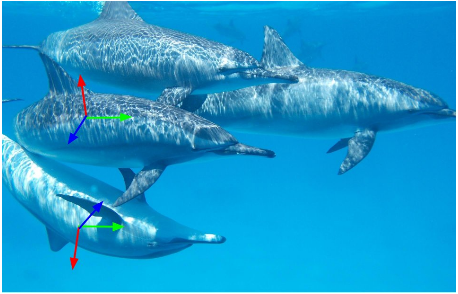

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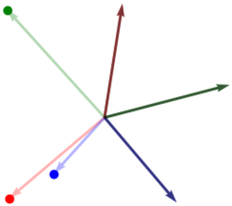
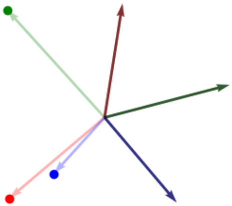
In this talk: spatially homogeneous model.

# Individual mechanisms: noise and alignment

$\mathrm{d}A = \rho \nabla (A \cdot A_0)\mathrm{d}t + 2\, P_{T_A} \circ \mathrm{d}B_t,\ \ \rho = 1$



$\mathrm{d}A = \rho \nabla (A \cdot A_0)\mathrm{d}t + 2\, P_{T_A} \circ \mathrm{d}B_t,\ \ \rho = 10$



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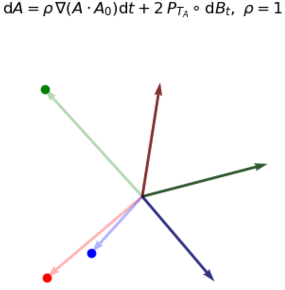
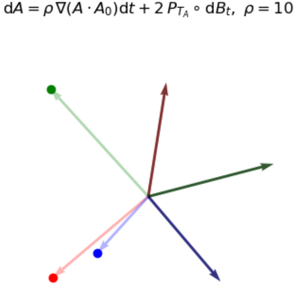


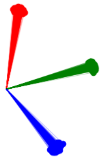




**Interacting particles (orientations only, mean-field, strength $\frac{\rho}{N}$)**

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

# How to measure alignment ?

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



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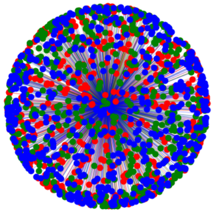

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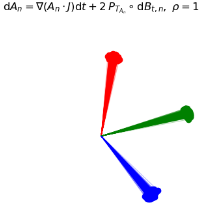
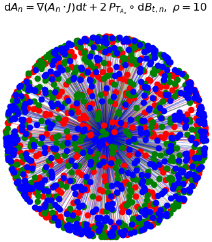
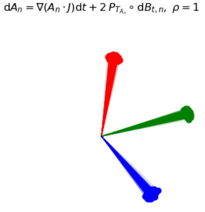
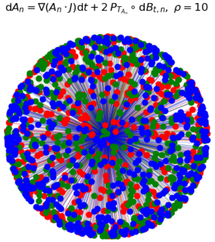


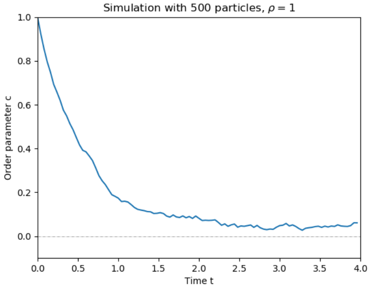



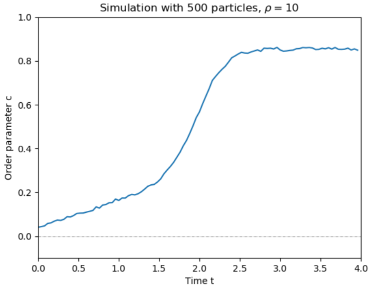

Variance: $\langle \|A\|^2 \rangle - \|\langle A \rangle\|^2 = \frac{3}{2} - (\frac{\|J\|}{\rho})^2 \in [0, \frac{3}{2}]$.
Therefore $c = \sqrt{\frac{2}{3}\mathrm{Tr}(\langle A \rangle \langle A \rangle^T)} = \frac{\sqrt{2}}{\sqrt{3}\rho}\|J\|$ is an order parameter: $c \in [0, 1]$,
concentration $\Leftrightarrow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

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

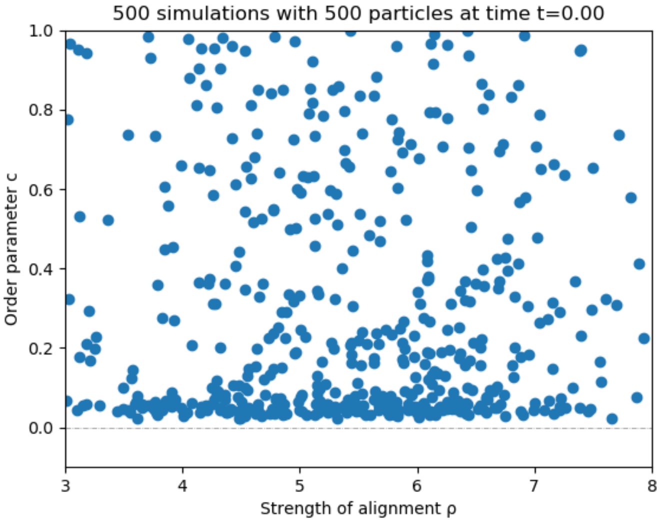


# Numerical evidence of a first order phase transition



# Mean-field limit: propagation of chaos

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

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LLN: if $(A_k)$ follows the SDE system (+ independence of noises, initial conditions), then $\frac{1}{N}\sum_k \delta_{A_k} \rightharpoonup \mu$.

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If now $J = \frac{\rho}{N}\sum_k A_k$, no more independence, but when $N \to +\infty$, 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

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

# Equilibria of the space-homogeneous kinetic equation

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

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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: $\partial_t f = \nabla_A \cdot \Big[M_{J_f} \nabla_A\big(\frac{f}{M_{J_f}}\big)\Big]$.

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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

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

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

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

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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].
"Polymères" 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) $D = \mathrm{diag}(d_1, d_2, d_3)$ and $P, Q \in SO_3(\mathbb{R})$ (non unique) such that

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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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Uniform ? First case.
Stability ?

# Dynamical study: BGK instead of Fokker-Planck

**A simplified model**

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

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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 $\mathbb{R}^3$).

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

# Gradient flow and long time behavior, BGK

## The equation is a gradient flow

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

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

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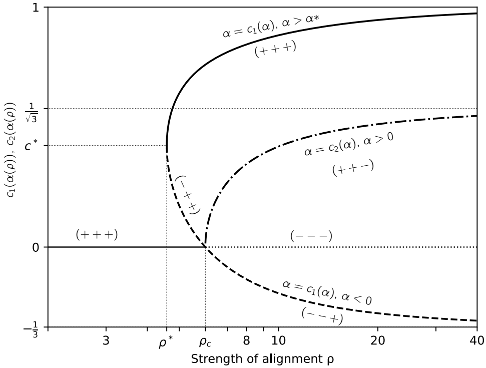
Bonus: we know the signature of the Hessian of $V$ (restricted to diagonal matrices) !



# Using BGK for the stability for Fokker–Planck [Fro21]

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

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

$$\mathcal{D}[f] = \int_{SO_3(\mathbb{R})} f(A) \|\nabla_A(\ln f - A \cdot J_f)\|^2 \mathrm{d}A.$$

$$\widetilde{\mathcal{D}}[f] = \int_{SO_3(\mathbb{R})} (f - \rho M_{J_f})\big(\ln f - \ln(\rho M_{J_f})\big)\mathrm{d}A \geqslant 0.$$

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

$\nabla W(J) = 0 \Leftrightarrow \nabla V(J) = 0 \Leftrightarrow J$ 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.**

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

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- $\mathcal{F}[f] - \mathcal{F}[f_{\mathrm{eq}}] = \mathcal{H}(f|\rho M_{J_f}) + V(J_f) - V(J_{\mathrm{eq}})$,
- $\mathcal{H}(f|f_{\mathrm{eq}}) = \mathcal{F}[f] - \mathcal{F}[f_{\mathrm{eq}}] + \frac{1}{2}\|J_{\mathrm{eq}} - J_f\|^2$,
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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 $\delta > 0$, $\widetilde{\lambda} > 0$, and $C > 0$ such that if there exists $f_{\mathrm{eq},0} \in \mathcal{E}_\infty$ with $\mathcal{H}(f_0|f_{\mathrm{eq},0}) < \delta$, then there exists $f_\infty \in \mathcal{E}_\infty$ such that

$$\forall t \geqslant 0, \mathcal{H}(f(t,\cdot)|f_\infty) \leqslant C\, e^{-2\widetilde{\lambda} t}\, \mathcal{H}(f_0|f_{\mathrm{eq},0}).$$

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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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