Hydrodynamic models for collective behavior of rigid bodies.

Amic Frouvelle – CEREMADE (Université Paris Dauphine)

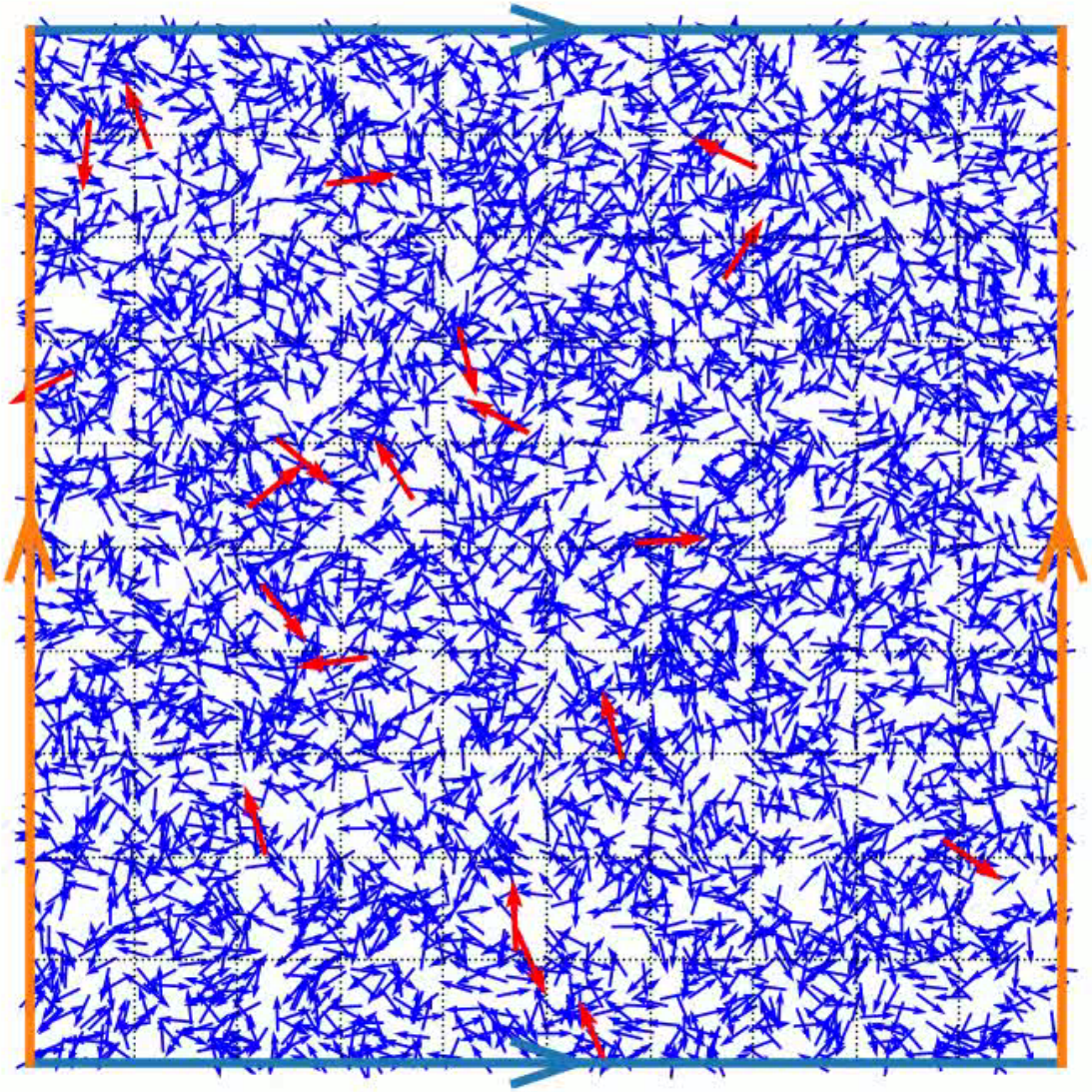
Asymmetry in interacting particle systems, microscopic and macroscopic effects

Lille, October 5th, 2021

From collaborations with Pierre Degond (Toulouse), Antoine Diez (London), Sara Merino-Aceituno (Vienna), Ariane Trescases (Toulouse) [DFMA17, DFMAT19, DDFMA20, DFMAT22]

Motivation: “active matter”

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



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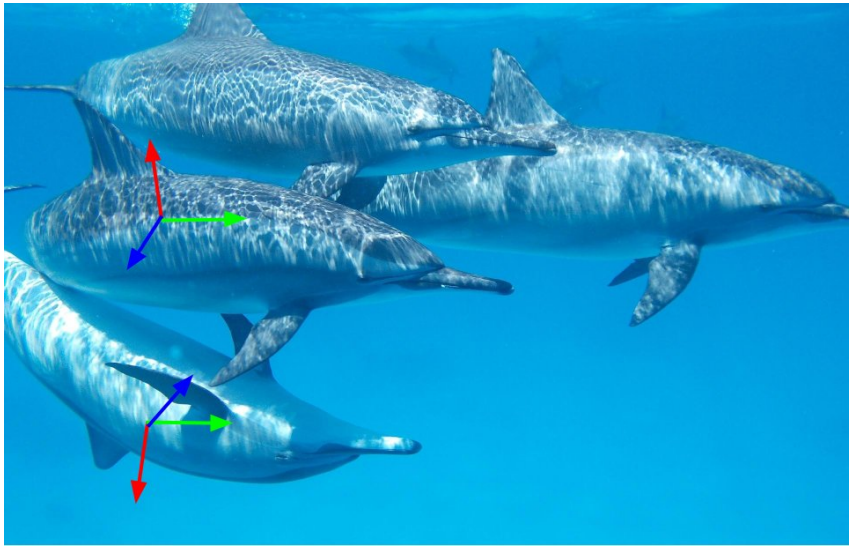

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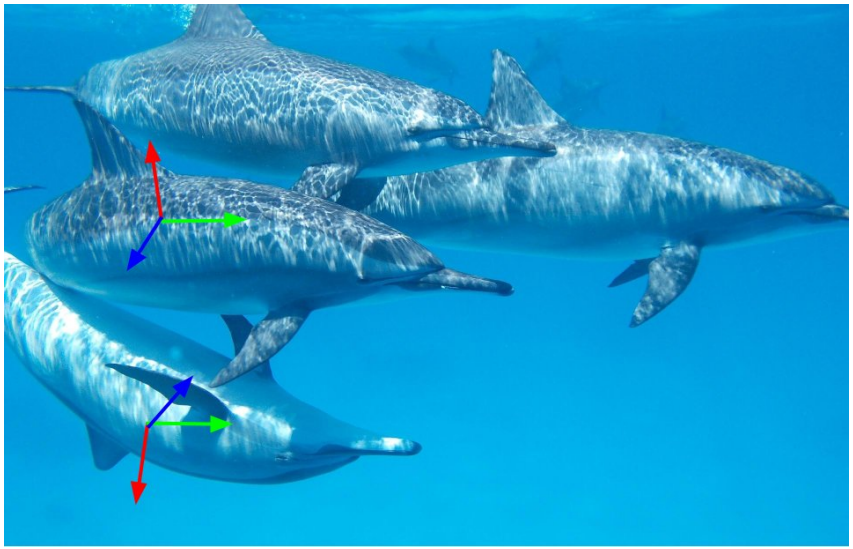

Aligning rotation matrices ?

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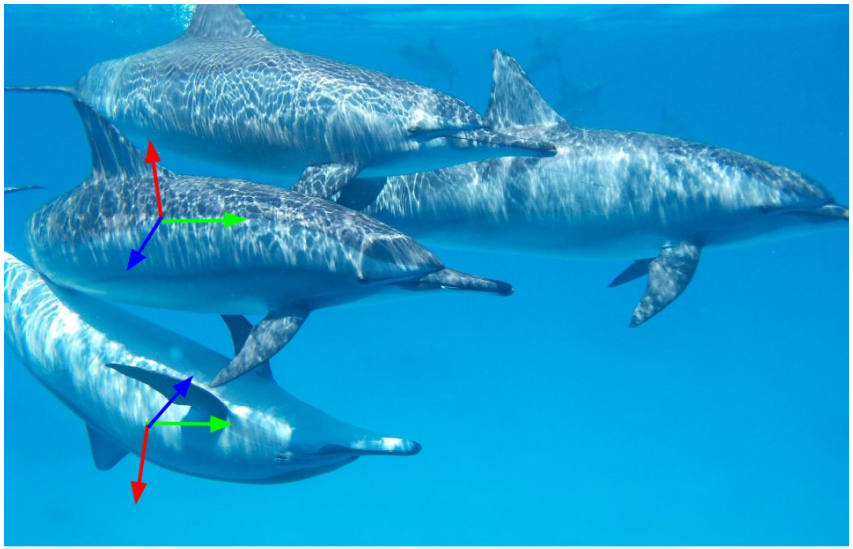

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$$\frac{\mathrm{d}A_k}{\mathrm{d}t} = -\sum_{j\sim k} \nu_{j,k} \nabla_{A_k} \left(\tfrac{1}{2}\|A_k - A_j\|^2\right)$$

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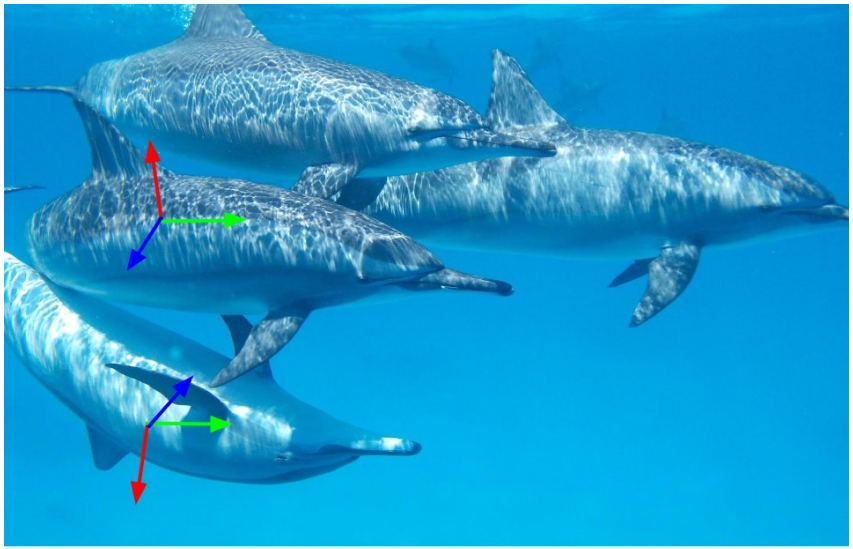

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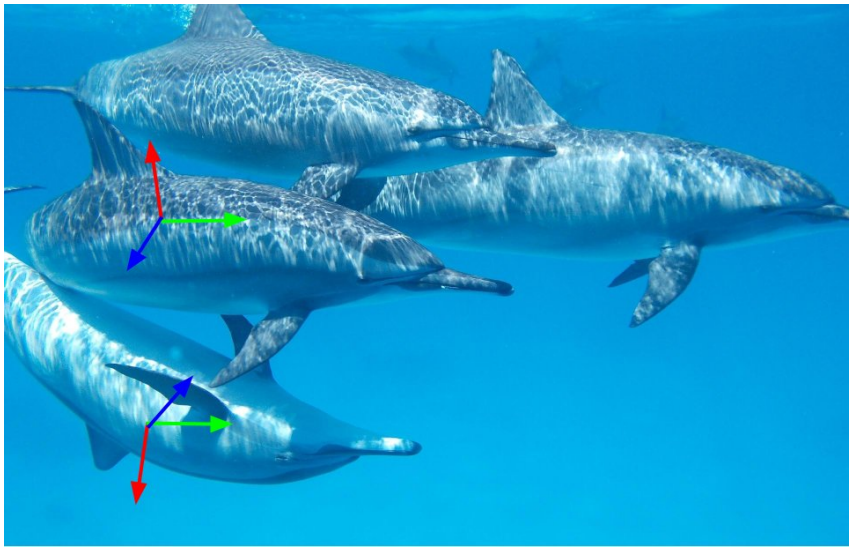

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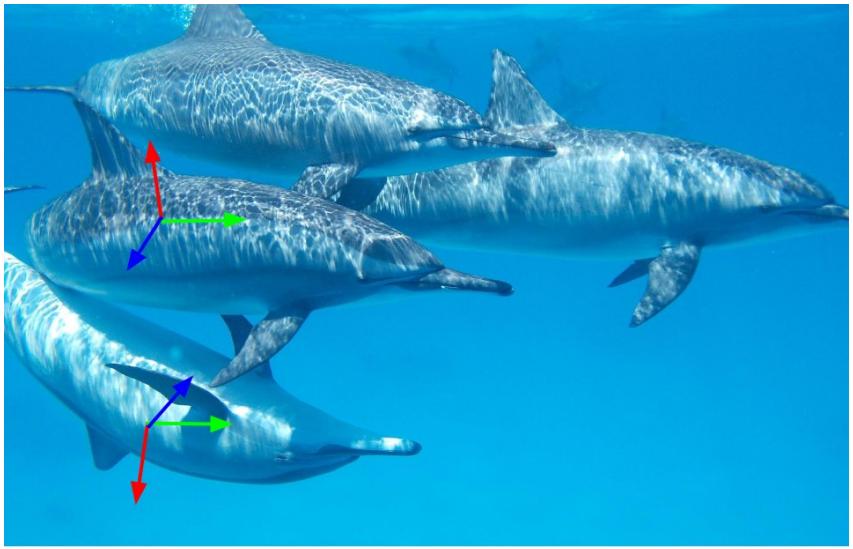

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Self-propelled particles aligning their body orientation [DFMA17]

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

$$\begin{cases} \mathrm{d}X_k = V_k \mathrm{d}t, \quad V_k = A_k e_1 \\ \mathrm{d}A_k = \nu \nabla_{A_k}(A_k \cdot \mathbb{A}(\mathcal{J}_k))\mathrm{d}t + \sqrt{2\tau} P_{T_{A_k}} \circ \mathrm{d}B_{t,k}, \quad \mathcal{J}_k = \sum_{j\sim k} \nu_{j,k} A_j \end{cases}$$

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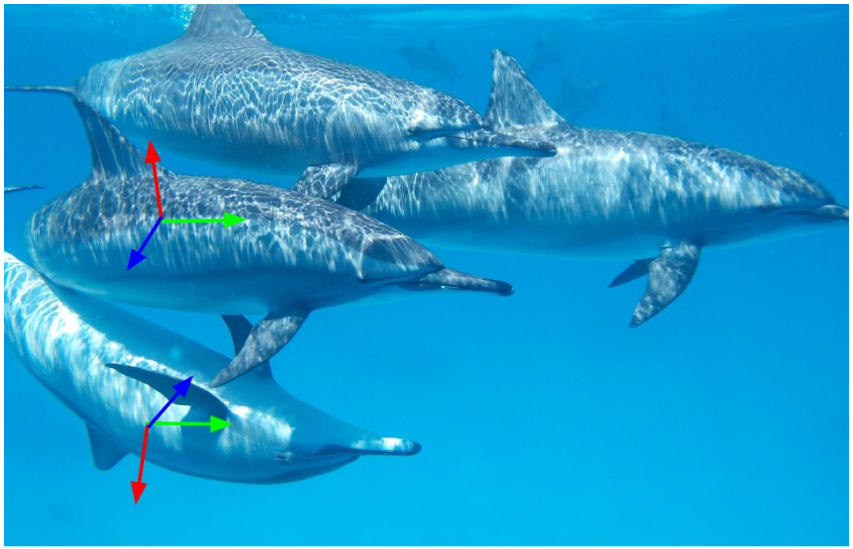

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Mean-field : $\nu_{j,k} = \frac{1}{N} K(|X_j - X_k|)$.

Mean-field limit: propagation of chaos

Given $\mathbb{A}(x,t) \in M_3(\mathbb{R})$, the law μ of $\begin{cases} \mathrm{d}X = V\mathrm{d}t, \quad V = Ae_1 \\ \mathrm{d}A = \kappa\nabla_A(A\cdot\mathbb{A})\mathrm{d}t + \sqrt{2}P_{T_A}\circ\mathrm{d}B_t \end{cases}$ satisfies the Vlasov–Fokker–Planck equation:

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For $\mathbb{A}(\mathcal{J}(X_k))$, $\mathcal{J}(x) = \frac{1}{N}\sum_j K(|x-X_j|)A_j$, no more indep., but we get asymptotic indep. when $N\to+\infty$: propagation of chaos [Szn91].

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

If $f^N = \frac{1}{N}\sum_k \delta_{X_k}\otimes\delta_{A_k}$, where (X_k, A_k) is the solution of the coupled SDE system, then for fixed $T>0$, $f^N \rightharpoonup f$ on $[0,T]$, where

$$\begin{cases} \partial_t f + (Ae_1)\cdot\nabla_x f + \kappa\nabla_A\cdot[\nabla_A(A\cdot\mathbb{A}(\mathcal{J}_f))f] = \Delta_A f \\ \mathcal{J}_f(x) = \int_{\mathbb{R}^3\times SO_3(\mathbb{R})} K(|x-y|)A\,f(A)\mathrm{d}A\mathrm{d}y. \end{cases}$$

Local equilibria of the kinetic equation

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Compatibility equation on $M_3(\mathbb{R})\ldots$

Equilibria are functions of the form $f=\rho M_{\mathbb{A}_0}$ such that $\mathbb{A}_0 = \mathbb{A}(\mathcal{J}_f)$.

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When $\mathbb{A}(\mathcal{J})=\mathcal{J}\in M_3(\mathbb{R})$, another story [DDFMA20, Fro21] (first order phase transition) ! But if $\mathbb{A}$ is the polar decomposition, automatically satisfied for any $\mathbb{A}_0\in SO_3(\mathbb{R})$: $\mathcal{J}_{M_{\mathbb{A}_0}} = c_1(\kappa)\mathbb{A}_0$.

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A simplified model (with same local equilibria)

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From particles ? Run and tumble (exponential clocks, PDMP) ! [Die20]

$$\begin{cases} X_k(t) = X_k(t_n) + (t - t_n) A_k(t_n) e_1, \ \ t \in [t_n, t_{n+1}) & \text{(ballistic)} \\ A_k(t) = A_k(t_n), \ \ t \in [t_n, t_{n+1}), \quad A_k(t_{n+1}) \sim M_{\mathbb{A}(\mathcal{J}_k(t_{n+1}^-))} & \text{(sampling)} \end{cases}$$

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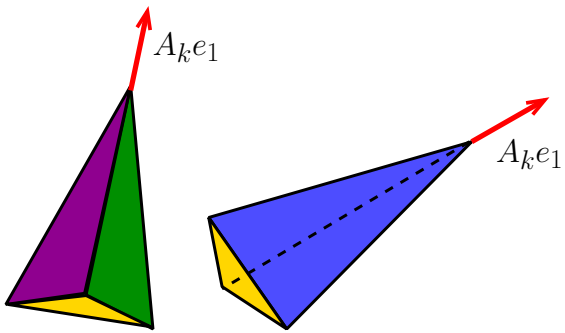
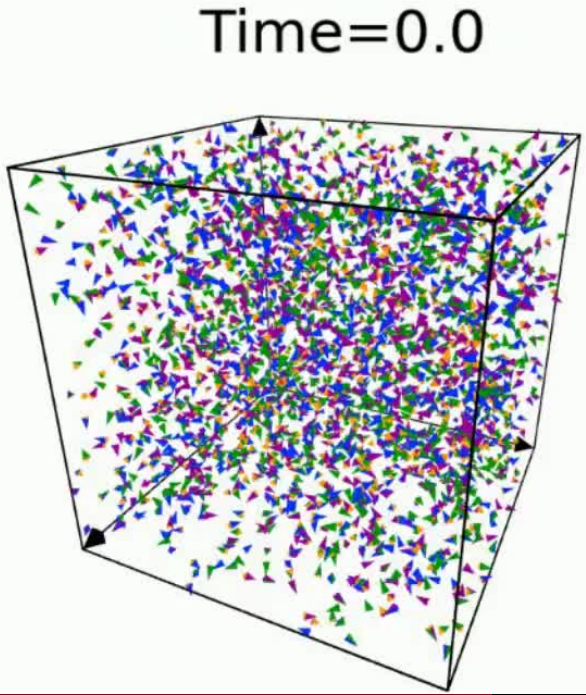


Simulations by Antoine Diez (Suppl. Mat. of [DDN22]).



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$$\partial_t f^\varepsilon + Ae_1 \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} \begin{cases} \nabla_A \cdot \left[M_{\mathbb{A}(J_{f^\varepsilon})} \nabla_A \left(\frac{f}{M_{\mathbb{A}(J_{f^\varepsilon})}} \right) \right] \\ (\rho M_{\mathbb{A}(J_{f^\varepsilon})} - f^\varepsilon) \end{cases} + O(\varepsilon).$$

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$$\partial_t \rho + \nabla_x \cdot (J_{\rho M_\Theta} e_1) = \partial_t \rho + \nabla_x \cdot (c_1(\kappa)\Theta e_1) = 0.$$

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Trouble : no other conservation...

Generalized collisional invariants [DFMA17, DFMAT19]

For $\partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon)$, fix $\Theta \in SO_3(\mathbb{R})$ and find invariants of the form $\psi_\Theta(A)$ such that

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Theorem : formal hydrodynamic limit

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$$\partial_t \rho + \nabla_x \cdot (c_1 \rho \Omega_1) = 0,$$
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where $\mathbb{W} = F \wedge \Omega_1 - c_4\, \rho\, \nabla_x \wedge \Omega_1$, and $F = -c_3\, \nabla_x \rho - c_4\, \rho\, \Theta \nabla_x \cdot \Theta$. The constants are explicit (BGK) and $c_3 > 0$.

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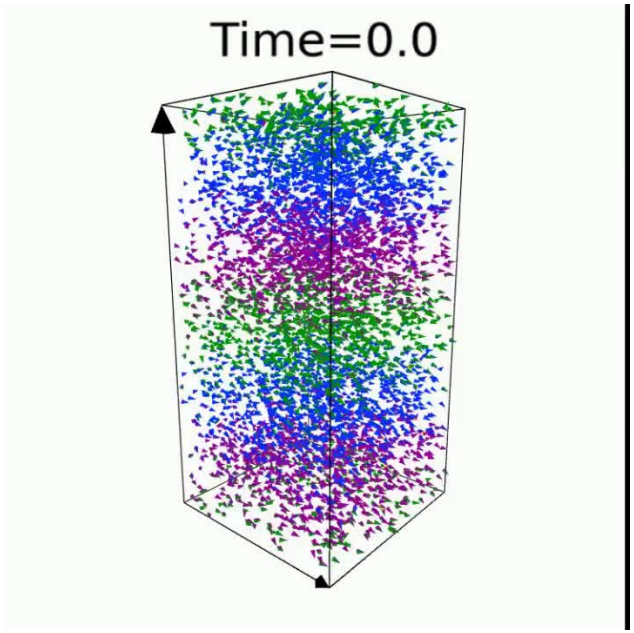
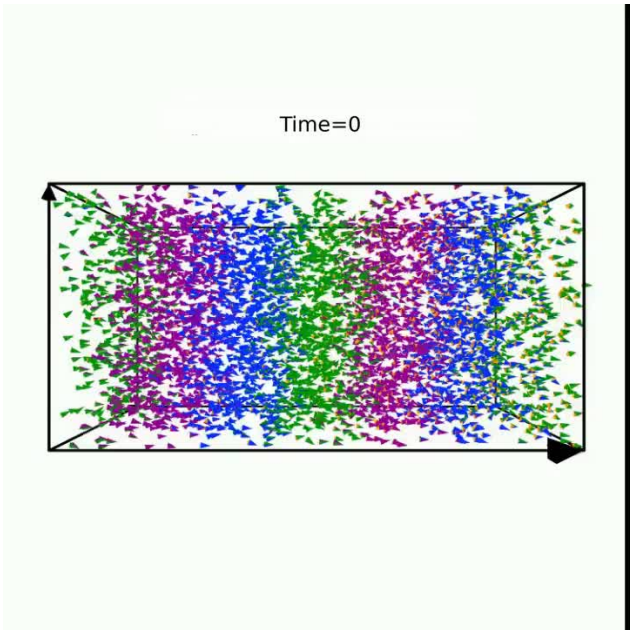
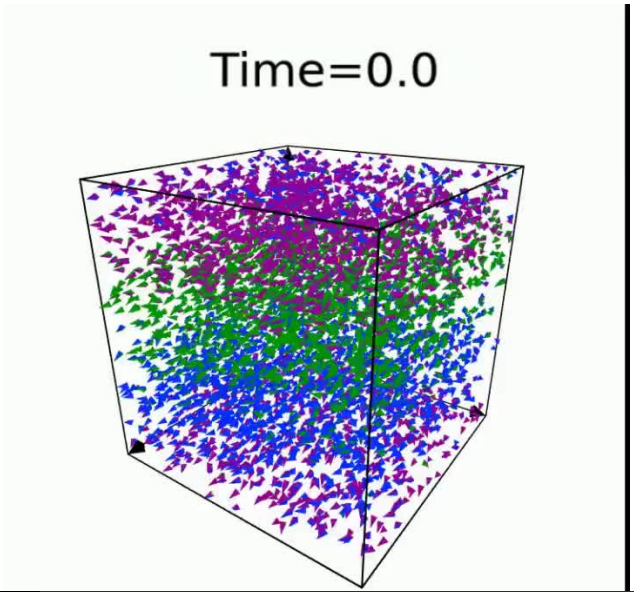
BGK for $SO_n(\mathbb{R})$: [DDF21].

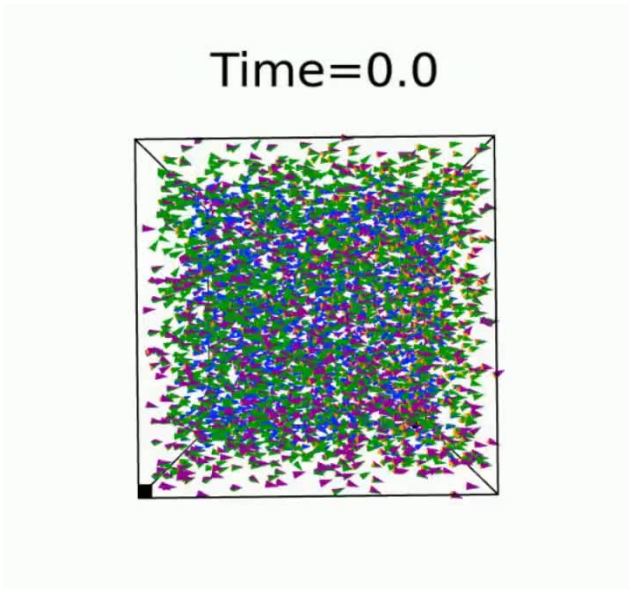
Is it useful ? [DDN22]

Exact (interesting) periodic solutions found at the macroscopic level.









Is it well-posed ? Numerically tractable ? [DFMAT22]

Hyperbolicity when $c_3 > 0$. Uses some invariance by change of frame of the linearized equation. In $SO_n(\mathbb{R})$, decouples in a 2×2 system, $(n-2)$ similar 2×2 systems, and $\binom{n-2}{2}$ scalar equations.

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By essence, non-conservativity. How to manage discontinuities ?

- Relaxation schemes. Systems of first order PDES
  for $\rho > 0$, $M \in M_3(\mathbb{R})$, conservative + source term inducing M to converge to $\Theta \in SO_3$ when a small parameter $\alpha \to 0$, and the solution of the system to a solution of the original one.

$$\partial_t \rho + c_1 \nabla_x \cdot (\rho M e_1) = 0$$

$$\partial_t(\rho M) + \nabla_x \cdot (\mathbf{F}(\rho, \rho M)) + \lambda \nabla_x \rho \otimes e_1 = -\frac{1}{\alpha} \rho (M M^T - I) M$$

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- Larger interaction scaling : $R = O(\sqrt{\varepsilon})$.
  Now $\mathcal{J}_{f^\varepsilon} = J_{f^\varepsilon} + \varepsilon \alpha \Delta_x J_{f^\varepsilon} + O(\varepsilon^2)$. Same strategy of generalized collisional invariants lead to

$$\partial_t \rho + \nabla_x \cdot (c_1 \rho \Omega_1) = 0,$$

$$\rho\big(\partial_t + c_2\, \Omega_1 \cdot \nabla_x\big)\Theta - \mathbb{W}\Theta = \alpha P_{T_\Theta} \Delta_x(\rho \Theta).$$

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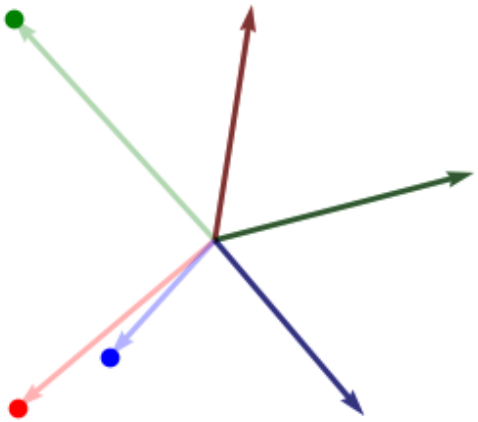
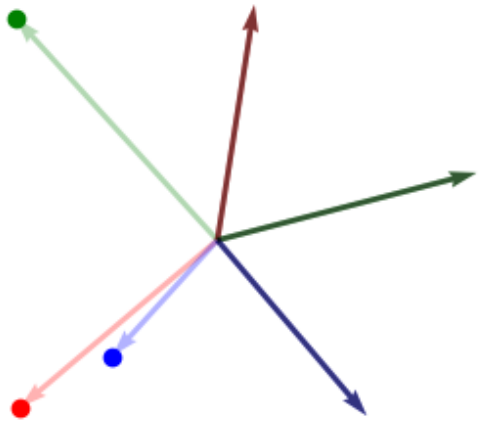
Individual mechanisms: noise and alignment

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



$$dA = \rho \nabla(A \cdot A_0)dt + 2\, P_{T_A} \circ dB_t,\ \rho = 10$$



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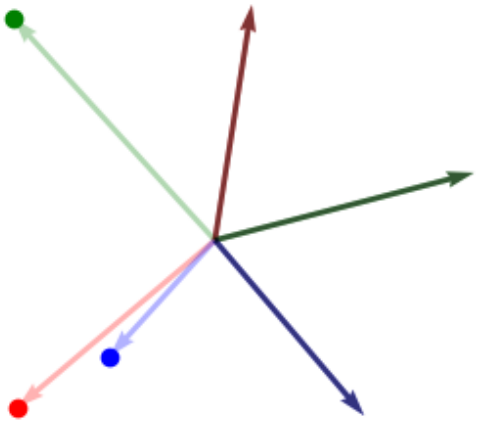

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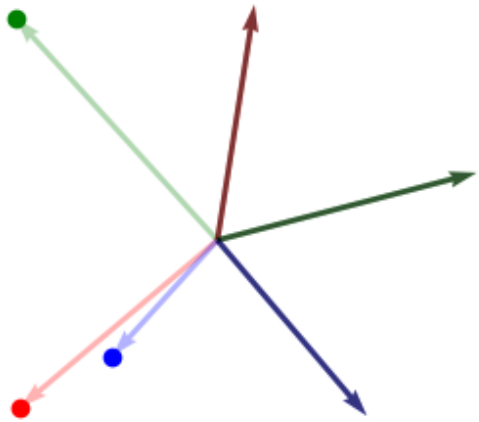
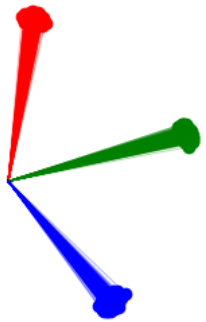


Interacting particles (orientations only, mean-field, strength $\frac{\rho}{N}$)

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

How to measure alignment ?

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



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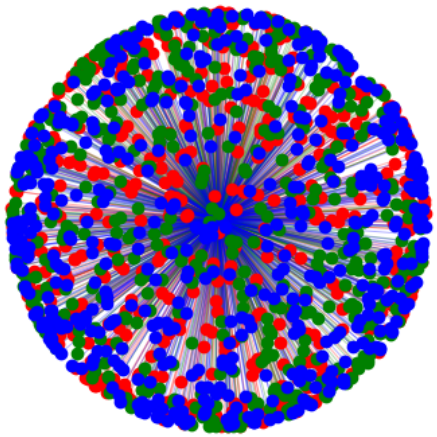

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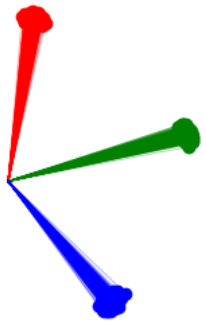

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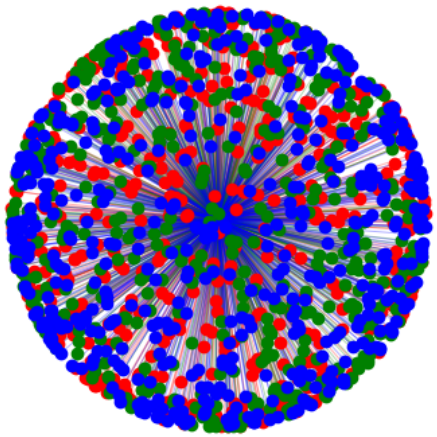
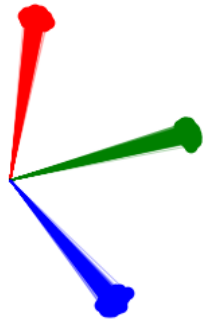


How to measure alignment ? $c = \sqrt{\frac{2}{3}\mathrm{Tr}(\langle A\rangle\langle A\rangle^T)} = \frac{\sqrt{2}}{\sqrt{3}\rho}\|J\|$

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



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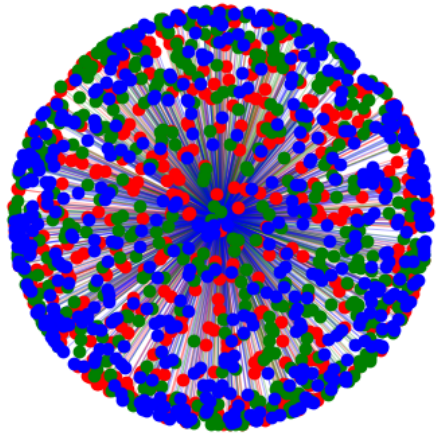

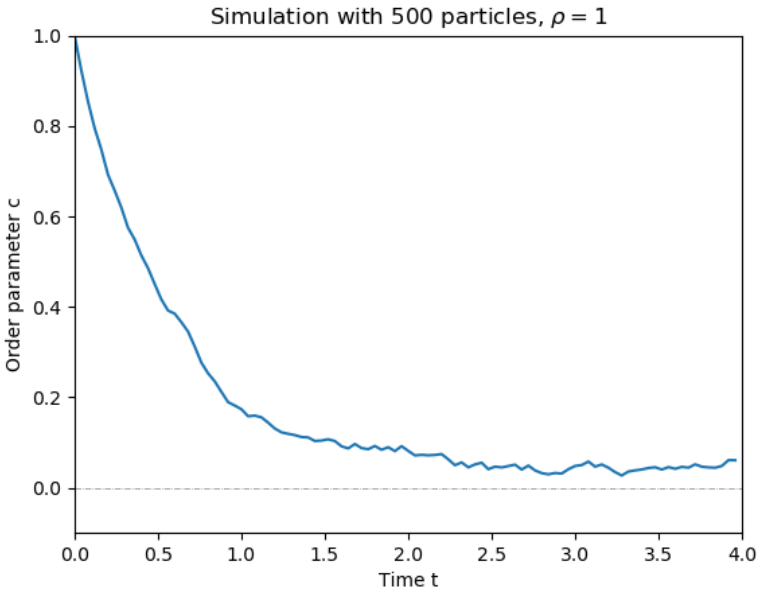

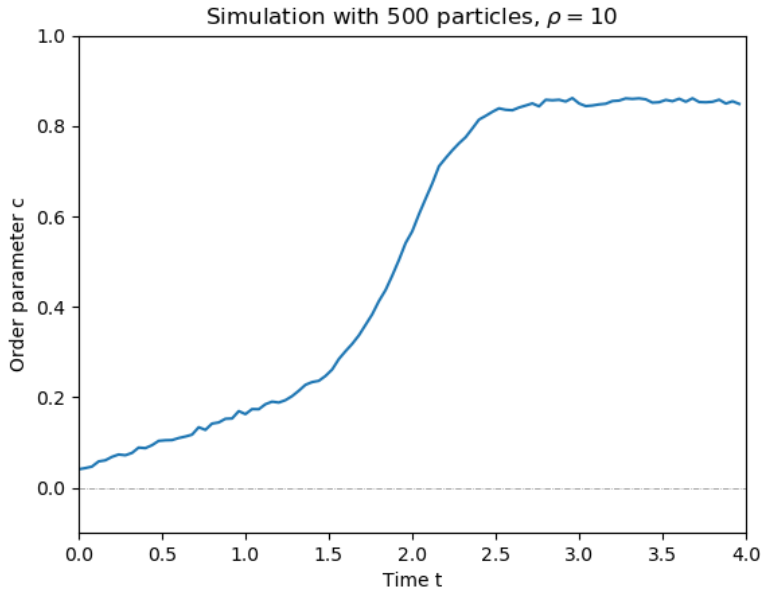

Numerical evidence of a first order phase transition