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

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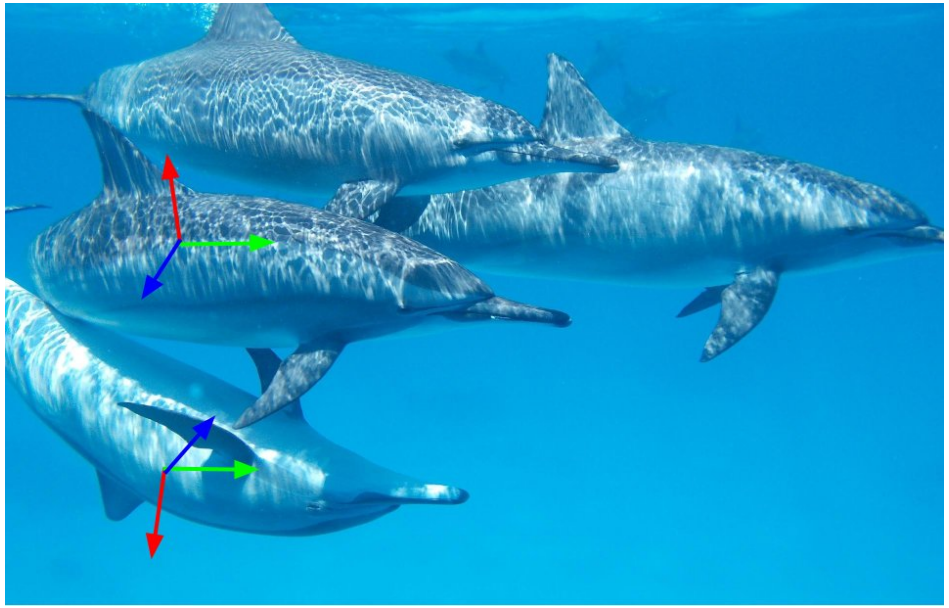
From collaborations with Pierre Degond (London), Antoine Diez (London), Sara Merino-Aceituno (Vienna), Ariane Trescases (Toulouse)
[DFMA17, DFMAT18, DFMAT19, DDFMA20]

Motivation



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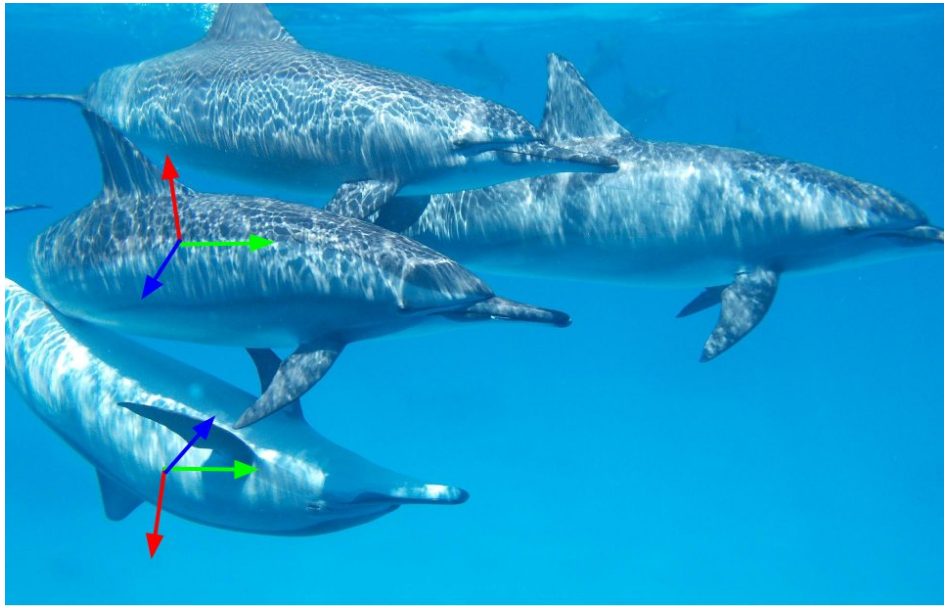


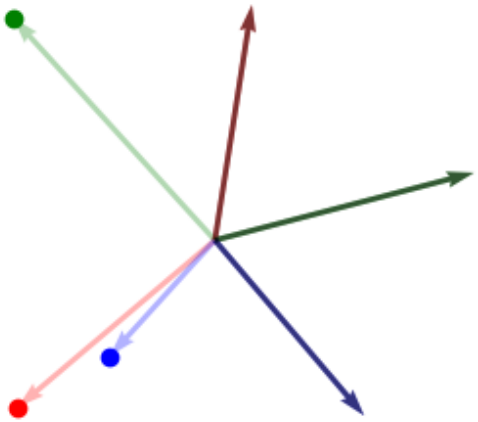
Self-propelled particles aligning their body orientation [DFMA17]

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

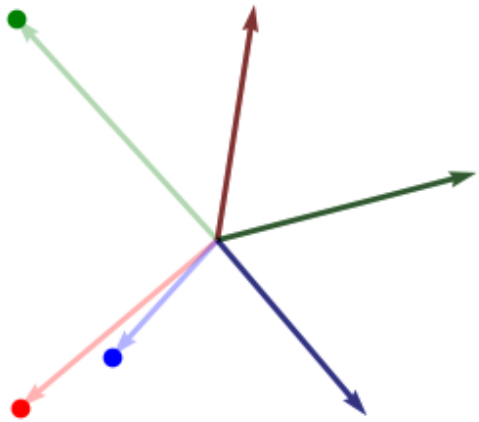
$$\begin{cases} \mathrm{d}X_k = A_k e_1 \mathrm{d}t \\ \mathrm{d}A_k = -\sum_{j \sim k} \nu_{j,k} \nabla_A (\frac{1}{2} \|A_k - A_j\|^2) \mathrm{d}t + 2\sqrt{\tau} P_{T_{A_k}} \circ \mathrm{d}B_{t,k} \end{cases}$$

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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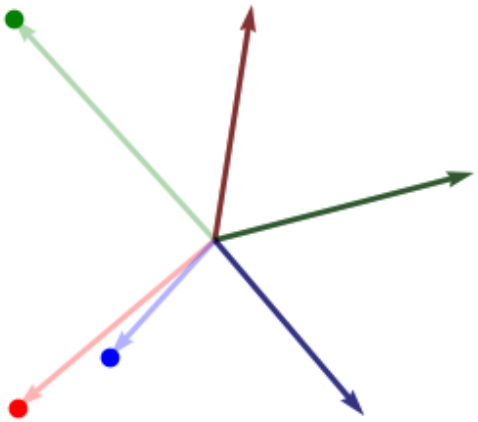

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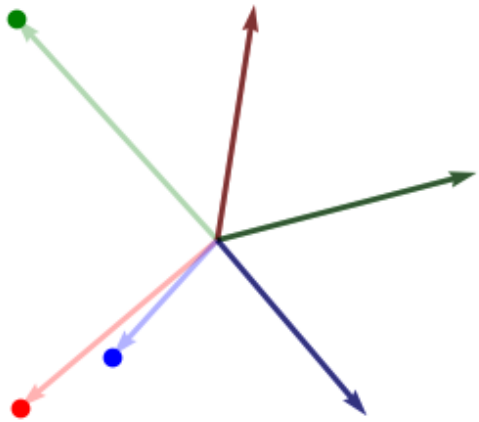
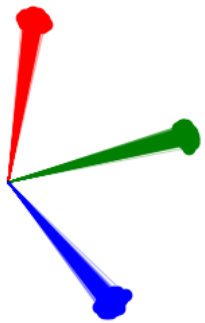


Interacting particles (orientations only, mean-field, strength $\frac{\rho}{N}$)

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

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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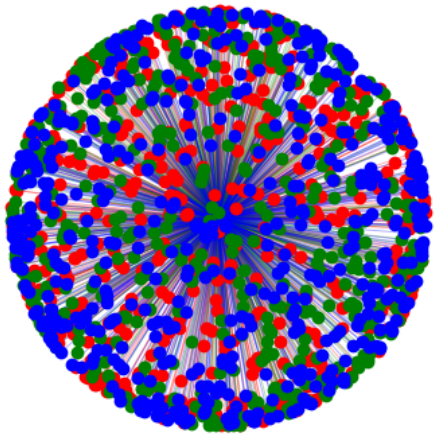

How to measure alignment ? $c = \sqrt{\frac{2}{3}\mathrm{Tr}(\langle A\rangle\langle A\rangle^T)} = \frac{\sqrt{2}}{\sqrt{3}\rho}\|J\|$

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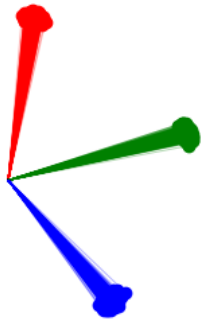

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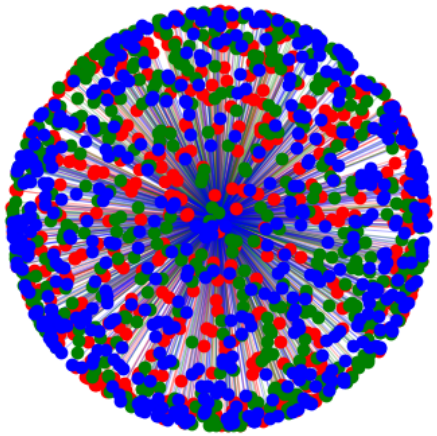
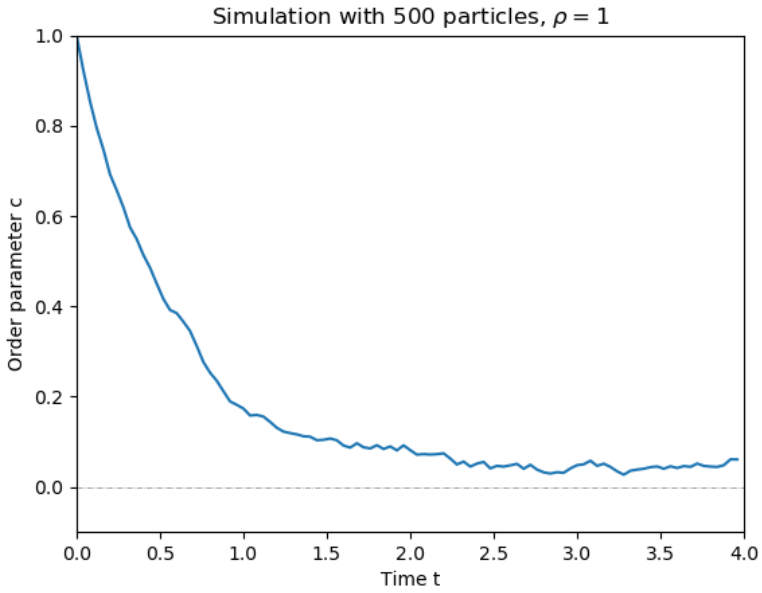
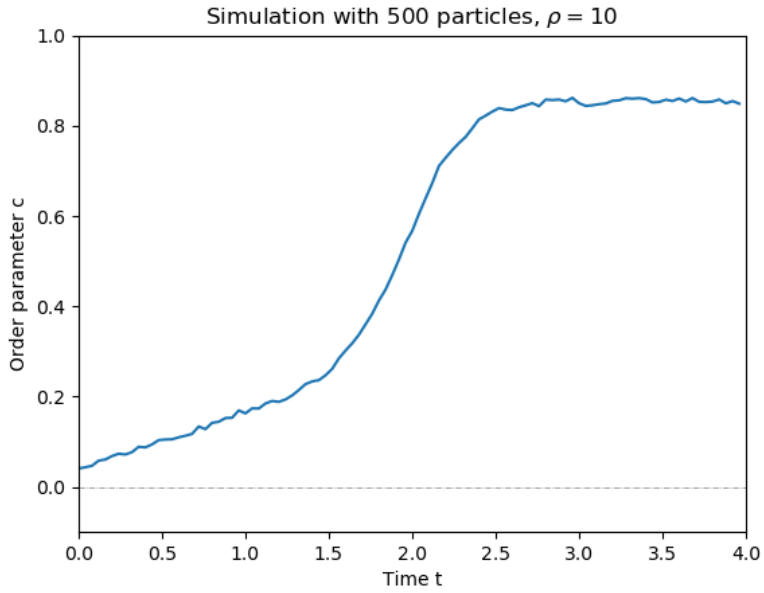
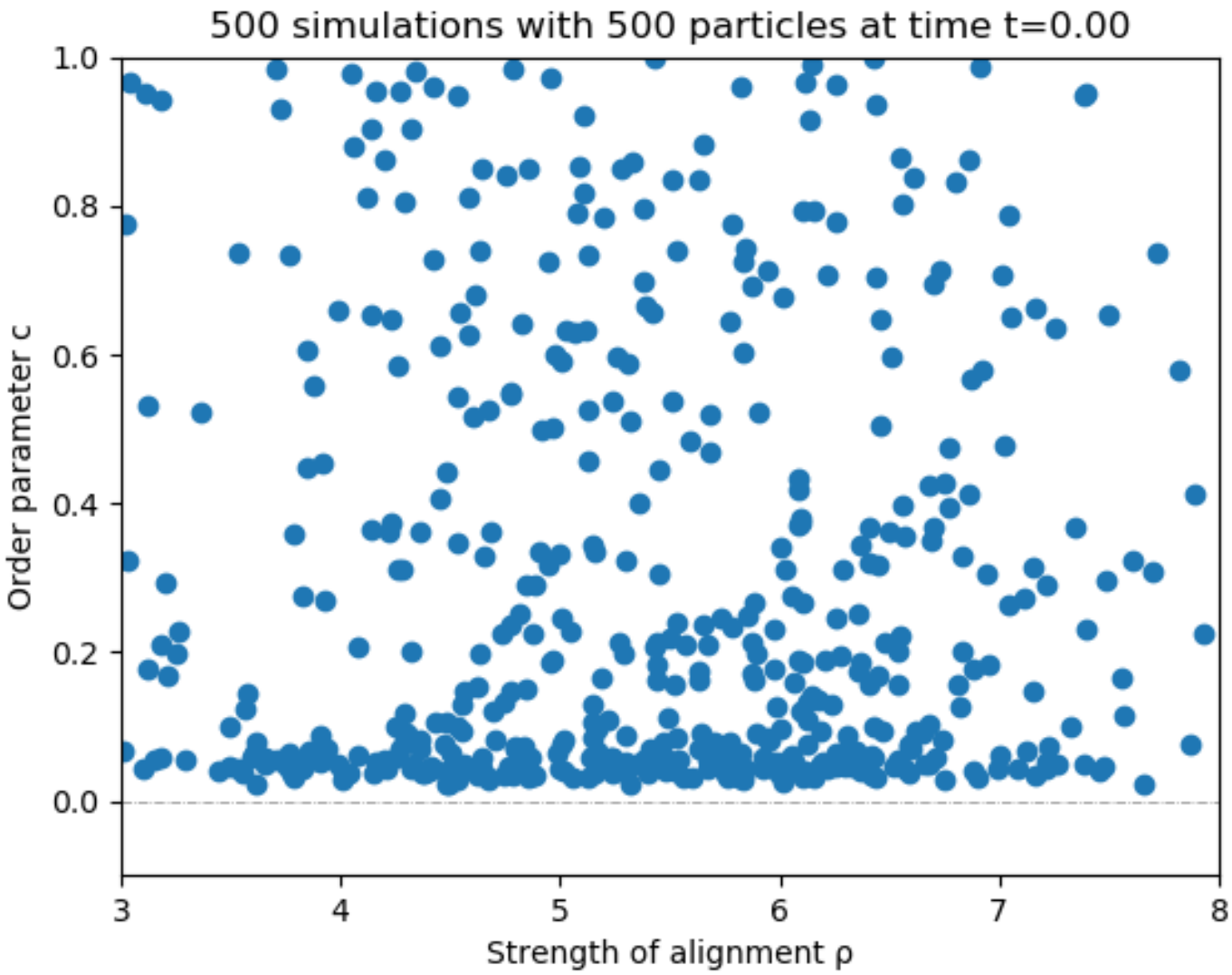






Numerical evidence of a first order phase transition



Equilibria of the space-homogeneous kinetic equation

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

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

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

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

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

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

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Higher dimensional polymers : theorem of Wang and Hoffmann [WH08].

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

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

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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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Dynamical study : BGK instead of Fokker-Planck

A simplified model

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

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

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Duhamel's formula : if $J_f \to J_\infty$ as $t \to +\infty$, then $f \to \rho M_{J_\infty}$.

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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

The equation is a gradient flow

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

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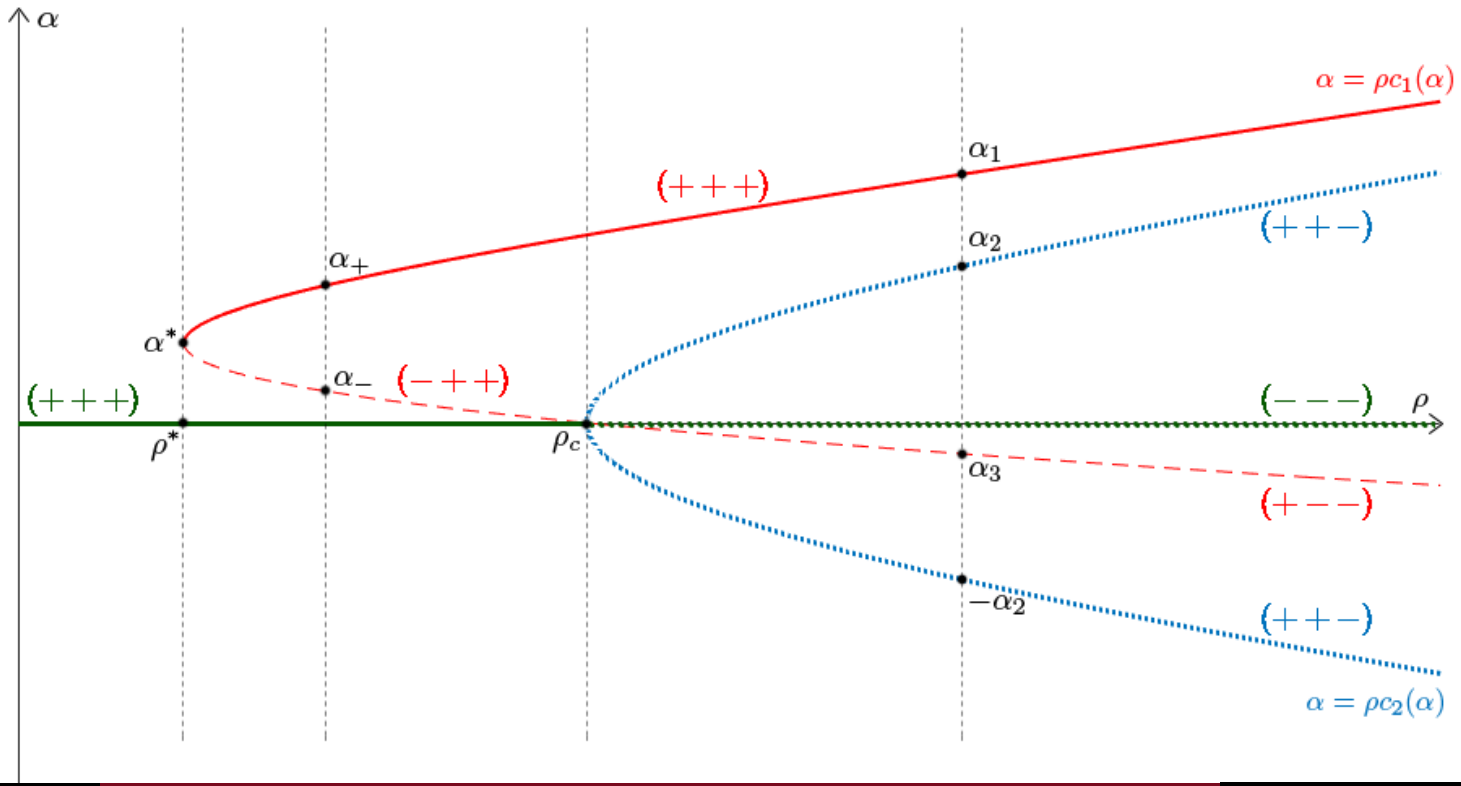
Bonus : we know the behavior of the Hessian of V !



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