A new flocking model through body attitude coordination

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ETH Zürich, November 2016
Transport phenomena in collective dynamics:
from micro to social hydrodynamics

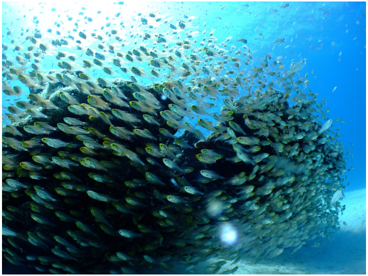
EPSRC
Engineering and Physical Sciences
Research Council

Imperial College
London

Section 1

Introduction

Emergent phenomena: auto-organisation



Many agents
Local interactions

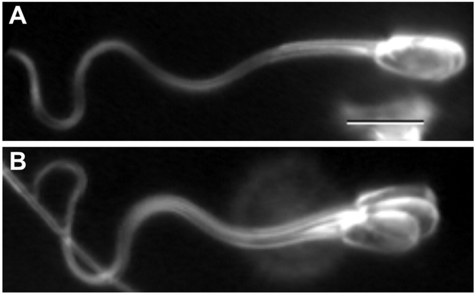


Figure: Scale bar, 10 μm. Source: *'A study of synchronisation between the flagella of bull spermatozoa, with related observations'*, David M. Woolley, Rachel F. Crockett, William D. I. Groom, Stuart G. Revell Journal of Experimental Biology 2009 212: 2215-2223.

Description of the system to model

Vicsek model

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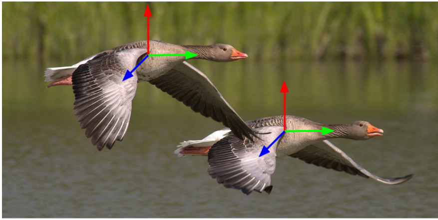
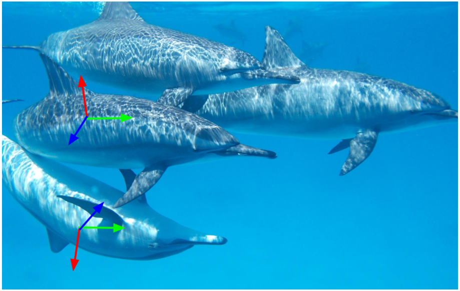


Body attitude coordination



Previous results for the Vicsek model

Equations at different scales

Vicsek model [Degond, Motsch,'08]

$(X_i(t), \omega_i(t)) \in \mathbb{R}^n \times \mathbb{S}^n$, $i = 1, \ldots, N$

$$\begin{cases} dX_i = c\omega_i dt, \quad c > 0 \\ d\omega_i = P_{\omega_i^\perp} \circ \left(\nu \bar{\omega}_i + \sqrt{2D} B_t^i\right) \quad \nu, D > 0 \\ \bar{\omega}_i := \frac{J_i}{|J_i|}, \quad J_i := \sum^N K(|X_i(t) - X_j(t)|)\omega_j \end{cases}$$

Fokker-Planck type equation

Macroscopic eq. SOH

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$f_t^N = \frac{1}{N} \sum_{i=1}^N \delta_{x_i(t), \omega_i(t)}$

(empirical distribution)

↓ $N \to \infty$ [Bolley, Carrillo, Cañizo]

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$\rho^\varepsilon = \int f^\varepsilon\, dv \to \rho$

$\int_{\mathbb{S}^n} \omega' f^\varepsilon\, d\omega' \sim \Omega^\varepsilon \to \Omega$

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Macroscopic eq. SOH $\rho = \rho(t, x)$, $\Omega = \Omega(t, x)$

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (c_1 \rho \Omega) = 0, \\ \rho \left(\partial_t \Omega + c_2 (\Omega \cdot \nabla_x) \Omega \right) + c_3 P_{\Omega^\perp}(\nabla_x \rho) = 0 \end{cases}$$

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$\varepsilon \to 0$

$f^\varepsilon \to f = \rho(t, x) M_\Omega(\omega)$

(local equilibria)

[Jiang, Xiong, Zhang]

Generalised Collision Invariant Simulation by Sébastien Motsch (ASU)

Section 2

New results: body attitude coordination

Derivation of the Individual Based Model

$(X_i, A_i)_{i\in\{1,\dots,N\}}$, $X_i \in \mathbb{R}^3$, $A_i \in SO(3)$. Averaged body orientation:

$$M_k(t) := \frac{1}{N}\sum_{i=1}^{N} K(|\mathbf{X}_i(t) - \mathbf{X}_\mathbf{k}(t)|)A_i(t). \quad (1)$$

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Lemma (Polar decomposition of a square matrix, Golub '12)

Given a matrix $M \in \mathcal{M}$, if $\det(M) \neq 0$ then there exists a unique orthogonal matrix A (given by $A = M(\sqrt{M^T M})^{-1}$) and a unique symmetric positive definite matrix S such that $M = AS$.

The matrix A minimizes the quantity
$\frac{1}{N}\sum_{i=1}^{N} K(|\mathbf{X}_i(t) - \mathbf{X}_\mathbf{k}(t)|)\|A_i(t) - A\|^2$ among the elements of $SO(3)$.

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The equations:

$$d\mathbf{X_k}(t) = v_0 A_k(t)\mathbf{e_1}\,dt \tag{2}$$

$$dA_k(t) = P_{T_{A_k}} \circ \left[\nu \mathrm{PD}(M_k)dt + 2\sqrt{D}dW_t^k\right] \tag{3}$$

Mean-field limit

Proposition (Formal)

When the number of agents in (2)-(3) $N \to \infty$, its corresponding empirical distribution

$$f^N(x, A, t) = \frac{1}{N} \sum_{k=1}^{N} \delta_{(X_k(t), A_k(t))}$$

converges weakly to $f = f(x, A, t)$, $(x, A, t) \in \mathbb{R}^3 \times SO(3) \times [0, \infty)$ satisfying

$$\partial_t f + v_0 A \mathbf{e_1} \cdot \nabla_x f = D \Delta_A f - \nabla_A \cdot (f F[f]) \tag{4}$$

$$F[f] := \nu P_{T_A}(\bar{M}[f])$$

$$\bar{M}[f] = PD(M[f]), \; M[f](x, t) := \int_{\mathbb{R}^3 \times SO(3)} K\left(x - x'\right) f(x', A', t) A' dA' dx'$$

where $PD(M[f])$ corresponds to the orthogonal matrix obtained on the Polar Decomposition of $M[f]$.

Macroscopic limit

Adimensional analysis and rescaling:

$$\partial_t f^\varepsilon + A\mathbf{e_1} \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon) + \mathcal{O}(\varepsilon) \tag{5}$$

$$F_0[f] := \nu \, P_{T_A}(\Lambda[f])$$

$$\Lambda[f] = \mathrm{PD}(\lambda[f]), \quad \lambda[f](x,t) := \int_{SO(3)} f(x, A', t) A' dA'$$

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with equilibria given by $\rho(t,x) M_\Lambda(A)$:

$$M_\Lambda(A) = \frac{1}{Z} \exp\left(\frac{\nu(A \cdot \Lambda)}{D} \right), \quad \int_{SO(3)} M_\Lambda(A)\, dA = 1, \quad \Lambda \in SO(3), \tag{6}$$

Consistency relation: $\lambda[M_{\Lambda_0}] = c_1 \Lambda_0$ where $c_1 \in (0, 1)$.

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Consistency relation: $\lambda[M_{\Lambda_0}] = c_1 \Lambda_0$ where $c_1 \in (0,1)$.
As $\varepsilon \to 0$, $f^\varepsilon \to f = f(t,x,A) = \rho M_\Lambda(A)$,
$\Lambda = \Lambda(t,x) \in SO(3)$, $\rho = \rho(t,x) \geq 0$.

Key steps of the proof: the continuity equation and the non-conservation of 'momentum'

$$\partial_t f^\varepsilon + A\mathbf{e_1}\cdot\nabla_x f^\varepsilon = \frac{1}{\varepsilon}Q(f^\varepsilon) + \mathcal{O}(\varepsilon)$$

By conservation of mass:

$$\partial_t \rho_\varepsilon + \nabla_x \cdot \underbrace{\int_{SO(3)} A\mathbf{e_1} f_\varepsilon \, dA}_{=:j[f_\varepsilon]} = \mathcal{O}(\varepsilon), \quad \rho_\varepsilon(t,x) := \int_{SO(3)} f_\varepsilon(x,A,t)\, dA$$

in the limit (formally) $\rho_\varepsilon \to \rho$ (remember that $f^\varepsilon \to \rho M_\Lambda$)

$$j[f_\varepsilon] \to \rho \int_{SO(3)} A\mathbf{e_1} M_\Lambda(A)\, dA =: j$$

by the consistency relation, we have that

$$j = \rho c_1 \Lambda \mathbf{e_1}.$$

Conclude:

$$\partial_t \rho(t,x) + \nabla_x \cdot (\rho(t,x)\, c_1 \Lambda(t,x)\mathbf{e_1}) = 0.$$

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$$\partial_t f^\varepsilon + A\mathbf{e_1} \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon) + \mathcal{O}(\varepsilon)$$

Equation for Λ? By the consistency relation:

$$\int_{SO(3)} A M_\Lambda(A)\, dA = c_1 \Lambda$$

but the 'momentum' is not conserved!

$$\frac{1}{\varepsilon} \int_{SO(3)} A Q(f^\varepsilon)(A)\, dA \neq 0$$

The Generalised Collision Invariant

Define the operator

$$\mathcal{Q}(f, \Lambda_0) := \nabla_A \cdot \left(M_{\Lambda_0} \nabla_A \left(\frac{f}{M_{\Lambda_0}} \right) \right)$$

notice in particular that

$$Q(f) = \mathcal{Q}(f, \Lambda[f]).$$

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Using this operator we define:

Definition (Generalised Collision Invariant)

For a given $\Lambda_0 \in SO(3)$ we say that a real-valued function $\psi : SO(3) \to \mathbb{R}$ is a Generalised Collision Invariant associated to Λ_0, $\psi \in GCI(\Lambda_0)$ for short, if

$$\int_{SO(3)} \mathcal{Q}(f,\Lambda_0)\psi \, dA = 0 \quad \text{for all } f \text{ s.t } P_{T_{\Lambda_0}}(\lambda[f]) = 0.$$

Why this helps? Consider $\psi_f \in GCI(\Lambda_f)$, then

$$\begin{aligned}\int_{SO(3)} \left[\partial_t f^\varepsilon + A\mathbf{e_1} \cdot \nabla_x f^\varepsilon\right] \psi_f \, dA &= \frac{1}{\varepsilon} \int_{SO(3)} Q(f^\varepsilon) \psi_f \, dA + \mathcal{O}(\varepsilon) \\ &= \frac{1}{\varepsilon} \int_{SO(3)} \mathcal{Q}(f^\varepsilon, \Lambda_f) \psi_f \, dA + \mathcal{O}(\varepsilon) \\ &= \mathcal{O}(\varepsilon)\end{aligned}$$

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&= \frac{1}{\varepsilon} \int_{SO(3)} \mathcal{Q}(f^\varepsilon, \Lambda_f) \psi_f \, dA + \mathcal{O}(\varepsilon) \\
&= \mathcal{O}(\varepsilon)
\end{aligned}$$

Reference: Ning Jiang, Linjie Xiong, Teng-Fei Zhang, *Hydrodynamic limits of the kinetic self-organized models*;
Existence of the GCI: Lax-Milgram;
Computation of the GCI: differential geometry in $SO(3)$

Computation of the GCI

Proposition (Equation for the GCI)

We have that $\psi \in GCI(\Lambda_0)$ *if and only if*

$$\textit{exists } C \in T_{\Lambda_0} \textit{ such that } \nabla_A \cdot (M_{\Lambda_0} \nabla_A \psi) = C \cdot A M_{\Lambda_0}. \tag{7}$$

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For a given $B \in T_\Lambda$ *fixed, there exists a unique* $\psi_B \in H^1(SO(3))$ *up to a constant, satisfying the relation* (7).

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Proposition (Change of variables)

Let $\bar{\psi}(B) := \psi(\Lambda B)$. *Then* $\bar{\psi}$ *satisfies*

$$\nabla_B \cdot \left(M_{Id} \nabla_B \bar{\psi}\right) = P \cdot B M_{Id}, \quad P \in \mathcal{A}. \tag{8}$$

Proposition (Non-constant GCI)

Let $P \in \mathcal{A}$, then the unique solution $\bar{\psi} \in H_0^1(SO(3))$ of (8) is given by

$$\bar{\psi}(B) = P \cdot B\, \bar{\psi}_0(\tfrac{1}{2}\mathrm{tr}(B)). \tag{9}$$

Going back to the GCI $\psi(A)$, we can write it as

$$\psi(A) = P \cdot (\Lambda^T A)\bar{\psi}_0(\Lambda \cdot A) \tag{10}$$

where $\bar{\psi}_0$ is constructed as follows: Let $\tilde{\psi}_0 : \mathbb{R} \to \mathbb{R}$ be the unique solution to

$$\frac{1}{\sin^2(\theta/2)}\partial_\theta\left(\sin^2(\theta/2)m(\theta)\partial_\theta\left(\sin\theta\tilde{\psi}_0\right)\right) - \frac{m(\theta)\sin\theta}{2\sin^2\theta/2}\tilde{\psi}_0 = \sin\theta m(\theta) \tag{11}$$

where $m(\theta) = M_{\mathrm{Id}}(B) = \exp(d^{-1}\sigma(\frac{1}{2} + \cos\theta))/Z$.
Then $\tilde{\psi}_0(\theta) = \bar{\psi}_0(\frac{1}{2}\mathrm{tr}(B))$ by the relation $\frac{1}{2}\mathrm{tr}(B) = \frac{1}{2} + \cos\theta$. $\tilde{\psi}_0$ is 2π-periodic, even and negative.

Back to the limit

$$\partial_t f^\varepsilon + A\mathbf{e_1} \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} Q(f^\varepsilon) + \mathcal{O}(\varepsilon).$$

With GCI $\psi_\Lambda^P(A) = (P \cdot \Lambda^T A)\psi_0(\Lambda \cdot A)$ for any P antisymmetric:

$$\int_{SO(3)} [\partial_t(\rho M_\Lambda) + A\mathbf{e_1} \cdot \nabla_x(\rho M_\Lambda)] \left[P \cdot \Lambda^T A\right] \psi_0(\Lambda \cdot A)\, dA = 0 \text{ for all } P \in \mathcal{A}$$

therefore

$$X := \int_{SO(3)} [\partial_t(\rho M_\Lambda) + A\mathbf{e_1} \cdot \nabla_x(\rho M_\Lambda)] (\Lambda^T A - A^T \Lambda)\psi_0(\Lambda \cdot A)\, dA = 0.$$

since

$$\mathcal{M} = \mathcal{P} \oplus \mathcal{S}$$

$\mathcal{P}$: antisymmetric matrices, $\mathcal{S}$, symmetric matrices.

Compute the value of each term.

The macroscopic equations

Theorem ((Formal) macroscopic limit)

When $\varepsilon \to 0$ *in the kinetic equation it holds that*

$$f_\varepsilon \to f = f(x, A, t) = \rho M_\Lambda(A), \qquad \Lambda = \Lambda(t,x) \in SO(3),\ \rho = \rho(t,x) \geq 0.$$

Consider the orthogonal basis $\{\Lambda \mathbf{e_1} =: \Omega, \Lambda \mathbf{e_2} =: \mathbf{u}, \Lambda \mathbf{e_3} =: \mathbf{v}\}$, *where* $\{\mathbf{e_1}, \mathbf{e_2}, \mathbf{e_3}\}$ *is the canonical basis. The equation for* Λ *expressed as the evolution of this basis is*

$$\rho D_t \Omega + P_{\Omega^\perp}\left(c_3 \nabla_x \rho + c_4 \rho \mathbf{r}\right) = 0, \tag{12}$$

$$\rho D_t \mathbf{u} - \mathbf{u} \cdot \left(c_3 \nabla_x \rho + c_4 \rho \mathbf{r}\right)\Omega + c_4 \rho \delta \mathbf{v} = 0, \tag{13}$$

$$\rho D_t \mathbf{v} - \mathbf{v} \cdot \left(c_3 \nabla_x \rho + c_4 \rho \mathbf{r}\right)\Omega - c_4 \rho \delta \mathbf{u} = 0, \tag{14}$$

where

$$D_t := \partial_t + c_2(\Omega \cdot \nabla_x), \tag{15}$$

$$\delta := [(\Omega \cdot \nabla_x)\mathbf{u}] \cdot \mathbf{v} + [(\mathbf{u} \cdot \nabla_x)\mathbf{v}] \cdot \Omega + [(\mathbf{v} \cdot \nabla_x)\Omega] \cdot \mathbf{u}, \tag{16}$$

$$\mathbf{r} := (\nabla_x \cdot \Omega)\Omega + (\nabla_x \cdot \mathbf{u})\mathbf{u} + (\nabla_x \cdot \mathbf{v})\mathbf{v}. \tag{17}$$

Proposition (Properties of δ and $\mathbf{r}$)

Let $\Lambda = \Lambda(x) : \mathbb{R}^3 \to SO(3)$ *be a function taking values on* $SO(3)$*. It holds that*

$$\delta_\Lambda = \delta_{\Lambda A} \quad \text{and} \quad \mathbf{r}_\Lambda = \mathbf{r}_{\Lambda A} \qquad \text{for any } A \in SO(3). \tag{18}$$

where δ_Λ *and* $\mathbf{r}_\Lambda$ *correspond to the expressions in* (16) *and* (17)*, respectively.*
Suppose now that $\Lambda = \Lambda(x) = \exp\left([\mathbf{b}(x)]_\times\right)\Lambda(x_0)$ *where* $\mathbf{b} = \mathbf{b}(x) : \mathbb{R}^3 \to \mathbb{R}^3$ *is a smooth function around a fixed* $x_0 \in \mathbb{R}^3$ *where* $\mathbf{b}(x_0) = 0$*, then*

$$\begin{aligned} \delta_\Lambda(x_0) &= \left(\nabla_x \cdot \mathbf{b}\right)(x_0), \\ \mathbf{r}_\Lambda(x_0) &= \left(\nabla_x \times \mathbf{b}\right)(x_0). \end{aligned}$$

Future work

- Simulations; new modelling using quaternions: joint with Pierre Degond (Imperial College London), Amic Frouvelle (Université Paris Dauphine) and Ariane Trescases (University of Cambridge).
- Study emergent structures. Compare them with the ones appearing in the Vicsek model (sperm dynamics).
- Some preliminary results: Maciek Biskupiak's video.

  Simulation by Maciek Biskupiak

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AND

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KI-NET & FIM at ETH Zürich

Summary: body attitude coordination

Equations at different scales

Individual Based Model

$(X_i(t), A_i(t)) \in \mathbb{R}^3 \times SO(3)$, $i = 1, \ldots, N$

$$\begin{cases} dX_i = v_0 A_i \mathbf{e_1} dt, \quad v_0 > 0 \\ dA_i = P_{T_{A_i}} \circ \left(\nu PD(M_k) dt + 2\sqrt{D} dW_t^i \right) \\ M_i(t) := \frac{1}{N} \sum_{k=1}^{N} K(|\mathbf{X}_k(t) - \mathbf{X_i}(t)|) A_k(t). \end{cases}$$

Fokker-Planck type equation $f = f(t, x, A)$

$$\begin{cases} \partial_t f^\varepsilon + c\omega \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon} \nabla_A \cdot \left(M_{\Lambda[f]} \nabla_A \frac{f^\varepsilon}{M_{\Lambda[f]}} \right) + \mathcal{O}(\varepsilon) \\ M_\Lambda(A) \sim \exp\left(\frac{\nu}{D} A \cdot \Lambda \right) \text{ (von-Mises eq. } SO(3)) \\ \Lambda^\varepsilon[f] \sim \int_{SO(3)} A' f^\varepsilon(t, x, A')\, dA' \end{cases}$$

Macroscopic eq. $\rho = \rho(t, x)$, $\Lambda = \Lambda(t, x)$

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (c_1 \rho \Lambda \mathbf{e_1}) = 0, \\ \rho D_t \Omega + P_{\Omega^\perp} (c_3 \nabla_x \rho + c_4 \rho \mathbf{r}) = 0, \\ \rho D_t \mathbf{u} - \mathbf{u} \cdot (c_3 \nabla_x \rho + c_4 \rho \mathbf{r}) \Omega + c_4 \rho \delta \mathbf{v} = 0, \\ \rho D_t \mathbf{v} - \mathbf{v} \cdot (c_3 \nabla_x \rho + c_4 \rho \mathbf{r}) \Omega - c_4 \rho \delta \mathbf{u} = 0, \end{cases}$$

Relations

$f_t^N = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_i(t), A_i(t)}$

(empirical distribution)

$N \to \infty$ (↓)

$f^\varepsilon = f^\varepsilon(t, x, v)$

$\rho^\varepsilon = \int f^\varepsilon \, dv \to \rho$

NON conserved quant.

Consistency relation:

$\int A' f^\varepsilon \, dA' = c_1 \Lambda^\varepsilon \to \Lambda$

$\varepsilon \to 0$ (↓)

$f^\varepsilon \to f = \rho(t, x) M_\Lambda(A)$