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Kinetic modeling for motion of Myxobacteria with nematic alignment

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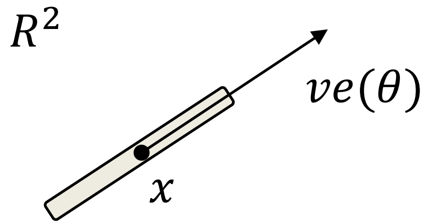
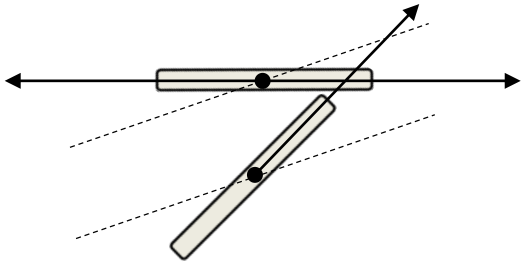
Models of Myxobacteria Motion

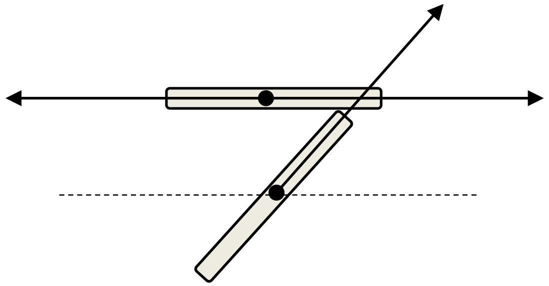
- Self-propelled elongated rods $(l \times w)$ in 2-d media
- Move along the longer axis (direction $e(\theta) \in S^2$ and speed v)
- Nematic alignment on collisions (timescale of alignment l/v):



(a) type I binary alignment (symmetric)



(b) type II binary alignment (asymmetric)

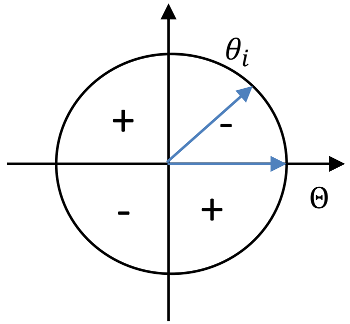


- Reversals and tumbled motion
- Chemotaxis and slime following

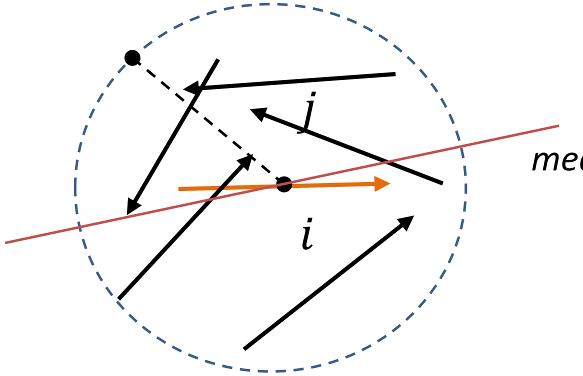
Phenomenological Models of Multi-Cell Alignment (Vicsek-type models)

- Alignment to the local mean director:

$$e^{2i\Theta(x,t)} = \frac{\sum_{j:|x_i - x_j|<l} e^{2i\theta_j}}{\left|\sum_{j:|x_i - x_j|<l} e^{2i\theta_j}\right|},$$



$$\frac{d\theta_i}{dt} = \gamma \sin(2(\Theta - \theta_i))$$



- γ – strength of alignment, l – interaction radius

- References

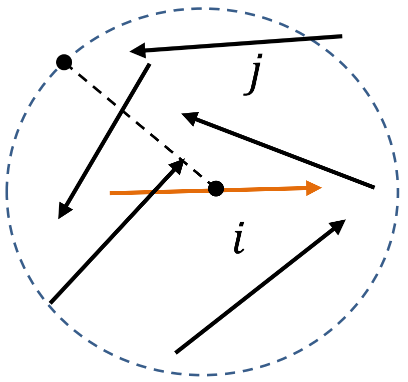
Peruani Deutch Bar A mean field theory for self-propelled particles interacting by velocity alignment mechanism (2008)
Ginelli Peruani Bar large-scale collective properties of self-propelled rods (2010)
Degond Manhart Yu A continuum model for nematic alignment (2017)
Degond Merino-Aceituno Nematic alignment of self-propelled particles: from particle to microscopic dynamics (2020)
Frouvelle Liu Dynamics in a kinetic model of oriented particles with phase transition (2011)

Phenomenological Models of Multi-Cell Alignment (Vicsek-type models)

- Mean-field model of alignment in liquid crystals (Maier-Saupe theory)

- Interaction potential for pair of cells:

$$U(\theta_i, \theta_j) = -cos^2(\theta_j - \theta_i)$$



- Aggregated potential: $\sum_{j:|x_i - x_j|<l} U(\theta_i, \theta_j)$

- Alignment along the gradient of the aggregated potential:

$$\frac{d\theta_i}{dt} = -\gamma \sum_{j:|x_i - x_j|<l} \nabla U(\theta_i, \theta_j) = \gamma \sum_{j:|x_i - x_j|<l} \sin(2(\theta_j - \theta_i))$$

- Equivalent to the mean director model with $\gamma = \gamma | \sum_{j:|x_i - x_j|<l} e^{2i\theta_j} |$

Phenomenological Models of Multi-Cell Alignment

- *Peruani-Deutch-Bar EPJ 2008* A mean field theory for self-propelled particles interacting by velocity alignment mechanism

- LC-model: N point particles (x_i, θ_i), each moving with velocity $ve(\theta_i)$ and orientation angles changes according to some averaging rule:

$$\frac{dx_i}{dt} = ve(\theta_i)$$

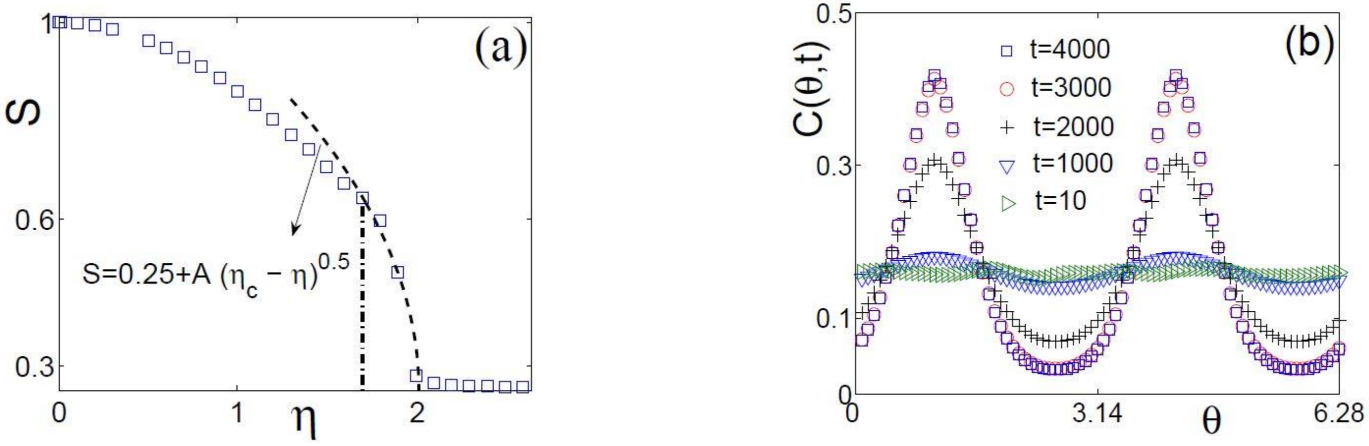
$$\frac{d\theta_i}{dt} = \gamma \sum_{j:|x_i - x_j| < l} \sin(2(\theta_j - \theta_i)) + \text{noise}$$

Phenomenological Models of Multi-Cell Alignment

- Fokker-Planck equation for the density of cells (f) in the in the phase space (x, θ)

$$\partial_t f + ve(\theta)\cdot\nabla f = \gamma N \partial_\theta \left(f \int_{|y-x|<r} \int_{-\pi}^{\pi} \sin(2(\theta-\theta_1)) f(y,\theta_1,t)\, d\theta_1 dy \right) + D\partial_\theta^2 f$$

- Application: phase transition to an aligned state (order parameter *S* , $\eta =$ diffusivity/density) parameter.



From *Peruani-Deutch-Bar EPJ 2008*

Can LC-model for myxobacteria alignment be derived from a model based on binary collisions?

Boltzmann Equation for Rarefied Gas

- f(x,v,t) – density of distribution of hard spheres in (x,v) space
- Nondimensional Boltzmann equation

$$\partial_t f + v \cdot \nabla f = \frac{Nl^2}{L^2} Q(f,f) + O\left(\frac{Nl^3}{L^3}\right)$$

N – number of spheres
l – radius
L – macroscopic length
T – macroscopic time
v = L/T – macroscopic speed

- Q(f,f) – Boltzmann operator (leading term of the collision operator)
- Inverse of Knudsen number: $Kn^{-1} = \frac{Nl^2}{L^2} = \frac{L}{d}$, d – mean free path,
- $\frac{Nl^3}{L^3} = \frac{l}{d}$

Air at 25 deg C, 1 atm, L=1m
$\frac{Nl^2}{L^2} \approx 10^7$ $\frac{Nl^3}{L^3} \approx 10^{-3}$

- Assumptions leading to the Boltzmann equation: large N, small l/L, small l/d, binary collisions, independence of two particle distribution (molecular chaos)

Boltzmann Equation for Rarefied Gas

- Boltzmann equation :

$$\partial_t f + v \cdot \nabla f = \frac{Nl^2}{L^2} Q(f, f)$$

- Short mean-free-path limit:

$$\frac{Nl^2}{L^2} \to \infty$$

- Equilibria are solutions of Q(f,f)=0. Equilibrium densities are Maxwellians

$$f(x, v, t) = \frac{\rho(x, t)}{(2\pi T(x, t))^{3/2}} e^{-\frac{|v-u(x,t)|^2}{2T(x,t)}}$$

- Collisions preserve number of particles, momentum and energy (3 moments of Q(f,,f) are zeros)
- Euler equations of Gas Dynamics for $\rho(x, t), u(x, t), T(x, t)$

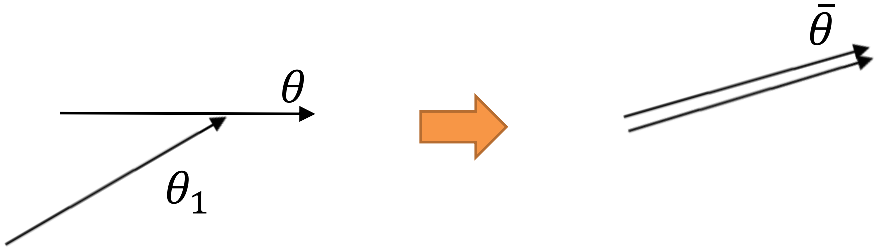
Boltzmann-type models for self-propelled rods

- **Bertin/Droz/Gregoire** Boltzmann and hydrodynamic description for self-propelled particles Phys Rev E   2018)
- **Hittmeir/Kanzler/Manhart/Schmeiser** Kinetic modeling of colonies of Myxobacteria KRM 2022)

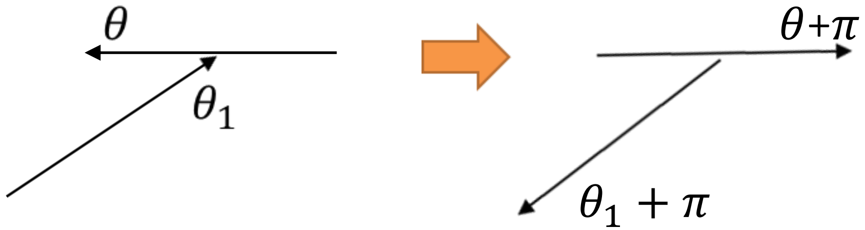
Kinetic modeling of colonies of Myxobacteria (Hittmeir/Kanzler/Manhart/Schmeiser KRM 2022)

- Cells are thin rods of length l with orientation $e(\theta)$ (unit vector) moving with velocity $ve(\theta)$

- Co-oriented collisions (angle between $e(\theta)$ and $e(\theta_1)$ is less than $\frac{\pi}{2}$



- Anti-oriented collisions (angle between $e(\theta)$ and $e(\theta_1)$ is more than $\frac{\pi}{2}$



- Number of cells and total (sum) angle are preserved in collisions

- Assumptions
  1. Binary collisions
  2. Two-particle independence

- Kinetic equation

$$\partial_t f + e(\theta)\cdot\nabla f = \frac{Nl}{L}\big(Q_{al}(f,f) + Q_{rev}(f,f)\big) + O\left(\frac{Nl^2}{L^2}\right)$$

- Limit of $N \to \infty,\ \frac{l}{L} \to 0,\ \frac{Nl}{L} \to \infty$ and $\frac{Nl^2}{L^2} \to 0$
- Equilibrium: $Q_{al}(f,f) + Q_{rev}(f,f) = 0$

$$\Leftrightarrow \quad f_{eq}(x,\theta,t) = \rho_+(x,t)\delta\big(\theta - \theta_+(x,t)\big) + \rho_-(x,t)\delta(\theta - \theta_+(x,t) - \pi)$$

Kinetic modeling of colonies of Myxobacteria (Hittmeir/Kanzler/Manhart/Schmeiser KRM 2022)

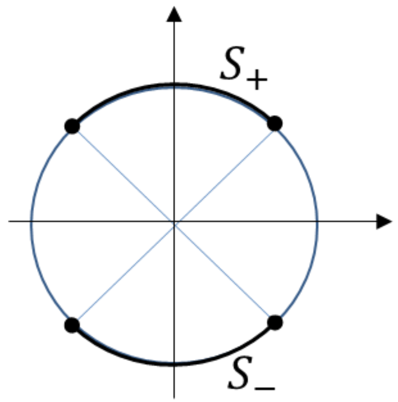
- Collision and Reversal operators

$$Q_{al}(f,f) = -\int_{\theta-\frac{\pi}{2}}^{\theta+\frac{\pi}{2}} |\sin(\theta-\theta_1)| f(x,\theta,t) f(x,\theta_1,t)\, d\theta_1 + 2\int_{\theta-\frac{\pi}{4}}^{\theta+\frac{\pi}{4}} |\sin(\theta-\theta_1)| f(x,2\theta-\theta_1,t) f(x,\theta_1,t)\, d\theta_1$$

$$Q_{rev}(f,f) = -\int_{\theta+\frac{\pi}{2}}^{\theta+\frac{3\pi}{2}} |\sin(\theta-\theta_1)| f(x,\theta,t) f(x,\theta_1,t)\, d\theta_1 + \int_{\theta+\frac{\pi}{2}}^{\theta+\frac{3\pi}{2}} |\sin(\theta-\theta_1)| f(x,\theta+\pi,t) f(x,\theta_1+\pi,t)\, d\theta_1$$

Kinetic modeling of colonies of Myxobacteria (Hittmeir/Kanzler/Manhart/Schmeiser KRM 2022)

- Two-group orientation geometry is invariant under collisions
- Orientation groups, S_+, S_-, are invariant in transport and collisions
- Number of cells in each group, S_+, S_-, is preserved in collisions
- 3 conserved quantities and 3 parameters in equilibrium density
- Applications: existence/uniqueness/convergence to equilibrium for space homogeneous eq for “Maxwellian cells”

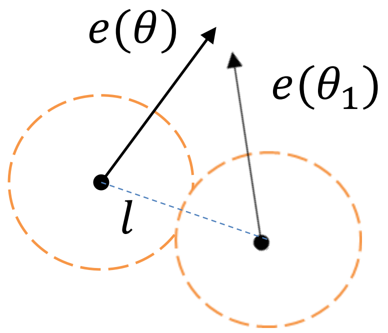


$$\partial_t \rho_+ + \nabla \cdot (\rho_+ e(\theta_+)) = 0$$
$$\partial_t \rho_- - \nabla \cdot (\rho_- e(\theta_+)) = 0$$
$$\partial_t ((\rho_+ + \rho_-)\theta_+) + \nabla \cdot ((\rho_+ + \rho_-)\theta_+ e(\theta_+)) = 0$$

Hyperbolic system of PDEs

Boltzmann and hydrodynamic description for self-propelled partiles (Bertin/Droz/Gregoire Phys Rev E 2018)

- Two point particles moving with velocities $ve(\theta)$ and $ve(\theta_1)$ interact when distance between particles < l
- New orientations



$$\hat{\theta} = \bar{\theta} + \eta$$
$$\hat{\theta}_1 = \bar{\theta} + \eta_1$$
$$\bar{\theta} = \mathrm{Arg}(\mathrm{e}(\theta) + \mathrm{e}(\theta_1))$$

η, η_1- independent Gaussians (noise)

- Diffusion: random adjustments to orientation as a Poisson process with frequency λ: $\hat{\theta} = \theta + \eta_d$

- Binary collisions, Two-particle independence, $\mathrm{N} \to \infty$, $\frac{l}{L} \to 0$, $\frac{\lambda L}{v} \approx 1$, $\frac{Nl}{L} \approx 1$ and $\frac{Nl^2}{L^2} \to 0$

$$\partial_t f + e(\theta) \cdot \nabla f = Q_{diff}(f, f) + Q_{al}(f, f)$$

Macroscopic parameters: density ρ and momentum w

$$\rho(x,t) = \int_{-\pi}^{\pi} f(x, \theta, t) d\theta$$
$$w(x,t) = \int_{-\pi}^{\pi} e(\theta) f(x, \theta, t)\, d\theta$$
$$= \int_{-\pi}^{\pi} e^{i\theta} f(x, \theta, t)\, d\theta$$

Boltzmann and hydrodynamic description for self-propelled partiles (Bertin/Droz/Gregoire Phys Rev E 2018)

- Conservation of number of cells in collisions

$$\partial_t \rho + \nabla \cdot w = 0$$

- First moment

$$\partial_t w = \int_{-\pi}^{\pi} e(\theta)\left(-e(\theta)\cdot\nabla f + Q_{al} + Q_{diff}\right) d\theta$$

- Fourier modes $f = \sum f_k e^{ik\theta}$ with

$$f_0 \approx \rho, \qquad f_1 \approx w$$

- Asymptotic regime of small macroscopic velocity:

$$\rho \approx O(1), |w| = \varepsilon,\ |f_k| \approx O\left(\varepsilon^{-|k|}\right),\ \varepsilon \ll 1$$

Limiting macroscopic equations

$$\partial_t \rho + \nabla \cdot w = 0$$

$$\partial_t w + \gamma(w\cdot\nabla)w = -\frac{1}{2}\nabla(\rho - k w\cdot w) + (\mu - \xi w\cdot w)w + \nu\Delta w - k(\nabla\cdot w)w$$

- Application: stability of homogeneous state

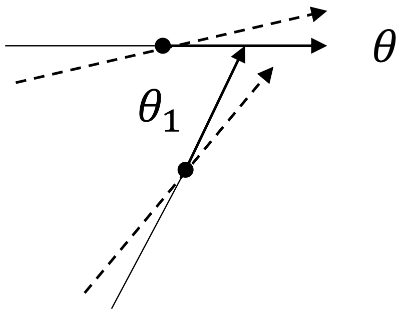
$$\partial_t w = (\mu - \xi w\cdot w)w$$

If $\mu < 0$, the only steady state w=0 (stable)

if $\mu > 0$, non-zero steady states $w = \sqrt{\frac{\mu}{\xi}}\, e(\theta)$

A mean-field model for nematic alignment of self-propelled rods (MP/Murphy/Igoshing/Timofeyev to appear in Phys Rev E 2022)

- Symmetric alignment in binary collisions

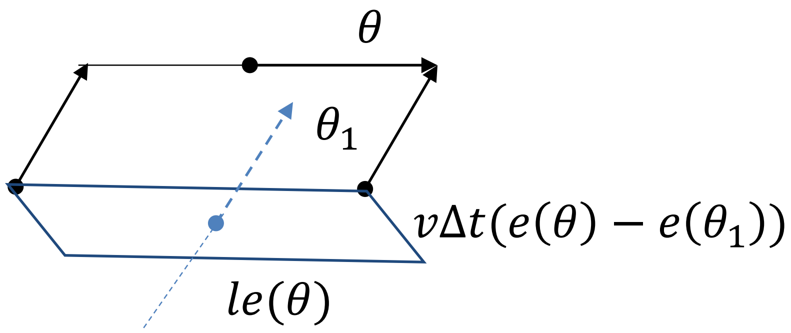


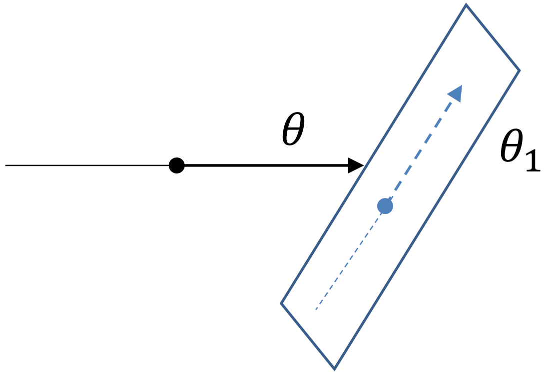
- δ – small parameter

$$\theta' = \theta + \delta \sin(2(\theta_1 - \theta))$$
$$\theta_1' = \theta_1 - \delta \sin(2(\theta_1 - \theta))$$

- Assumptions: binary collisions, two-particle independence

- Geometry of interactions in time Δt





- Area of interaction parallelograms:

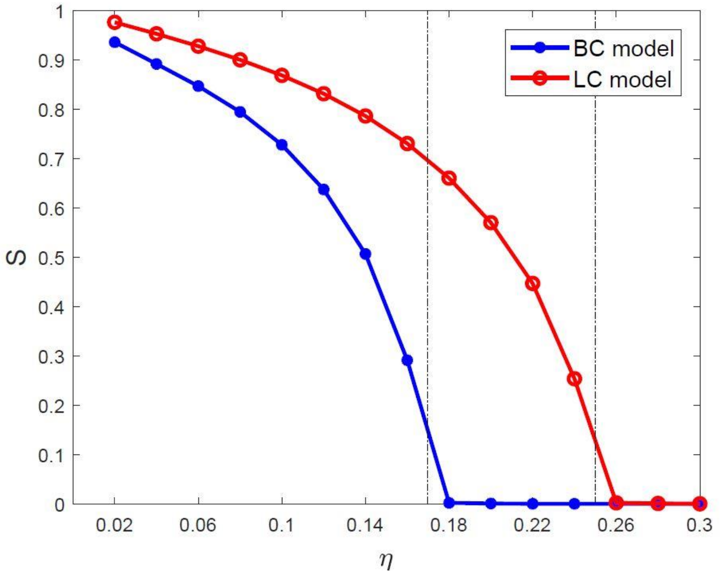
$$lv\Delta t|\sin(\theta - \theta_1)|$$

A mean-field model for nematic alignment of self-propelled rods

- Balance of probability + Scaling + Asymptotic expansion:

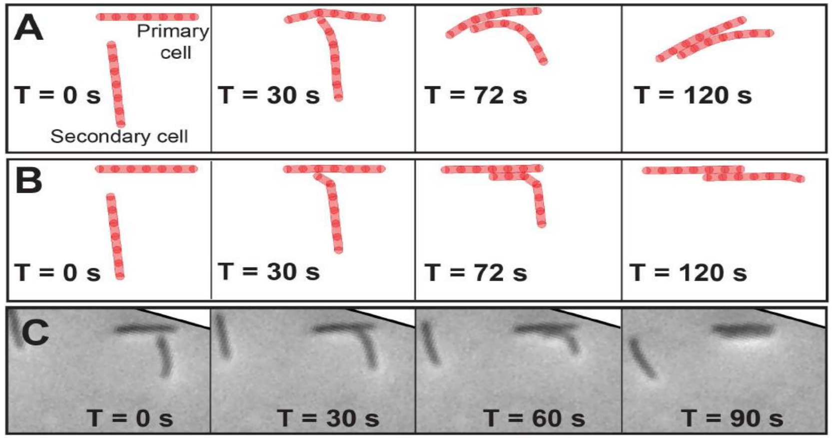
$$\partial_t f + v(\theta)\cdot\nabla f = -\frac{(N-1)l\delta}{L}\partial_\theta\left(f(x,\theta,t)\int_{-\pi}^{\pi}|\sin(\theta_1'-\theta)|\phi(\theta_1'-\theta)f(x,\theta_1',t)\,d\theta_1'\right) + O\left(NlL^{-1}\delta^2\right) + O\left(Nl^2L^{-2}\delta\right).$$

- $\delta \ll 1,\ \frac{l}{L} \ll 1,\ \ \mathrm{N} \gg 1$
- $\frac{Nl\delta}{L} = \delta\frac{N}{L^2}(lL) = 1$: (amount of alignment per collision)x(cell density)x("interaction area" over characteristic distance L)=(amou of alignment per collision)x(# of collisions over characteristic distance L)=1
- Large number of collisions over characteristic distance L
- Conclusion: Liquid crystal model of myxocell alignment can be derived on the basis of purely collisional model, in the limit of the zero interaction distance and large number of cells



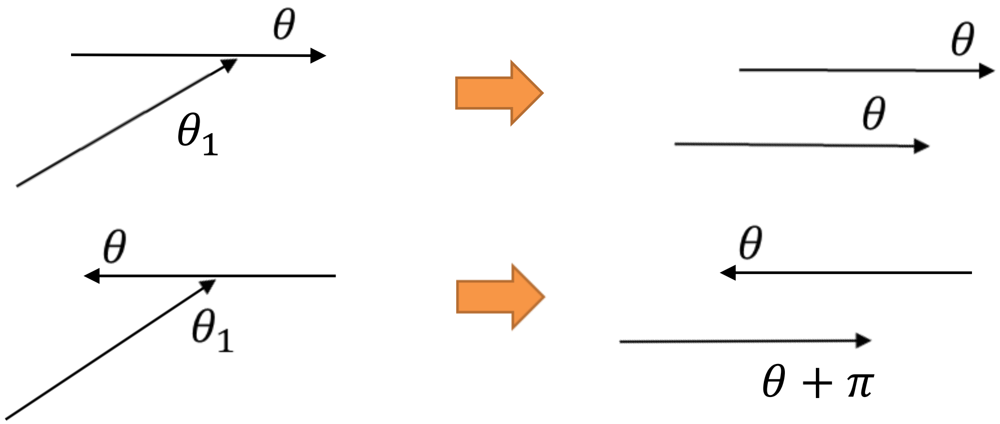
- Application: phase transition to an aligned state

Asymmetric Alignment



Mechanical interactions between two cells during head-to-side collision. From Balagam et al. PLOS Comp. Bio. 2014.

Pre-collision: Post-collision:



Kinetic equation

$$\partial_t f + e(\theta) \cdot \nabla f = \frac{Nl}{L} Q_o(f,f) + \frac{Nl^2}{L^2} Q_1(f,f)$$

Physical range: $\frac{Nlw}{L^2} < 1$

Length (l) = 3µm, width (w) = 0.5µm: $\frac{Nl^2}{L^2} < 6$

N = 1,000-10,000 L = 500µm

$\frac{Nl}{L} = 6..60$ $\frac{Nl^2}{L^2} = 0.036..0.36$

- Initial set of orientations and their reflections is preserved in collisions and transport

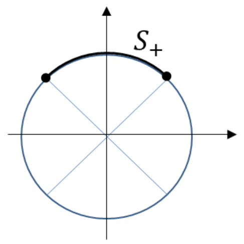
- Assumptions:
  1. Binary collisions
  2. Two-particle independence
  3. $\frac{Nl}{L} \gg 1,\ \frac{Nl^2}{L^2} \approx 1$

Interaction Operators

$$Q_0(f,f) = \int_{\theta-\frac{\pi}{2}}^{\theta+\frac{\pi}{2}} |\sin(\theta-\theta_1)|(f(x,\theta+\pi,t)f(x,\theta_1,t) - f(x,\theta,t)f(x,\theta_1+\pi,t))\,d\theta_1$$

$$Q_1(f,f) = \int_{\theta-\frac{\pi}{2}}^{\theta+\frac{\pi}{2}} |\sin(\theta-\theta_1)|\,(f(x,\theta_1,t)e(\theta_1)\cdot\nabla_x f(x,\theta,t) - f(x,\theta,t)e(\theta)\cdot\nabla_x f(x,\theta_1,t)$$
$$+ f(x,\theta_1,t)e(\theta_1)\cdot\nabla_x f(x,\theta+\pi,t) - f(x,\theta,t)e(\theta)\cdot\nabla_x f(x,\theta_1+\pi,t))\,d\theta_1$$

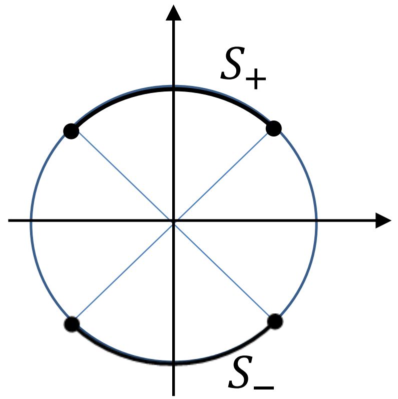
- Asymmetry (key property): $Q_0(f,f)(x,\theta+\pi,t) = -Q_0(f,f)(x,\theta,t)$
- Equilibria: $Q_0(f,f) = 0$
- One co-oriented group:
  $f(x,\theta,t)$ supported on S_+



- Two co-oriented groups:

$$f(x,\theta,t) = \begin{cases} f_+(x,\theta,t), & \theta \in S_+ \\ \lambda(x,t)f_+(x,\theta+\pi), & \theta \in S_- \end{cases}$$

(the only equilibrium for two nematic orientations)



Singular Limit and Macroscopic Equations

Limit of $\mathrm{N} \to \infty$, $\frac{\mathrm{l}}{\mathrm{L}} \to 0$, $\frac{\mathrm{Nl}}{\mathrm{L}} \to \infty$, and $\frac{\mathrm{Nl}^2}{\mathrm{L}^2} \approx 1$

- Implications:
  1. $Q_0(f, f) \to 0$
  2. If initial data are nematically co-oriented then so is $f(x, \theta, t)$ for any (x, t)
  3. Assuming finite set of m initial orientations $\theta_1, \ldots, \theta_m$,

$$f(x, \theta, t) = \sum_k \rho_k(x, t)\delta(\theta - \theta_k) + \lambda(x, t)\rho_k(x, t)\delta(\theta - \theta_k - \pi)$$

(m+1) macroscopic parameters

- Equations:
  1. conservation of total number of cells
  2. m asymmetry conditions

Examples of Macroscopic Equations

- One co-oriented group with two angles θ_1, θ_2:

$$\partial_t \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix} + A(\rho)\partial_x \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix} = 0,$$

where $A(\rho)$ is a 2×2 matrix

$$A(\rho) = \begin{bmatrix} e(\theta_1)_1 - |\sin(\theta_1 - \theta_2)| e(\theta_2)_1 \rho_2 & |\sin(\theta_1 - \theta_2)| e(\theta_1)_1 \rho_1 \\ |\sin(\theta_1 - \theta_2)| e(\theta_2)_1 \rho_2 & e(\theta_2)_1 - |\sin(\theta_1 - \theta_2)| e(\theta_1)_1 \rho_1 \end{bmatrix}$$

- Two nematically co-oriented group with two angles:

$$\partial_t \begin{bmatrix} \rho_1 \\ \rho_2 \\ \lambda \end{bmatrix} + A(\rho)\partial_x \begin{bmatrix} \rho_1 \\ \rho_2 \\ \lambda \end{bmatrix} = 0,$$

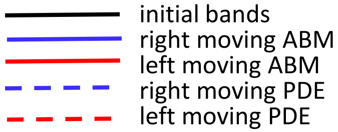
$A(\rho)$ is a 3x3 matrix

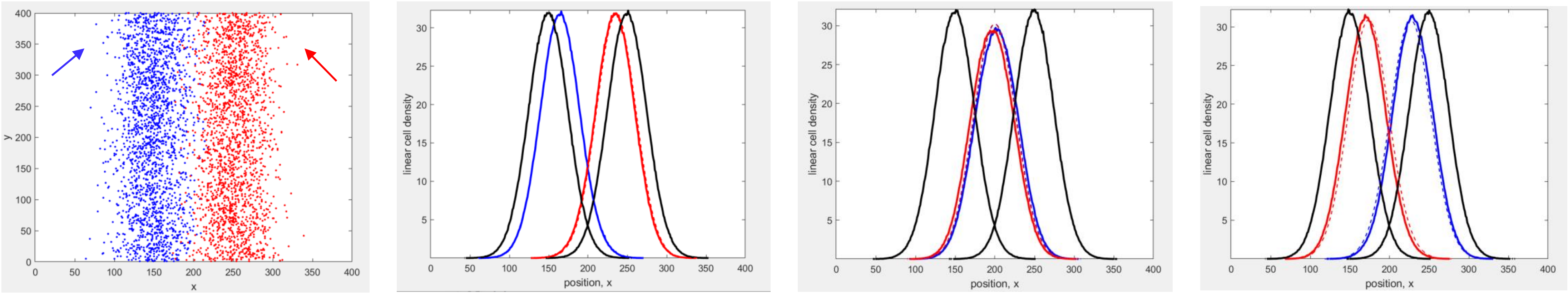
$$\begin{bmatrix} \frac{1-\lambda+(1-\lambda^2)\rho_2}{\sqrt{2}(1+\lambda)} + \frac{\sqrt{2}\lambda\rho_1}{(1+\lambda)(\rho_1+\rho_2)} & \frac{(1-\lambda)\rho_1}{\sqrt{2}} - \frac{\sqrt{2}\lambda\rho_1}{(1+\lambda)(\rho_1+\rho_2)} & \frac{-\rho_1+2(1-\lambda)\rho_1\rho_2}{\sqrt{2}(1+\lambda)} + \frac{\rho_1(\rho_1-\rho_2)}{\sqrt{2}(1+\lambda)(\rho_1+\rho_2)} \\ -\frac{(1-\lambda)\rho_2}{\sqrt{2}} + \frac{\sqrt{2}\lambda\rho_2}{(1+\lambda)(\rho_1+\rho_2)} & -\frac{1-\lambda+(1-\lambda^2)\rho_1}{\sqrt{2}(1+\lambda)} - \frac{\sqrt{2}\lambda\rho_2}{(1+\lambda)(\rho_1+\rho_2)} & \frac{-\rho_2-2(1-\lambda)\rho_1\rho_2}{\sqrt{2}(1+\lambda)} + \frac{\rho_2(\rho_1-\rho_2)}{\sqrt{2}(1+\lambda)(\rho_1+\rho_2)} \\ -\frac{\sqrt{2}\lambda}{(\rho_1+\rho_2)} & \frac{\sqrt{2}\lambda}{(\rho_1+\rho_2)} & -\frac{(\rho_1-\rho_2)}{\sqrt{2}(\rho_1+\rho_2)} + \frac{\sqrt{2}\lambda\rho_2}{(1+\lambda)(\rho_1+\rho_2)} \end{bmatrix}$$

- Hyperbolic system of PDES

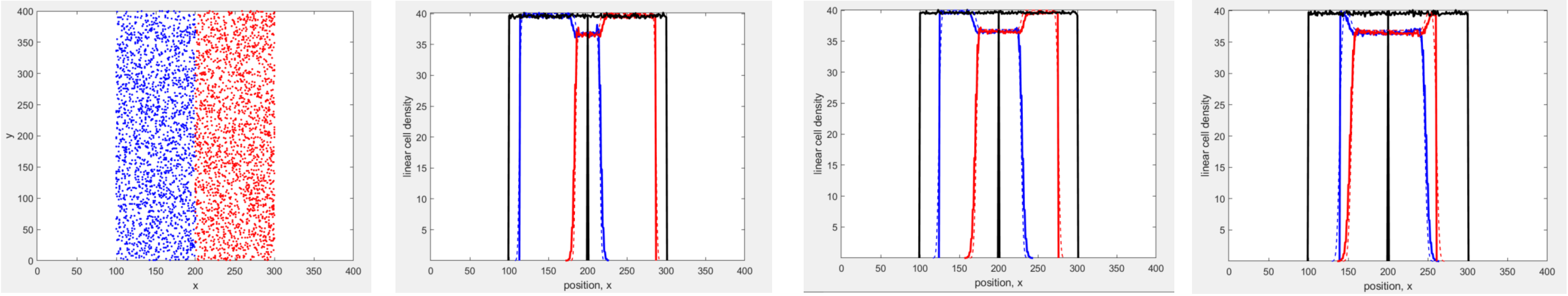
ABM and PDE simulations

- Two orientations θ_1, θ_2, N=4000 cells, square domain of side L=400μm, average over 1000 simulations





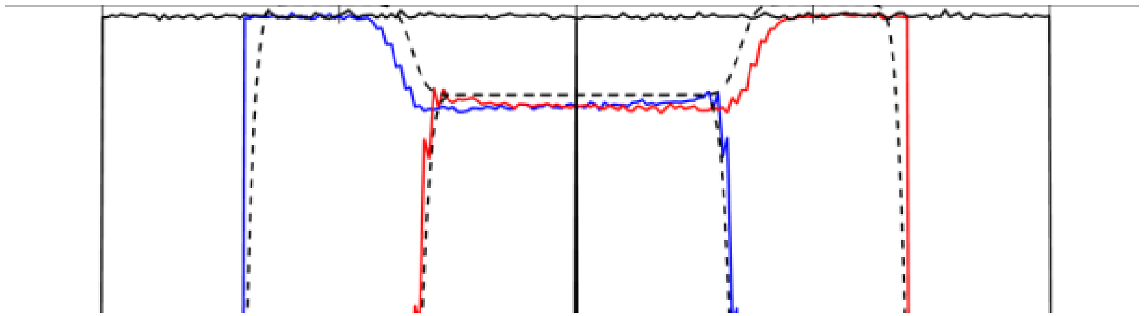
Gaussian bands



Uniform bands

ABM and PDE simulations

- Interaction of uniform bands
- ABM (solid line) vs. PDE (dotted line)

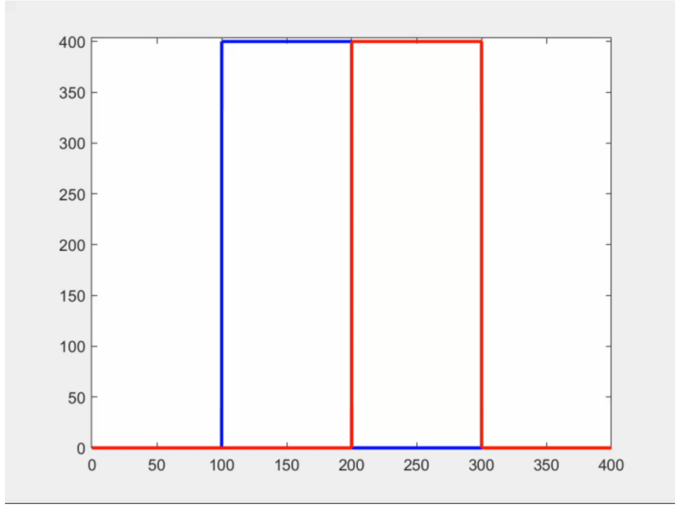


PDEs $(c_1, c_2 > 0)$

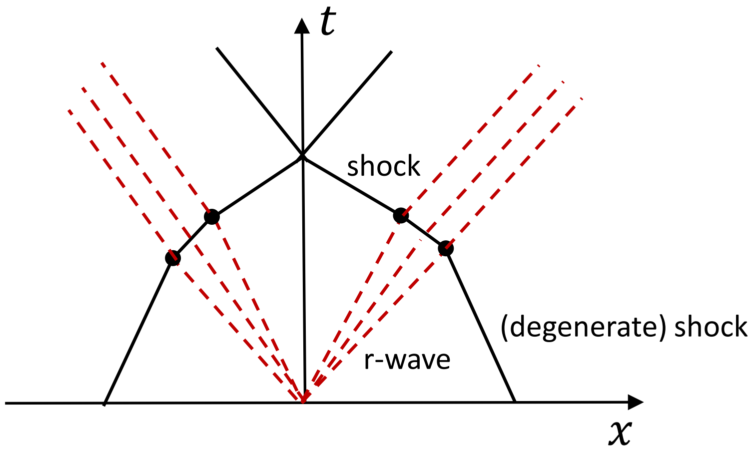
$$\partial_t \rho_1 + c_1 \partial_x(\rho_1(1 + c_2\rho_2)) = 0$$
$$\partial_t \rho_2 - c_1 \partial_x(\rho_2(1 + c_2\rho_1)) = 0$$

Numerical solution of PDE model (Lax-Friedrichs scheme)

- Interaction of uniform bands (numerical solution of PDEs)



- Wave structure in the interaction of two uniform bands



Further Comments

I. Summary

- Boltzmann-type PDE model gives reasonable qualitative approximation of agent-base dynamics
- Higher order terms in the Boltzmann equation must be accounted for

II. Difficulties

- PDEs are generically non-conservative
- Agent-based dynamics exhibit growth of correlations (clustering due to short mean-free path)
- Two-particle independence hypothesis is violated in a long run
- Boltzmann-type PDE model is valid in transient regimes

III. Future Work

- Different closures for the kinetic function (f)
- Models with Reversals and Refraction period
- Different geometries of alignment (for ex. turning trough the head of a cell)