Macroscopic models for collective sperm-cells dynamics and cells inclination

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Joint work with Pierre Degond

ANR Motimo
Workshop "Collective dynamics of active particles, swimmers, motile cells"
IMFT, Toulouse, 23 September 2015

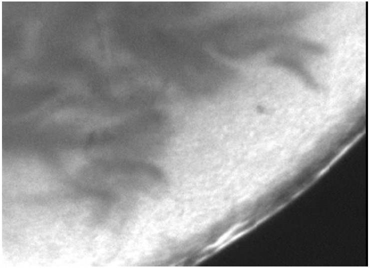
ANR Motimo

→ spermatozoa in seminal liquid

- 5.10^9 cells per cm^3
- volume ratio 50%

→ collective movement

- mass motility
- dark waves
- fertility measure



[X. Druart]

Spermatozoa : collective movement and cell geometry

- cell geometry
  - head : flat ellipsoids
  - flagella : neglected
- head inclination $\Rightarrow$ dark zone

Collective displacements

system of interacting particles

$$(x_k(t), v_k(t)),\ k \in \{1, \dots, N\}$$

$$\Downarrow$$

macroscopic model

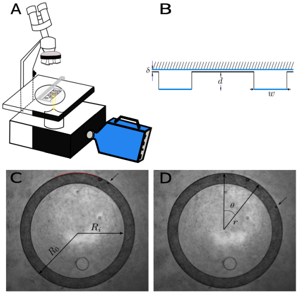
$$(\rho(x,t), u(x,t))$$

Interactions

- hydrodynamic interactions
- volume-exclusion interactions
  predominant at large density

  $\Rightarrow$ **local alignment** for self-propelled elongated particles [Peruani, 2006]

  $\Rightarrow$ experiment validation : spontaneous rotation [Creppy et al.]



[Creppy et al., to appear]

Modeling assumptions

- self-propulsion
- local alignment interactions with neighbors
  (volume-exclusion interactions)
- geometry : flat disks

Context

- system of interacting particles
- self-propelled dynamics with alignment interactions :
  Vicsek dynamics, phase transition, band formation [Vicsek, Chaté, etc.]
- derivation of macroscopic model with kinetic theory [Degond, Motsch, 2008]

Plan

1. Particle model
2. Derivation of the macroscopic model
3. Macroscopic model
4. Numerical simulations
5. Conclusion

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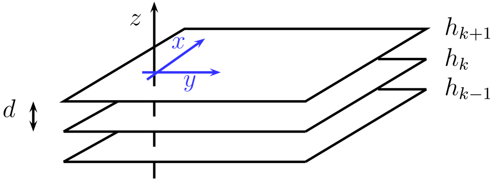
Particle model

- **2D flow**

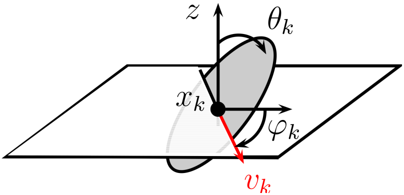
  Displacements in layers

  Layers : horizontal planes with inter-distance d



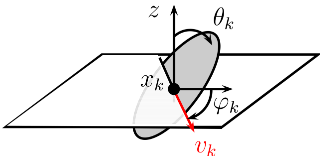
- Motion inside layers

(altitude) $h_k \in \mathbb{R}$
(position) $x_k(t) \in \mathbb{R}^2$
(velocity) $v_k(t) \in \mathbb{S}^1 \to \varphi_k(t) \in [0, 2\pi]$



- Spatial configuration of disks

$v_k \in$ Disk plane
(inclination) $\theta_k(t) \in [0, \pi]$



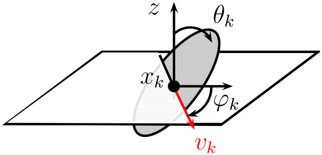
Microscopic model

$$\frac{dx_k}{dt} = v(\varphi_k),$$

$$d\varphi_k = -\nu \sin(\varphi_k - \bar{\varphi}_k)\, dt + \sqrt{2D}\, dB_t^{\varphi,k} \quad \text{modulo } 2\pi,$$

$$d\theta_k = (-K \sin(2(\theta_k - \bar{\theta}_k)) + \mu T_k)\, dt + \sqrt{2\delta}\, dB_t^{\theta,k} \quad \text{modulo } \pi,$$

- **self-propulsion : unit speed** $(v_k = v(\varphi_k) = (\cos\varphi_k, \sin\varphi_k)^T)$



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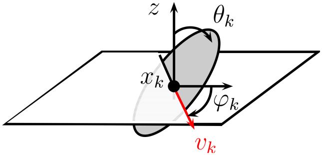
  → local alignment with the disks of the same layer
  → local alignment with the disks the neighboring layers



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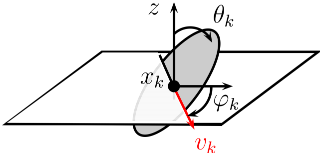
  → nematic alignment with disks of the same layer : relax to $\bar{\theta}_k$
  → with disks of the neighboring layers : torque w.r.t to $\langle v_k \rangle$: T_k

$$T_k = \sum_{\substack{j, h_j = h_k \pm 1, \\ |X_j - X_k| \leqslant R}} T_{kj} \qquad T_{kj} = \text{sign}(h_j - h_j)\,(v_k \times v_j) \cdot \hat{z}$$



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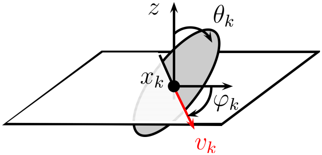

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⇒ several parameters : ν, μ, K, D, δ

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Mean-field kinetic equation

- $f(x,\varphi,\theta,h,t)$ distribution function in phase space
  $x \in \mathbb{R}^2, \varphi \in [0,2\pi], \theta \in [0,\pi], h \in \mathbb{N}$

- Mean-field model

$$\partial_t f + \nabla_x \cdot (v(\varphi) f) = -\partial_\varphi \Big(-\nu \sin(\varphi - \bar{\varphi}_f) f \Big) + D\, \partial_\varphi^2 f$$
$$- \partial_\theta \Big((-K \sin(2(\theta - \bar{\theta}_f)) + \mu\, T_f) f \Big) + \delta\, \partial_\theta^2 f$$

with $v(\varphi) = (\cos\varphi, \sin\varphi)^T$.

Mean inclination angle $\bar{\theta}_f$:

$$e^{2i\bar{\theta}_f} = \frac{J^\theta_{R,f}}{|J^\theta_{R,f}|} \quad J^\theta_{R,f}(x,h,t) = \int_{\substack{\theta\in[0,\pi],\varphi\in[0,2\pi],\\ y\in\mathbb{R}^2, |y-x|\leqslant R}} e^{2i\theta} f(y,\varphi,\theta,h,t)\, dy\, d\varphi\, d\theta$$

Rescaling

- Large time and space scale (hydrodynamic rescaling)

$$\tilde{x} = \varepsilon x, \quad \tilde{t} = \varepsilon t, \quad \varepsilon \ll 1$$

- interaction frequency inside layers

  $\gg$ interaction frequency between neighboring layers

  $\to \mu = \varepsilon \mu'$, with $\mu' = O(1)$
  $\to \beta = \varepsilon \beta'$, with $\beta' = O(1)$

$$\varepsilon \Big(\partial_t f^\varepsilon + \nabla_x \cdot (v(\varphi) f^\varepsilon) + \overbrace{\partial_\theta(\mu T_{f^\varepsilon} f^\varepsilon) + \partial_\varphi \big(S_{f^\varepsilon} f^\varepsilon \big)}^{\text{interactions with nb. layers}} \Big)$$
$$= \underbrace{K\, \partial_\theta \big(\sin(2(\theta - \bar{\theta}_{f^\varepsilon})) f^\varepsilon \big) + \delta \partial_\theta^2 f^\varepsilon + \nu\, \partial_\varphi \big(\sin(\varphi - \bar{\varphi}_{f^\varepsilon}) f^\varepsilon \big) + D \partial_\varphi^2 f^\varepsilon}_{\text{interactions inside layers}}$$

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$$\varepsilon \Big(\partial_t f^\varepsilon + \nabla_x \cdot (v(\varphi) f^\varepsilon) + \overbrace{\partial_\theta (\mu \, T_{f^\varepsilon} f^\varepsilon) + \partial_\varphi \big(S_{f^\varepsilon} f^\varepsilon \big)}^{\text{interactions with nb. layers}} \Big) = \underbrace{Q(f)}_{\text{interactions inside layers}}$$

- Operator $Q(f)$:

$$Q(f^\varepsilon) = K \, \partial_\theta \big(\sin(2(\theta - \bar{\theta}_{f^\varepsilon})) f^\varepsilon \big) + \delta \partial_\theta^2 f^\varepsilon + \nu \, \partial_\varphi \big(\sin(\varphi - \bar{\varphi}_{f^\varepsilon}) f^\varepsilon \big) + D \partial_\varphi^2 f^\varepsilon$$

Equilibria

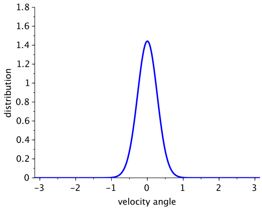
- $Q(f)$ non-linear tensorial Fokker-Planck operator
- Convergence to local equilibra for velocity/inclination distribution

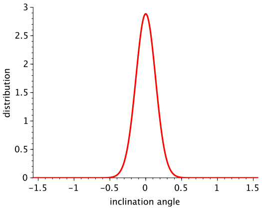
$$\mathcal{E} = \{f, Q(f) = 0\} = \left\{\rho M_{\bar{\varphi},\bar{\theta}} \quad | \quad \rho \in \mathbb{R}^+, \bar{\varphi} \in [0, 2\pi],\, \bar{\theta} \in [0, \pi]\right\}$$

with $M_{\bar{\varphi},\bar{\theta}}$ product of von-Mises function

$$M_{\bar{\varphi},\bar{\theta}}(\varphi, \theta) = \frac{1}{Z} \exp\left(\frac{\nu}{D} \cos(\varphi - \bar{\varphi})\right) \exp\left(\frac{K}{\delta} \cos(2(\theta - \bar{\theta}))\right)$$

with Z : renormalization constant.





- macroscopic dynamics of $\rho, \bar{\varphi},\ \bar{\theta}$

Moment method

- Dynamics of ρ : mass conservation

$$\partial_t \rho + \nabla_x \cdot (c_1 \rho \, v(\bar{\varphi})) = 0$$

- Dynamics of $\bar{\varphi}$, $\bar{\theta}$?

  → No conservation of momentum ⇒ lack of collisional invariants

  dimension of $\mathcal{E} = 3 >$ dimension of collisional invariants $= 1$

  → [Degond,Motsch,2008] Generalized collisional invariants

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Theorem (Macroscopic system)

[density $\rho(x,h,t)$] $$\partial_t \rho + c_1 \nabla_x \cdot (\rho\, v(\bar\varphi)) = 0$$

[mean velocity angle $\bar\varphi(x,h,t)$] $$\rho\Big(\partial_t \bar\varphi + c_2\, (v(\bar\varphi)\cdot\nabla_x)\bar\varphi\Big) + \frac{1}{\kappa_1}\, v(\bar\varphi)^\perp \cdot \nabla_x \rho = \frac{\nu\beta'}{c_3}\, v(\bar\varphi)^\perp \cdot \mathcal{S}$$

[mean inclination angle $\bar\theta(x,h,t)$] $$\rho\Big(\partial_t \bar\theta + c_1\, (v(\bar\varphi)\cdot\nabla_x)\bar\theta\Big) = \frac{\mu'}{c_4}\, (c_1 \rho v(\bar\varphi))^\perp \cdot \mathcal{T}$$

- Left-hand side :
  Self-Organized Hydrodynamics (SOH) model $(\rho, \bar\varphi)$ + transport $(\bar\theta)$
- Right-hand side : interaction between layers

$$\mathcal{S} = \sum_{k,\, k-h=\pm 1} \langle g M_2 M_2\rangle(\bar\theta, \bar\theta_k)\, c_1 \rho_k v(\bar\varphi_k)$$

$$\mathcal{T} = \sum_{k,\, k-h=\pm 1} \mathrm{sign}(k-h)\langle g M_2 M_2 \partial_\theta I_2\rangle(\bar\theta, \bar\theta_k)\, c_1 \rho_k v(\bar\varphi_k)$$

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- c_1, c_2, c_3, c_4 : weighted averages of von-Mises equilibria

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- g overlap function $\Rightarrow$ strong coupling between velocity and inclination

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Numerical method

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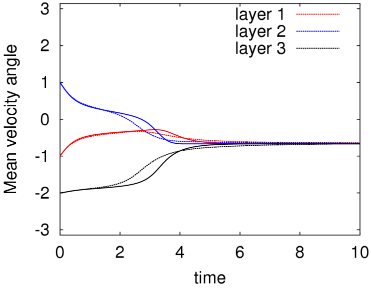
Difficulties :

- no momentum conservation ⇒ non-conservative hyperbolic system
- [Motsch, Navoret] Relaxation scheme : at each time step
  1. solve the left-hand side with a finite volume scheme
  2. add the source term
  3. renormalized the velocity vector field

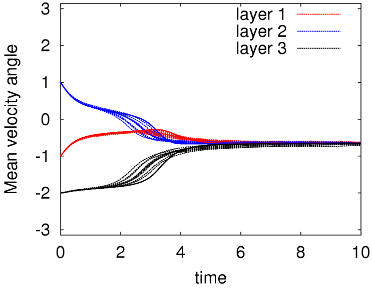
Comparison between particle and macroscopic simulations

micro-macro comparisons

Space homogeneous simulation : 3 layers, **velocity angle** $\bar{\varphi}$



macro / micro (averaged over 20 runs)



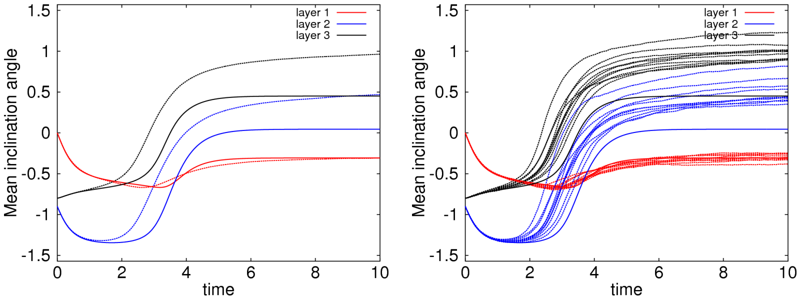
macro / micro (10 runs)

- relaxation to a unique velocity angle
- good agreement micro/macro

Parameters : 25000 particles per layer

micro-macro comparisons

Space homogeneous simulation : 3 layers, **inclination angle** $\bar{\theta}$



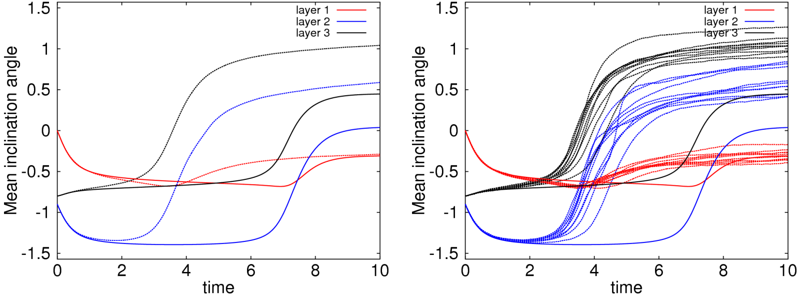
macro / micro (averaged over 20 runs) macro / micro (10 runs)

- relaxation in two steps
- stochastic fluctuations (finite number of particles)
  $\rightarrow$ second relaxation earlier for micro simulations
- after second relaxation : constant inclination

Parameters : 25000 particles per layer, $d = 0.02 = R$

micro-macro comparisons

Space homogeneous simulation : 3 layers, inclination angle $\bar{\theta}$



macro / micro (averaged over 20 runs) macro / micro (10 runs)

- relaxation in two steps
- stochastic fluctuations (finite number of particles)
  $\rightarrow$ second relaxation earlier for micro simulations
- after second relaxation : constant inclination

Parameters : 25000 particles per layer, $d = 0.0205 > R = 0.02$

micro-macro comparisons

2D Taylor-Green test-case

→ velocity : normalized and translated Taylor Green vortex

$$v(\bar{\varphi}) = \frac{(u_1, u_2)}{\|(u_1, u_2)\|}$$

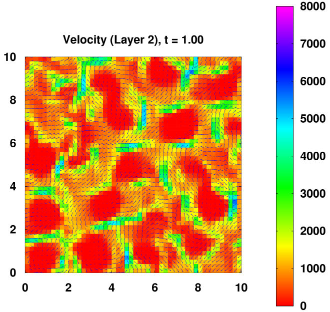
$$u_1(x, y) = \frac{1}{3}\sin\left(\frac{\pi}{5}x\right)\cos\left(\frac{\pi}{5}y\right) + \frac{1}{3}\sin\left(\frac{3\pi}{10}x\right)\cos\left(\frac{3\pi}{10}y\right) + \frac{1}{3}\sin\left(\frac{\pi}{2}x\right)\cos\left(\frac{\pi}{2}y\right)$$

$$u_2(x, y) = -\frac{1}{3}\cos\left(\frac{\pi}{5}x\right)\sin\left(\frac{\pi}{5}y\right) - \frac{1}{3}\cos\left(\frac{3\pi}{10}x\right)\sin\left(\frac{3\pi}{10}y\right) - \frac{1}{3}\cos\left(\frac{\pi}{2}x\right)\sin\left(\frac{\pi}{2}y\right)$$

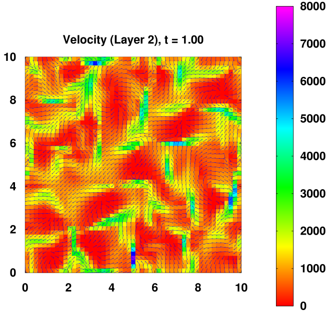
→ inclination : space homogeneous

micro-macro comparisons

2D Taylor-Green test-case : 3 layers, **density**



micro (averaged over 20 runs)



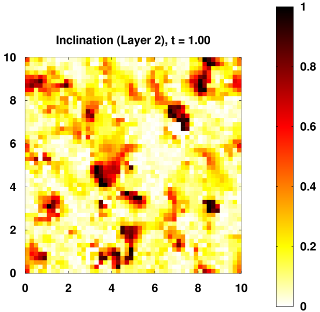
macro

- Layer 2 : intermediate layer
- good agreement
- except in low density region
- macro : more diffuse

Parameters : 10^5 particles per layer

micro-macro comparisons

2D Taylor-Green test-case : **cosine of the inclination angle**



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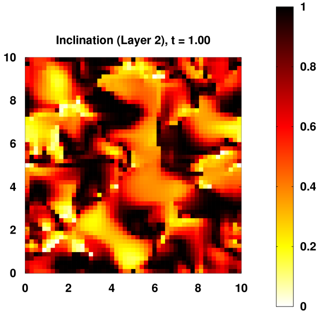

macro

- uniform at $t = 0 \Rightarrow$ non uniform
- large differences between micro/macro
- aligned inclinations do not necessarily match regions of uniform densities

Parameters : 10^5 particles per layer

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Conclusion

- Tensorial alignment problem (velocity, inclination)
- Macroscopic model : hyperbolic system with source terms
- Some deviations for the inclination dynamics but general good agreement between particle/macroscopic simulations

To do :

- characterize the macroscopic motion
- model refinement (density constraint, etc.)
- annular ring geometry

Advertisement

Master 2 of Cell Physics (Université de Strasbourg)

$$2\eta v_{\alpha\beta} = \left(1 + \tau\frac{D}{Dt}\right)\left\{\sigma_{\alpha\beta} + \zeta\Delta\mu q_{\alpha\beta} + \tau A_{\alpha\beta} - \frac{\nu_1}{2}\left(p_\alpha h_\beta + p_\beta h_\alpha - \frac{2}{3}h_\gamma p_\gamma \delta_{\alpha\beta}\right)\right\}$$

$$\frac{D}{Dt}p_\alpha = \frac{1}{\gamma_1}h_\alpha + \lambda_1 p_\alpha \Delta\mu - \nu_1 v_{\alpha\beta} p_\beta - \bar{\nu}_1 v_{\beta\beta} p_\alpha, \; r = \Lambda\Delta\mu + \zeta p_\alpha p_\beta v_{\alpha\beta} + \bar{\zeta} v_{\alpha\alpha} + \lambda_1 p_\alpha h_\alpha.$$

Direction : D. Riveline (IGBMC)