Stationary particle currents in sedimenting active matter wetting a wall

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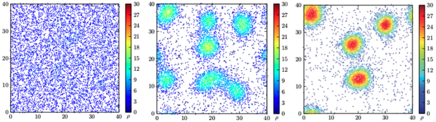
Thursday, March 21st

DPG Meeting - Berlin 2024 (DY 43.10)

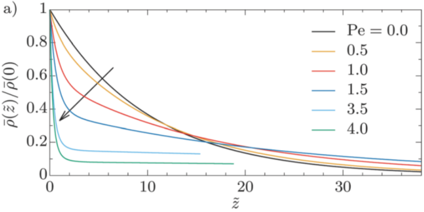
Short review on properties of self-propelled particles

Motility-Induced Phase Separation



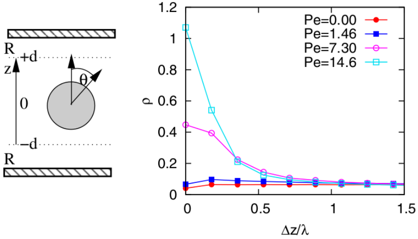
Cates and Tailleur, EPL (2013)

Active ideal sedimentation



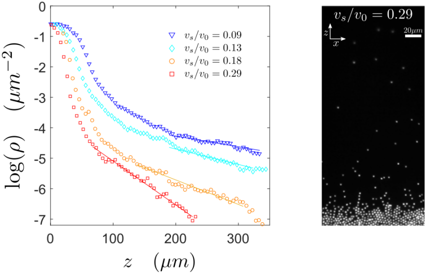
Hermann and Schmidt, Soft Matter (2018)

Wall accumulation of self-propelled spheres



Elgeti and Gompper, EPL (2013)

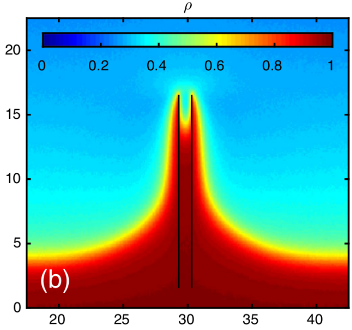
Sedimentation of self-propelled Janus colloids



Ginot et al., New Journal of Physics (2018)

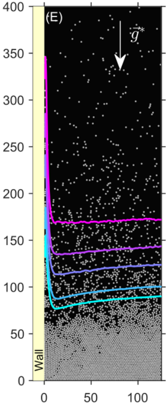
Short review on properties of self-propelled particles

Capillary action in scalar active matter



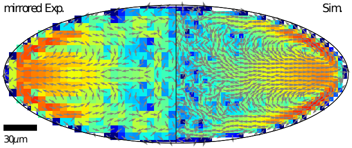
Wysocki and Rieger, PRL (2020)

Active colloids on vertical walls



Carreira et al, Nat. Comm. (2024)

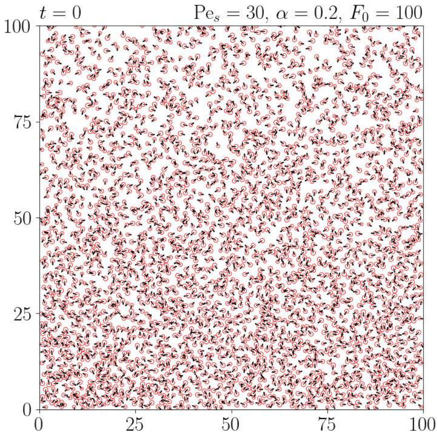
Emergent probability fluxes of motile cells



Cammann et al., PNAS (2021)

Interacting ABPs: the model

- N circular active Brownian particles in a $L_x \times L_y$ box with reflecting boundaries.
- Poly-disperse ABPs with diameters uniformly distributed in $2R_i/a \in [0.8, 1.2]$.



- Self-propulsion velocity $v_s \hat{\mathbf{e}}_i = v_s(\cos\theta_i, \sin\theta_i)$.
- Sedimentation velocity $-v_g \hat{\mathbf{y}}$.
- Rotational diffusion D_r.
- Interacting force: $\mathbf{F}_i = \sum_{j=1}^{m} \mathbf{F}_{ij} + \mathbf{F}_i^{\mathrm{wall}}$ with

$$\mathbf{F}_{ij} = \begin{cases} k(R_i + R_j - r_{ij})\hat{\mathbf{r}}_{ij}, & \forall\ r_{ij} < R_i + R_j \\ 0, & \text{otherwise} \end{cases}$$

- Langevin equations:

$$\dot{\mathbf{r}}_i = v_s \hat{\mathbf{e}}_i - v_g \hat{\mathbf{y}} + \frac{\mathbf{F}_i}{\gamma}, \qquad \dot{\theta}_i = \sqrt{2D_r}\eta.$$

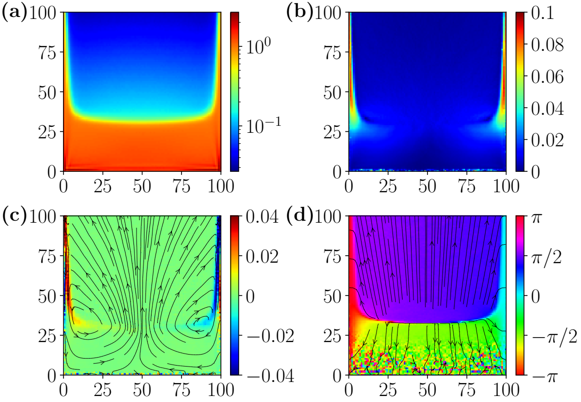
- Parameters: $\mathrm{Pe}_s = v_s/aD_r$, $\alpha = v_g/v_s = \mathrm{Pe}_g/\mathrm{Pe}_s$ and $F_0 = ka/\gamma v_s$.
- Constants: $N = 5000$ particles in a 100×400 box ($a = 1$). Average density: $\rho_0 = 0.125$, global packing fraction: $\phi = 0.098$.

Interacting ABPs: steady-state profiles

- Steady-state particle density $\rho(\mathbf{r})$, polarization vector $\mathbf{P}(\mathbf{r})$, and current density $\mathbf{J}(\mathbf{r})$:

$$\rho(\mathbf{r}) = \frac{1}{N}\sum_{i=1}^{N}\langle\delta(\mathbf{r}-\mathbf{r}_i(t))\rangle_t, \quad \mathbf{P}(\mathbf{r}) = \frac{1}{N}\sum_{i=1}^{N}\langle\hat{\mathbf{e}}_{\mathbf{i}}(t)\,\delta(\mathbf{r}-\mathbf{r}_i(t))\rangle_t, \quad \mathbf{J}(\mathbf{r}) = \frac{1}{N}\sum_{i=1}^{N}\langle\dot{\mathbf{r}}_i(t)\,\delta(\mathbf{r}-\mathbf{r}_i(t))\rangle_t.$$

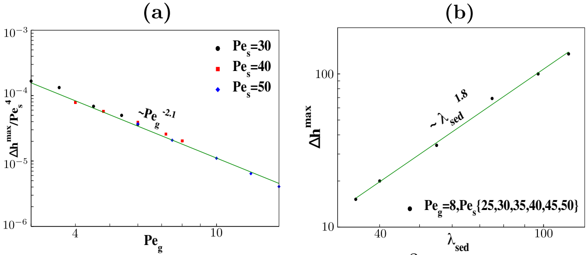
- MIPS (dilute/solid phases) and particle accumulation on vertical walls.
- Current vortices present on the meniscus.



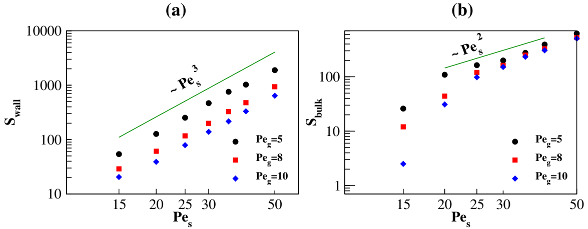
(a) Particle density ρ. (b) Modulus of the current density $|\mathbf{J}|$. (c) Curl amplitude $A = \partial_x J_y - \partial_y J_x$. (d) Average particle orientation.

Interacting ABPs: maximal wetting height and vortex areas

- Bulk density profile: $\rho(y) \sim \exp(-y/\lambda_{\mathrm{sed}})$, with the sedimentation length: $\lambda_{\mathrm{sed}} \sim \dfrac{\mathrm{Pe}_s^2}{\mathrm{Pe}_g}$.
- Maximal wetting height: $\Delta h_{\max} \sim \dfrac{\mathrm{Pe}_s^4}{\mathrm{Pe}_g^{2.1}} \sim \lambda_{\mathrm{sed}}^{1.8}$.

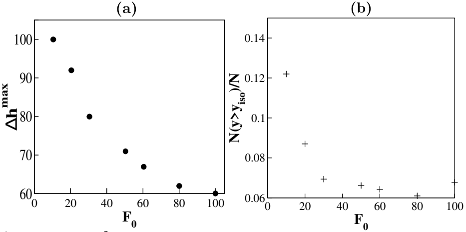


- Areas of the largest curl clusters ($A > 0.01$): $S_{\mathrm{wall}} \sim \mathrm{Pe}_s^3$ (area in the wetting layer) and $S_{\mathrm{bulk}} \sim \mathrm{Pe}_s^2$ (area near the meniscus).

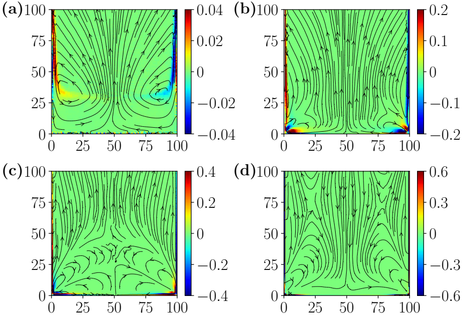


Interacting ABPs: interaction strength dependence

- Maximal wetting height and number of particles in the dilute phase decreases.



- Current vortices migrate to the corners.



(a) $F_0 = 100$, (b) $F_0 = 3$, (c) $F_0 = 0.3$, and (d) $F_0 = 0$.

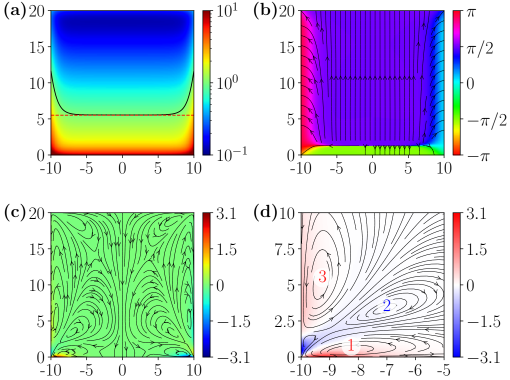
Non-interacting ABPs: equations for $F_0 = 0$ and steady-state profiles

- Langevin equations: $\dot{\mathbf{r}} = v_s \mathbf{e}_\theta - v_g \hat{\mathbf{y}} + \sqrt{2D_t}\boldsymbol{\eta}_\mathbf{r}$, $\dot{\theta} = \sqrt{2D_r}\eta_\theta$.
- Corresponding Fokker-Planck equation for the prob. dens. func. $p(\mathbf{r}, \theta; t)$:

$$\partial_t p = \nabla \cdot \left[D_t \nabla p - \left(v_s \mathbf{e}_\theta - v_g \hat{\mathbf{y}}\right) p\right] + D_r \partial_\theta^2 p.$$

- Steady-state particle density $\rho(\mathbf{r})$, polarization vector $\mathbf{P}(\mathbf{r})$, and current density $\mathbf{J}(\mathbf{r})$:

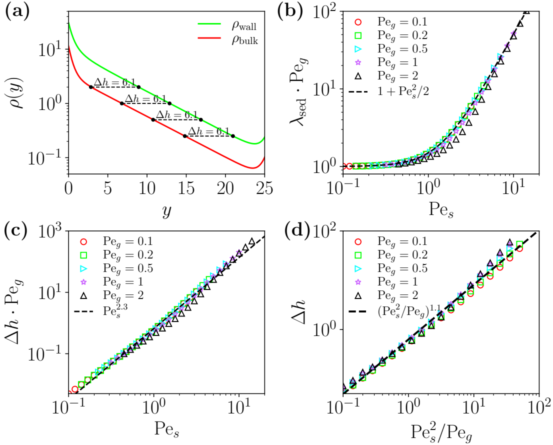
$$\rho(\mathbf{r}) = \int d\theta\ p(\mathbf{r}, \theta), \quad \mathbf{P}(\mathbf{r}) = \int d\theta\ \mathbf{e}_\theta p(\mathbf{r}, \theta), \quad \mathbf{J}(\mathbf{r}) = -D_t \nabla \rho + v_s \mathbf{P} - v_g \rho \hat{\mathbf{y}}.$$



(a) Particle density ρ. (b) Average particle orientation. (c) Curl amplitude $A = \partial_x J_y - \partial_y J_x$.
(d) Zoomed-in version of the bottom-left corner.

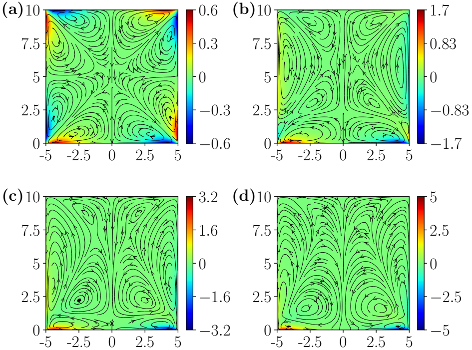
Non-interacting ABPs: wetting height

- Density profile: $\rho(x,y) \sim f(x)\exp(-y/\lambda_{\text{sed}})$, sedimentation length: $\lambda_{\text{sed}} \sim \dfrac{1+0.5\text{Pe}_s^2}{\text{Pe}_g}$.
- Wetting height: $\Delta h \sim \left(\dfrac{\text{Pe}_s^2}{\text{Pe}_g}\right)^{1.1} \sim \lambda_{\text{sed}}^{1.1}$.

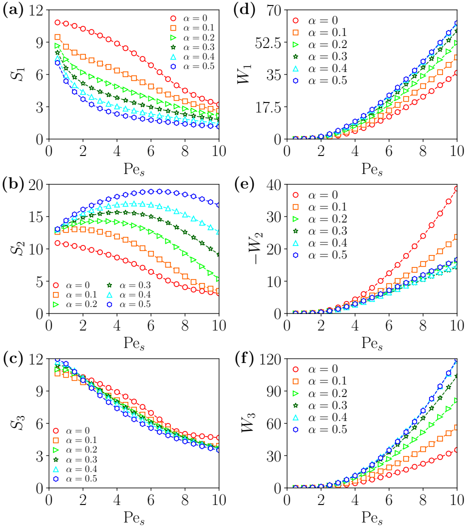


(a) Density profiles at $x = x_{\text{bulk}}$ and $x = x_{\text{wall}}$. (b) Sedimentation length. (c-d) Wetting height.

Non-interacting ABPs: dependence of current vortices on gravity



(a) $\alpha = 0$. (b) $\alpha = 0.25$. (c) $\alpha = 0.5$. (d) $\alpha = 0.75$.



(a-c) Vortex areas. (d-f) Circulation $W_i = \int dS_i A$.

Conclusion

Interacting active Brownian particles:

- Presence of motility-induced phase separation (dilute/solid phases).
- Particle accumulation on vertical walls, with maximal wetting height $\Delta h_{\max} \sim \lambda_{\text{sed}}^{1.8}$.
- Current vortices on the meniscus, with areas following $S_{\text{wall}} \sim \text{Pe}_s^3$ and $S_{\text{bulk}} \sim \text{Pe}_s^2$.
- When $F_0 \to 0$, the maximal wetting height increases, and current vortices migrate to the corners.

Non-interacting active Brownian particles ($F_0 = 0$):

- No motility-induced phase separation but particle accumulation on vertical walls, with wetting height $\Delta h \sim \lambda_{\text{sed}}^{1.1}$.
- Presence of current vortices at the corners of the box. Their geometry is modified with increasing gravity (increasing circulations, decreasing areas).

Thank you for your attention !

Previous presentations:

- Wednesday 20 at 15:00: M. Mangeat *et al.*, Flocking of two unfriendly species (DY 32.13).
- Thursday 21 at 10:00: S. Chatterjee *et al.*, Metastability of ordered phase in discretized flocking (DY 43.2).

References:

- M. Mangeat, S. Chakraborty, A. Wysocki, and H. Rieger, *Stationary particle currents in sedimenting active matter wetting a wall*, Phys. Rev. E **109**, 014616 (2024).
- A. F. Carreira, A. Wysocki, C. Ybert, M. Leocmach, H. Rieger, and C. Cottin-Bizonne, *How to steer active colloids up a vertical wall*, Nat. Comm. **15**, 1710 (2024).
- A. Wysocki and H. Rieger, *Capillary Action in Scalar Active Matter*, Phys. Rev. Lett. **124**, 048001 (2020).