Statistical Physics of Active Particles: from effective temperature to motility-induced phase separation

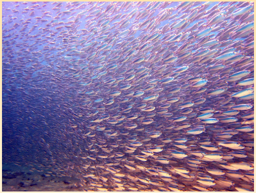
J. Tailleur

Laboratoire MSC
CNRS - Université Paris Diderot

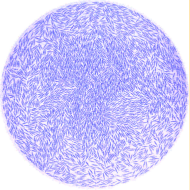
Active Matter: Cytoskeleton, Cells, Tissues and Flocks

Active Matter: a wide class of non-eq. systems

“Soft active systems are exciting examples of a new type of condensed matter where stored energy is continuously transformed into mechanical work at microscopic length scales.” [Marchetti & Liverpool, PRL 97, 268101 (2006)]



Fish shoals



Vibrated rods

Birds flocks

- Rich phenomenology
- Simple models
- Experimental realisations

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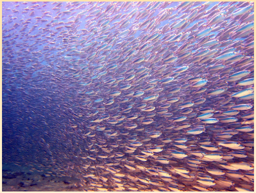

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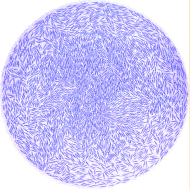

Vibrated rods

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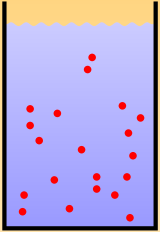
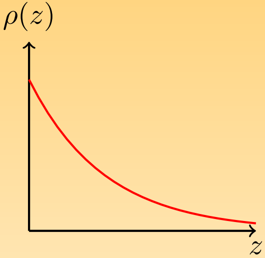
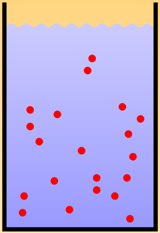
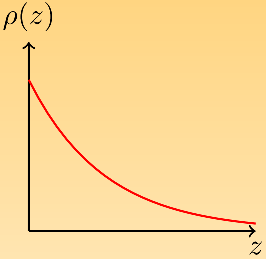
- Simple models ⟶ Generic description?
- Experimental realisations

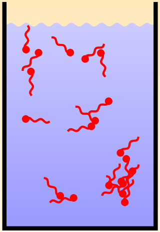


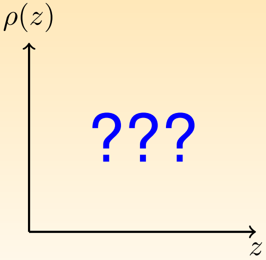


$\rho(z)$
z









Similar physics ?

Similar methods ?

Outline

- Run-and-Tumble Bacteria and Active Brownian Particles
- External potential in dilute suspensions
- Interacting particles: Motility-Induced Phase Separation

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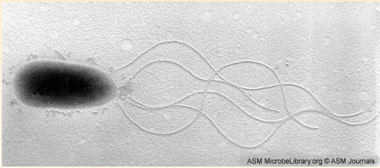
Run-and-Tumble bacteria

- *Escherichia coli* – Unicellular Organism $(1\mu m \times 3\mu m)$
- Flagella (few μm long)
- Electron microscopy



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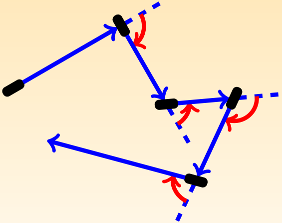

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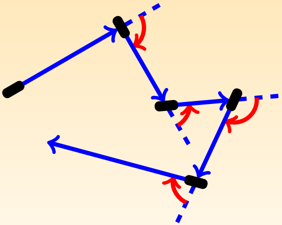
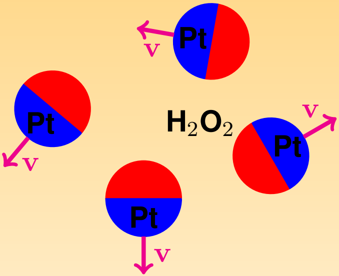


- Diffusion at large scale $D = \frac{v^2}{d\alpha} \sim 100\, \mu m^2.s^{-1}$

Self-propelled colloids

- Colloids with asymmetric coating
- Self [diffusio-] phoresis
- Self propulsion $\mathbf{v}$



$$v \simeq 1\mu m.s^{-1}; \qquad D_t \simeq 0.3\mu m^2.s^{-1}; \qquad D_{\text{eff}} \simeq 1-4\mu m^2.s^{-1}$$

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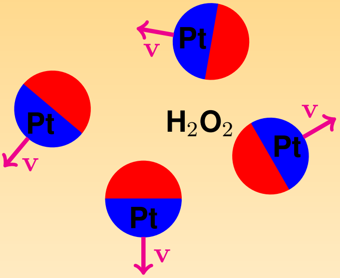

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- Rotational diffusion crucial

- Light-controlled [Palacci *et al.* Science **339**, 936 (2013)] •

Common large scales properties ?

- ABP: v_A, D_t, D_r
- RTP: v_R, α
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- Adjust v_A, D_t, D_r, v_R, α, ν so that D and V are the same ?

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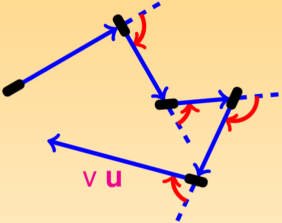
Microscopic Dynamics



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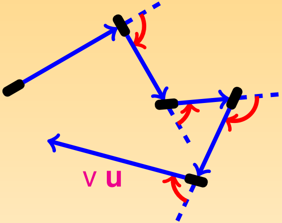

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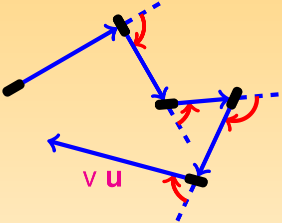

$$\dot{P}(x,\mathbf{u}) = -\nabla \cdot [P(x,\mathbf{u})\mathbf{v}] - \alpha(\mathbf{u})P(x,\mathbf{u}) + \frac{1}{\Omega}\int d\mathbf{u}'\alpha(\mathbf{u}')P(x,\mathbf{u}')$$

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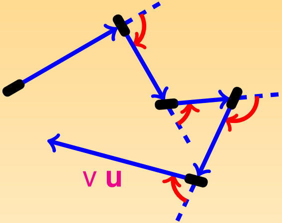

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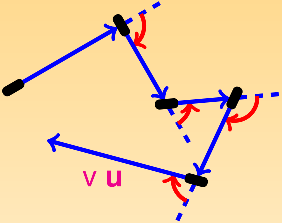

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Diffusive limit

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$$\dot{\rho} = \int \dot{P}(x, \mathbf{u}) d\mathbf{u} \simeq D_0 \Delta \rho; \qquad D_0 = D_t + \frac{v^2}{\alpha d + d(d-1) D_r}$$

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- Equivalence ABP - RTP - Hot colloids

External potential $V_{ext}(x)$

- $\alpha(\mathbf{u}) = \alpha \qquad D_r(\mathbf{u}) = D_r$
- $\mathbf{v}(\mathbf{u}) = v\mathbf{u} + \mathbf{v}_\tau$ with $\mathbf{v}_\tau = -\mu \nabla V_{ext}$

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- $\mathbf{v}(\mathbf{u}) = v\mathbf{u} + \mathbf{v}_\tau$ with $\mathbf{v}_\tau = -\mu \nabla V_{ext}$
- Colloids at equilibrium $P \propto \exp[-V_{ext}/kT]$
- Bacteria? ABP?

Sedimentation RTP ($D_t = D_r = 0$)

- Exact solution for $\mathbf{v}(\mathbf{u}) = v\mathbf{u} + \mathbf{v}_\tau$ $\mathbf{v}_\tau = -\mu\,\delta m\,g\,\mathbf{u_z}$
  [Tailleur & Cates EPL 2009]

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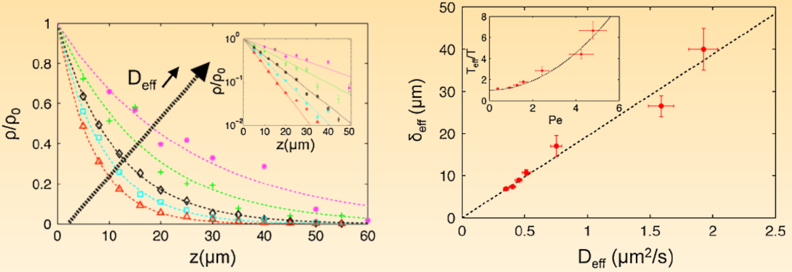
- Effective Temperature for $v_\tau \ll v$ $kT_{eff} = \frac{D_0}{\mu}$ (Einstein)
  Holds for generic potential

Sedimentation: experiments ($\alpha = 0$)

- Active colloids [Palacci *et al.* PRL **105**, 088304 (2010)]



$$\rho(x) \propto \exp\left(-\frac{v_\tau x}{D_{\text{eff}}}\right)$$

Trapping bacteria (1d)

- Quadratic potential $\longrightarrow v_{L,R} = v \pm \lambda x$

$$P_{ss}(x) \propto \left|1 - \frac{x^2\lambda^2}{v^2}\right|^{\frac{\alpha}{2\lambda}-1}$$

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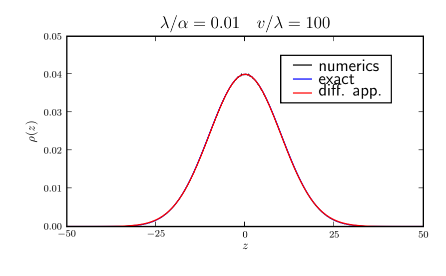

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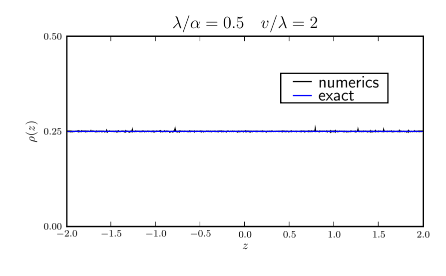

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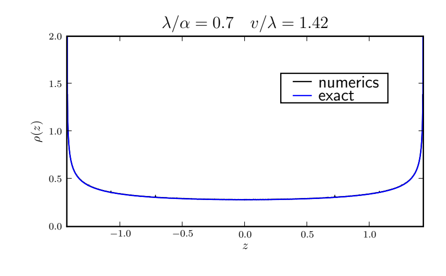

Harmonic trap in 3d

- Quadratic potential $V = -\lambda\frac{\vec{r}^2}{2} \longrightarrow$ $\vec{v}(\vec{r},\vec{u}) = v\vec{u} - \lambda\vec{r}$
- Effective temperature: $P(r) \propto r^2 e^{-\frac{3\alpha\lambda r^2}{2v^2}}$

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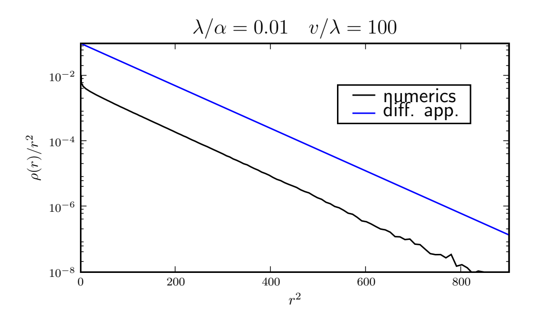

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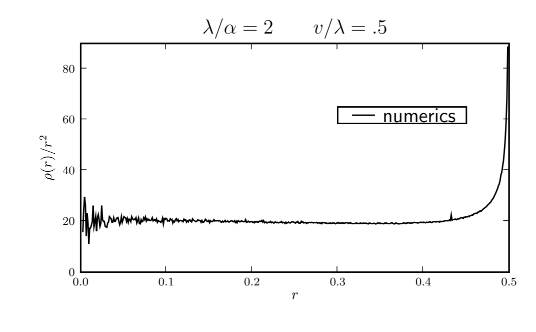

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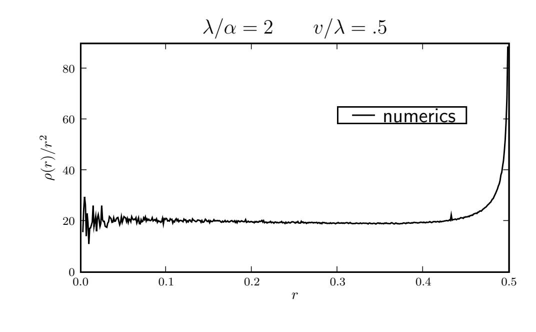
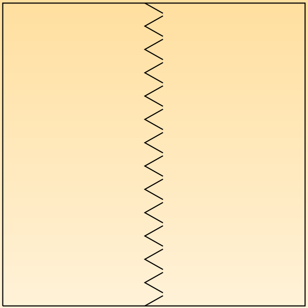


- **Strong non-perturbative effects** •

Fishing lobsters at the micrometer scale



[P. Galajda, J. Keymer, P. Chaikin, R. Austin, J. Bacteriol. **189**, 8704 (2007)]

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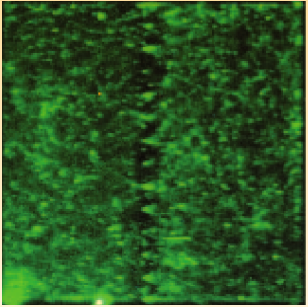
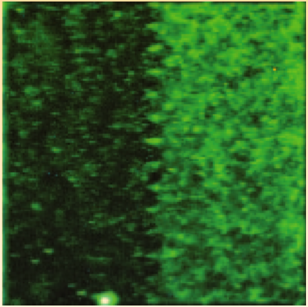


Colloids

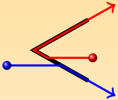
Fishing lobsters at the micrometer scale



Bacteria

Where does the ratchet effect come from ?

- Bacteria align with walls upon collisions ••



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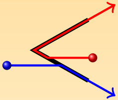
- Interactions with walls ⟶ no time-reversal symmetry



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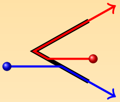
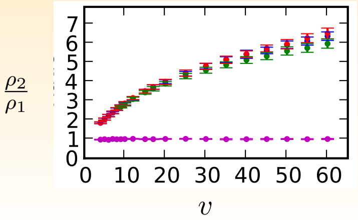


- Elastic collisions ⟶ No ratchet effect



Summary

- Effective temperature perturbatively
- Strong non-thermal effects otherwise
- Local order → Hydrodynamics matter
- Non-equilibrium effects do NOT come the active random-walk

Outline

- Run-and-Tumble Bacteria and Active Brownian Particles
- External potential in dilute suspensions
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Motility induced phase separation

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- Non-uniform speed $v(\mathbf{r})$

$$\dot{P}(\mathbf{r},\theta) = -\nabla[v(\mathbf{r})P(r,\theta)] + (\text{tumbles, rotational diff., etc.})$$

- Stationnary distribution $P(\mathbf{r},\theta) \propto 1/v(\mathbf{r})$ [Schnitzer PRE 1993]

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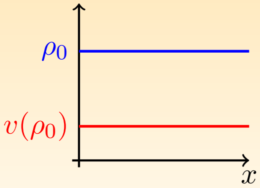
- IF $v'(\rho) < 0$ $\longrightarrow$ Feedback loop



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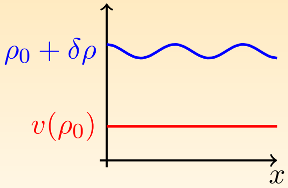

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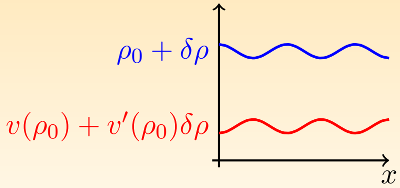

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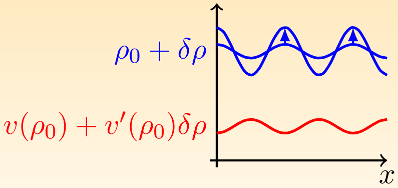

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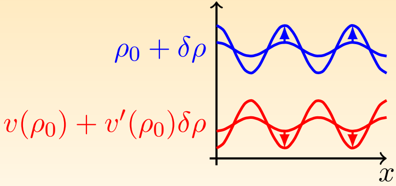

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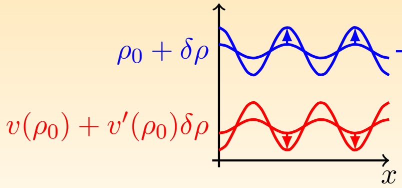

$$\longrightarrow \frac{1}{v(\rho_0)+v'(\rho_0)\delta\rho} \simeq \rho_0 - \rho_0 \frac{v'}{v}\delta\rho$$

- Linear instability if $\frac{v'}{v} \leq -\frac{1}{\rho} \longrightarrow$ MIPS

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◇ One active particle in a density ρ of other particles

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- More serious derivations [Stenhammar et al. 2013, Bialké et al. 2013]

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- RTP (α) ⟷ ABP $((d-1)D_r)$ ⟷̸ Hot eq. colloids

D and V mapped at the same time

[Cates, Tailleur, EPL **101**, 20010 (2013)]

Effective free energy $v[\rho(\mathbf{r})]$

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$$\mathbf{J} = -\rho\frac{v^2}{A}\nabla\frac{\delta\mathcal{F}}{\delta\rho}$$

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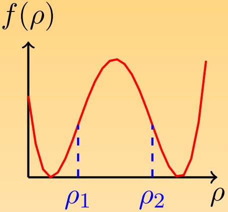

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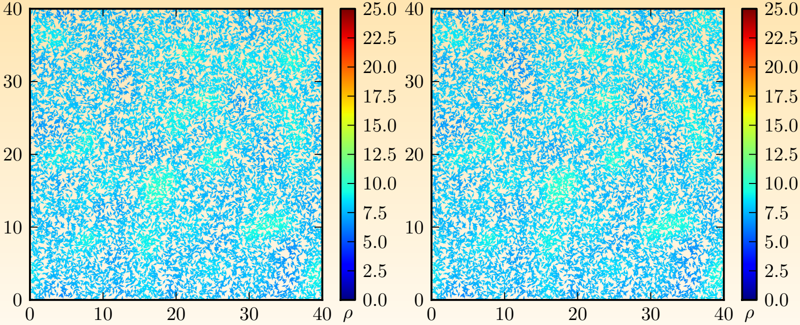

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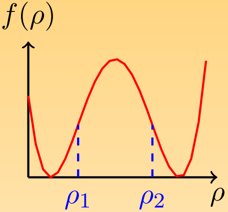

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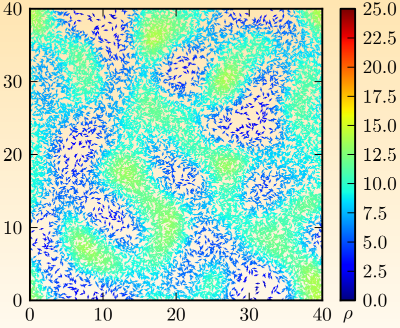

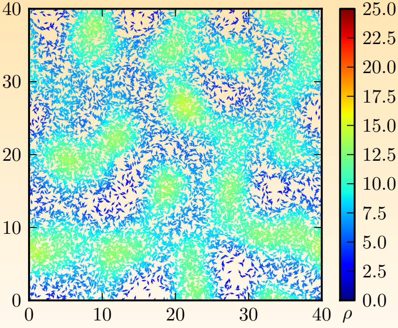

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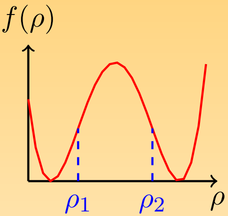

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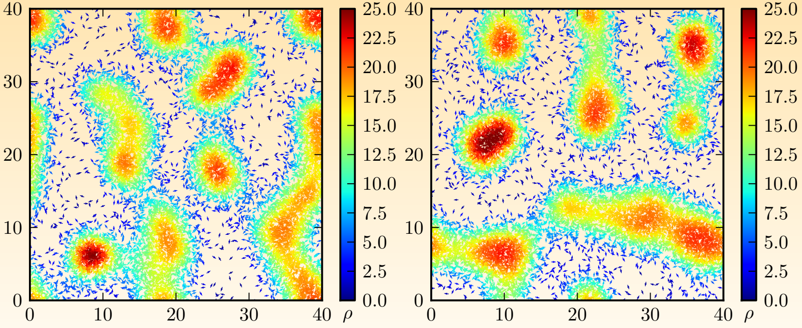

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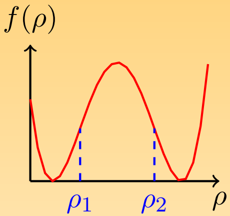

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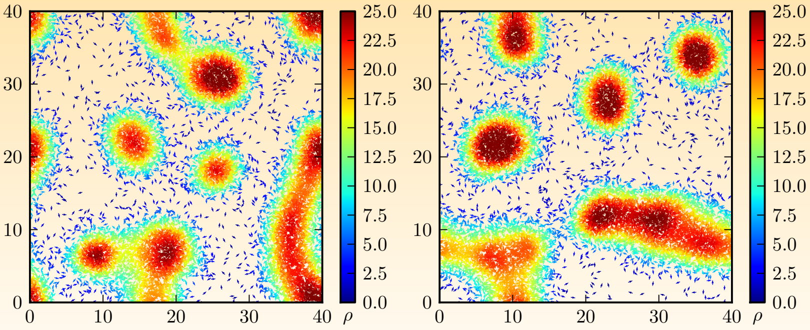

Coarsening: be wise, discretize!

- Lattice-gas model of run-and-tumble bacteria
- Excluded volume interactions (ASEP-like) $\longrightarrow$ MIPS

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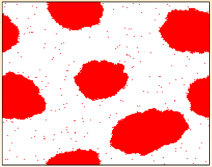

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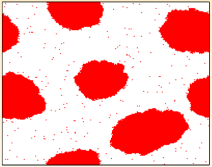
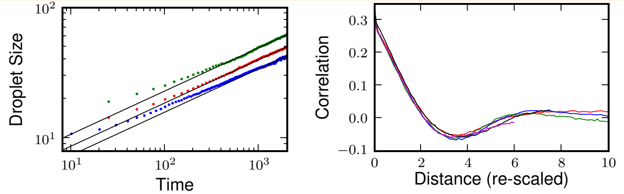
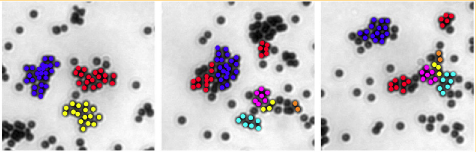




Experiments and perspective

- Active colloids (LPMCN, Lyon ; NYU •)



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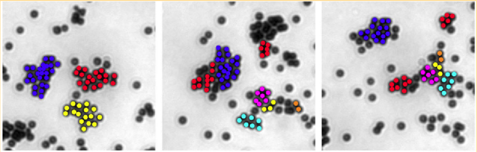


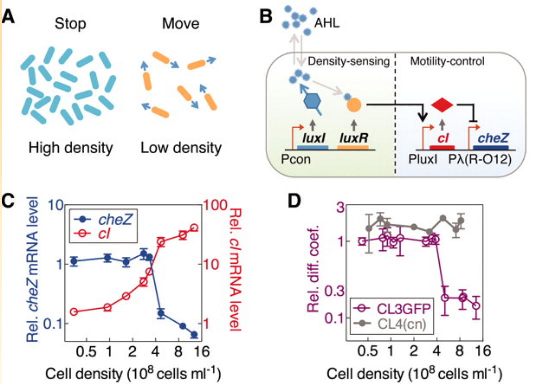
- Simulations [Thompson et al. 2011, Fily et al. 2012, Redner et al. 2012+2013, ...]

Our theory:
Mean-field based
Equilibirum-like Steady-states
No attractive interactions

Lots of things missing!
Coarsening dynamics
Higher order gradient terms
Beyond mean-field
Consider all interactions
Dense phases

Bacterial pattern formation

- Synthetic biology ⟶ drop of motility at large ρ •



[Liu et al. Science **334** 238 (2011)]

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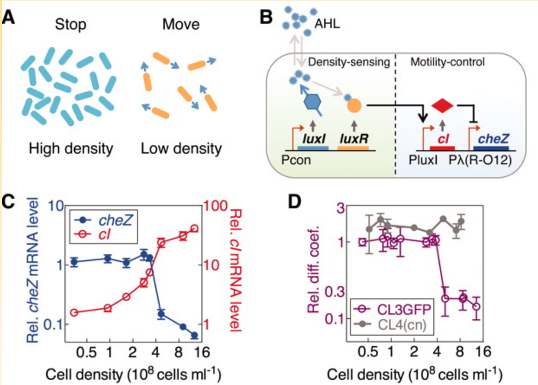

[Liu et al. Science **334** 238 (2011)]

- A different mechanism ?

Finite duration tumbles

- Tumble duration τ

$$D = \frac{v^2}{d\alpha(1+\alpha\tau)}; \qquad V = -\frac{v}{d\alpha}\nabla\frac{v}{1+\alpha\tau}$$

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- All can lead to MIPS when $D_{\rm eff.}(\rho) < 0$

Cells division and death

- Logistic growth

$$\dot{\rho} = \nabla[D_{\text{eff}}(\rho)\nabla\rho] + \boldsymbol{\alpha\rho(1-\rho/\rho_0)}$$

- $\rho \leq \rho_0$ $\longrightarrow$ division dominates ($\dot{\rho} > 0$)
- $\rho \geq \rho_0$ $\longrightarrow$ death dominates ($\dot{\rho} < 0$)

Birth-death vs phase separation

- $D'(\rho_0) < 0 \longrightarrow D_{\text{eff}}[\rho_0] < 0 \longrightarrow$ phase separation

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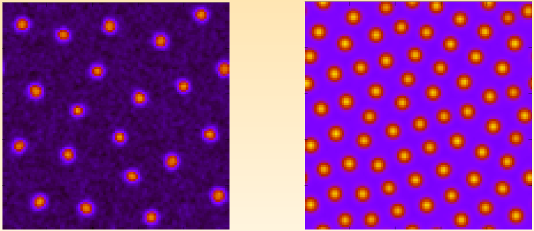

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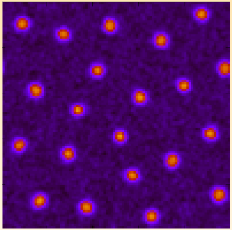
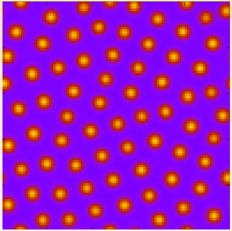
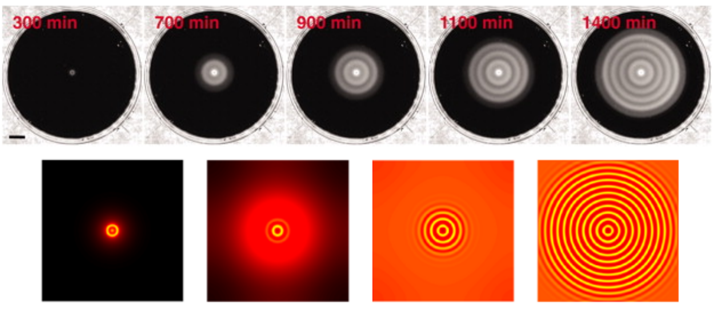




- Patterns found in liquid suspensions for *E. coli* or *S. Typhimurium*.

- Semi-solid-agar: central inocculum as a seed



- Reproduce experimental results qualitatively

Conclusion

- Classes of active particles allow for common large-scale description
- Some generic features
- Effective temperature perturbatively
- Motility-Induced Phase Separation
- Lots of open questions

Acknowledgements

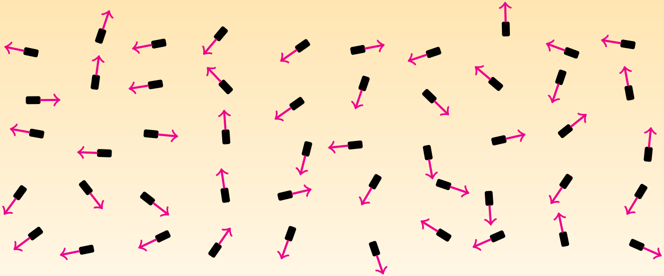
- R. Blythe, M. Cates, D. Marrenduzzo, R. Nash, I. Pagonabarraga, A. Thompson

- MIPS for RTP [J.T., M.E. Cates, PRL **100**, 218103 (2008)]
- Ext. Pot./ratchet [J.T., M.E. Cates, EPL **86**, 60002 (2009)]
- Hydrodynamics [R.W. Nash, R.Adhikari, J.T., M.E. Cates, PRL **104**, 258101 (2010)]
- Bacterial Pattern formation [M.E. Cates, D. Marenduzzo, I. Pagonabarraga, J.T., PNAS **107** 11715 (2010)]
- Lattice-gas model of R&T particles [A. G. Thompson, J. Tailleur, M. E. Cates, R. A. Blythe, JSTAT P02029 (2011)]
- Equivalence of RTP and ABP [M.E.C. Cates, J.T., EPL **101** 20010, (2013)]

Mesoscopic description

Spherical harmonics expansion

$$P(\mathbf{r},\mathbf{u},t) = \varphi(\mathbf{r}) + \mathbf{p}(\mathbf{r}).\mathbf{u} + \mathbf{Q}(\mathbf{r}) : (\mathbf{uu} - \mathbf{I}/d) + \dots$$



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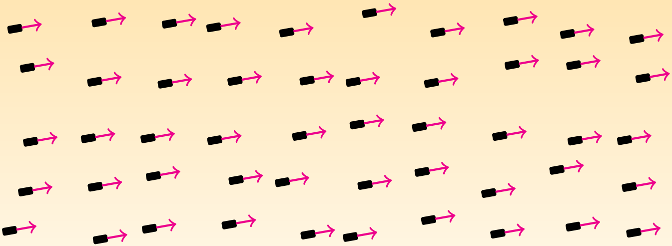

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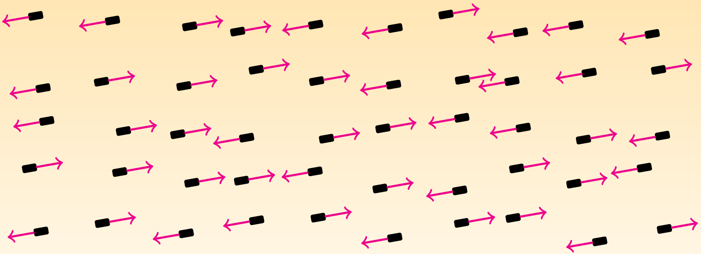

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Mesoscopic equations

- Allow for spatial variations of v, α, D_r, D_t

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Mesoscopic equations

- Allow for spatial variations of v, α, D_r, D_t

$$\dot{\varphi} = \nabla\Big[\Big(D_t + \frac{v^2}{D_r d(d-1) + d\alpha}\Big)\nabla\varphi + \frac{\varphi v}{D_r d(d-1) + d\alpha}\nabla v\Big]$$

$$p_a = -\frac{1}{D_r(d-1) + \alpha}\nabla_a(v\varphi) + \mathcal{O}(\nabla^2)$$

$$Q_{ab} \sim \nabla$$

- Gradient expansion + $t \gg D_r^{-1},\ \alpha^{-1}$
- $\mathbf{p}$ and $\mathbf{Q}$ are fast variables
- $\mathbf{Q} \sim \nabla$