# Collective Motion of Active Particles With and Without Hydrodynamics
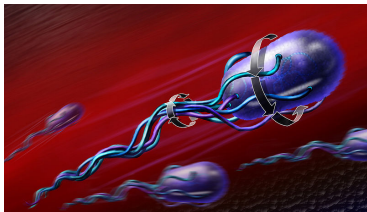
Gerhard Gompper

Theoretical Soft Matter and Biophysics
Institute of Complex Systems and Institute for Advanced Simulation
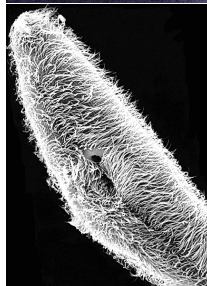Forschungszentrum Jülich

March 10, 2014

# Microswimmers and Self-Propelled Particles

- Many biological examples:
  bacteria, sperm, paramecium
- Interesting phenomena:
  surface adhesion, vortices,
  metachronal waves



Nicolle Rager Fuller, National Science Foundation

# Microswimmers and Self-Propelled Particles

- Many biological examples:
  bacteria, sperm, paramecium
- Interesting phenomena:
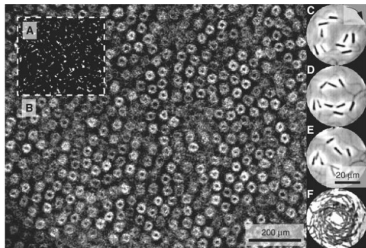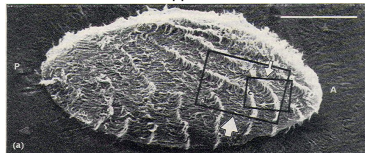  surface adhesion, vortices,
  metachronal waves



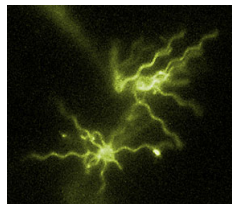Riedel et al., Science **309**, 300 (2005)



Kaupp et al.



Machemer, Cilia and Flagella (1974)

# Biological Microswimmers
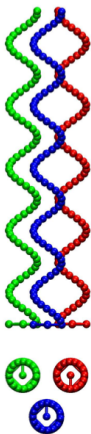
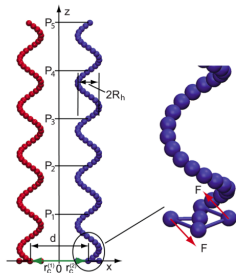Role of hydrodynamic interactions in

- Bundling of bacterial flagella
- Formation of metachronal waves
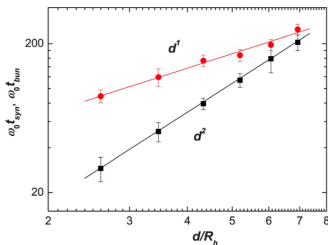- Sperm adhesion to surfaces



(Howard Berg Lab, Harvard)

# Bacterial Flagella: Synchronization & Bundling

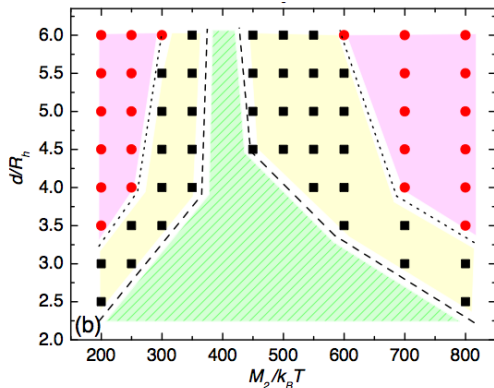Model: anchored flagella with torque



Synchronization and bundling times:



$t_{sync} \sim d$

($d$: distance between anchoring points)

S.-Y. Reigh, R.G. Winkler, G. Gompper, Soft Matter **8** (2012)

# Bacterial Flagella: Slippage & Unbundling

Dynamic phase diagram:



motor torque on flagellum 2

With increasing torque difference:

phase locking

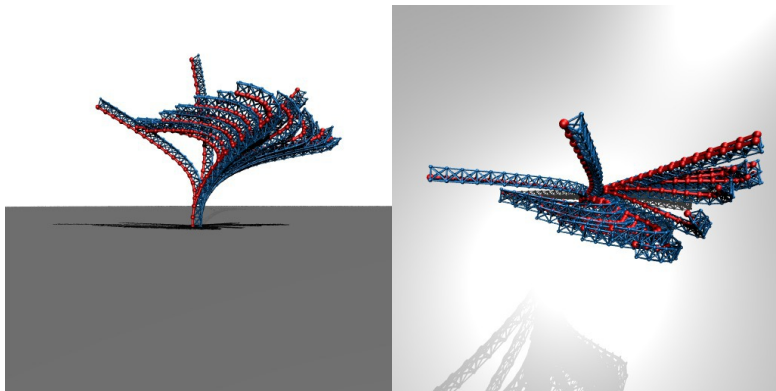phase slip

phase drift

Conclusion:
Bundle formation very robust to torque differences
$\longrightarrow$ important for "run"-phase of bacterium

S.-Y. Reigh, R.G. Winkler, and G. Gompper, PLoS ONE, **8**, e70868 (2013)
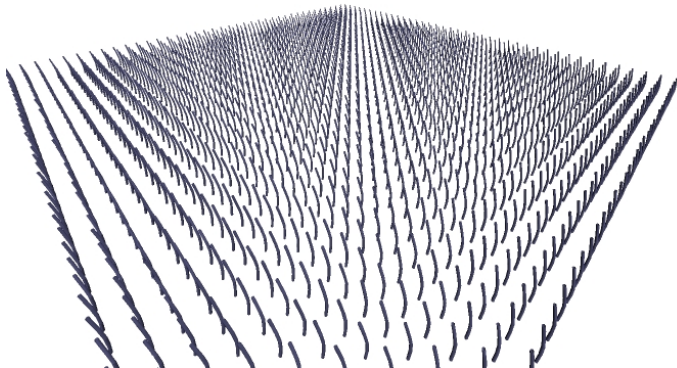
# Cilia and Metachronal Waves

Active elastic filament + power stroke + recovery stroke
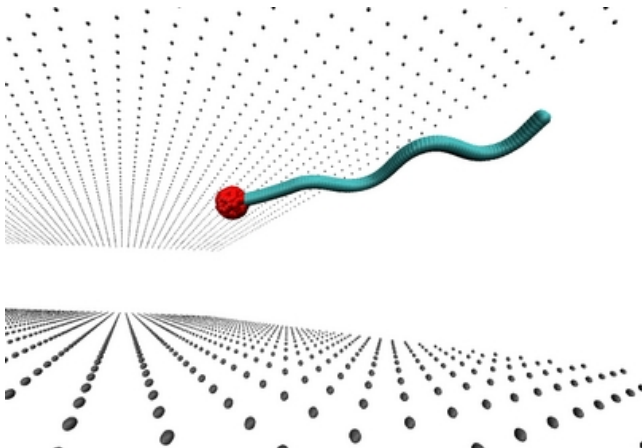+ "geometric clutch" + hydrodynamic interactions + noise



J. Elgeti & G. Gompper, Proc. Natl. Acad. Sci. USA **110**, 4470 (2013)

# Self-Organization of Metachronal Waves (MCWs)

# Sperm Swimming near Surfaces

- Sperm adheres to surface             (fluid particles not shown)
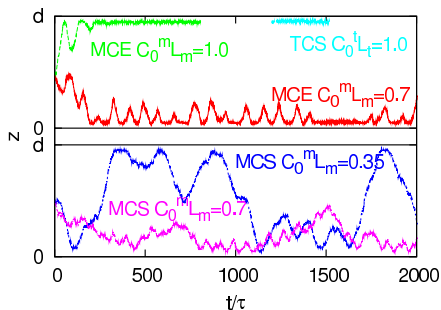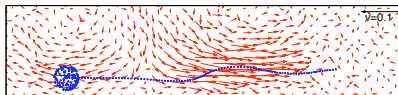- Chiral sperm swims in circles at surface

# Sperm Swimming near Surfaces

What keeps sperm at the wall?

- short-range hydrodynamic attaction (pusher)
- steric interactions
- elongated shape

**But:**

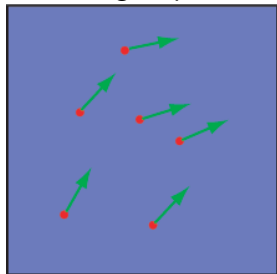Curved shape plus swimming can lead to detachment!



J. Elgeti, U.B. Kaupp, G. Gompper, Biophys. J. **99**, 1018 (2010)

# Mesoscale Hydrodynamics Simulations

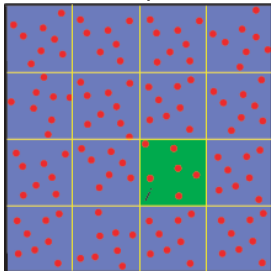Multi-Particle Collision Dynamics (MPC)

Fluid of point particles:

Streaming step



Ballistic motion
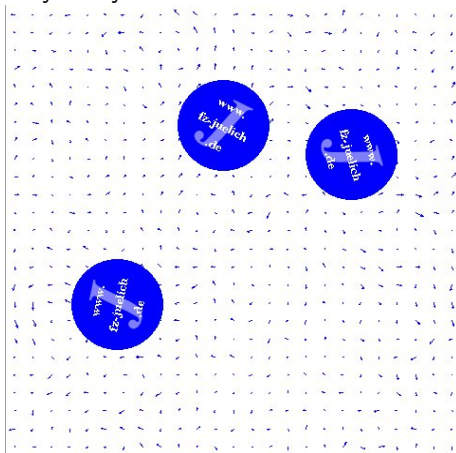
Collision step



In comoving frame of each cell:
rotation of relative velocities

Reviews: R. Kapral, Adv. Chem. Phys. **140**, 89 (2008);

G. Gompper, T. Ihle, D.M. Kroll, R.G. Winkler, Adv. Polym. Sci. **221**, 1 (2009)

Get a feeling for hydrodynamic interactions: Interactive Simulations



See webpage: http://www.fz-juelich.de/ics/ics-2/EN/
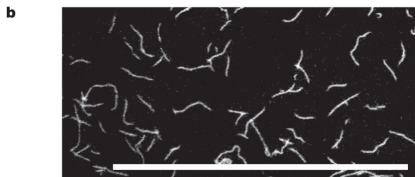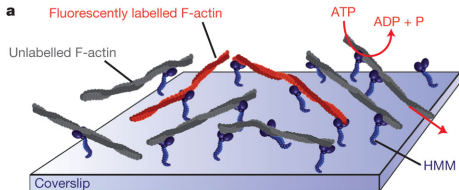Forschung/HydrodynamicsSimulation/_node.html

Collective Behavior of

- Self-Propelled Rods
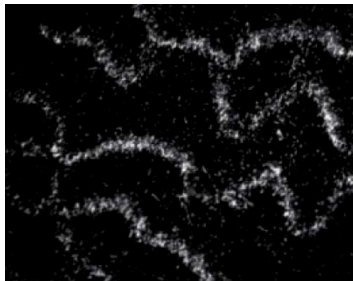- Self-Propelled Spheres
- Curved Flagella

Collective Motion of Self-Propelled Rod-Like Particles

# Collective Behavior in Motility Assays

Actin filaments on a carpet of propelling molecular motors



Density waves:



V. Schaller, C. Weber, C. Semmrich, E. Frey, and A. R. Bausch, Nature **467**, 73 (2010)

# Penetrable Rod Model in 2D

**Forces**:

1. Intrinsic swimming force ($F_{\mathrm{rod}}$)

2. Noise ($k_{\mathrm{B}}T$)

3. Soft repulsion between rods

   ↪ segment-wise via a separation-shifted Lennard-Jones (SSLJ) potential: energy barrier ($E$)
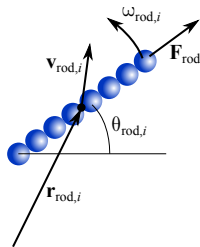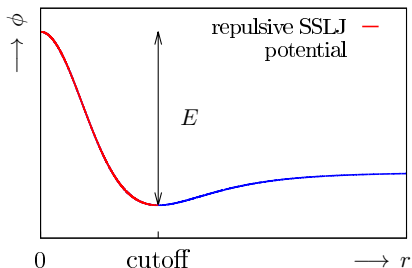


M. Abkenar, K. Marx, T. Auth, G. Gompper, Phys. Rev. E **88**, 062314 (2013)

# Penetrable Rod Model in 2D

**Forces**:

1. Intrinsic swimming force ($F_{\rm rod}$)
2. Noise ($k_{\rm B}T$)
3. Soft repulsion between rods: energy barrier ($E$)
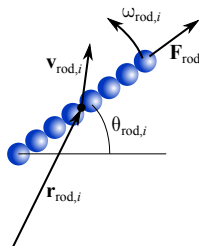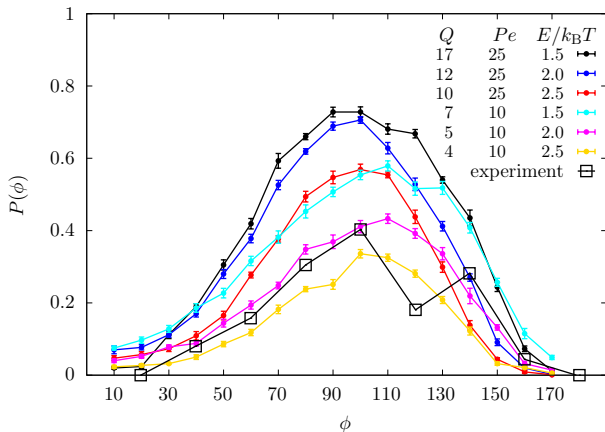


**Dimensionless parameters**:

- The Péclet number: $Pe = \dfrac{L_{\rm rod}F_{\rm rod}}{k_{\rm B}T}$
- Penetrability coefficient: $Q = \dfrac{L_{\rm rod}F_{\rm rod}}{E}$

Penetrating rods $\longrightarrow$ quasi-2D systems

M. Abkenar, K. Marx, T. Auth, G. Gompper, Phys. Rev. E **88**, 062314 (2013)

# Rod Crossing Probability

Crossing probability $P(\phi)$ versus collision angle $\phi$
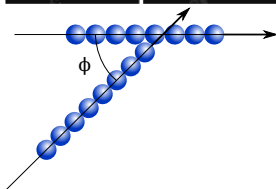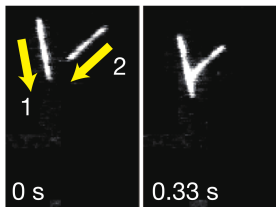


- Highest crossing probability near $\phi \simeq 90°$
- Function shape consistent with experiments with micro-tubules

Y. Sumino *et. al.*, Nature **483**, 448 (2012)

# Cluster Break-Up Phase
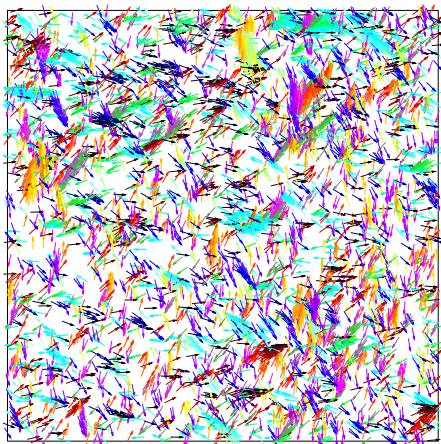


High penetrability $Q$:

- Single rods and small clusters pass through each-other
- When $F_{\text{swim}} > F_{\text{repulsion}}$

- There is a critical $Q$ for cluster break-up

$Q = 67, \quad Pe = 100, \quad \rho\, L_{\text{rod}}^2 = 5.1$

# Giant Cluster Phase



Low penetrability $Q$:

- Rods collide and align
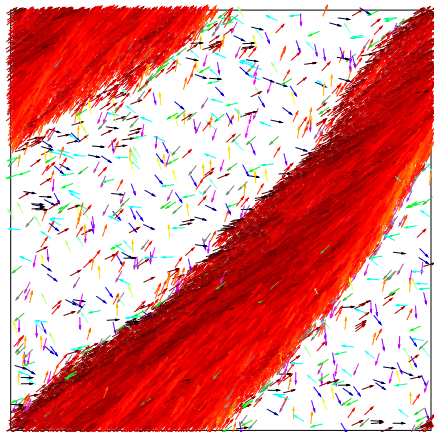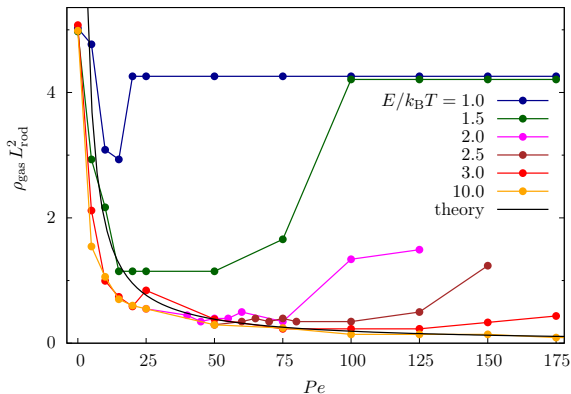- A gas of rods around the cluster, density $\rho_{\mathrm{gas}}$
- A rate equation gives $\rho_{\mathrm{gas}} = (192/\pi^2)(1/L_{\mathrm{rod}}^2 Pe)$

- Gas density independent of total density $\longrightarrow$ A vapor density for rods!

$Q = 17, \quad Pe = 25, \quad \rho\, L_{\mathrm{rod}}^2 = 10.2$

# Gas Density: Clustering Window

Giant clusters form at high enough $Pe$ and low enough $Q$



- Low gas density: larger clusters
- $\rho_{\mathrm{gas}}$ decreases, and then increases back
- $Pe = \frac{L_{\mathrm{rod}} F_{\mathrm{rod}}}{k_{\mathrm{B}} T}$, $Q = \frac{L_{\mathrm{rod}} F_{\mathrm{rod}}}{E}$

- There is a "clustering window" in propulsion strength
- At low $E$, noise also plays role in cluster break-up

# Gas Density: Clustering Window
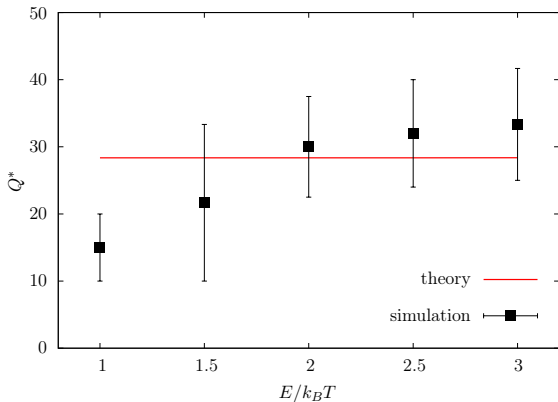
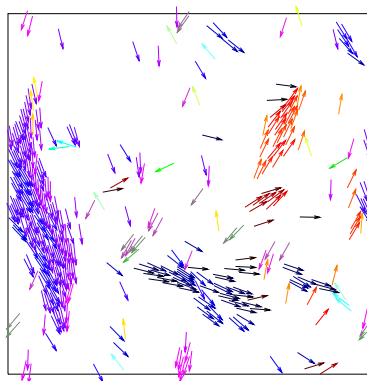Giant clusters form at high enough $Pe$ and low enough $Q$



- Low gas density: larger clusters
- $\rho_{\mathrm{gas}}$ decreases, and then increases back
- $Pe = \frac{L_{\mathrm{rod}} F_{\mathrm{rod}}}{k_{\mathrm{B}} T}$, $Q = \frac{L_{\mathrm{rod}} F_{\mathrm{rod}}}{E}$

- There is a "clustering window" in propulsion strength
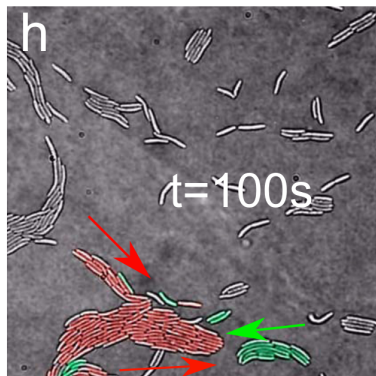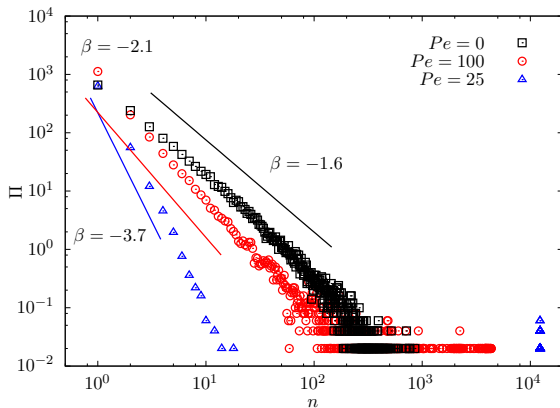- At low $E$, noise also plays role in cluster break-up

# Cluster Properties



- Polar clusters result from alignment interaction
- Cluster polarity and geometry similar to experiments with myxobacteria

Harvey *et. al.*, New Journal of Physics **15** (2013) 035029

# Cluster Size Distributions

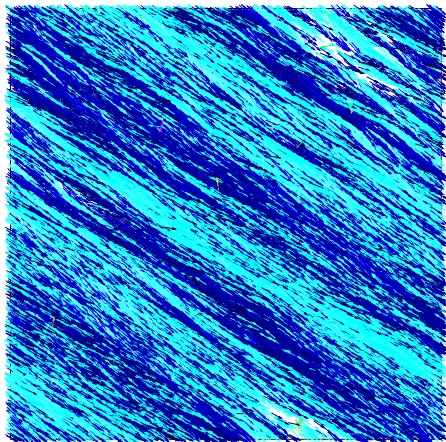Power-law decay in cluster size distributions



- $\Pi(n) \propto n^{\beta}$
- We obtain
  $-3.7 < \beta < -1.5$
- Exponents consistent with simulations of hard rods and experiments with myxobacteria

M. Abkenar, K. Marx, T. Auth, G. Gompper, Phys. Rev. E **88**, 062314 (2013)

Y. Yang, V. Marceau, and G. Gompper, *Phys. Rev. E* **82**, 031904 (2010)

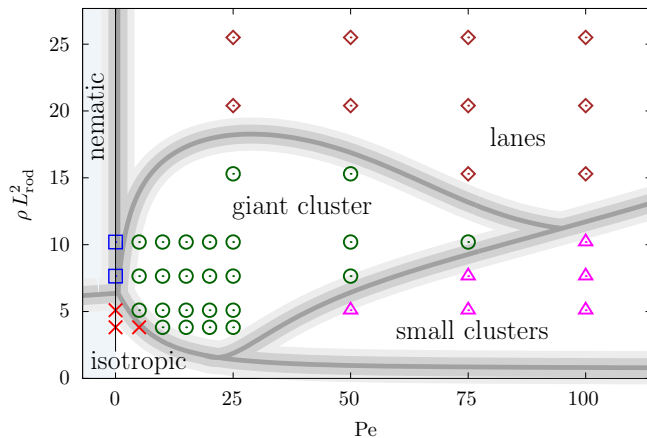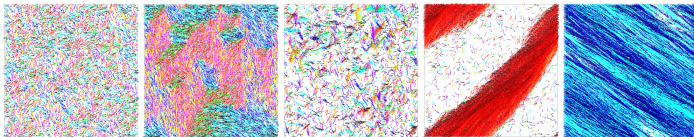F. Peruani *et. al.*, *Phys. Rev. Lett.* **108**, 098102 (2012)

# Laning Phase



$Q = 67, \quad Pe = 100, \quad \rho\, L_{\mathrm{rod}}^2 = 25.5$

- Very high density
- Streams of rods swimming in opposite directions
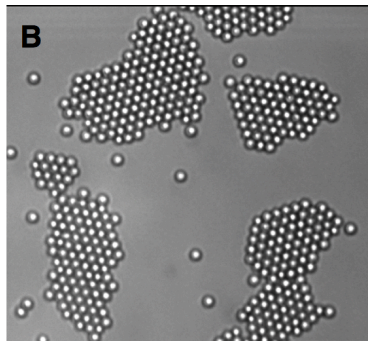
# Phase Diagram of Self-Propelled Rods

# Aggregation and Collective Dynamics

## of Self-Propelled Brownian Spheres
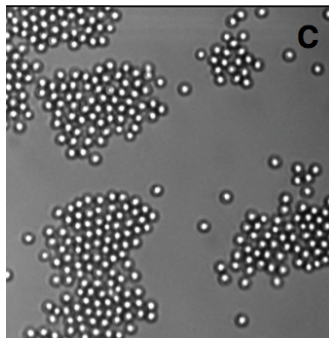
# Self-Propelled Spheres at Surfaces

Self-propelled Janus colloids (diffusiophoretic, thermophoretic)
(Theurkauff et at., PRL (2012), Buttinoni et al., PRL (2013), Palacci et al., Science (2013))



with propulsion

→ crystalline clusters

propulsion switched off

J. Palacci, S. Sacanna, A.P. Steinberg, D.J. Pine, and P.M. Chaikin, Science **339**, 936 (2013).

# Brownian Spheres in 3D: Aggregation

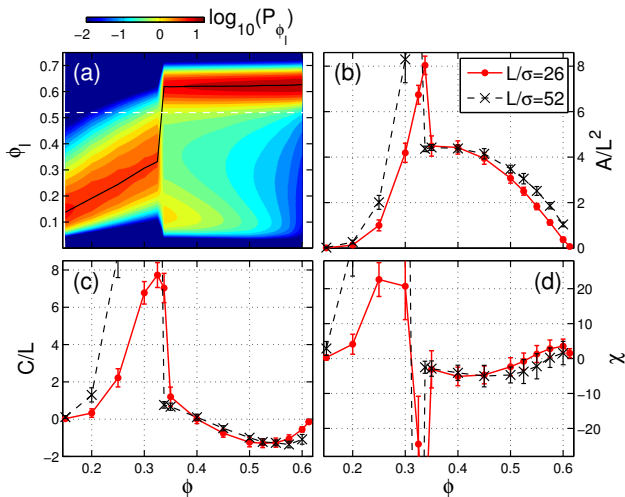Brownian spheres in three dimensions:

- No alignment mechanism – orientational diffusion
- At sufficiently high volume fraction and Pe: phase separation
- Dense phase is fluid
- Droplets $\rightarrow$ bicontinuous $\rightarrow$ gas bubbles
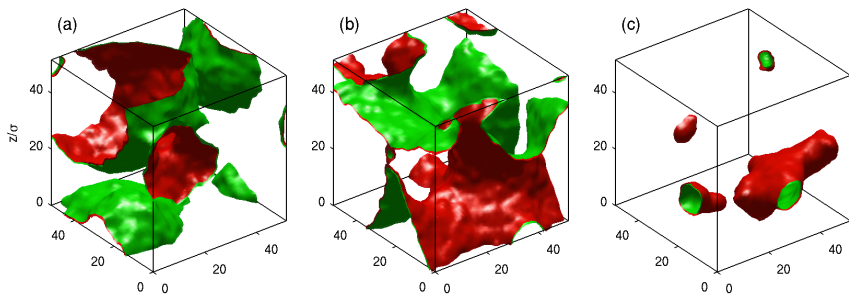


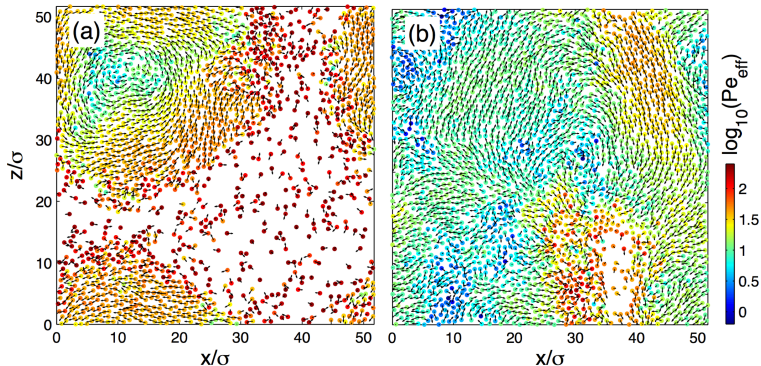A. Wysocki, R.G. Winkler, G. Gompper, EPL **105**, 48004 (2014)

# Brownian Spheres: Domain Geometry (Pe=270)



- Note high density of fluid phase $\phi = 0.62$, larger than (passive) glass transition!

Collective motion of self-propelled particles without aligning interactions
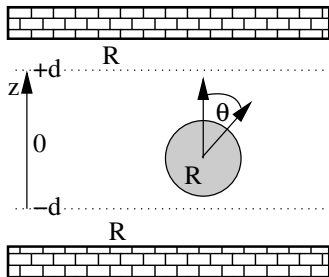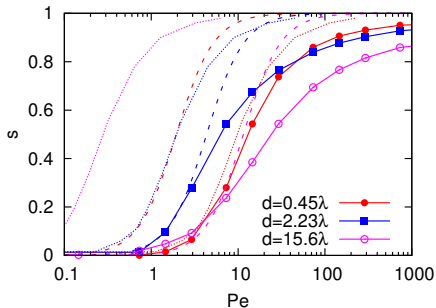


- Swirls and jets due to particle sorting

A. Wysocki, R.G. Winkler, G. Gompper, EPL **105**, 48004 (2014)

Consider single self-propelled Brownian sphere between hard walls



- Sphere shows strong surface adhesion

J. Elgeti & G. Gompper, EPL **101**, 48003 (2013)

# Intermezzo: Self-propelled Brownian Sphere between Walls

Solution of Fokker-Planck equation
for small Peclet numbers $Pe = v_0/\sqrt{DD_r}$:

$$
\begin{aligned}
\frac{\rho(z,\theta)}{\rho_0} &= 1 - \frac{Pe}{\sqrt{2}}\exp(-\sqrt{2}z/\lambda)Y_1^0(\theta) \\
&+ \frac{Pe^2}{6}\left[\sqrt{3}\exp(-\sqrt{6}z/\lambda) - \exp(-\sqrt{2}z/\lambda)\right]Y_2^0(\theta) \\
&+ \frac{Pe^2}{6}\exp(-\sqrt{2}z/\lambda) + \mathcal{O}(Pe^3)
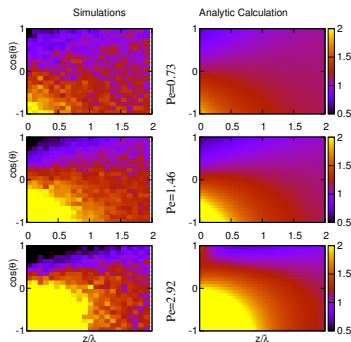\end{aligned}
$$

Polarization *towards* surface:

$$
\langle\cos\theta\rangle = -Pe\sqrt{2\pi/3}\,\exp(-\sqrt{2}z/\lambda) + \mathcal{O}(Pe^2)
$$

Surface excess:

$$
s = \frac{\lambda Pe^2}{6\sqrt{2}} + \mathcal{O}(Pe^4)
$$

Compare with simulation results



J. Elgeti & G. Gompper, EPL **101**, 48003 (2013)

Solution of Fokker-Planck equation for thin films, with $Pe_r = v_0/(D_r d) \to \infty$:
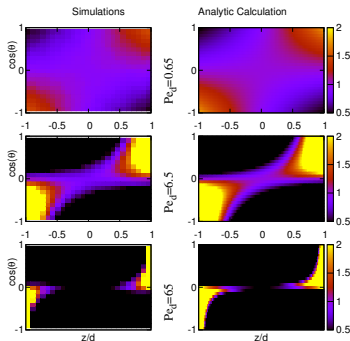
$$\rho(z, \theta) = \frac{Pe_d \rho_0 \cos(\theta)}{\pi \sinh(Pe_d \cos(\theta))} e^{Pe_d \cos(\theta) z}$$

where $Pe_d = v_0 d/D$.

Large $Pe_d$ gives complete sorting.

J. Elgeti & G. Gompper, EPL **101**, 48003 (2013)

Compare with simulation results

## Brownian Spheres: Collective Motion
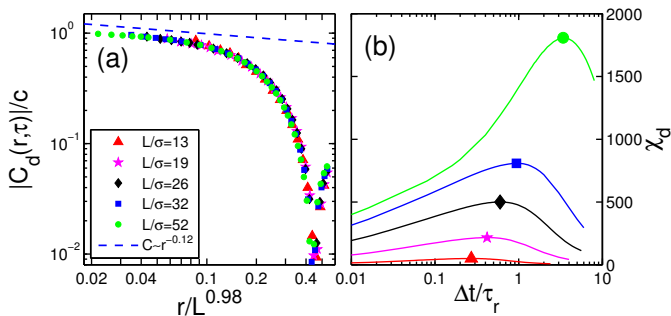
Displacement pair correlation function

$$C_d(r, \Delta t) = \frac{\left\langle \sum_{i,j \neq i} \mathbf{d}_i \cdot \mathbf{d}_j \, \delta(r - |\mathbf{r}_i - \mathbf{r}_j|) \right\rangle_t}{c_0 \left\langle \sum_{i,j \neq i} \delta(r - |\mathbf{r}_i - \mathbf{r}_j|) \right\rangle_t},$$

depends on time lag $\Delta t$ via displacement vector $\mathbf{d}_i = \mathbf{r}_i(t + \Delta t) - \mathbf{r}_i(t)$.

Global measure of cooperativity

$$\chi_d(\Delta t) = \int_\sigma^{L/2} C_d(r, \Delta t) \, \mathrm{d}^3 r.$$
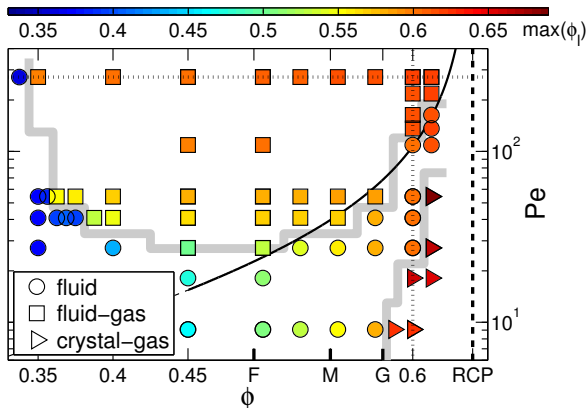
# Brownian Spheres: Collective Motion (Pe=270)



- Correlations very long ranged
- Build-up time $\tau$ required to reach maximum cooperativity!
- Correlation time $\tau$ strongly depends on system size.

A. Wysocki, R.G. Winkler, G. Gompper, EPL **105**, 48004 (2014)

- Minimum Peclet number $Pe_c \simeq 30$ required to generate phase separation!

Flagellar Vortices

# Sperm Vortices

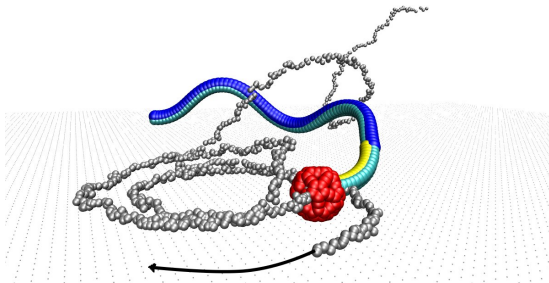Spermatozoa spontaneously form vortices at surfaces at high concentration
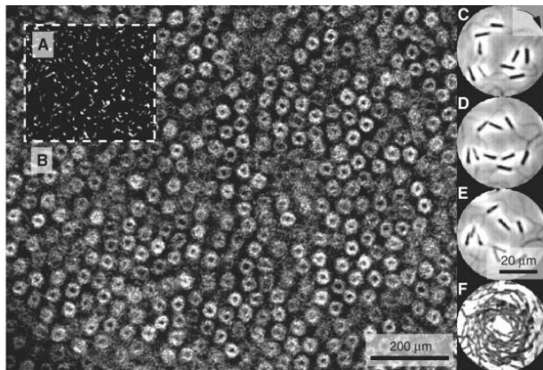


I.H. Riedel, K. Kruse, and J. Howard, Science **309**, 300 (2005)

# Single Sperm near Surfaces

Mesoscale hydrodynamics simulations show

- effective attraction of sperm to surfaces
- due to hydrodynamic interactions and elongated shape
- circular motion for chiral sperm shapes



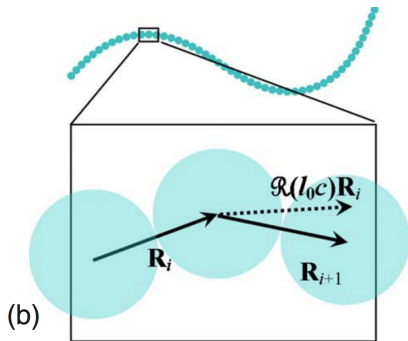J. Elgeti, U.B. Kaupp, and G. Gompper, Biophys. J. **99**, 1018 (2010)

Flagellum described as semi-flexible polymer

- chain of beads
- curvature elasticity
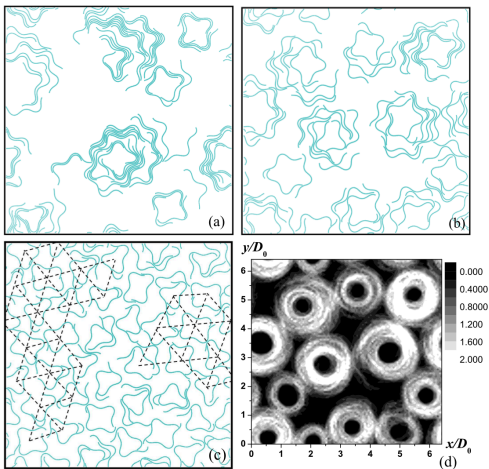- time-dependent spontaneous curvature

$$c(s,t) = A\sin(qs - 2\pi f_0 t)$$

with beat frequency $f_0$.



(b)

Y. Yang, V. Marceau, and G. Gompper, Phys. Rev. E **82**, 031904 (2013)

# Dense Flagella Systems in Two Dimensions
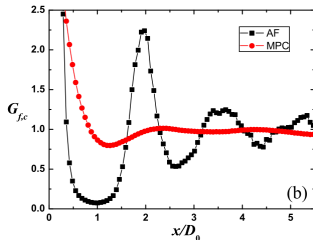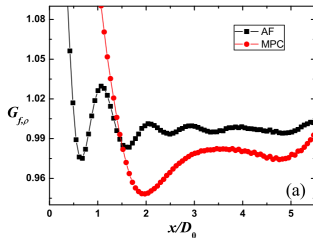


(a) with hydrodynamic interactions
(b) anisotropic friction, small curvature
(c) anisotropic friction, large curvature
(d) same as in (b), averaged over 30 beats.

Y. Yang, F. Qiu, and G. Gompper, Phys. Rev. E **89** 012720 (2014)

# Dense Flagella Systems in Two Dimensions

- much stronger correlations without hydrodynamics

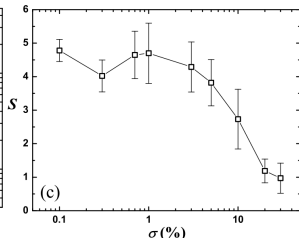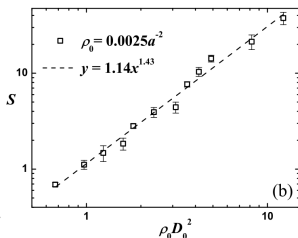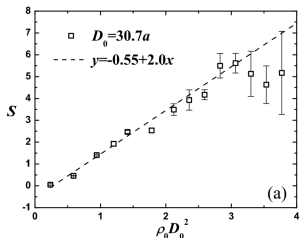- hydrodynamics in 2D over-estimates hydrodynamics near wall in 3D

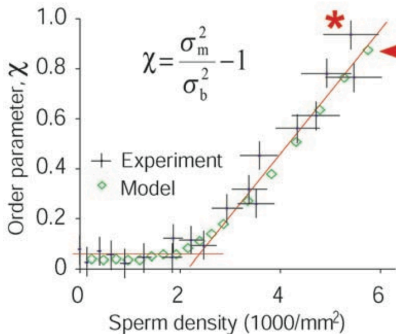Order parameter

$$S = \Delta^2/\Delta_0^2 - 1$$

where $\Delta^2$ is variance of trajectory centers in area $D_0^2$.


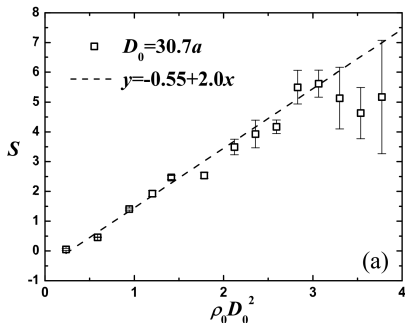
Y. Yang, F. Qiu, and G. Gompper, Phys. Rev. E **89** 012720 (2014)

# Dense Flagella Systems in Two Dimensions

Comparison with experiment:



$$\chi = \frac{\sigma_m^2}{\sigma_b^2} - 1$$

+ Experiment
◇ Model

Order parameter, $\chi$

Sperm density (1000/mm²)

I.H. Riedel, K. Kruse, and J. Howard,
Science **309**, 300 (2005)



$D_0 = 30.7a$

$y = -0.55 + 2.0x$

$S$

$\rho_0 D_0^2$

(a)

Y. Yang, F. Qiu, and G. Gompper,
Phys. Rev. E **89** 012720 (2014)

# Summary & Conclusions

- Shape, orientational fluctuations and hydrodynamics together determine dynamics of microswimmers
- Aggregation and clustering generic feature of self-propelled particles
- Penetrable self-propelled rods – motile polar clusters and laning
- Brownian spheres – phase separation and collective dynamics
- Sperm dynamics – wall adhesion and circular motion
- Multiple sperm dynamics – vortex formation


Masoud Abkenar


Jens Elgeti


Thorsten Auth


Adam Wysocki


Yingzi Yang


Roland Winkler