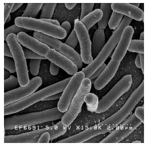
The role of fluid dynamics in micro-swimmer suspensions

Enkeleida Lushi
Brown University, Engineering

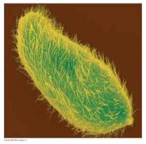
Collaborators:
Hugo Wioland & Raymond Goldstein,
DAMTP, University of Cambridge
& Vasily Kantsler
University of Warwick & SkolTech

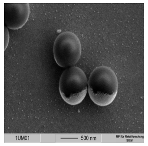
Active matter -> collective motion of self-propelled agents

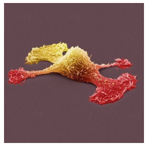

Bacteria


Alga


Sperm


Paramecium


Colloids


Cancer cell

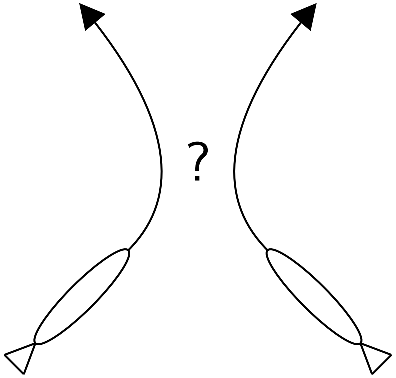

Cricket


Bristle Bot


Bird


Fish


Self-propelled unit



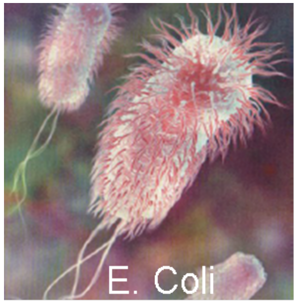
Interactions


Collective behavior

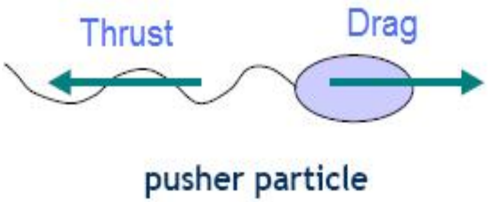
Background: swimming at low Reynolds number

In nature, several swimming mechanisms are observed:
e.g. flagellar propulsion (E Coli, B Subtilis, C. Rheinhardii…)

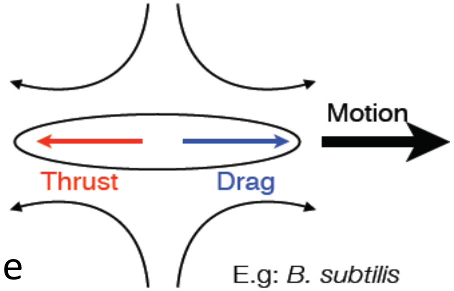
Reynolds number is very small ~ 10^(-4)

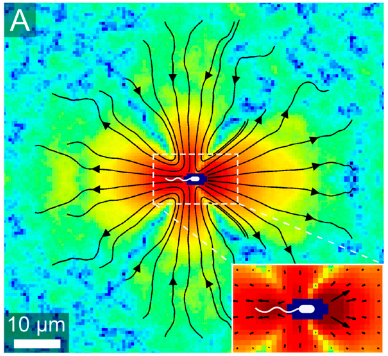


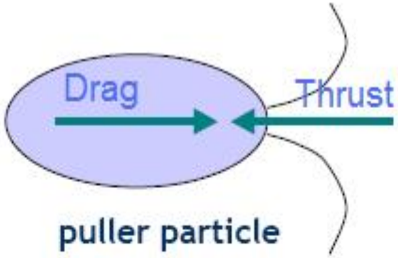
We look at micro-swimmers classified into **pusher** or **puller** types due to **the leading order** force dipole / stresslet they create due to locomotion.



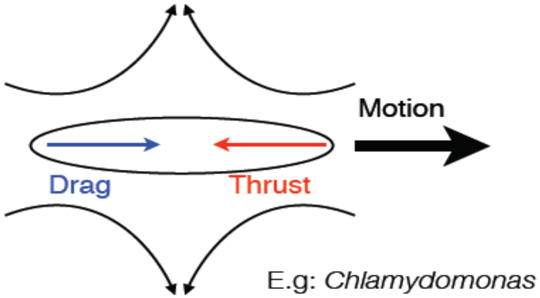
Extensile force dipole

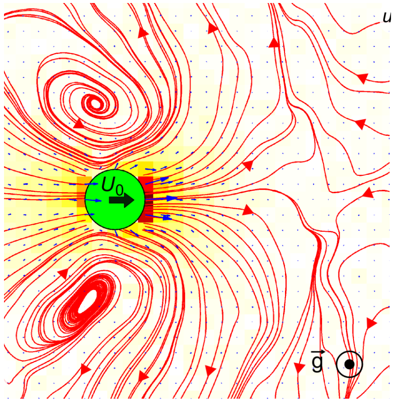




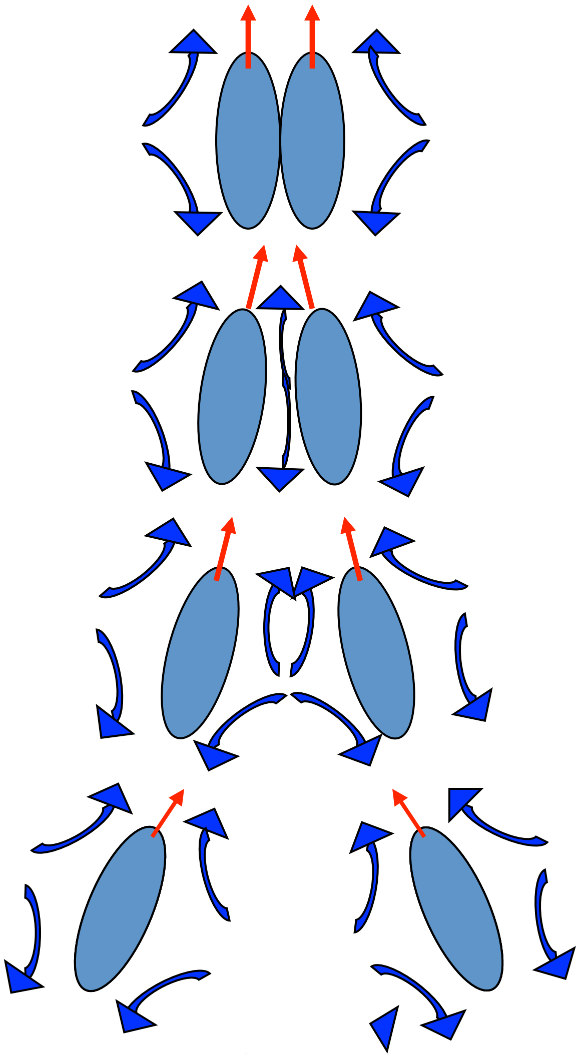


Contractile force dipole

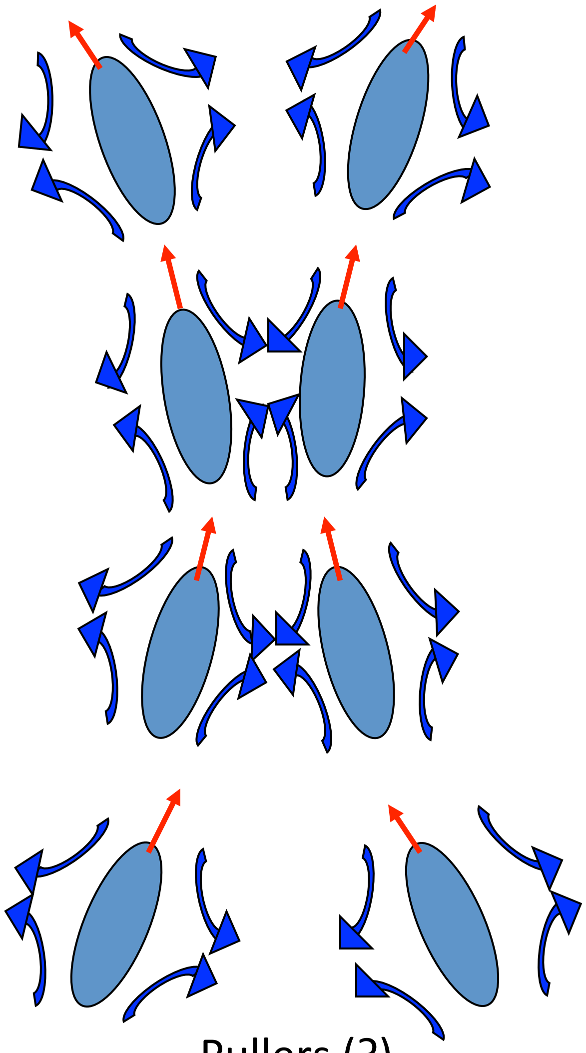




Schematic interaction of two swimmers



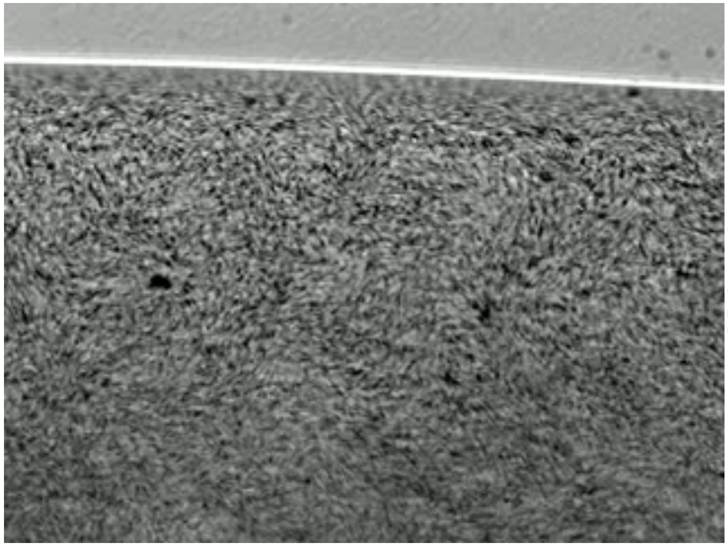
Pushers

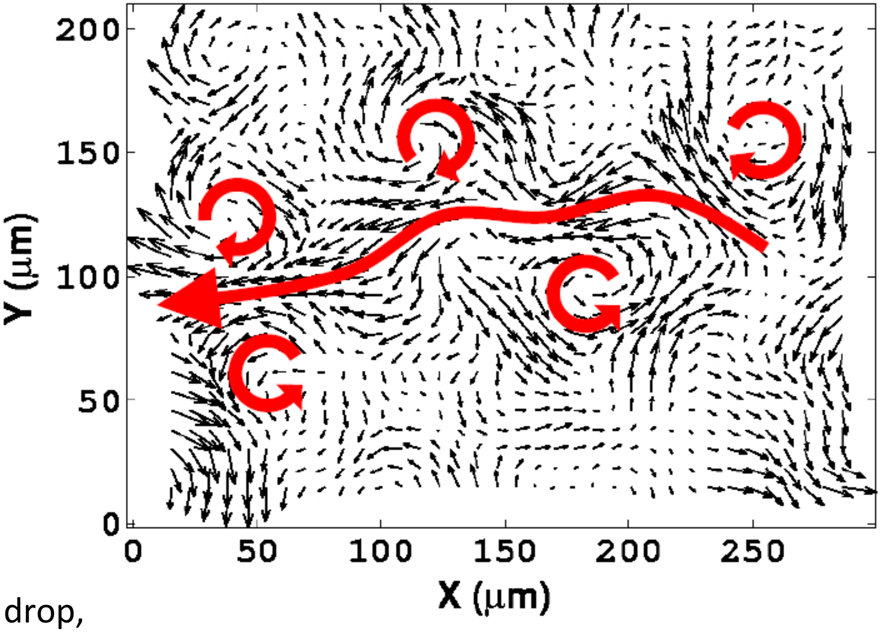


Pullers (?)

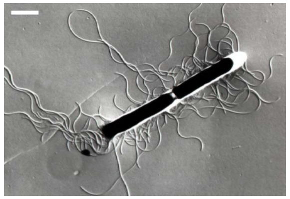
Interactions in suspensions of micro-swimmers

Bacterial ``turbulence''.





Bacterial bath: Colony of B. Subtilis in a pendant drop,
Dombrowski, Kessler and Goldstein, 2004

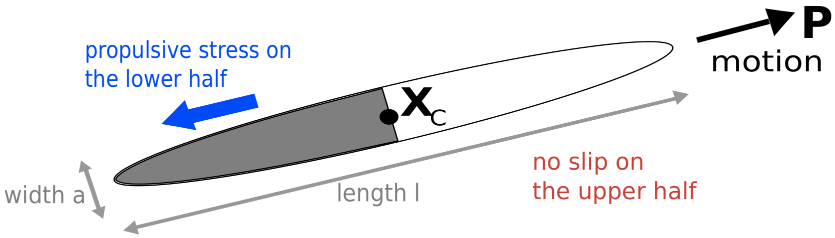


Bacterium Subtilis rod-shaped ~4 μm long
swimming speed 20-30 μm/sec
not much tumbling

Observations:

- collective behavior drives the fluid
- correlated motions over large length scales, collective speed ~10 times individual speed
- density fluctuations, self-organization -> jets, vortices
- enhanced transport and diffusion, etc.

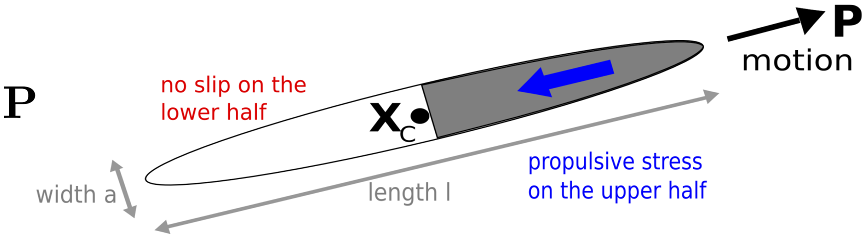
Minimal swimmer model: leading order dynamics in swimmer slenderness



Center of mass and orientation

$$\dot{\mathbf{X}}_i = \mathbf{u}\delta(\mathbf{x}-\mathbf{X}_i) + V\mathbf{P} + \frac{1}{2}(\mathbf{I}+\mathbf{P}_i\mathbf{P}_i^T)\sum_{j\neq i}^{M}\mathbf{F}^e_{ij}$$

$$\dot{\mathbf{P}}_i = (\mathbf{I}-\mathbf{P}\mathbf{P}^T)[\nabla\mathbf{u}\delta(\mathbf{x}-\mathbf{X}_i)]\mathbf{P} + 6\sum_{j\neq i}^{M}\mathbf{T}^e_{ij}\times\mathbf{P}$$



Low Re flow with extra stress (active + due pairwise steric interactions)

$$-\nabla^2\mathbf{u} + \nabla q = \nabla\cdot\boldsymbol{\Sigma}$$
$$\nabla\cdot\mathbf{u} = 0$$

$$\boldsymbol{\Sigma} = \sum_{i=1}^{M}\left[\mathbf{S}^a_i + \mathbf{S}^e_i\right]\delta(\mathbf{x}-\mathbf{X}_i)$$
$$\mathbf{S}^a_i = \alpha\mathbf{P}_i\mathbf{P}_i^T$$
$$\mathbf{S}^e_i = \sum_{j>i}^{M}\mathbf{F}^e_{ij}\mathbf{r}^T_{ij}$$

E. Lushi & C.S. Peskin, Comp. & Structures
122, 239-246 (2013)

Numerical Methodology

- Coupled dynamics of the micro-swimmers (Lagrangian) and the fluid equations (solved in an Eulerian grid)

- We use an Immersed Boundary Framework.

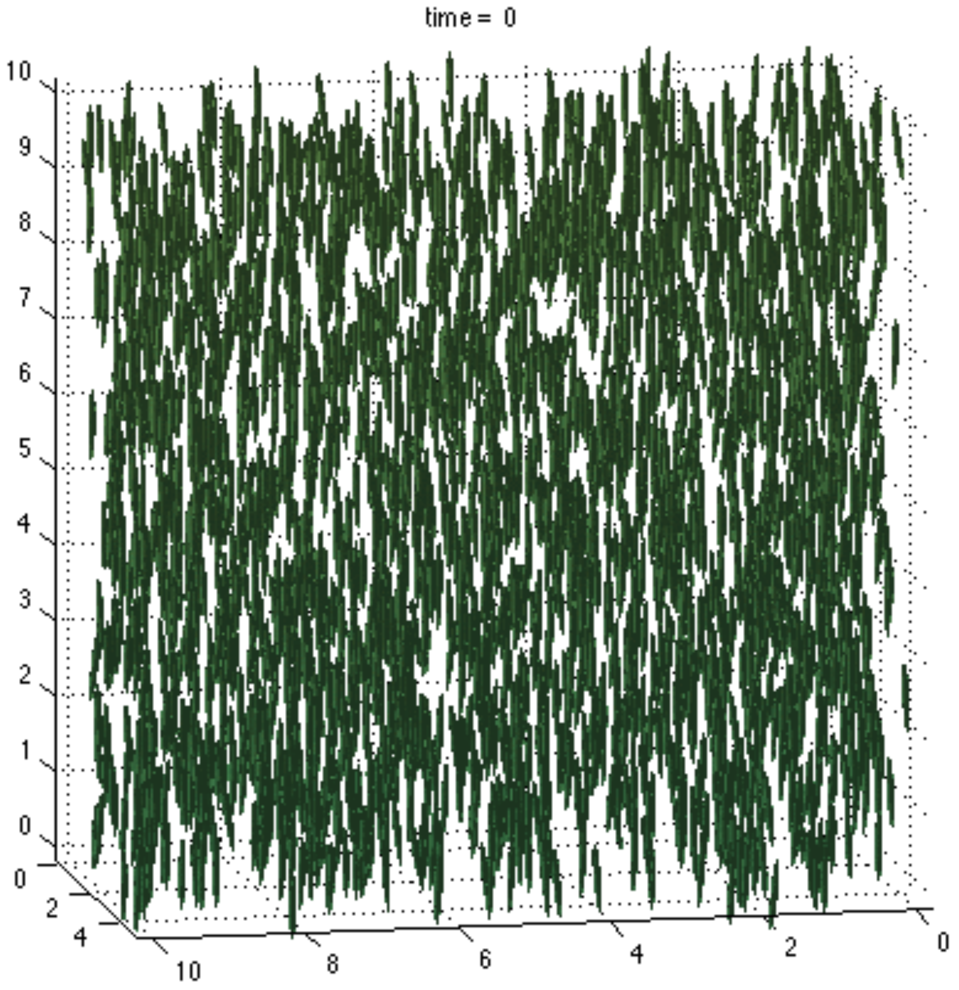
- Triply periodic fluid domain – we solve the fluid equations spectrally.

- Steric interactions done via a soft anisotropic potential.

- Computational cost O(N log N + M) with N the total number of mesh points, M total swimming particles.

- Methodology extendable to include domain boundaries (e.g. thin films), curved surfaces, obstacles, etc.
- The particles need not be uniform in speed, shape or type.

3D simulation: initially nearly-aligned pusher swimmers



10^3 box, triply-periodic
(slice of the domain shown)

4000 swimmers,
length 1, diameter 1/10,
initially nearly aligned in the vertical direction

volume fraction <10%

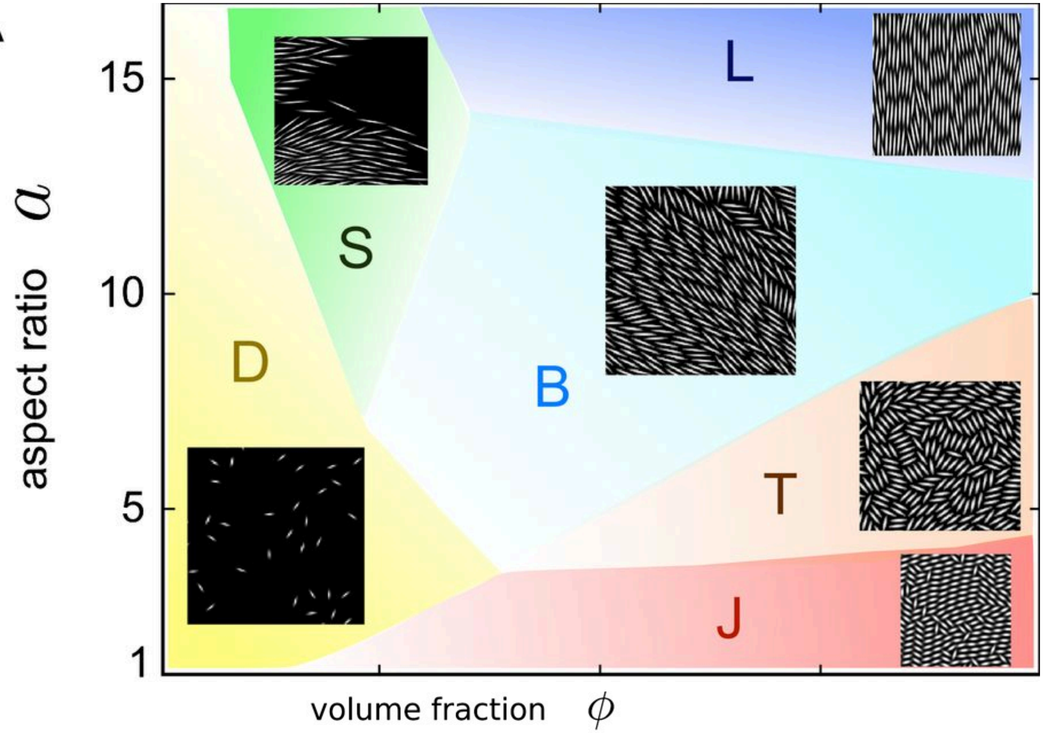
We observe the emergence of large-scale fluid flows.

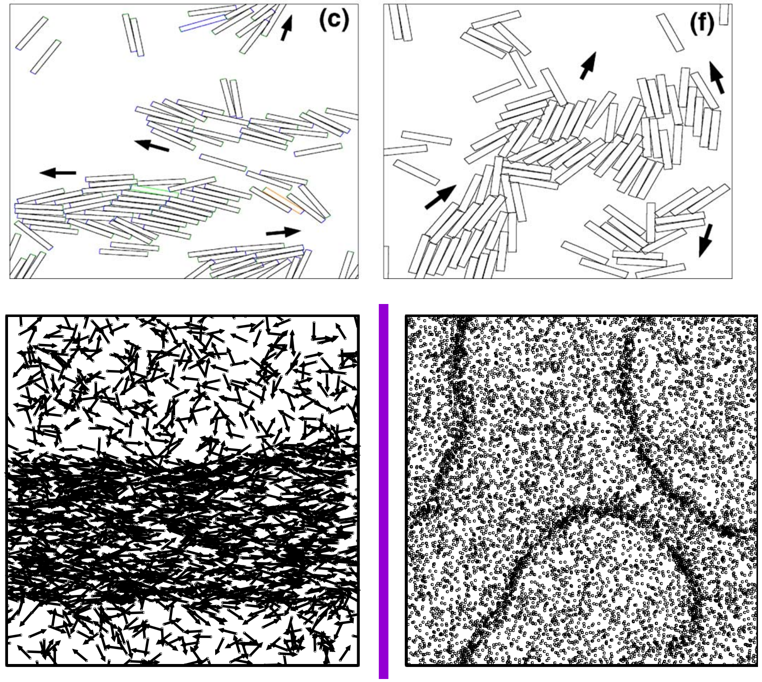
Suspension becomes isotropic on the whole, but swimmers locally align.

Collective dynamics of SPP-s

- Direct measurements of the flow field around a single micro-swimmer by Drescher et al PNAS 2011 indicate that direct collisions and noise are significant factors in the motion of such organisms, especially at short range.

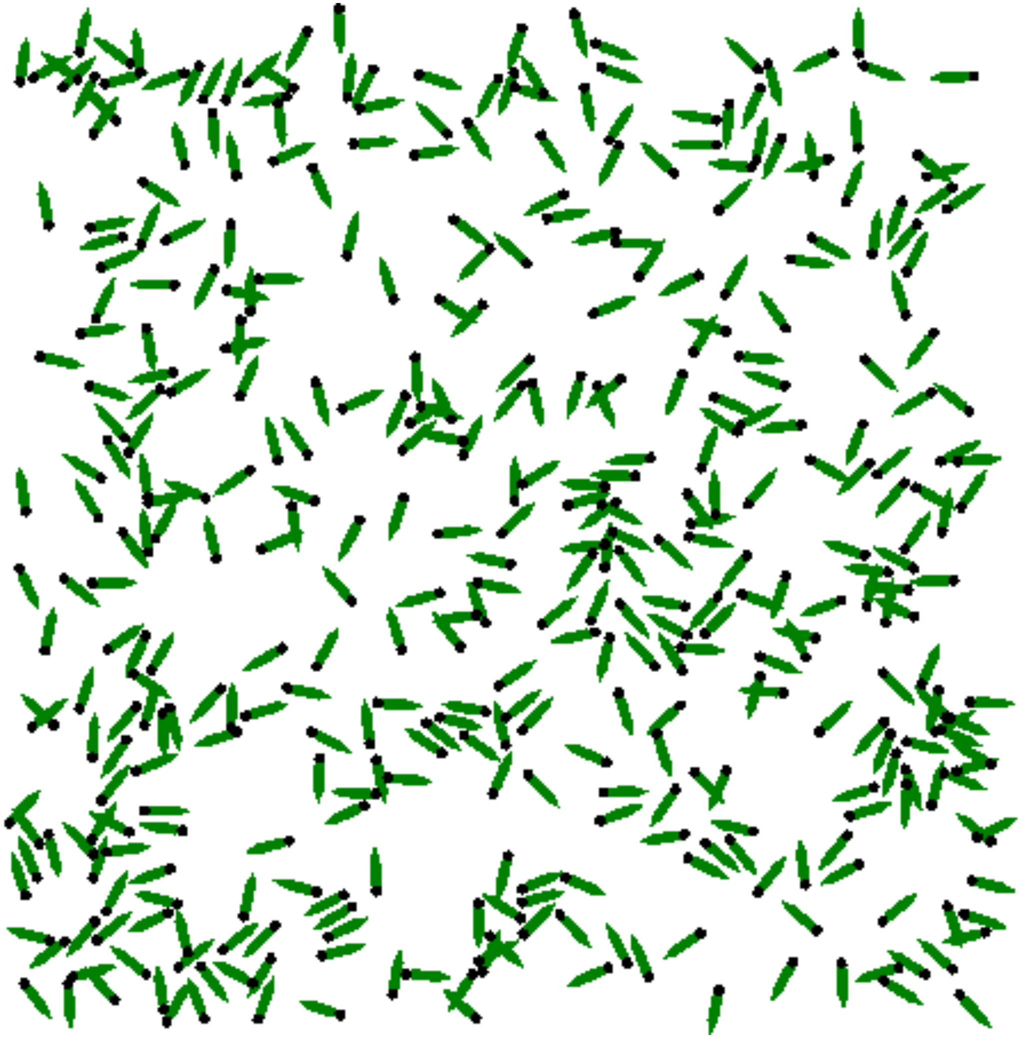
- Recently there have been many studies of suspensions of SPP (self-propelled particles) with no hydrodynamics but sometime with aligning interactions.

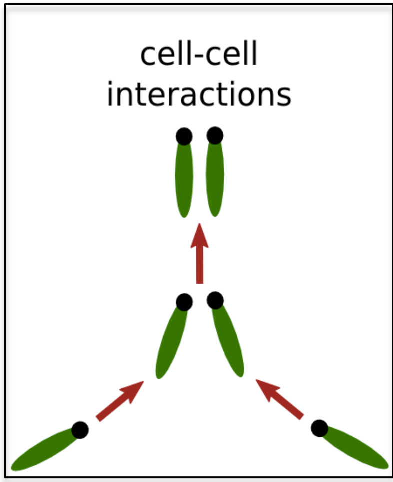




Wensink et al, PNAS 2012, Peruani et al, PRE 2007, Ginelli et a, PRL 2010

2D, dilute, NO hydrodynamics

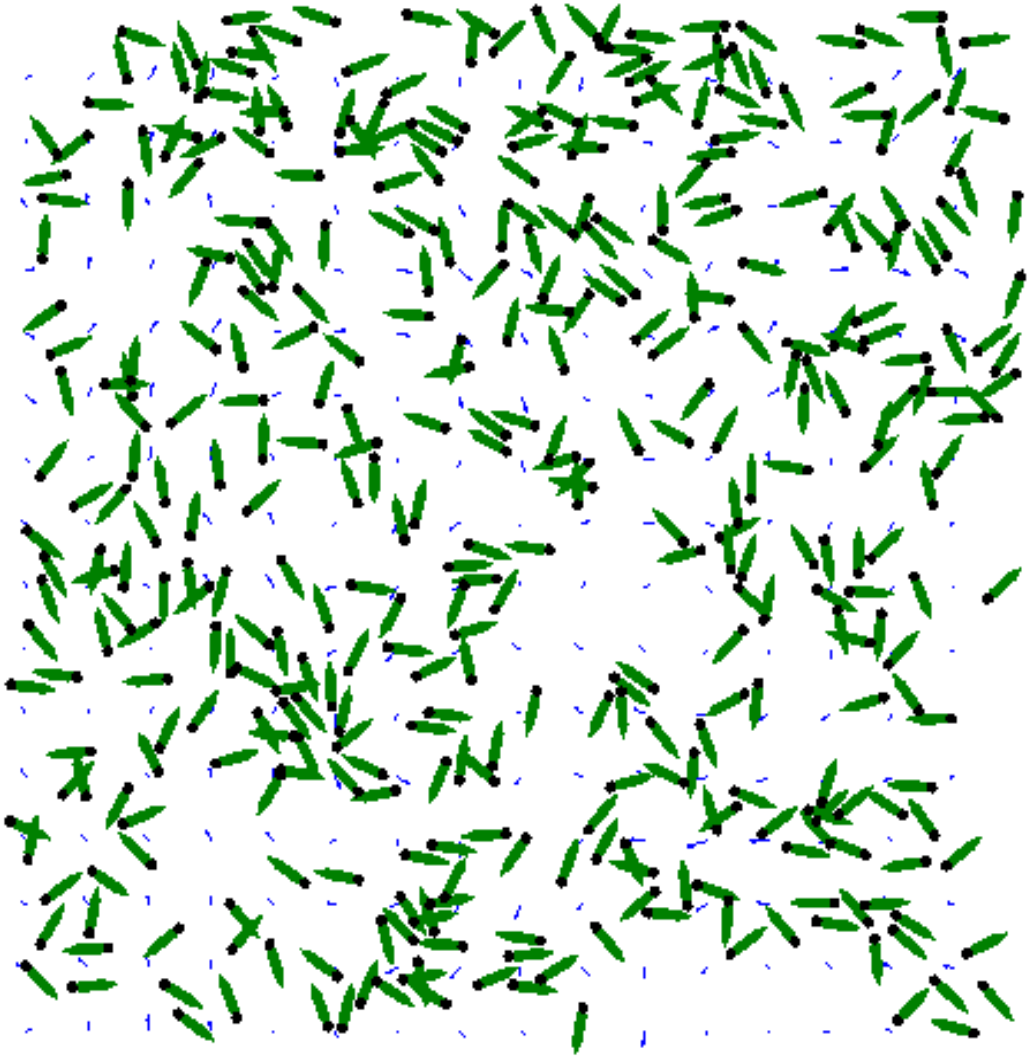


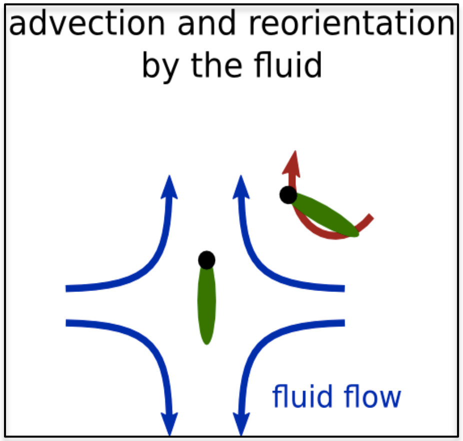


Bionematic or Swarming state

Observe large clusters co-moving.

2D, dilute, with hydrodynamics



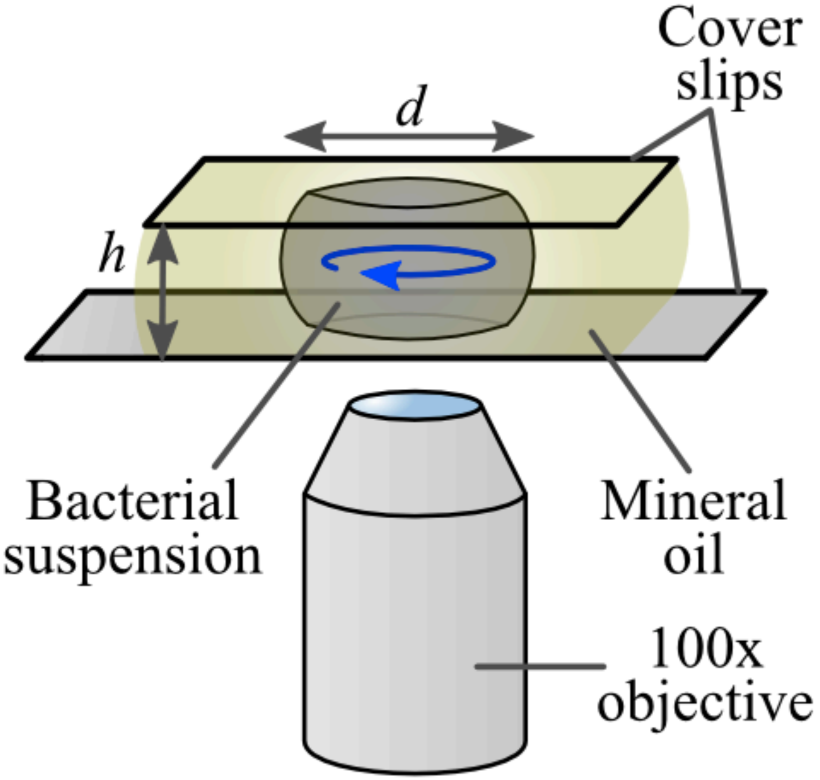

advection and reorientation by the fluid

Observe smaller and more dynamic clusters of swimmers.

So hydrodynamics makes a difference.

Organization in a bacterial drop

H. Wioland, F. Woodhouse, J. Dunkel, J. Kessler, R. Goldstein, PRL 110(26) 268102 (2013)

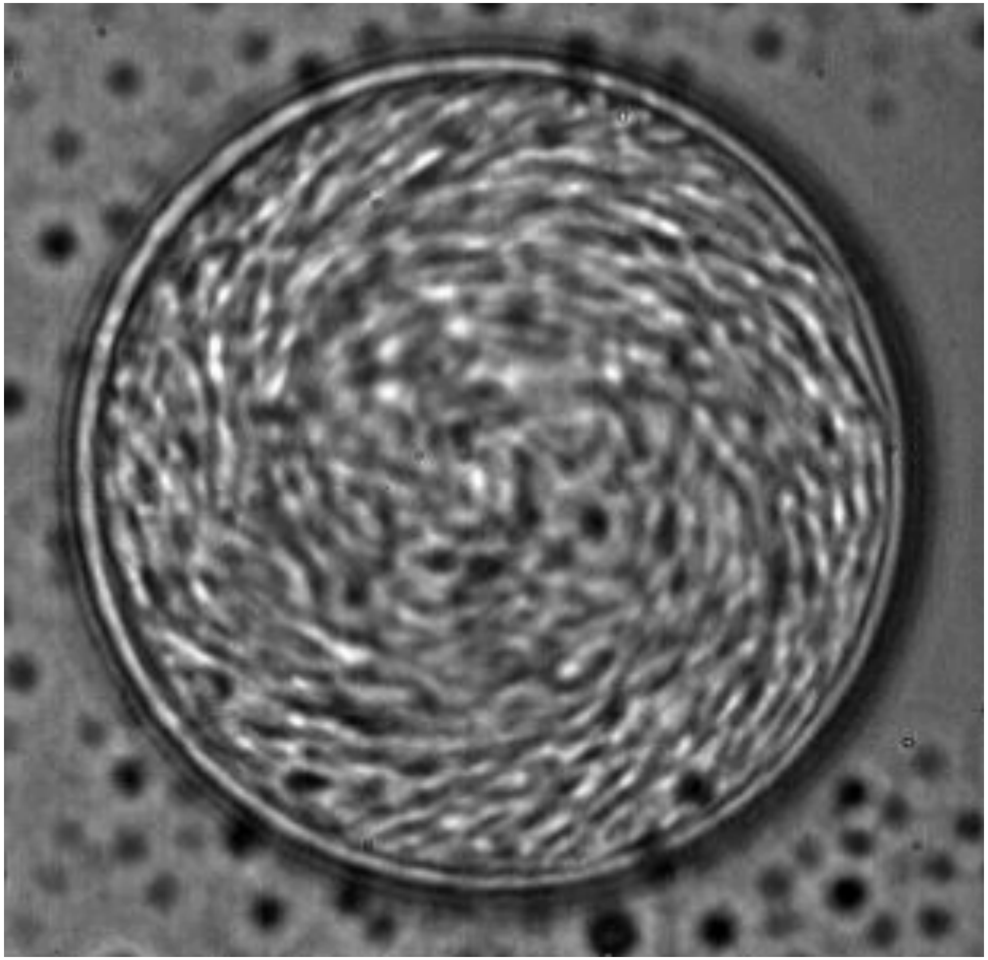


An emulsion of dense bacteria is confined between two coverslips to create flattened drops.

d = 10-100 µm;   h~25 µm.

Organization in a bacterial drop

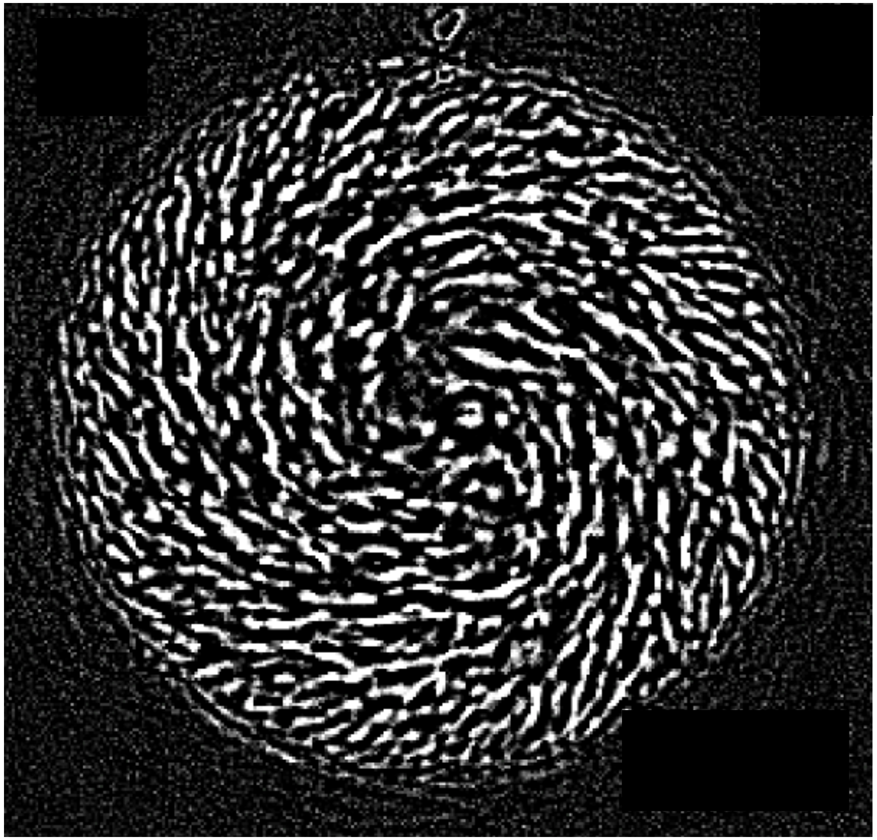
H. Wioland, F. Woodhouse, J. Dunkel, J. Kessler, R. Goldstein, PRL 110(26) 268102 (2013)



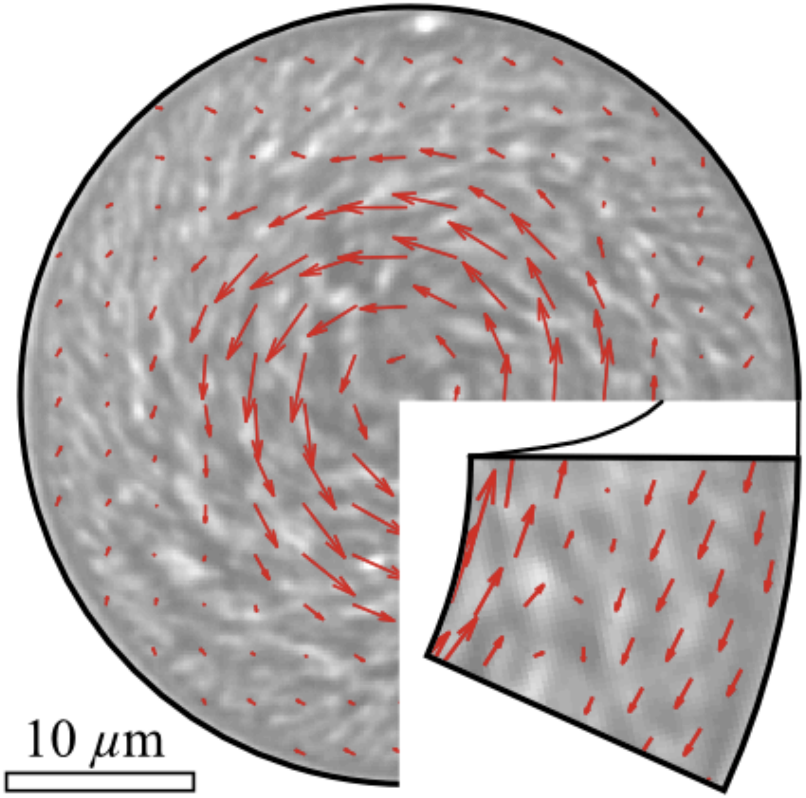
The suspension self-organizes into a spiral vortex, stable for tens of minutes.

Experiments: B. Subtilis in a drop

H. Wioland, F. Woodhouse, J. Dunkel, J. Kessler, R. Goldstein, PRL 110(26) 268102 (2013)

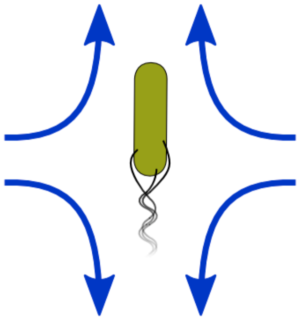


Spontaneous organization of the suspension into a spiral vortex.

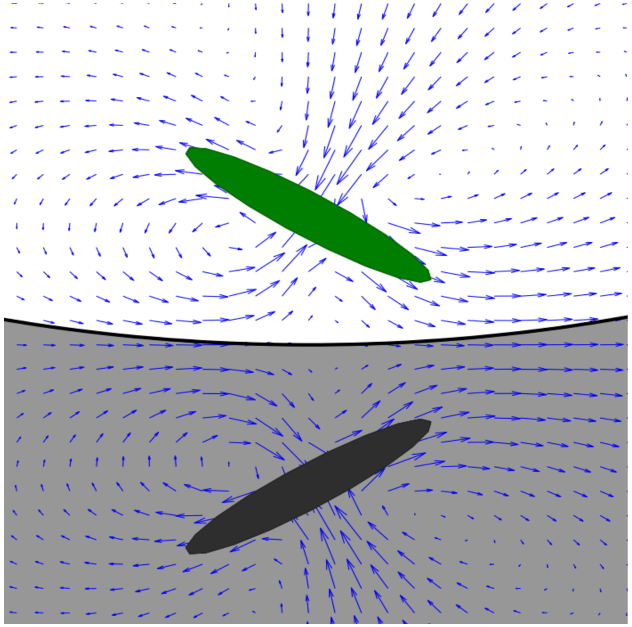


bacteria flow (PIV)

Modeling & Simulation Method



generated fluid flow



Swimmers are ellipsoidally-shaped, propel along their main axis, etc. Need to trace only their centers of mass **X** and orientations **P**.

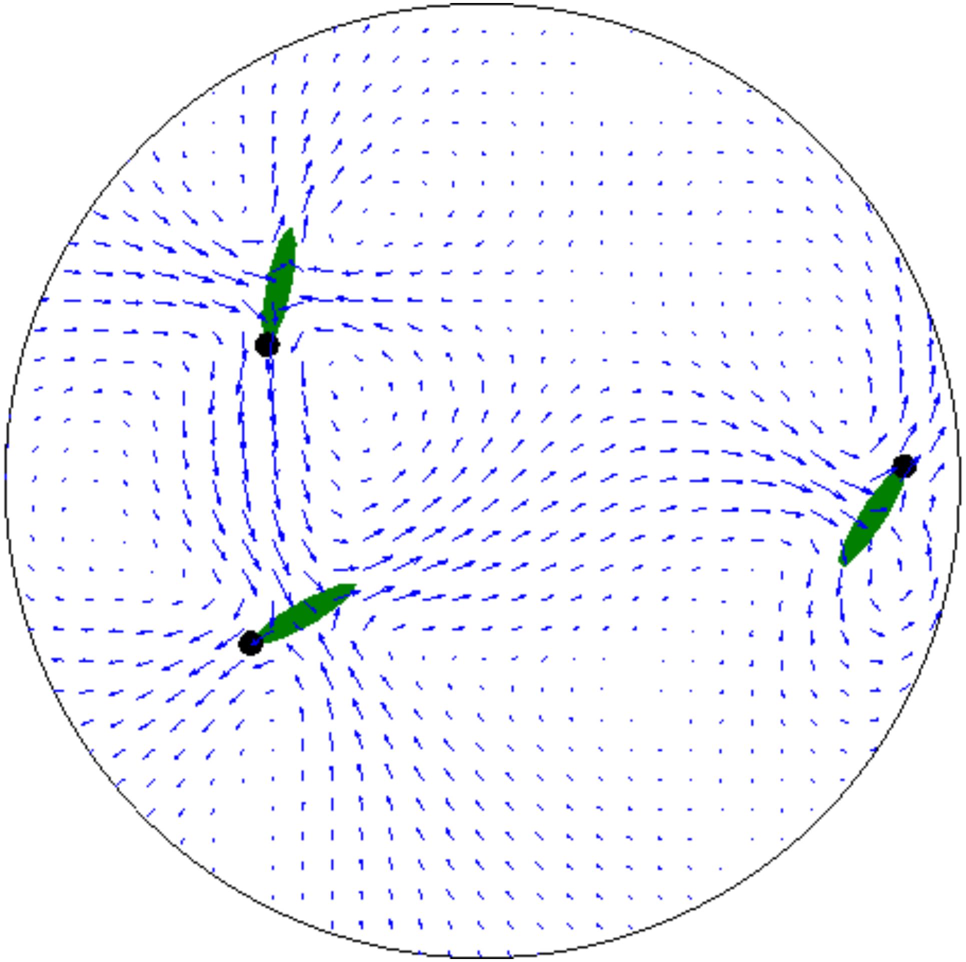
Each swimmer generates instantaneously a dipolar fluid disturbance.

Pair interactions between the swimmers are done via the repulsive part of a soft potential (so there can be some overlaps).

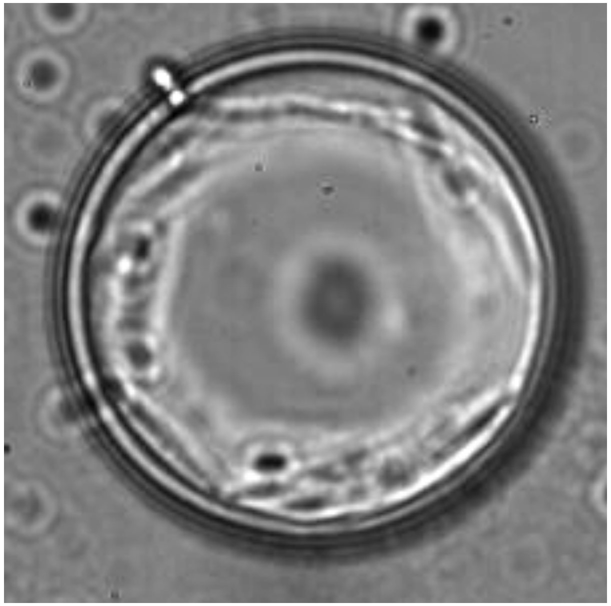
Near a boundary, use an image (this approximates a no-stress condition at the water-oil drop interface. Steric repulsions with the image swimmer effectively gives confinement.

In 2D, free space fluid flow u decays as 1/r. When there is a wall, u decays as 1/r^2.

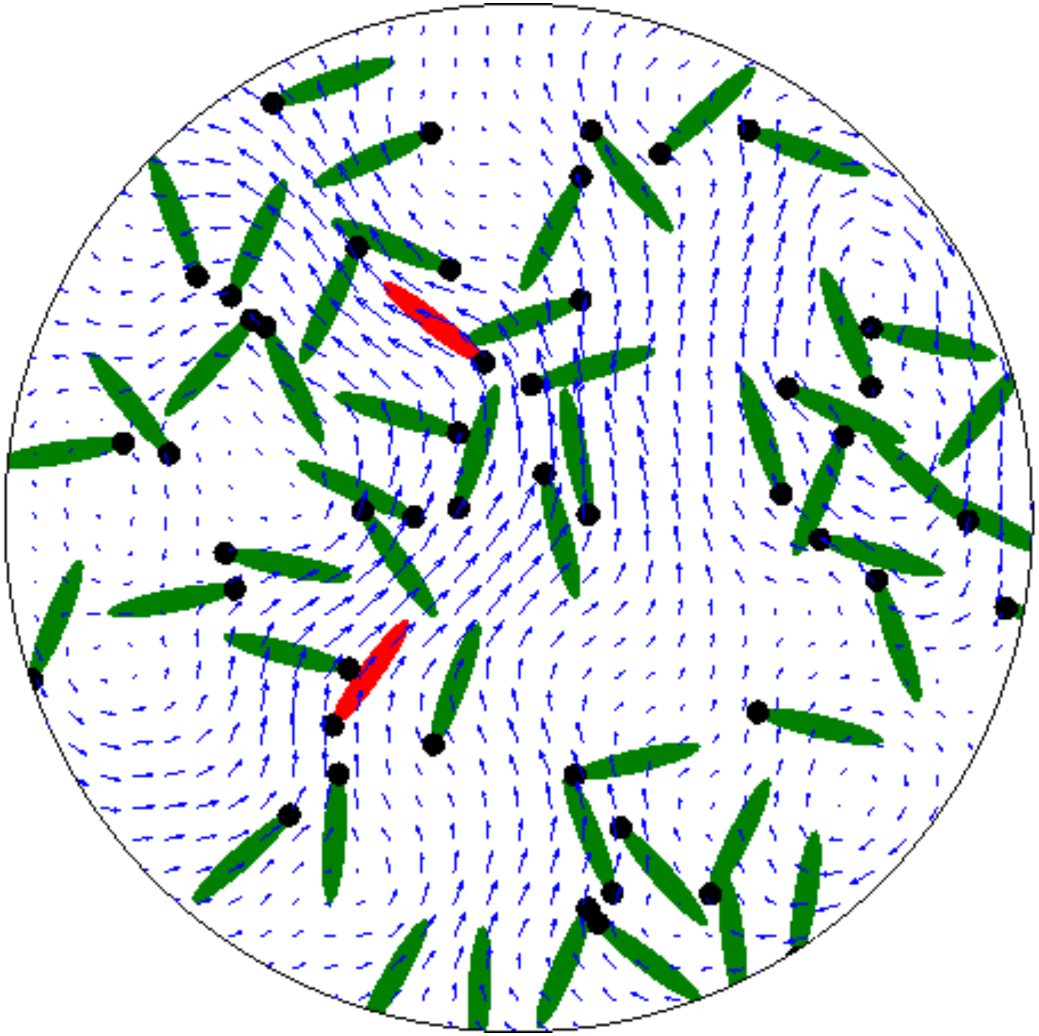
A Swimmer in a Circle



Swimmers end up at the boundary and swim at a very low angle.
Just as in the experiments.



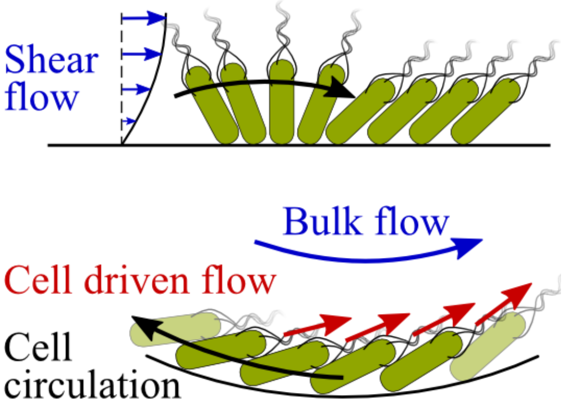
A Dilute Suspension



Swimmers head to the boundary and stay there.

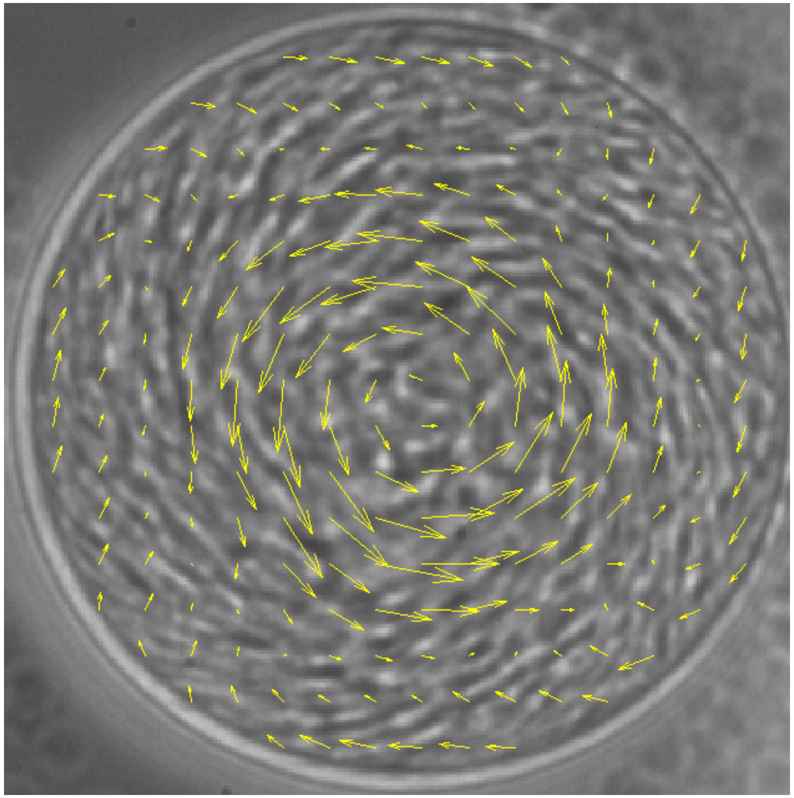
The outer layer forms first and then it is stable.

The pusher swimmers produce fluid flow in the opposite direction of their circulation.

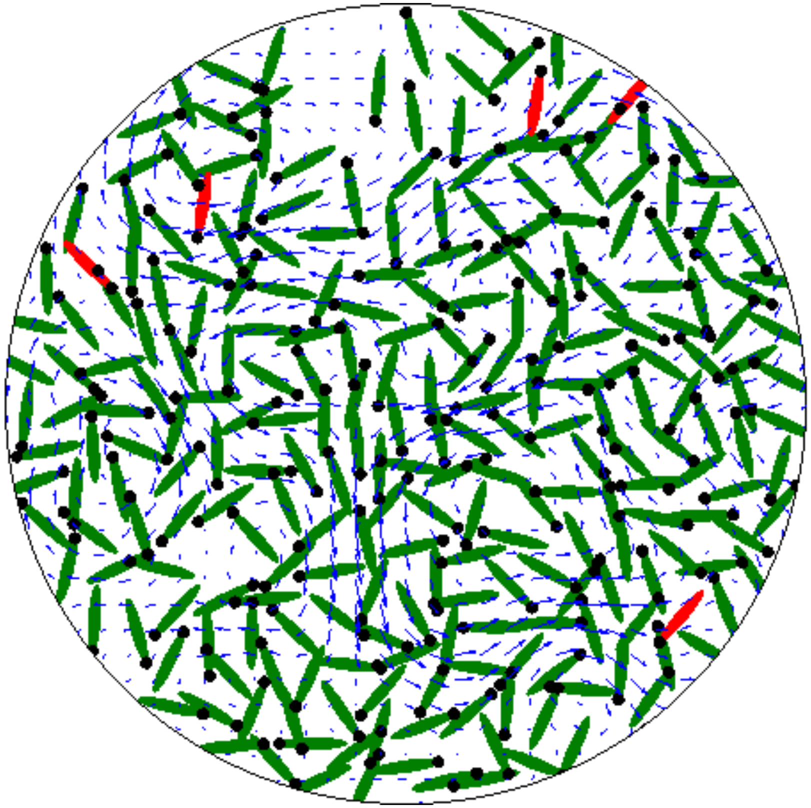


B. Subtilis in a drop, pushers in a disk

Experiments of H. Wioland et al. (2013)

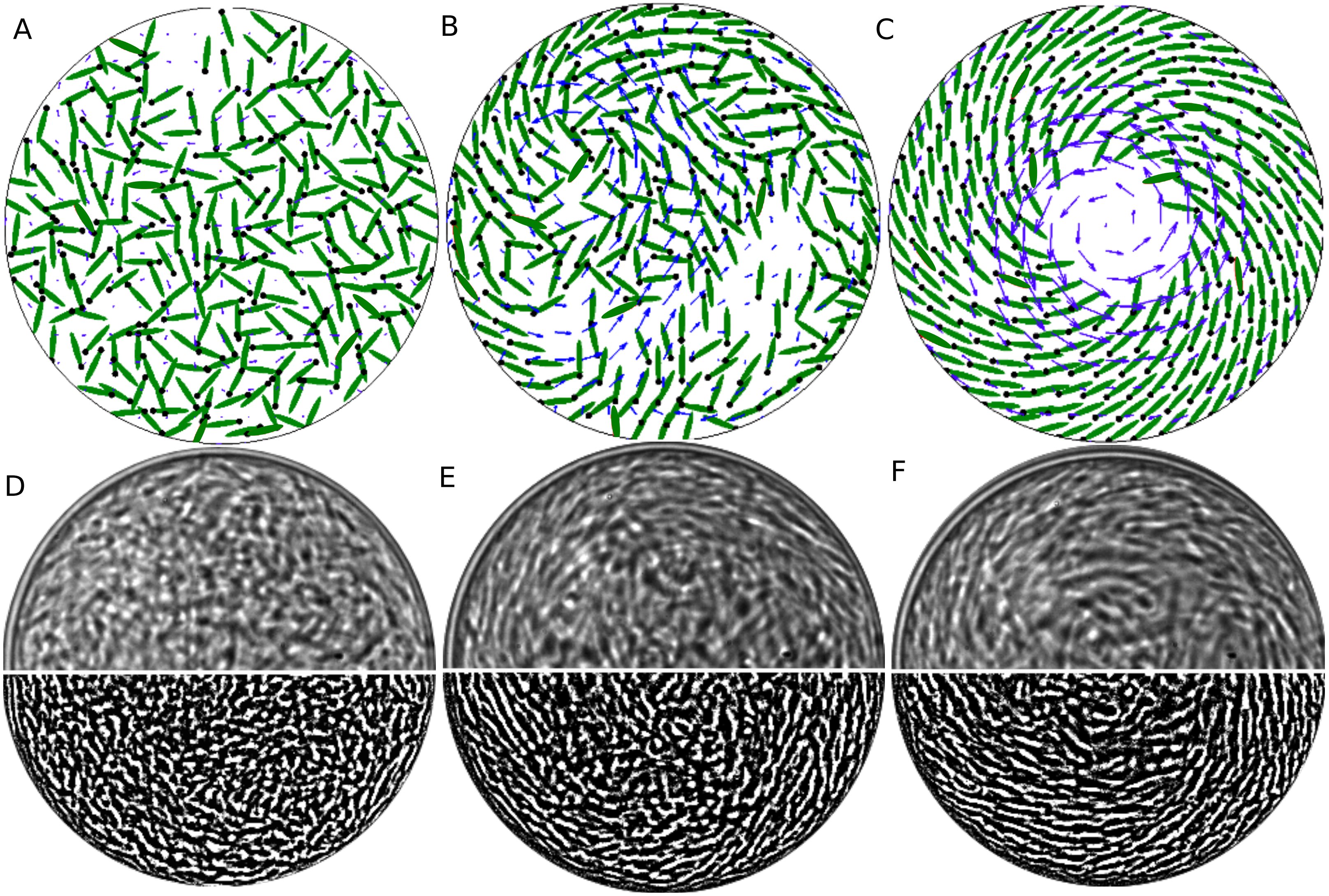


2D simulation



2D simulation captures dynamics → vortex flow, ordering of swimmers, etc.

Boundary-driven organization



Causes for the self-organization

The usual ingredients include confinement and self-propulsion.

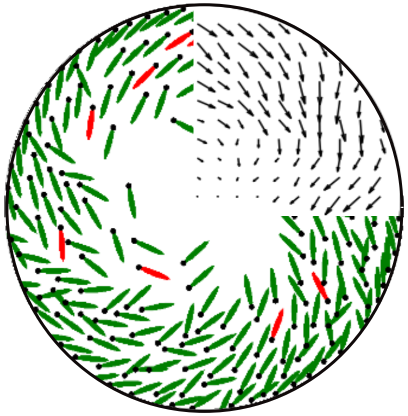
- Elongated swimmer shape (needed for steric interactions and boundary packing)
- Hydrodynamics (in some fashion)

- ? Noise ? Lubrication hydrodynamics? Some kind of other (prescribed) alignment ?

- Some previous studies have shown spontaneous vortex motion of self-propelled disk-like particles under some prescribed alignment, e.g. .Grossman et al, N. J. Phys. (2008).

- But the circulation in all of these is unidirectional.

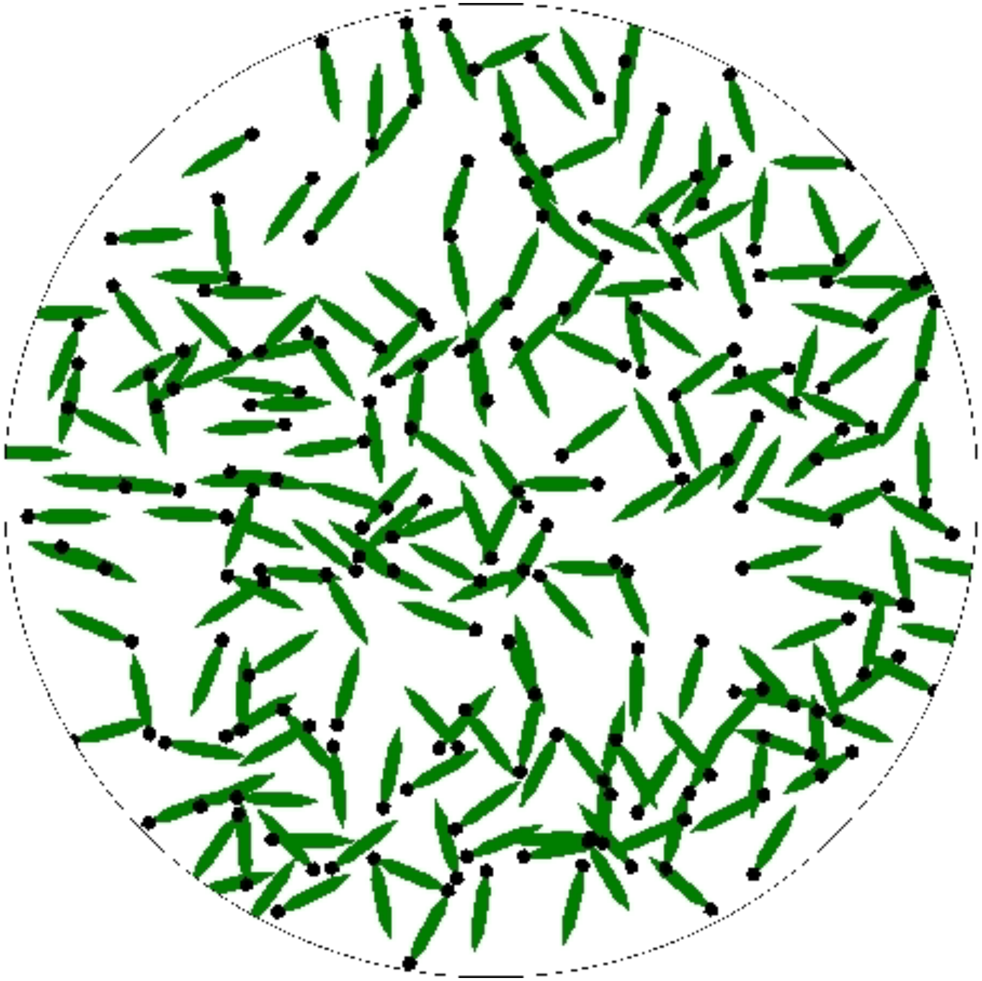
Investigate the causes



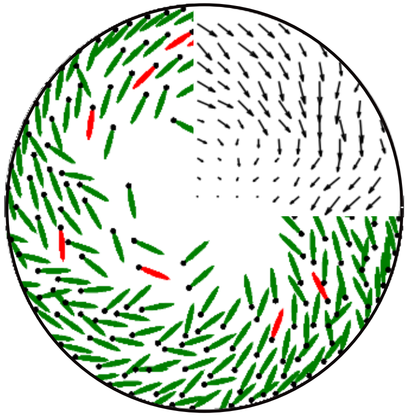
- self-propulsion
- elongated particles
- no hydro

-> (spiral) organization
-> slow unidirectional
circulation.

Investigate the causes

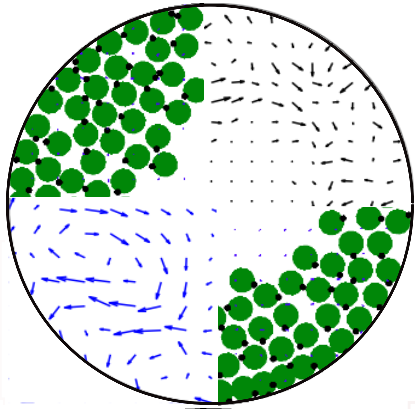


Investigate the causes



- self-propulsion
- elongated particles
- no hydro

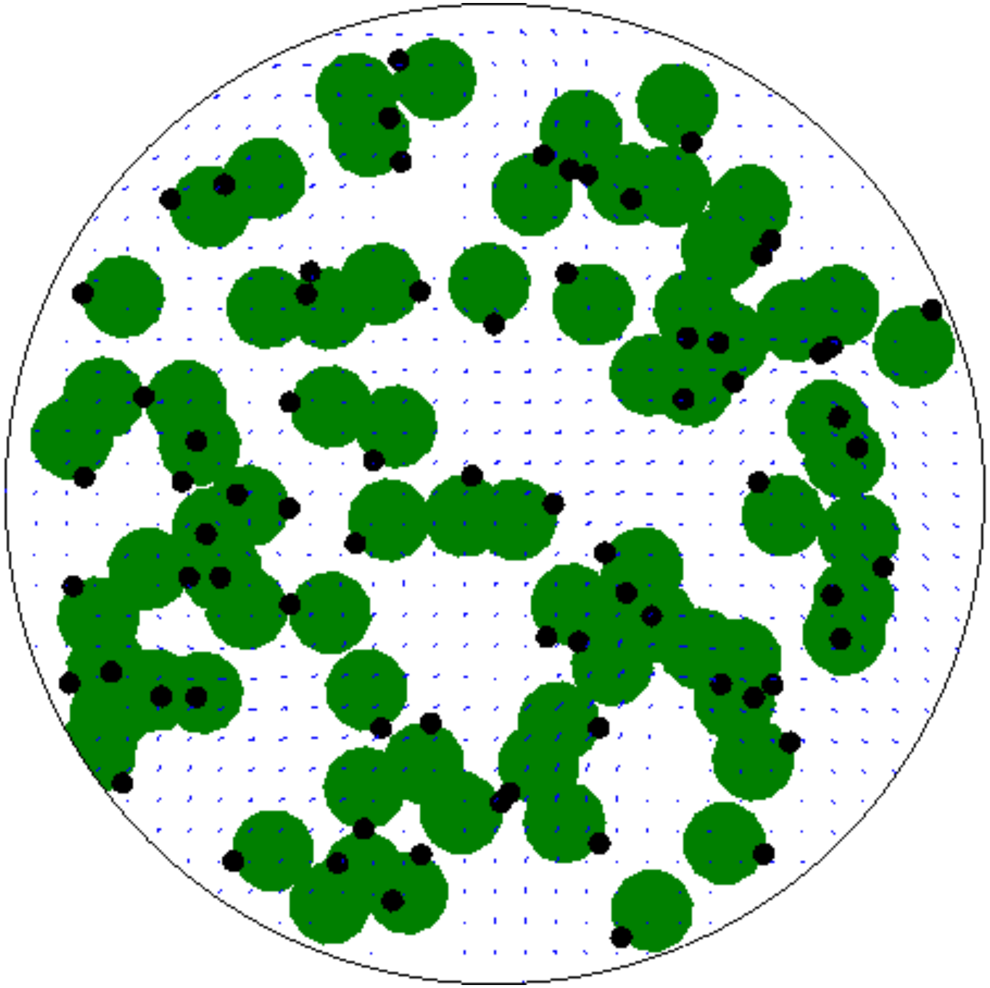
-> (spiral) organization
-> slow unidirectional circulation.



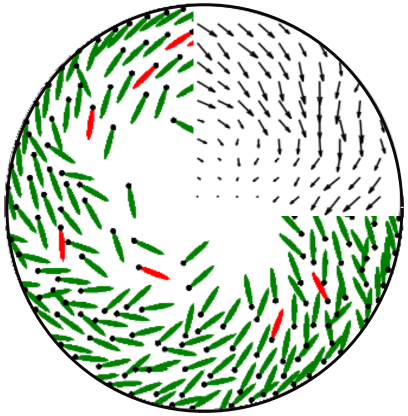
- self-propulsion
- disks
- with hydro

-> layers form
-> no organization
-> unstable circulation spurts

Investigate the causes

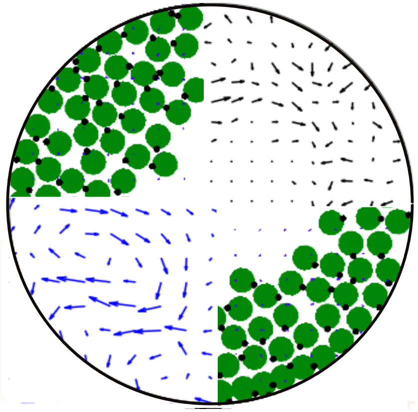


Investigate the causes



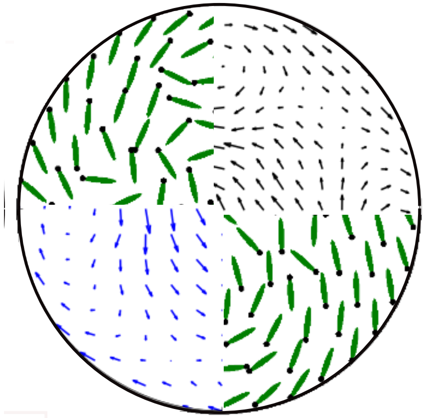
- self-propulsion
- elongated particles
- no hydro

-> (spiral) organization
-> slow unidirectional
circulation.



- self-propulsion
- disks
- with hydro

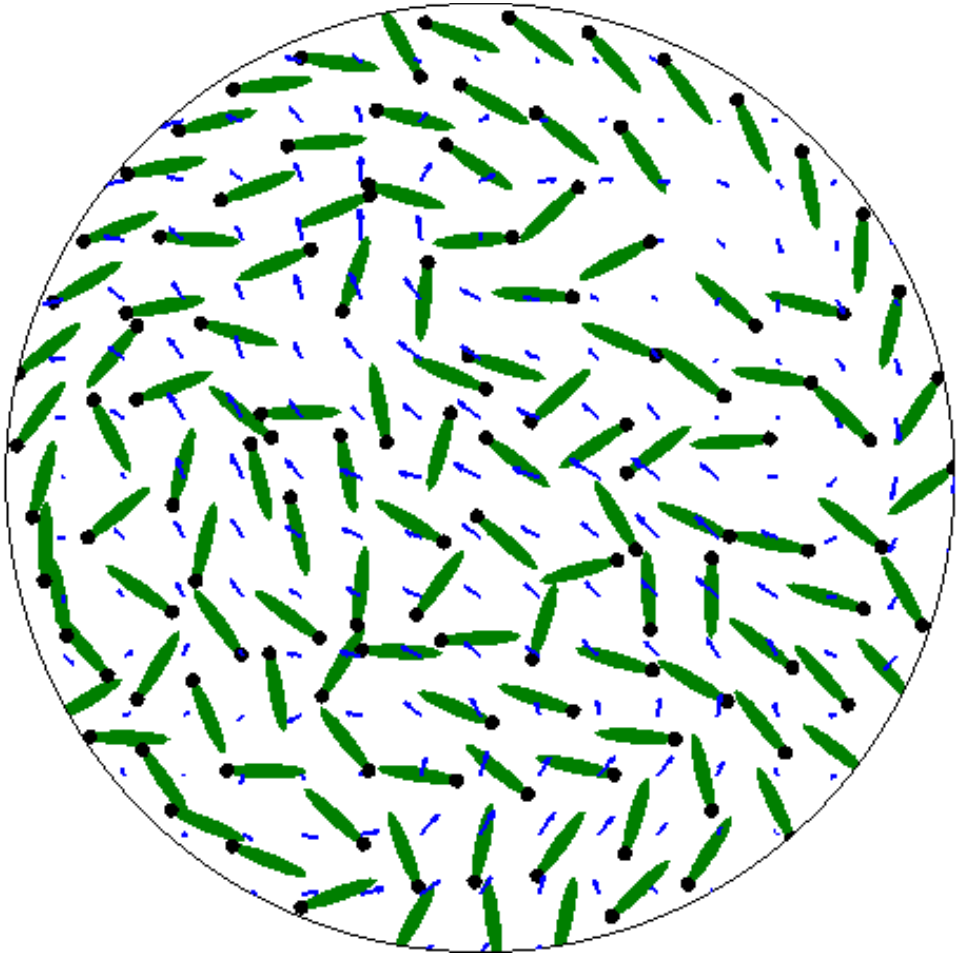
-> layers form
-> no organization
-> unstable
circulation spurts



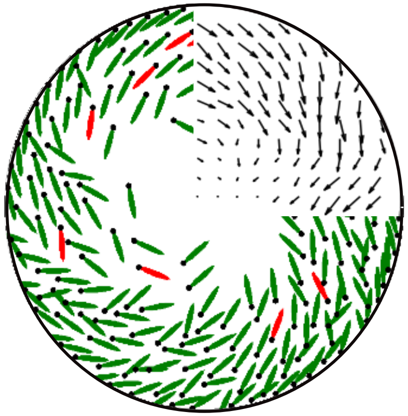
- self-propulsion
- elongated particles
- disk steric repulsions
- with hydro

-> layers form
-> spiral organization
-> double circulation
(so the ordering is due
to hydrodynamics!)

Investigate the causes

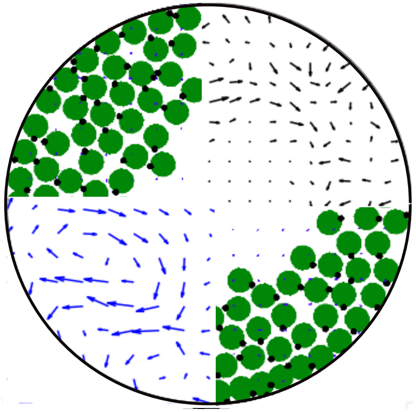


Investigate the causes



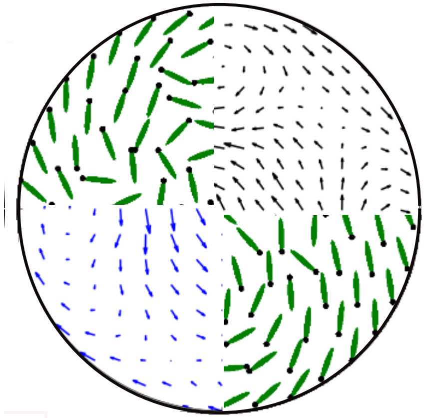
- self-propulsion
- elongated particles
- no hydro

-> (spiral) organization
-> slow unidirectional circulation.



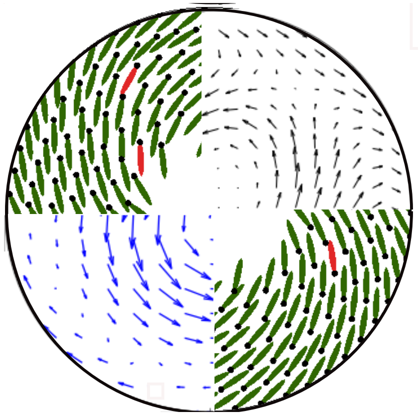
- self-propulsion
- disks
- with hydro

-> layers form
-> no organization
-> unstable circulation spurts



- self-propulsion
- elongated particles
- disk steric repulsions
- with hydro

-> layers form
-> spiral organization
-> double circulation
(so the ordering is due to hydrodynamics!)

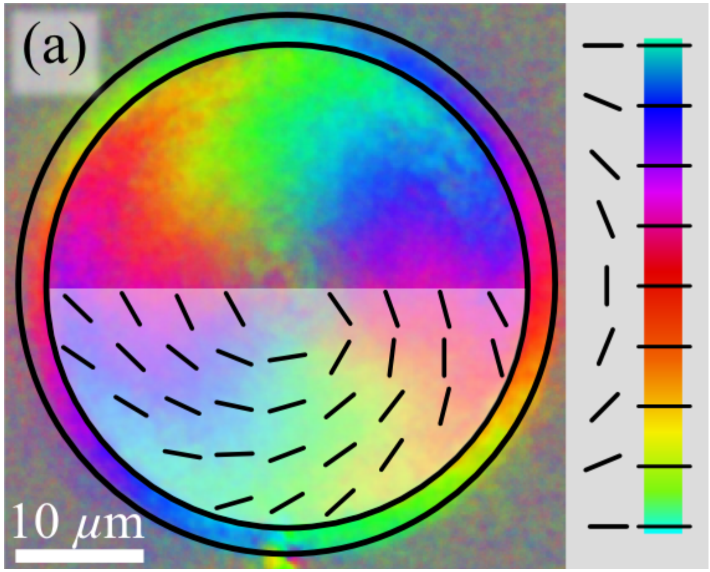


- self-propulsion
- elongated particles
- with hydro

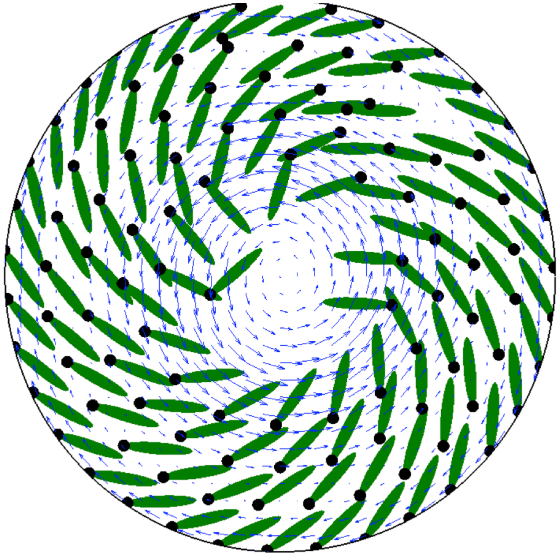
-> layers form
-> spiral organization
-> double circulation

Swimmer Orientation

Experiments: observe a spiral ordering

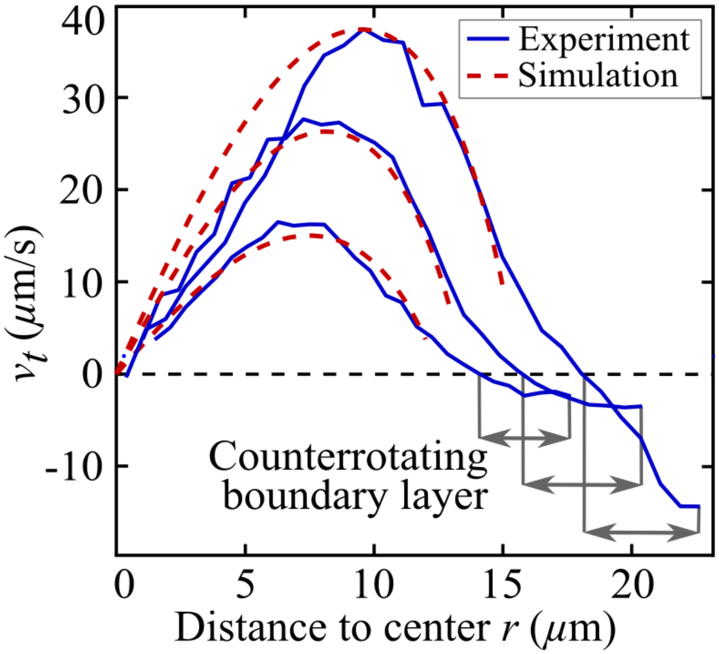


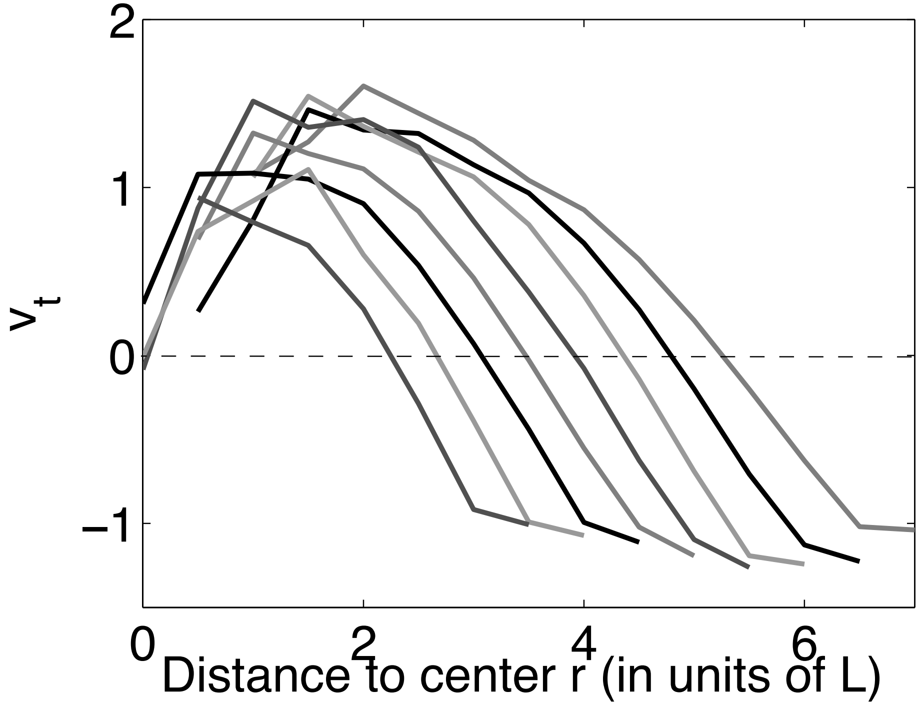
Direct simulations: spiral ordering there too.



Cells move at an angle to tangential

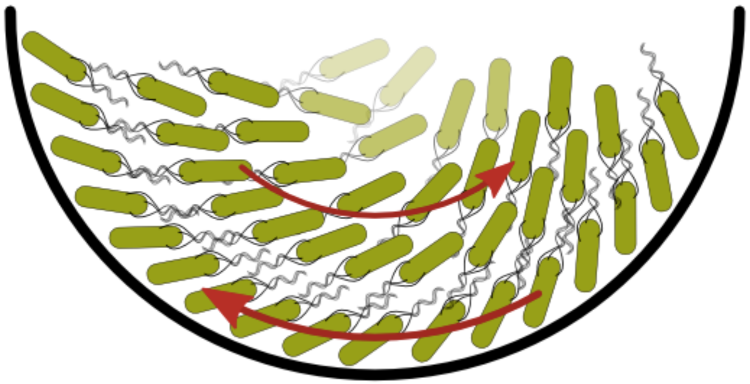
``Bacterial flow''


Experiments + continuum theory


Particle simulations

Counter-rotating boundary layer is about 1-2 swimmer lengths in both.
Counter-rotating bacterial flow magnitude about 0.5-1V (V is individual swimmer speed)
Max bulk bacterial flow magnitude about 1-2V.

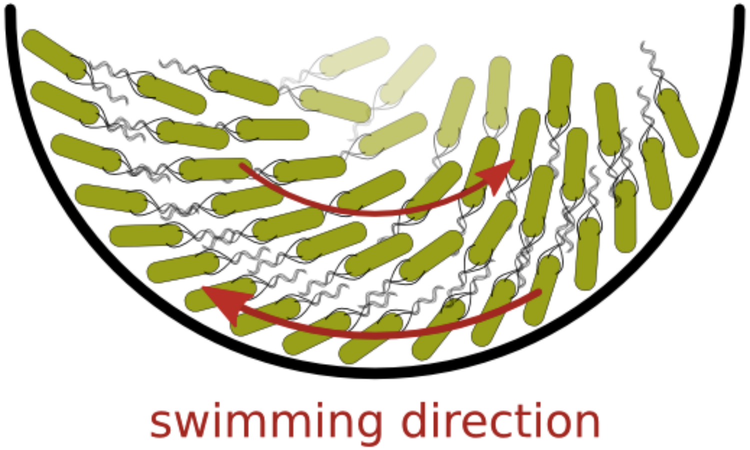
Swimming Orientation



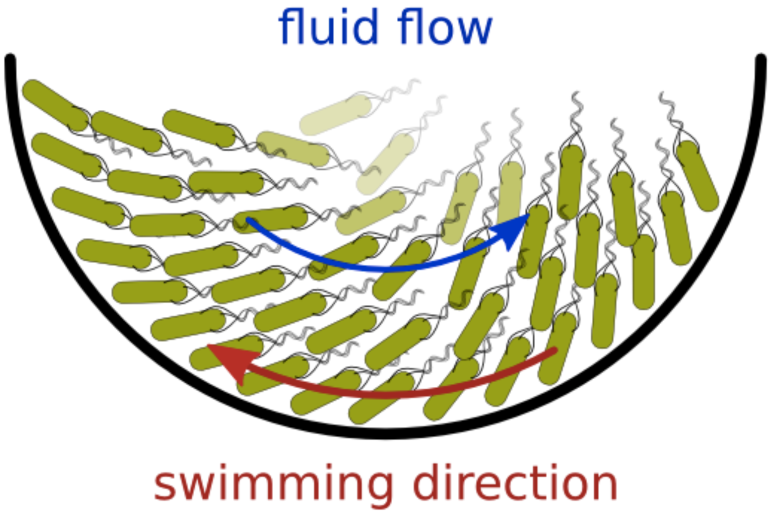
swimming direction

Initial interpretation of experiments (Wioland et al, PRL, 2013): cells in the bulk point inwards…

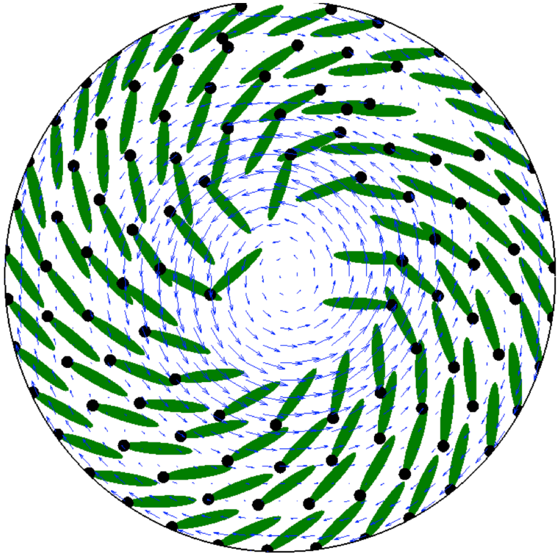
Swimming Orientation



Initial interpretation of experiments (Wioland et al, PRL, 2013): cells in the bulk point inwards…



Simulations however reveal that cells in the bulk point outwards…

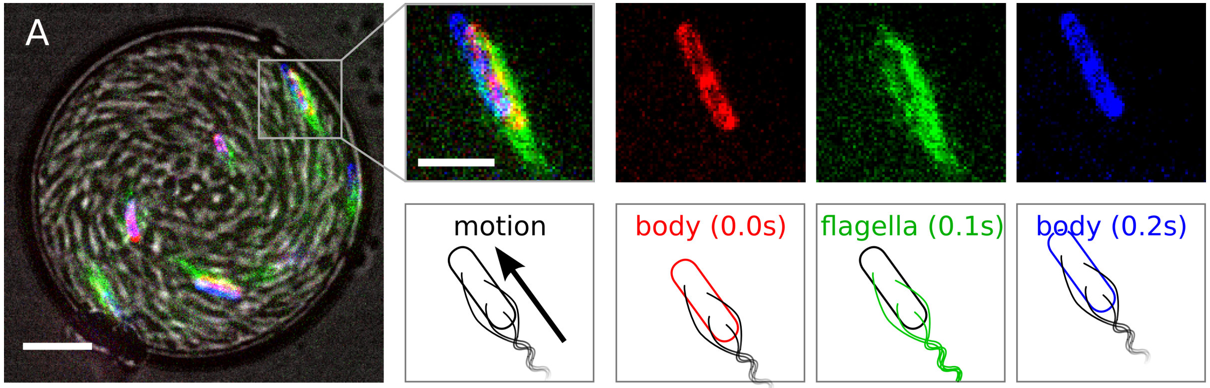


Motion of B. Subtilis at the Boundary and in the Bulk

New experiments to determine the configuration of the swimmers.

Mutant B. Subtilis (DS1919 3610) are labeled with Alexa Fluor 488 C5 maleimide on the flagella and FM4-64 on the cell membrane. These two-colored bacteria are mixed with a large amount of wild-type cells (strain 168) to form drops of dense suspensions.

Cell at boundary



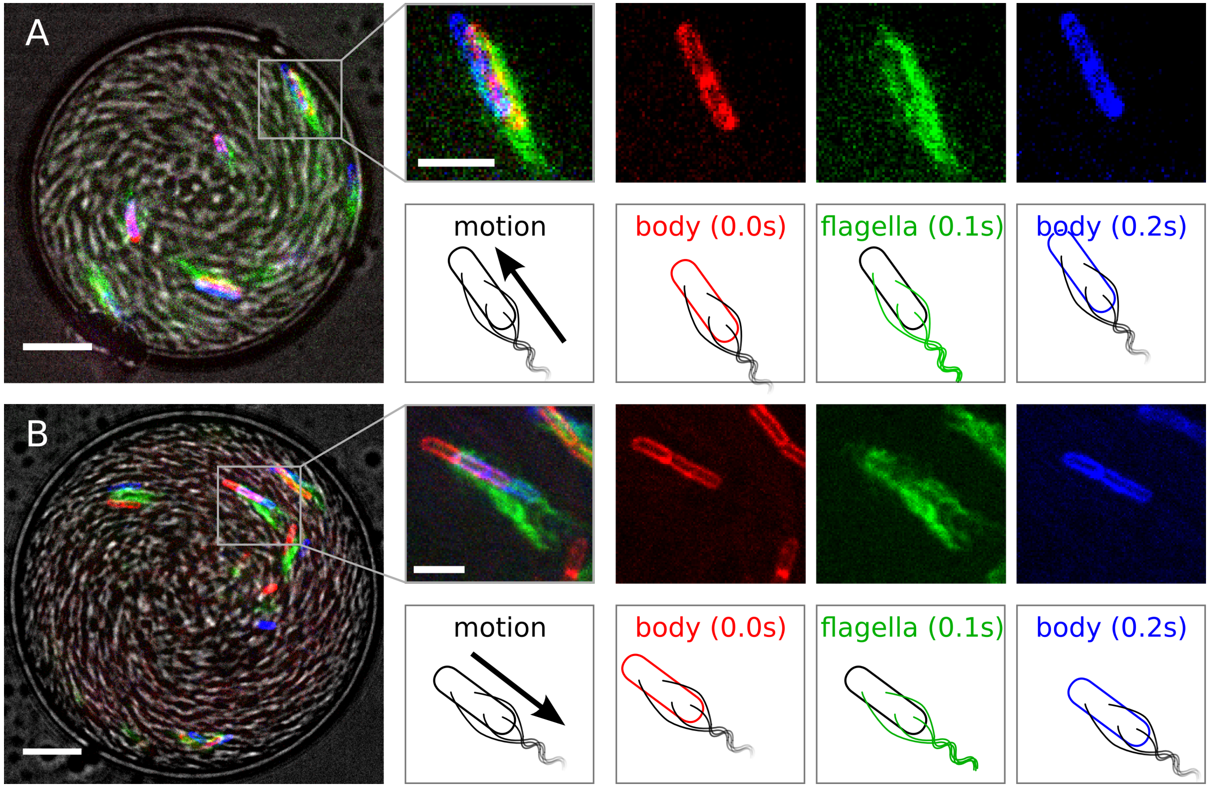
Motion of B. Subtilis at the Boundary and in the Bulk

New experiments to determine the configuration of the swimmers.

Mutant B. Subtilis (DS1919 3610) are labeled with Alexa Fluor 488 C5 maleimide on the flagella and FM4-64 on the cell membrane. These two-colored bacteria are mixed with a large amount of wild-type cells (strain 168) to form drops of dense suspensions.

Cell at boundary

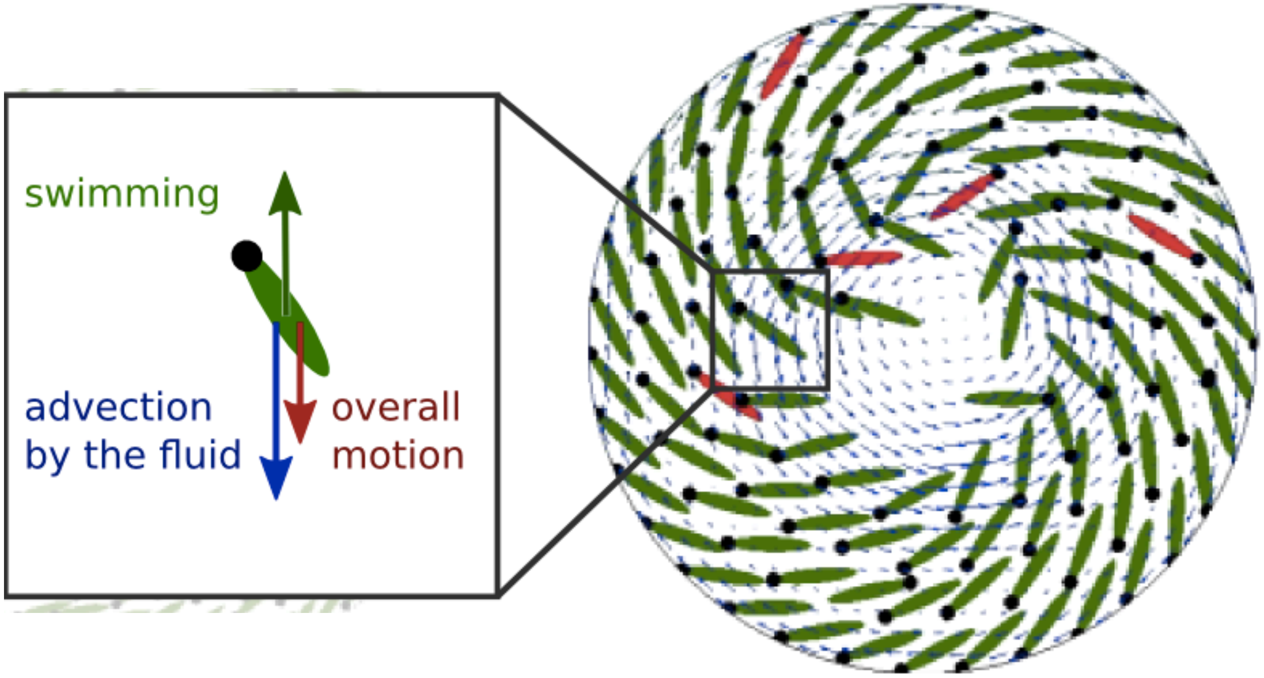
Cell in bulk



E. Lushi, H. Wioland, R.E. Goldstein, Proc. Nat'l Acad Sci. 111(27) 9733-9738 (2014)

Motion of B. Subtilis at the Boundary and in the Bulk

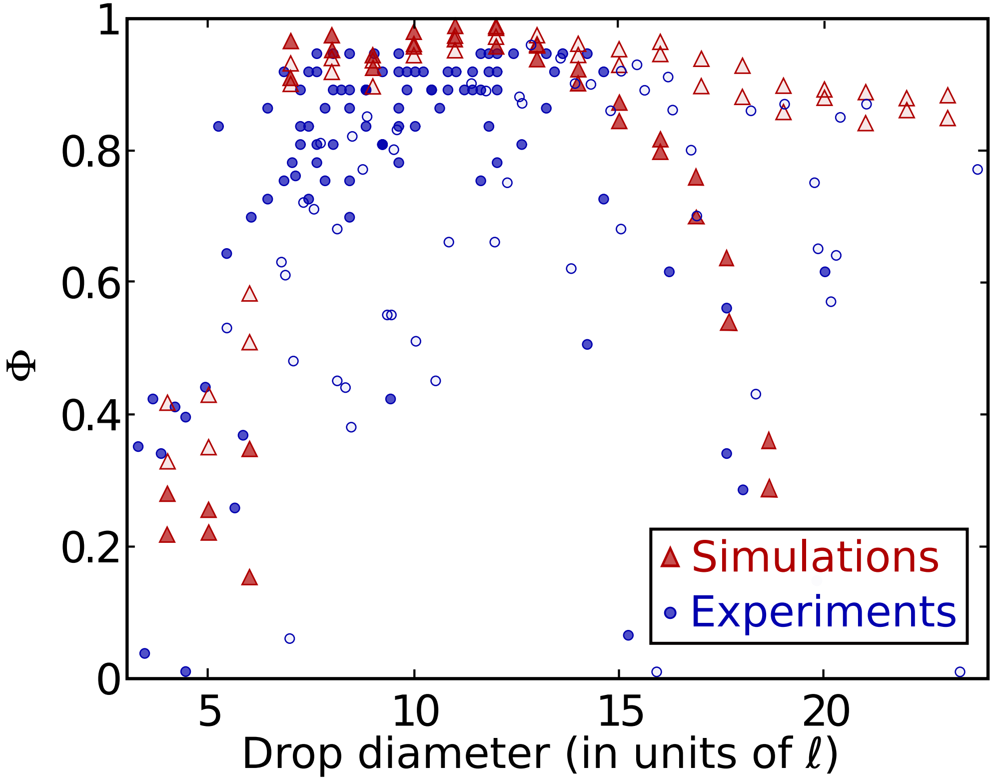
Cell-fluid interactions are necessary and sufficient to reproduce the organization and dynamic of the drop. Cells in the center move backward as the fluid flow is stronger than their swimming speed.



E. Lushi, H. Wioland, R.E. Goldstein, Proc. Nat'l Acad Sci. 111(27) 9733-9738 (2014)

Drop size range for self-organization

In experiments with drops 15 micron high the vortex emerges for drops with diameters ~30-70micron

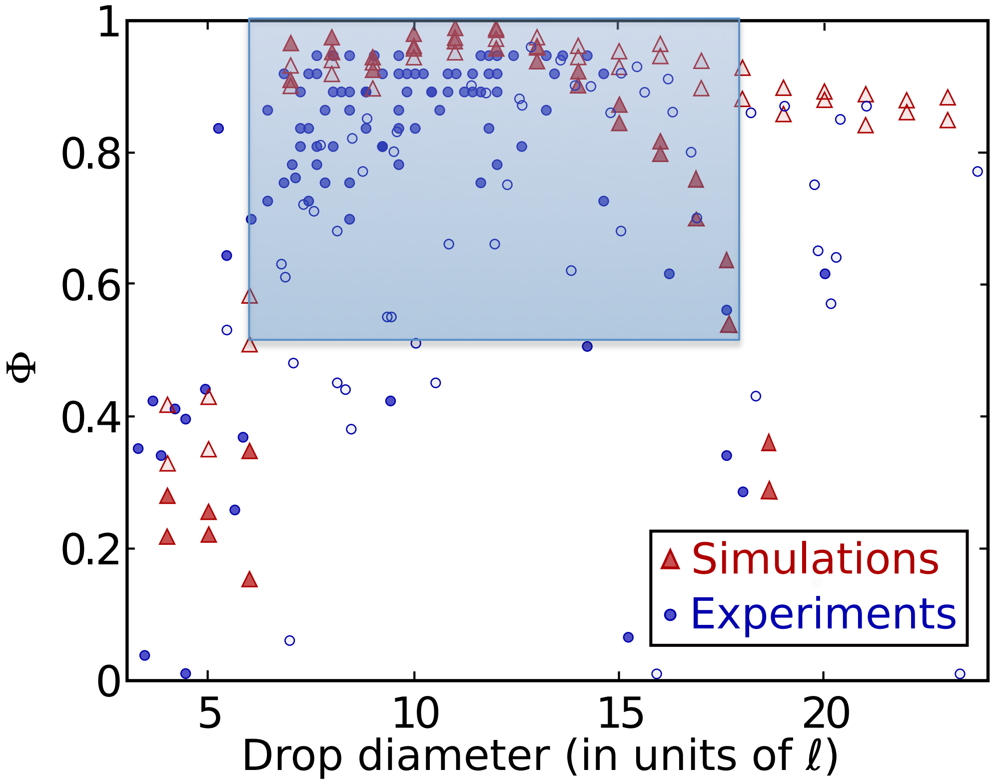


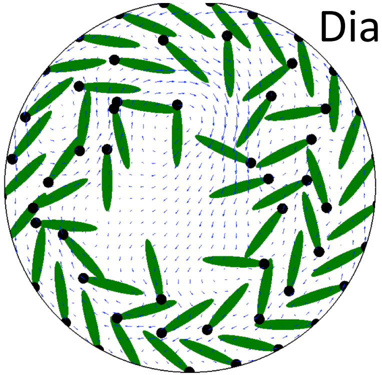
Vortex order parameter $\Phi = \dfrac{\sum_i |\mathbf{v}_i \cdot \mathbf{t}_i| / \sum_j ||\mathbf{v}_j|| - 2/\pi}{1 - 2/\pi}$ ~1 for a vortically-ordered suspension

Drop size range for self-organization

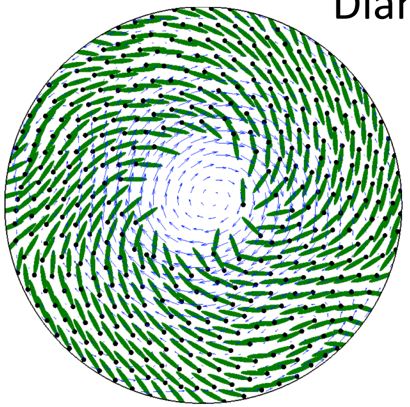
In experiments with drops 15 micron high the vortex emerges for drops with diameters ~30-70micron

In particle simulations the spiral vortex spontaneously emerges for circle diameters 7-16L





Diam=6L

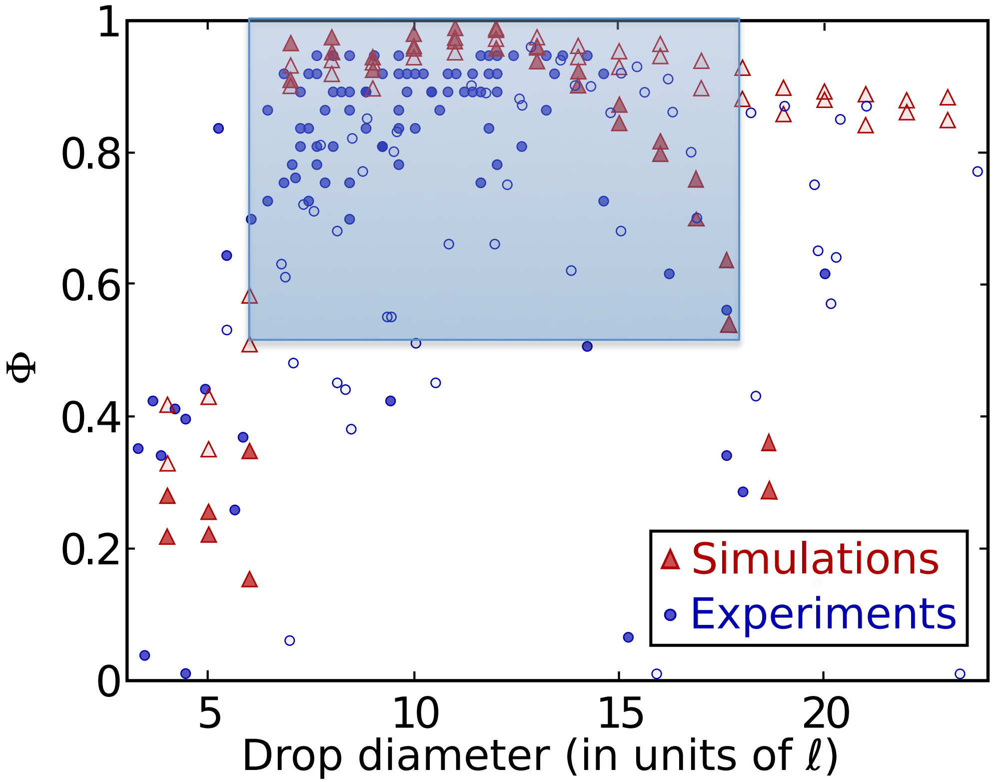


Diam=17L

Vortex order parameter $\Phi = \dfrac{\sum_i |\mathbf{v}_i \cdot \mathbf{t}_i| / \sum_j ||\mathbf{v}_j|| - 2/\pi}{1 - 2/\pi}$ ~1 for a vortically-ordered suspension

Drop size range for self-organization

In experiments with drops 15 micron high the vortex emerges for drops with diameters ~30-70micron



This suggests this length-scale range for confinement is important.

Indeed, it plays an important role in suspension self-organization <u>in other domain geometries</u> (current work with H. Wioland and R.E. Goldstein).

E. Lushi, H. Wioland, R.E. Goldstein, Proc. Nat'l Acad Sci. 111(27) 9733-9738 (2014)

Vortex order parameter $\Phi = \frac{\sum_i |\mathbf{v}_i \cdot \mathbf{t}_i| / \sum_j ||\mathbf{v}_j|| - 2/\pi}{1 - 2/\pi}$ ~1 for a vortically-ordered suspension

Summary and Discussion

- Minimalistic model that captures the physics of swimming and interactions. Fast numerical simulation allows us to trace a very large number of swimmers. Method is amendable for domains with static (or moving) boundaries, particles need not be uniform in shape, speed, etc.

- Method captures well the dynamics as observed in experiments.

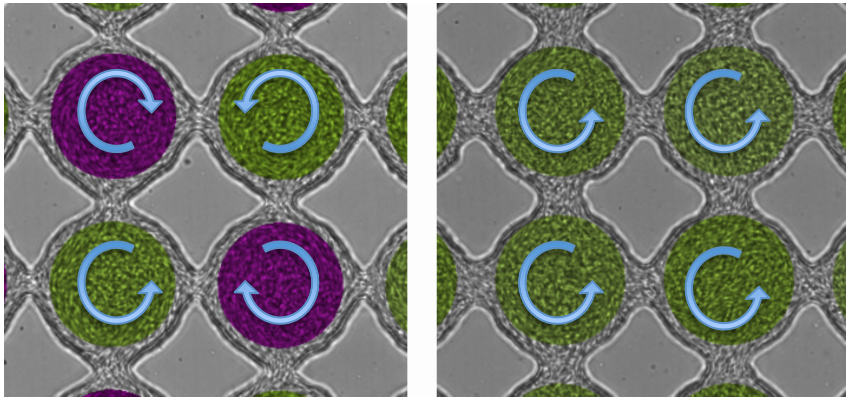
- In the bacterial drop case, the simulations correctly predicted what drives the dynamics and give new insights into the microscopic arrangement of the bacteria.

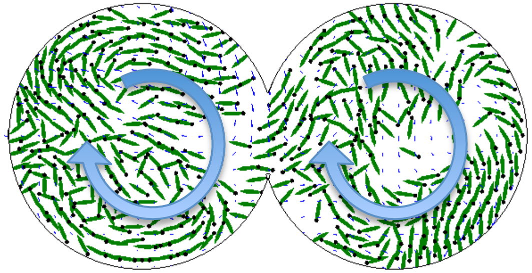
- Most importantly, that study clearly shows that hydrodynamics is crucial in obtaining and reproducing the bacterial organization observed in the experiments.

E. Lushi, H. Wioland, R.E. Goldstein, Proc. Nat'l Acad Sci. 111(27) 9733-9738 (2014)

Some other adaptations & current directions

- Interactions of many bacterial vortices, ferromagnetic & antiferromagnetic order in a vortex lattice. With H. Wioland, F. Woodhouse, J. Dunkel, R. Goldstein.

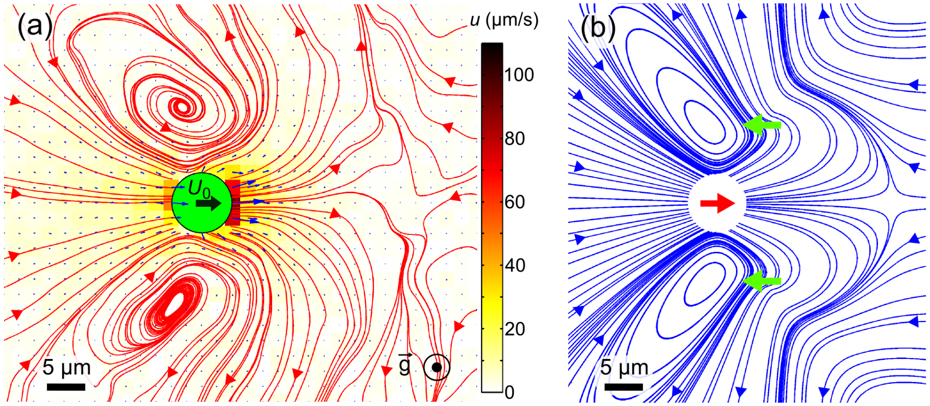




- Other geometries; directing collective motion. With H. Wioland, R. Goldstein.

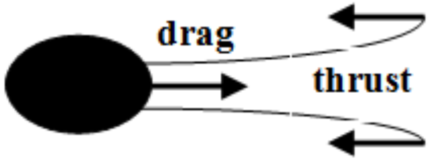
More ``realistic'' models for micro-swimmers

Inspired by the experimental observations of Drescher at al, PRL 2010

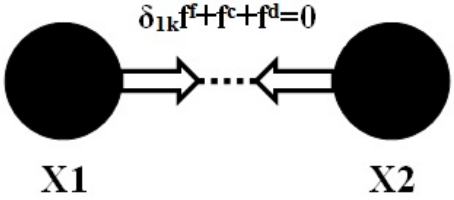


Develop <u>minimalistic mathemathical models</u> that correctly capture the essential dynamics of a microswimmer, in bulk or near boundaries.

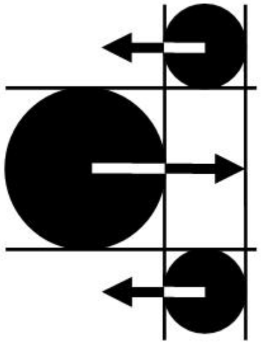
a) C. Rheinhardii



b) Forces on fluid



c) 2 beads model



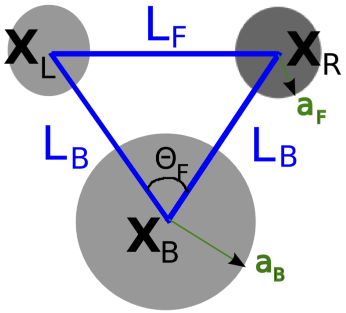
d) 3 beads model

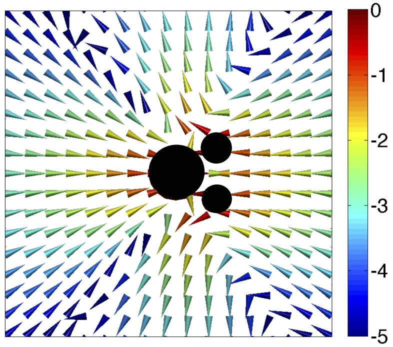
Behavior of a biflagellate near walls

Most minimal models of C. Rheinhardii neglect the fore-aft asymmetry of the swimmer and particulars of the geometry. But that can quite affect the near-wall dynamics.

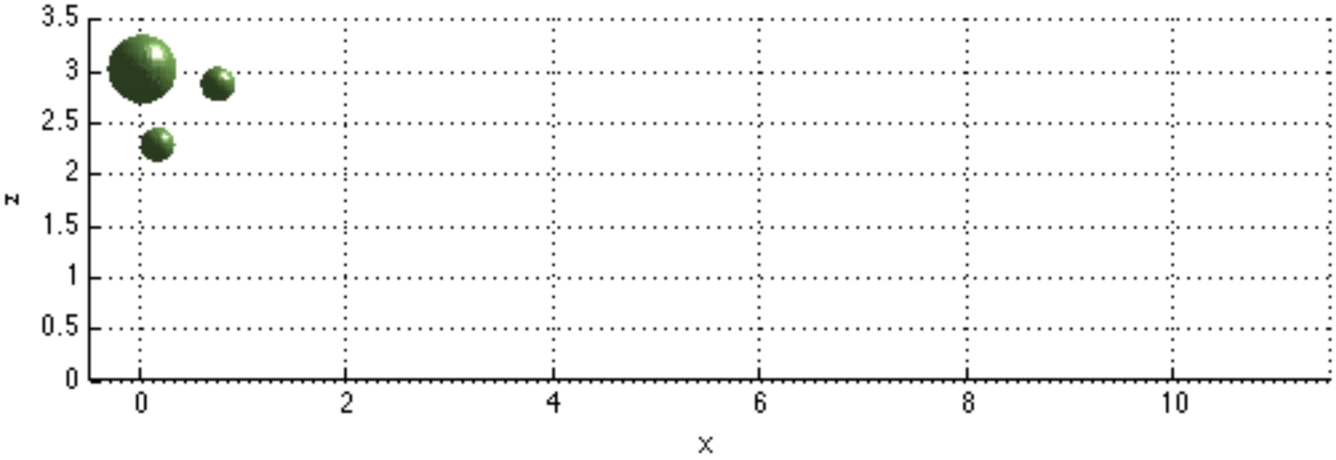
So we build a model that consists of **3** spherical beads connected by FENE springs

$$
\begin{aligned}
\frac{d\mathbf{x}_k}{dt} &= \frac{1}{\xi_k}\left[\delta_{k,(L,R)}\mathbf{f}_k^f + \mathbf{f}_k^c + \mathbf{f}_k^x\right] \\
&+ \sum_{j=(B,L,R)} G_{a_j}(\mathbf{x}_k,\mathbf{x}_j)\left[(1-\delta_{k,j})\mathbf{f}_j^c + \mathbf{f}_j^x\right] \\
&+ \sum_{j=(B,L,R)} \tilde{G}_{a_j}(\mathbf{x}_k,\mathbf{x}_j)\left(\mathbf{f}_j^c + \mathbf{f}_j^x\right)
\end{aligned}
$$



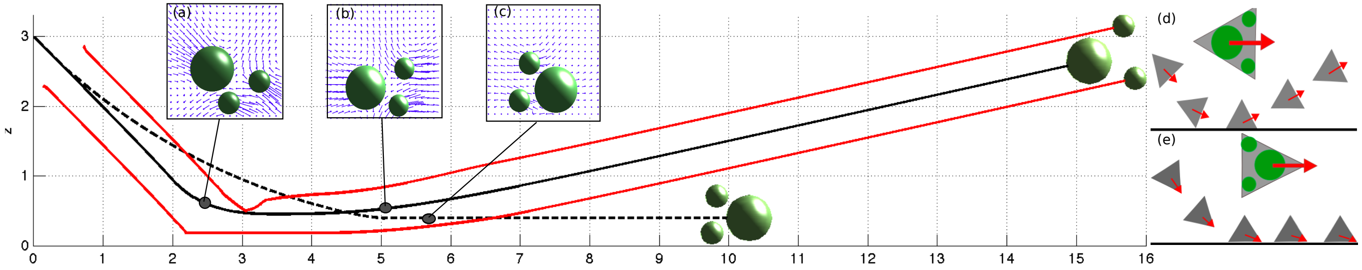


Direct interactions with walls done via the repulsive part of the LJ potential for spheres. Model captures what is seen in experiments of Kantsler et al, 110(4) 1187-1192 PNAS 2013.



Scattering from a wall

Turning chlamydomonas at a wall → ciliary contact with walls is important.

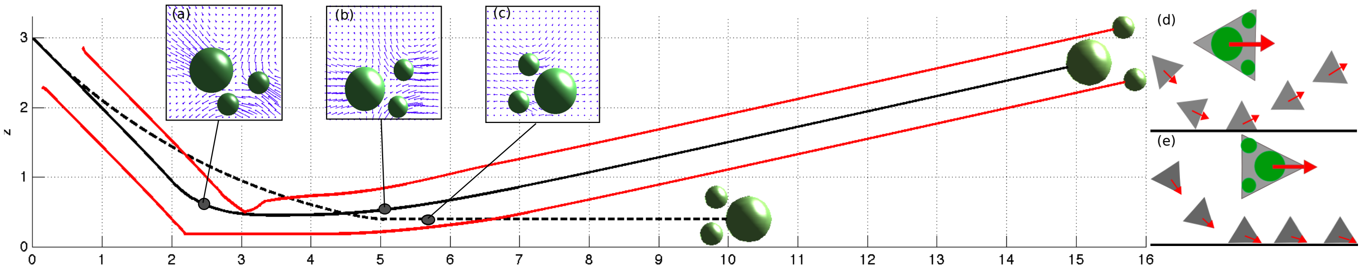


``Puller'' chlamy scatters off but at angle different from incident angle

``Pusher'' chlamy swims near wall

Scattering from a wall

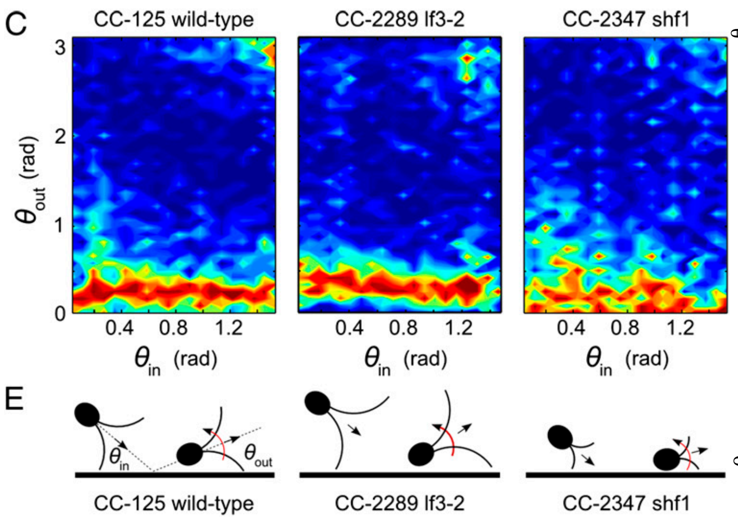
Turning chlamydomonas at a wall → ciliary contact with walls is important.

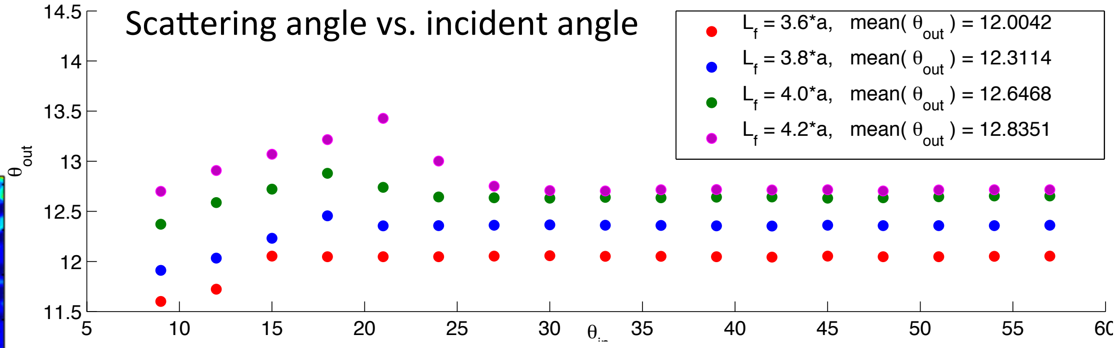


``Puller'' chlamy scatters off but at angle different from incident angle

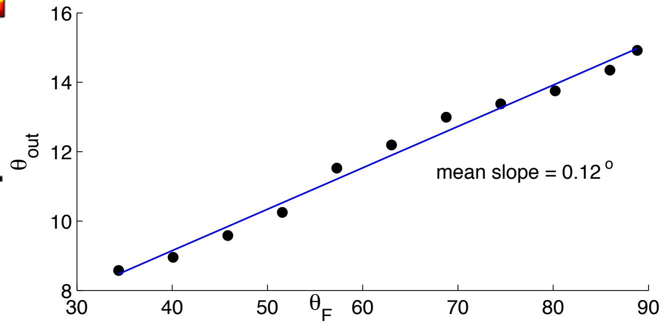
``Pusher'' chlamy swims near wall

Experiments of V. Kantsler et al, PNAS 2013




Scattering angle vs. incident angle

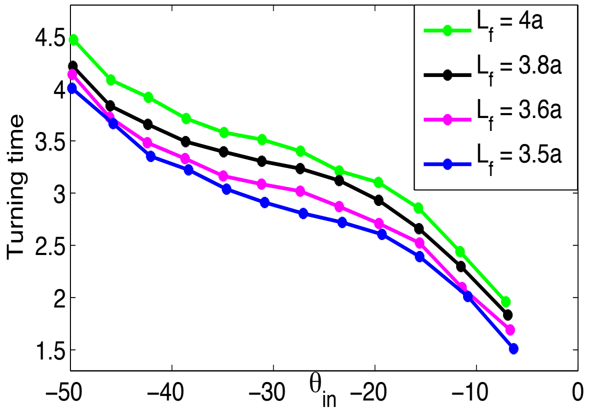
Scattering angle vs. inter-flagella angle



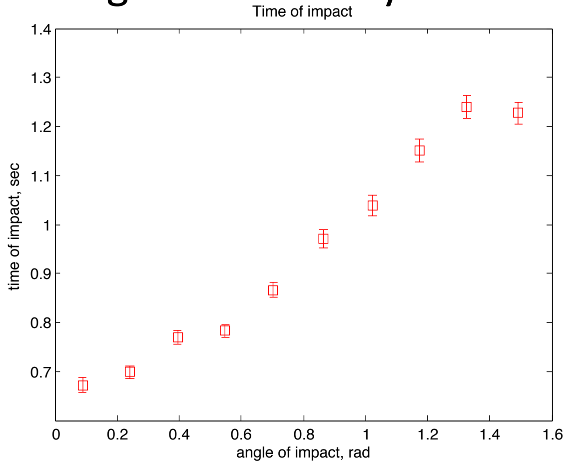
Scattering angle depends on length of flagella and the angle in-between them, but almost not at all on incident angle.

Turning Time & Trapping

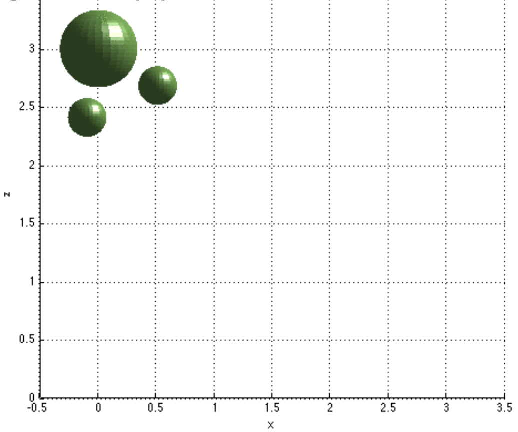
The time it takes a ``puller'' chlamy to turn at the wall vs. incident angle.



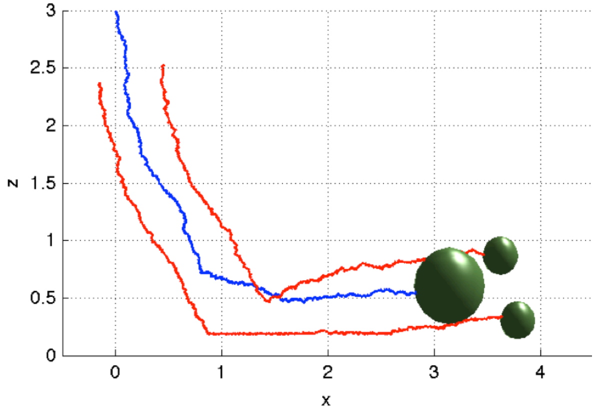
Depends on incident angle, approx. linearly. Flagella length makes very little difference.



If incident angle is too steep, the chlamy may get trapped at the wall.



Adding noise can help it escape (depending on noise strength).



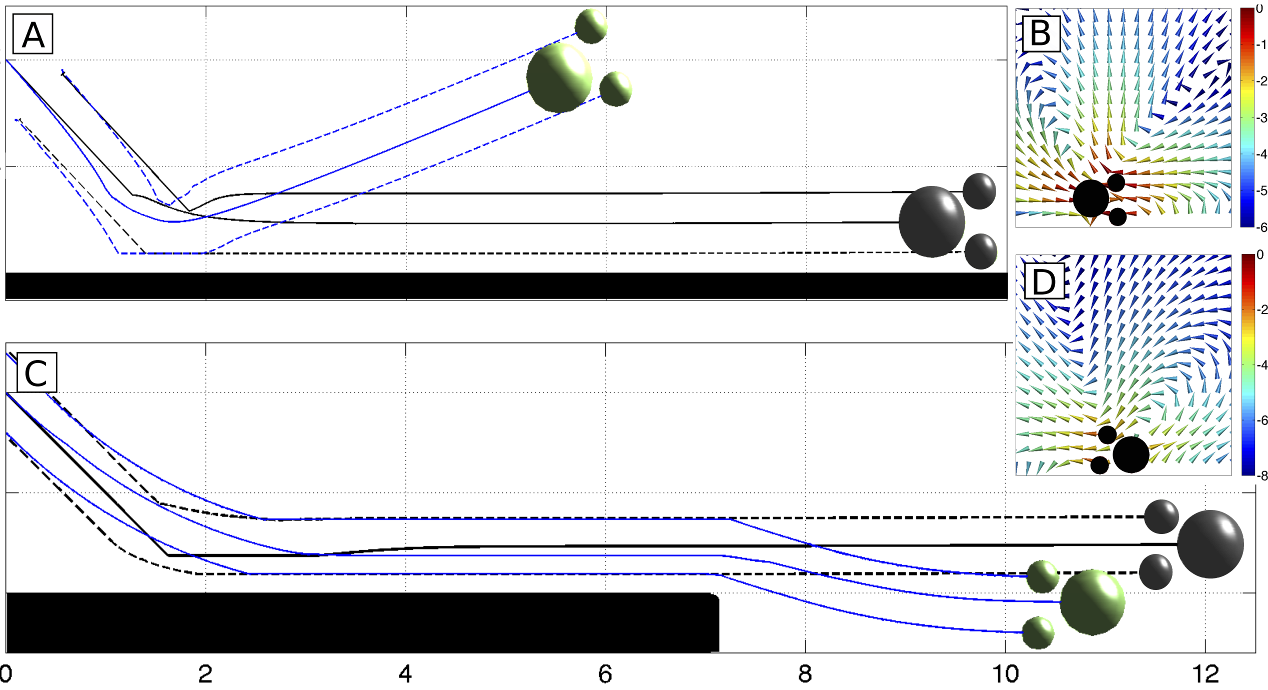
So does hydrodynamics matter?

``Puller'' chlamy, with and without hydrodynamics
(blue and black lines respectively

-- orientation gets affected
-- but so does the scattering!

``Pusher'' chlamy, with and without hydrodynamics
(blue and black lines respectively

-- orientation gets affected
-- but so does going off an edge!



Lushi, Kantsler, Goldstein, in preparation (2014).