Collective Motion in Active Systems

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Argonne NATIONAL LABORATORY

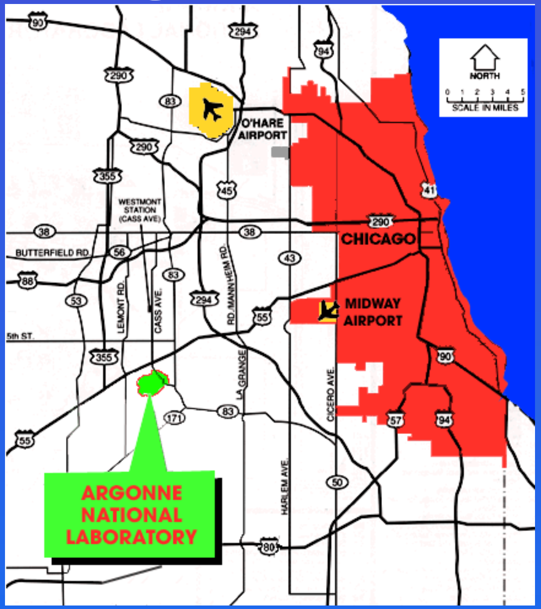
Outline of the course

- Overview of experiments
- Self-organization of active polar rods: application *in vitro* cytoskeletal networks
- Collective motion of interacting self-propelled particles

- Purpose: to teach a variety of research tools at the interface of mathematics, physics and biology

- **Introduction**
- **patterns in granular systems**
- ***in vitro* cytoskeletal networks**
- **suspensions of swimmers**

Where in the World is Argonne?



- World-Class Science
- Unique Scientific Facilities
- Free and Abundant Parking
- 25 min from Downtown Chicago
- White Deer (almost extinct)

Argonne National Laboratory

- Argonne is a multidisciplinary science and engineering research center
- Mission: address vital national challenges in clean energy, environment, technology and national security.
- Total 3,350 employees, 1250 scientists
- Budget: $800 million
- 15 research division, 6 national user facilities

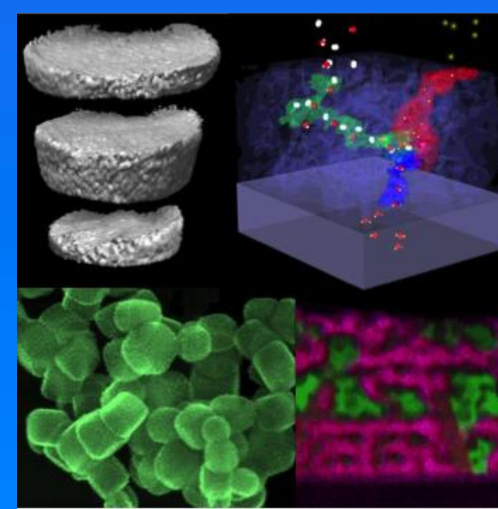
World-Class User Facilities

advanced photon source

center for nanoscale materials

leadership computing facility

electron microscopy center



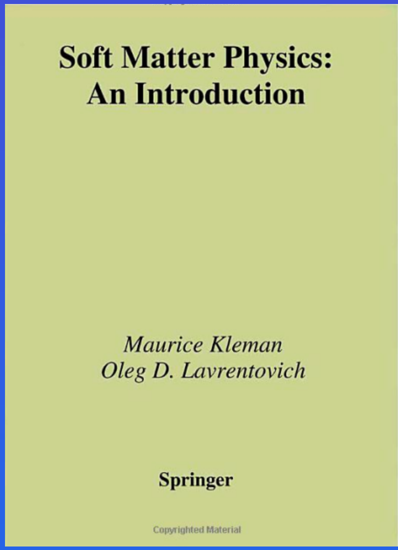
Definition of Soft Matter

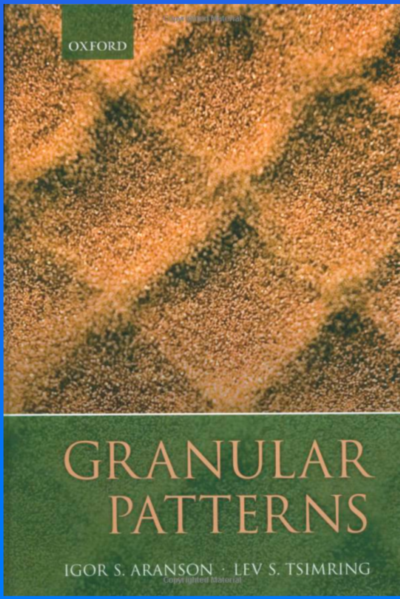
- Soft Matter - a subfield of condensed matter dealing with physical states that are easily deformable by thermal fluctuations and external stresses.

- Examples: complex liquids, colloids, gels, polymers, biological materials

- Simple introduction:

I Aranson, Collective Behavior in Out-of-Equilibrium Colloidal Suspensions, *Comptes Rendus Physique*, v14, 518 (2013)





Active Matter

- Active Matter - a new field of condensed matter physics focused on the physical and statistical properties of a wide class of systems actively consuming energy from environment, such as assemblages of active self-propelled particles. The particles have a propensity to convert energy stored in the medium to motion.
- Examples: suspensions of swimming bacteria and synthetic microswimmers, cytoskeletal networks, school of fish etc

- Simple introduction:

S. Ramaswamy, The mechanics and statistics of active matter. Ann Rev Condens Matter Phys **1**(1):323–345 (2010)

T. Vicsek, A Zafeiris, Collective Motion, Physics Reports, v517, 71, 2012

Dynamic Self-Assembly

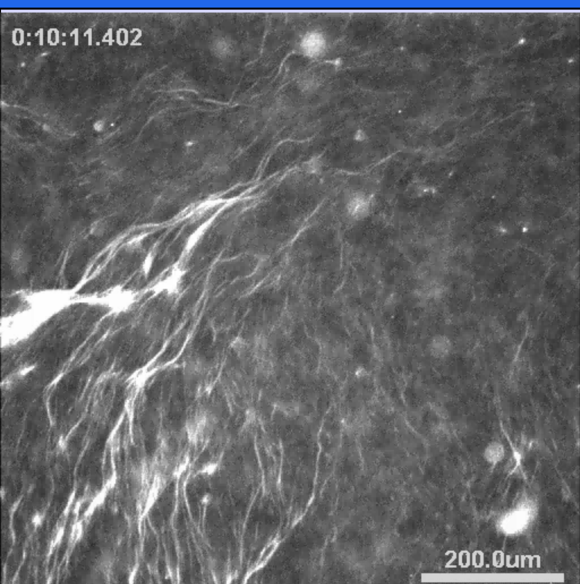
- **SA - natural tendency of simple building blocks to organize into complex functional architectures, from biomolecules to living cells**
- **unique opportunity for materials science – alternative to lithography**
- **self-assembled materials are intrinsically complex, with a hierarchical organization over nested length and time scales**
- **static (equilibrium) vs dynamic (active) self-assembly**
- **active (out of equilibrium) assembled emerging structures are not accessible under equilibrium conditions**

Introduction: G.M. Whitisides, B Grzybowski, Self-Assembly at all scales, *Science*, v295, 2418 (2002)

Collective Behavior in Living and Synthetic Matter

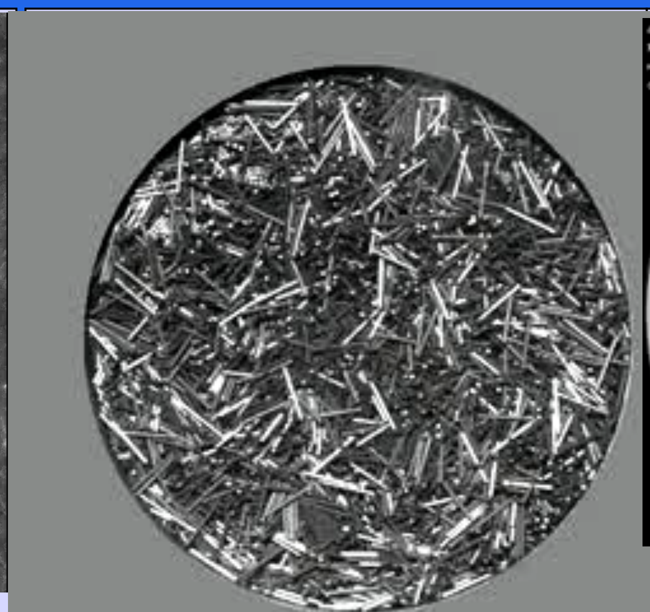
- **simple interactions – complex emergent behavior**
- **different mechanisms – similar patterns**
- **no obvious leader**

swirling ***microtubules***



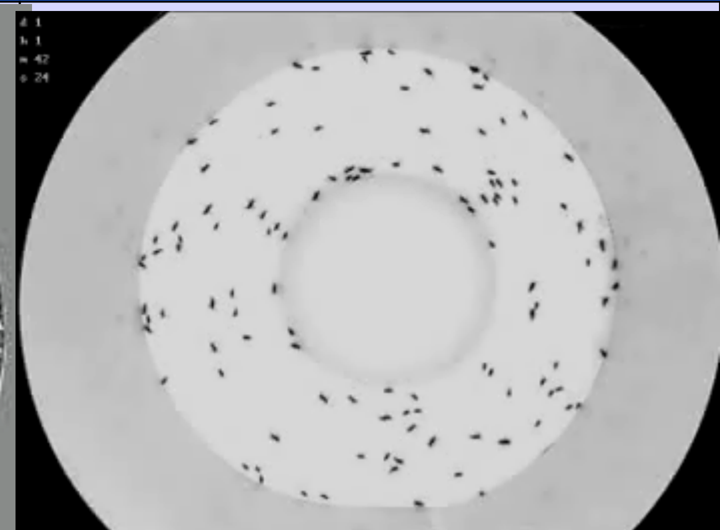
Sumino et al, Nature 2012

swirling granular rods



Blair, Kudrolli, 2003

swarming hungry locusts

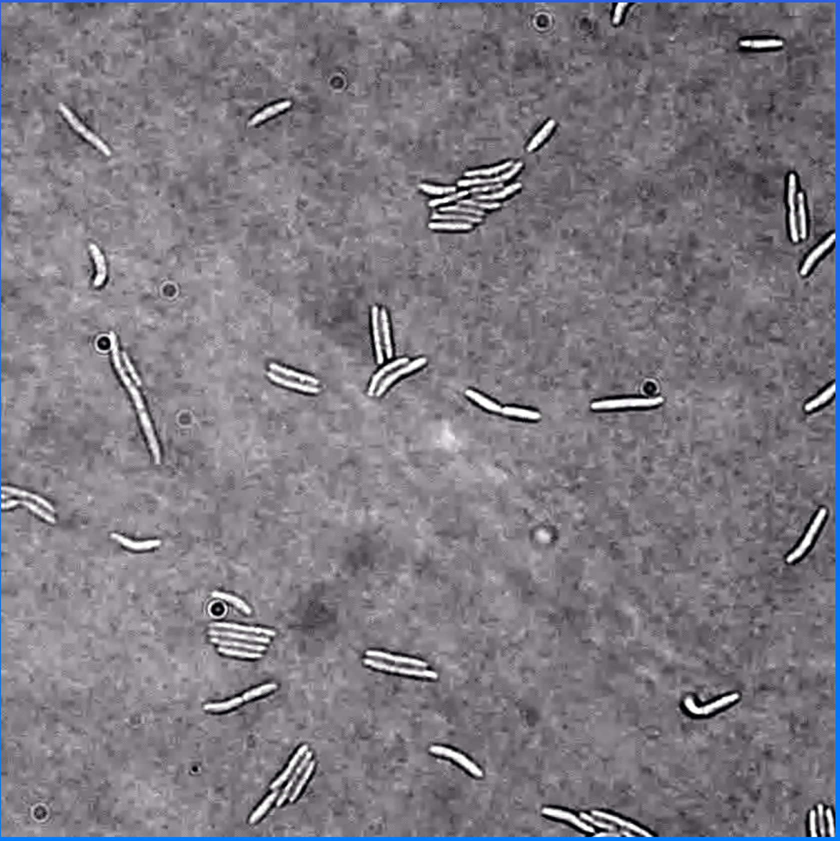


I. Cousin et al, Science, 2005

Seemingly Intelligent behavior

- **no obvious leader**
- **only local interactions between the individuals**

Myxobacteria

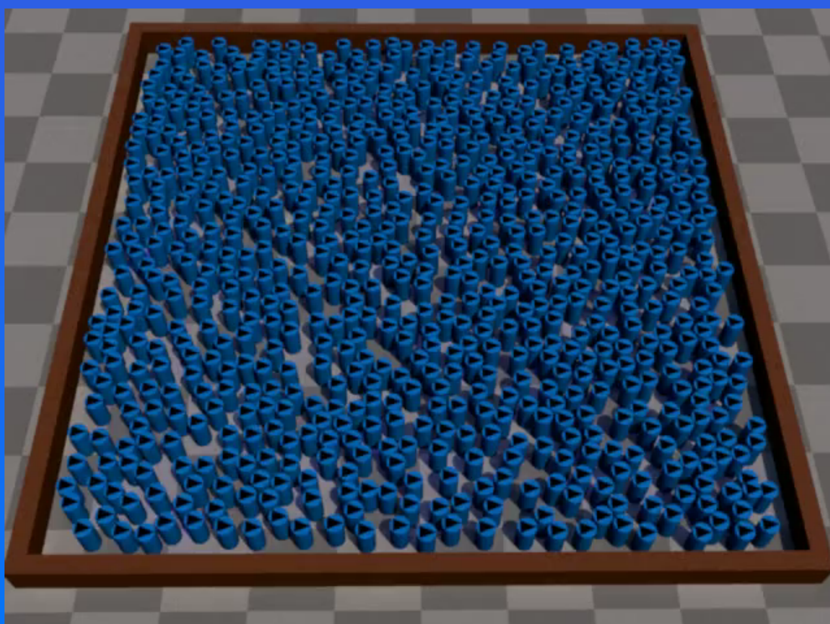


Starlings (birds)

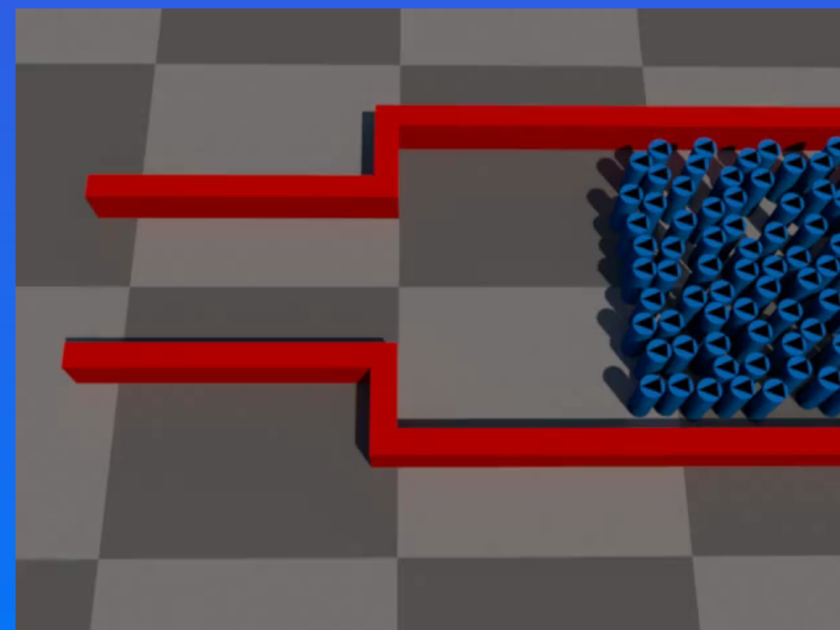
Opposite is also true!

- **Highly intelligent beings (humans) - simple behavior**

humans in a square room



bottleneck



Karamouzas, Skinner, Guy, Universal Law Governing Pedestrian Interactions, Phys Rev Lett, 2014

Vicsek Model: A Major Theoretical Milestone

•Point particles (*boids - birdoids*) move off-lattice

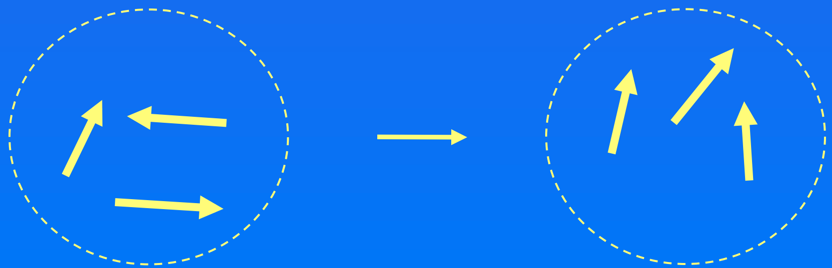
• Driven overdamped (no inertia effects) dynamics

•Strictly local interaction range

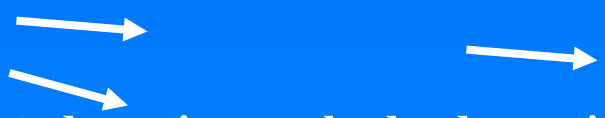
•Alignment according to average direction of the neighbors

•Simple update algorithm for the position/orientation of particles
•Not necessarily reproduce observed phenomenology
•Only two parameters – radius of interaction and noise magnitude

1. Polar orienting interaction in a noisy environment



2. Streaming: motion along the polar direction →



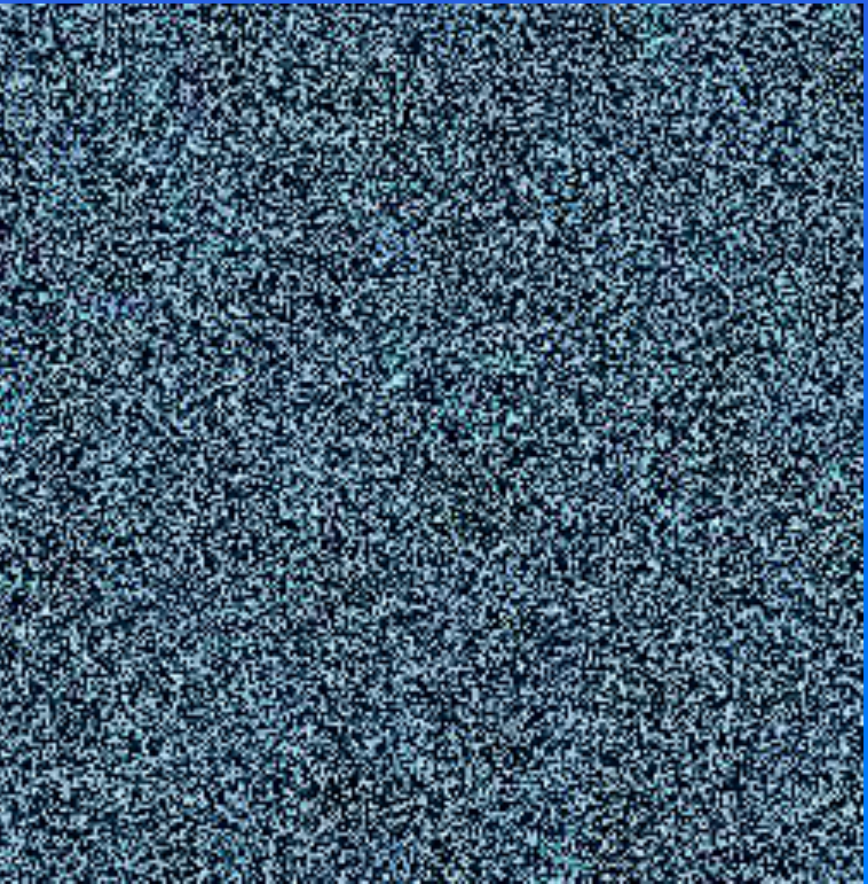
•More complicated continuum hydrodynamic models (Tu, Toner, Ramaswamy)

Simulations of Vicsek model

Chate and Gregoire,PRL 2004

1,000,000 boids

Fish school

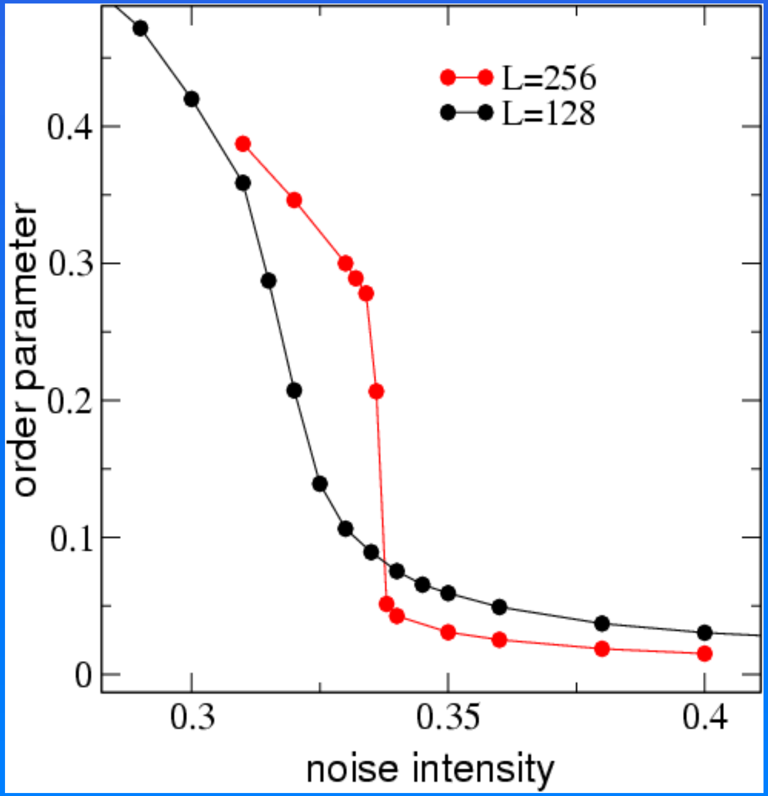


Simulations of Vicsek model: Phase transition

Order parameter:
Magnitude of average velocity
(similar to magnetization)

$$\varphi(t) = \frac{1}{N}\left|\sum_{i=1}^{N} v_i(t)\right|$$

at large size,
discontinuous transition



Fundamental issues we will investigate

- Similarity between collective behaviors in living and inanimate systems
- Role of long-range interactions vs short-range collisions
- Derivation of mathematical models from simple interaction rules

Active Systems are Complex

- **Focus on simple yet non-trivial systems such as *in vitro* cytoskeletal networks, bacterial suspensions, swimmers**
- **Fundamental interactions are simple and well-characterized**
- **Interactions are mostly of the "physical nature": inelastic collisions, self-propulsion, hydrodynamic entrainment, vs chemotaxis, visual signaling, intelligence, etc**
- **Derive continuum description from elementary interaction roles and connect observed patterns with experiment**

Multi-Scale Approach

- **Microscopic discrete models (self-propelled particles – Vicsek model)**

- **Mesoscale probabilistic Boltzmann/Fokker-Plank equations**

- **Continuum microscopic models (phenomenological theory by Toner and Tu, Ramaswamy) or derived from the Boltzmann equation (Boltzmann-Ginzburg-Landau Approach)**

- **Purpose: bridge 3 levels of description**

Active Matter and grand challenges in materials science

Understanding, controlling, and building complex hierarchical structures by

- ***mimicking nature's self- and directed-assembly approaches***

- ***design and synthesis of environmentally adaptive, self-healing materials and systems***

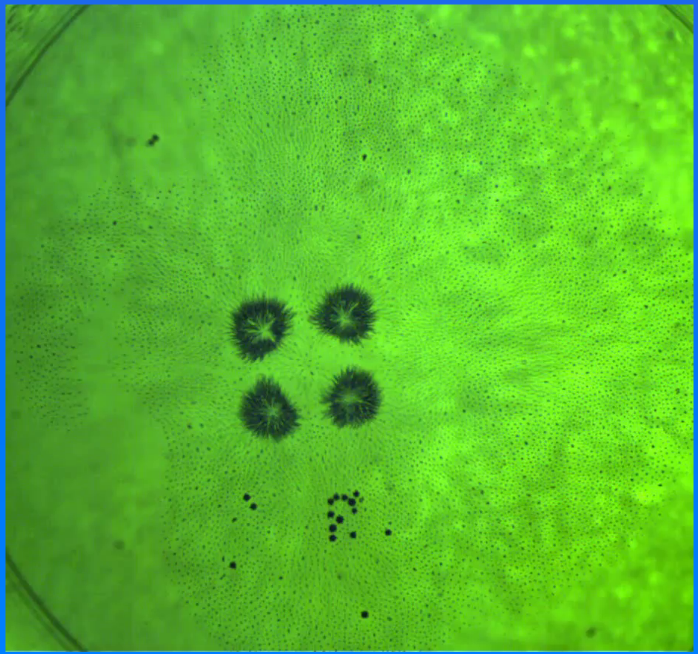
http://science.energy.gov/bes/mse/research-areas/biomolecular-materials/

Active Self-Assembled Systems – A Unique Opportunity for Materials Science

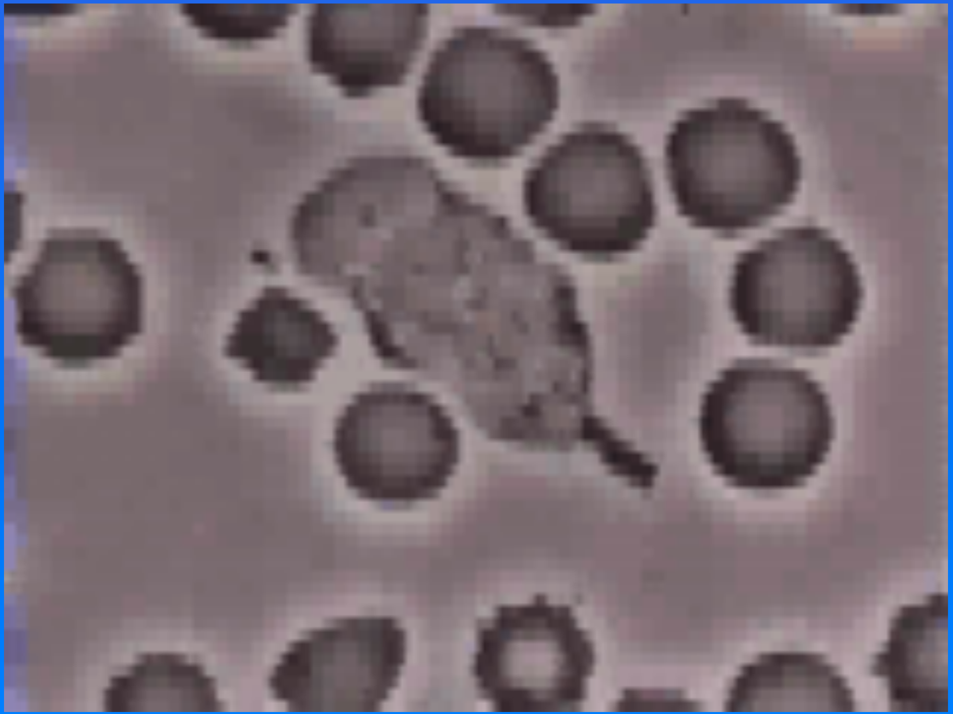
- ***<u>Design of active self-assembled structures with functionality not available under equilibrium conditions</u>***

self-assembled colloidal robot

Snezhko & I Aranson, Nature Materials, 2011



neutrophil chasing a bacterium

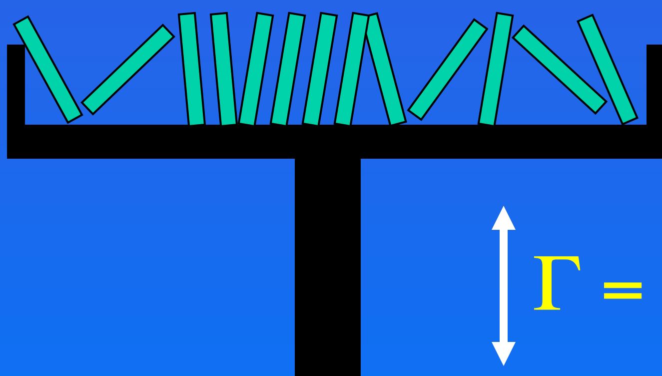


Survey of experimental systems

- Granular materials: vibration, friction, collisions
- Cytoskeletal networks: molecular motors, collisions, chemical interactions
- Suspensions of swimmers such as bacteria: rotation of flagella, hydrodynamic interactions, collisions

Blair-Neicu-Kudrolli experiment

vibration of long rods

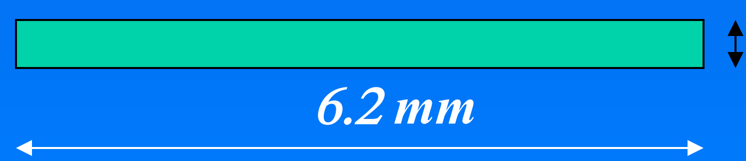


$$\Gamma = \Gamma_0 \sin(\omega t)$$

top view

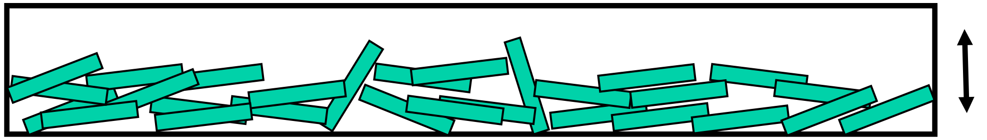
long Cu cylinders

# of particles 10^4

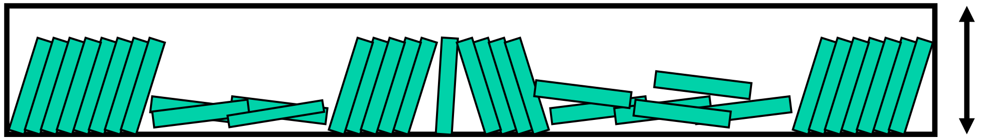


Phase transitions and vortices

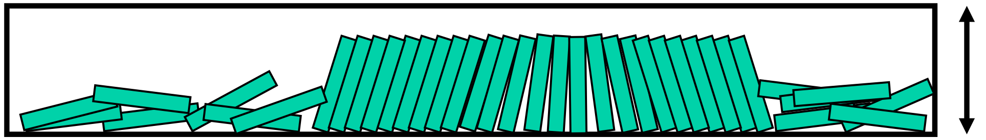
- *Weakly vibrated layer of rods*



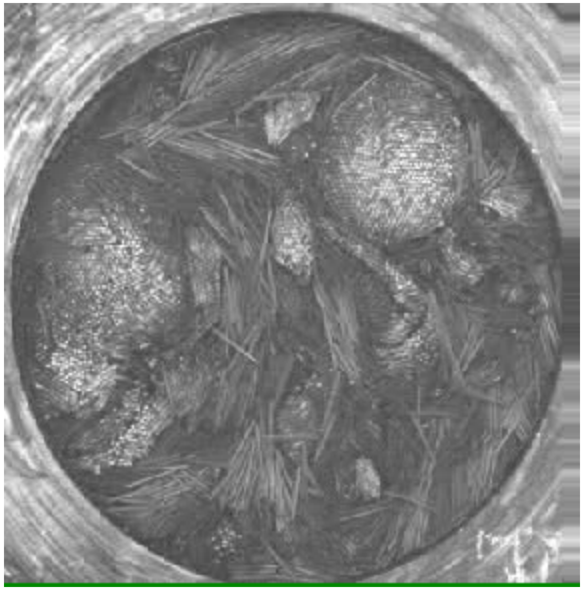
- *Phase transition*



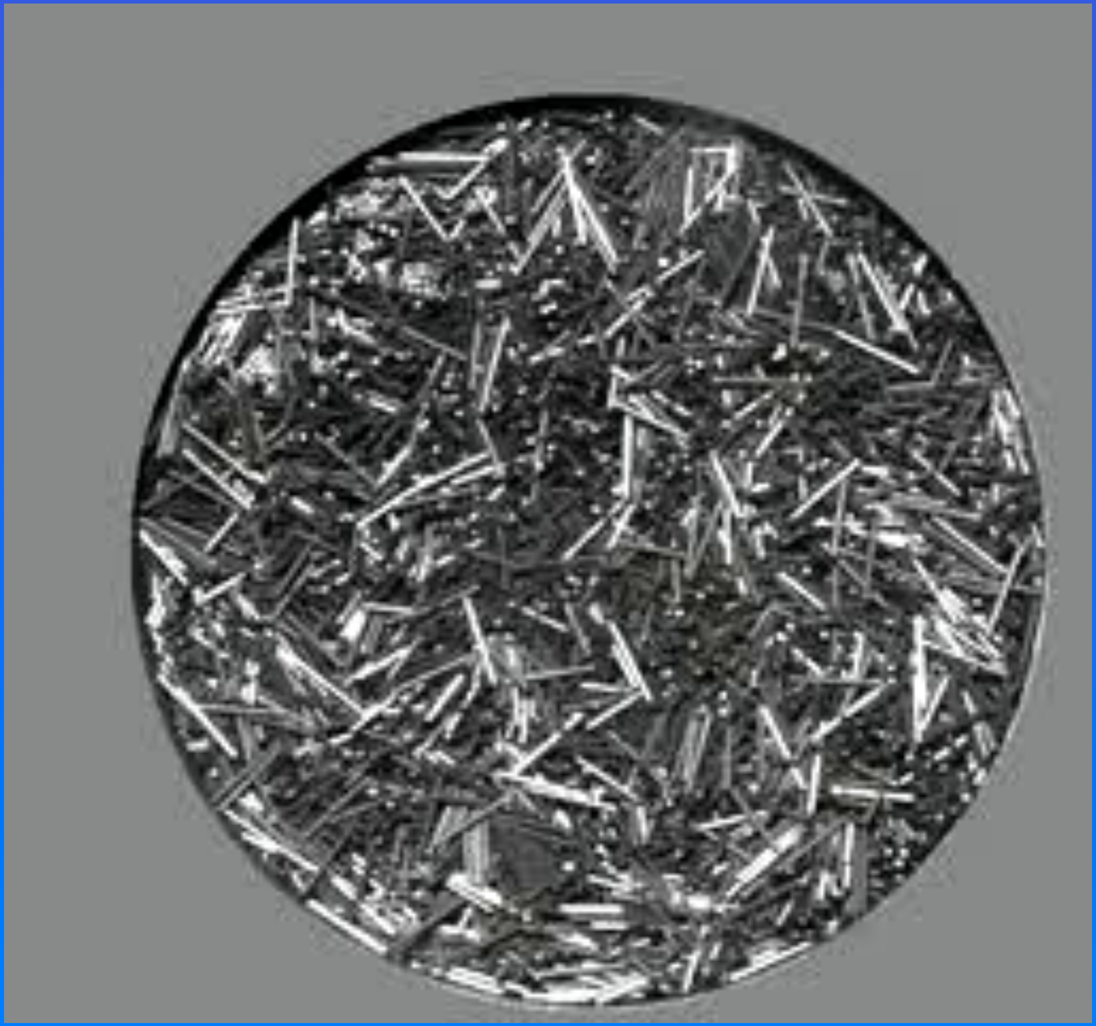
- *Coarsening*



- *Vortex motion*

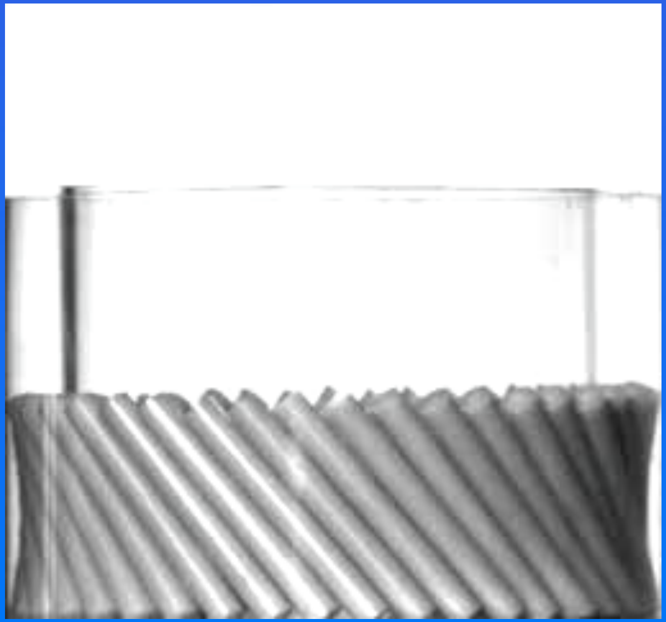


Long-Term Evolution

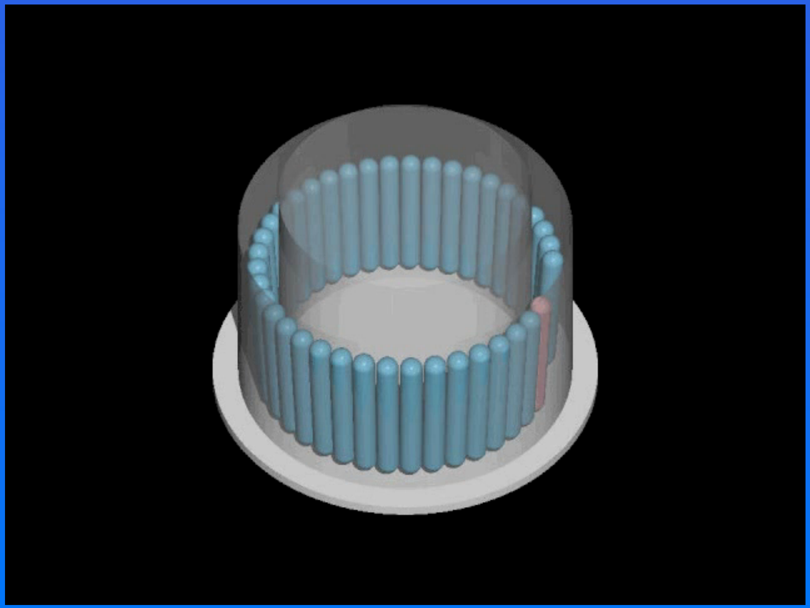


Origin of Motion

Experiment



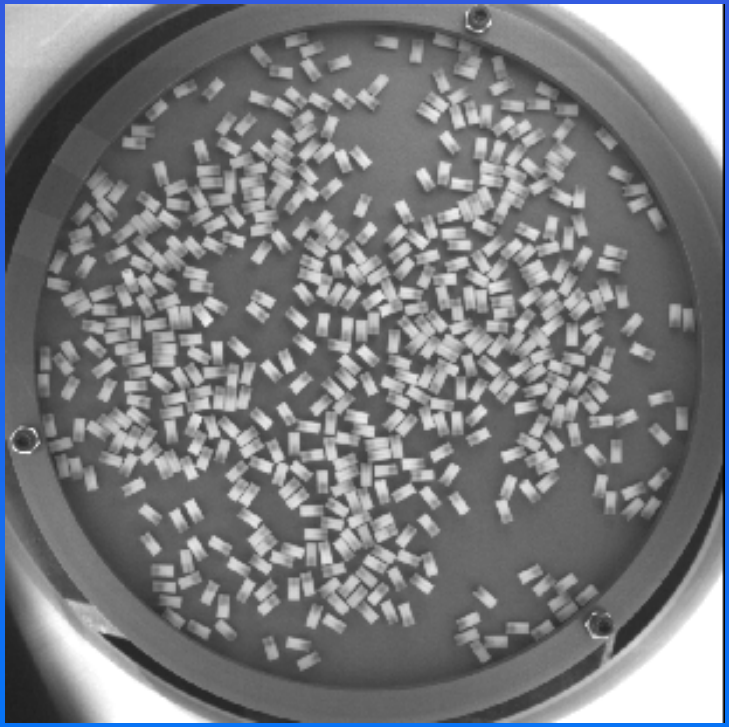
Simulations

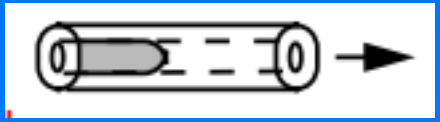


D Volfson, L Tsimring, A. Kudrolli , Phys Rev E (2004)

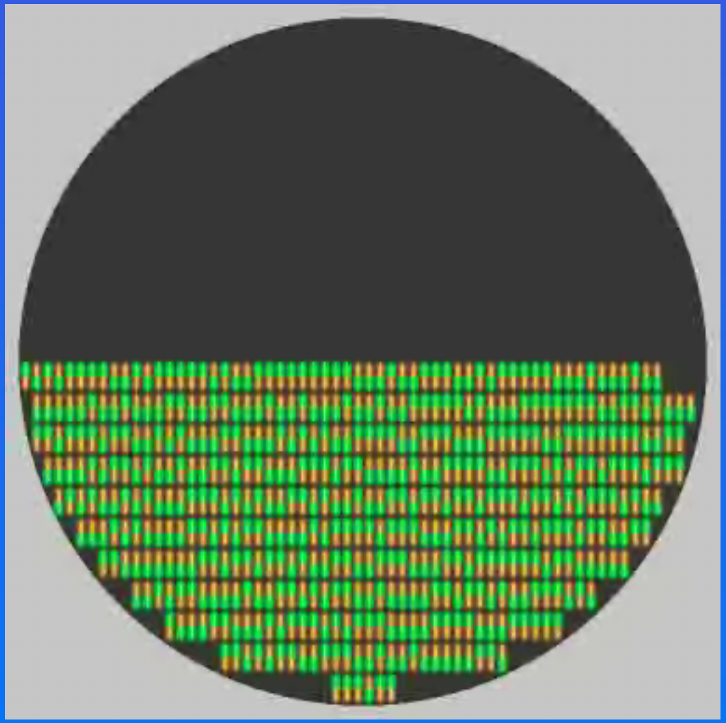
Swarming in Quasi-2D Experiments

Experiment, 500 asymmetric rods





Simulations, 500 rods

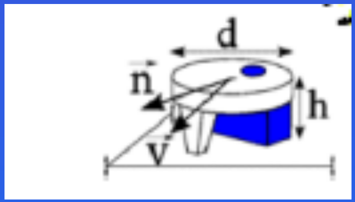


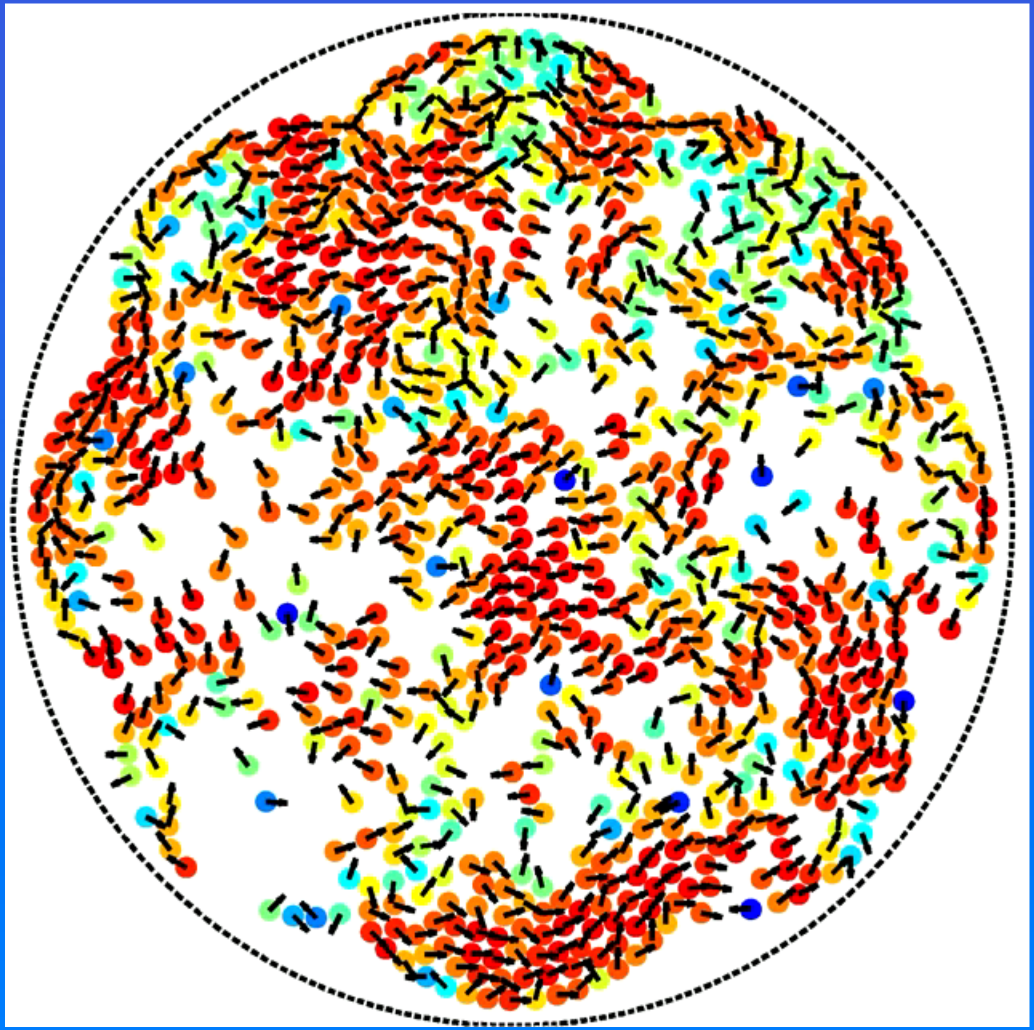
Lumay, D Volfson, L Tsimring, A. Kudrolli PRL 2008

Vibrated Polar Disks

Experiment, 1000 asymmetric disks

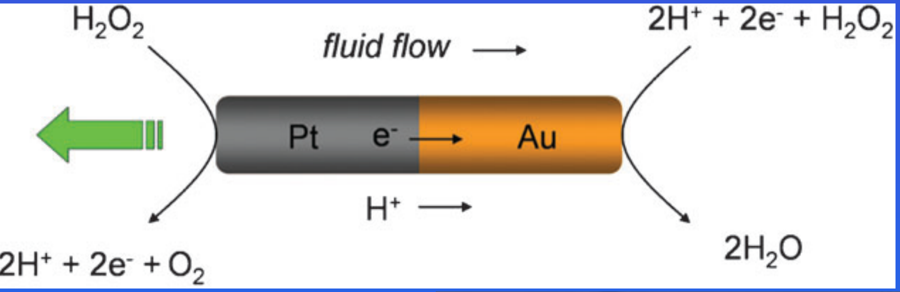
re-injecting boundary conditions (multi-petal dish)





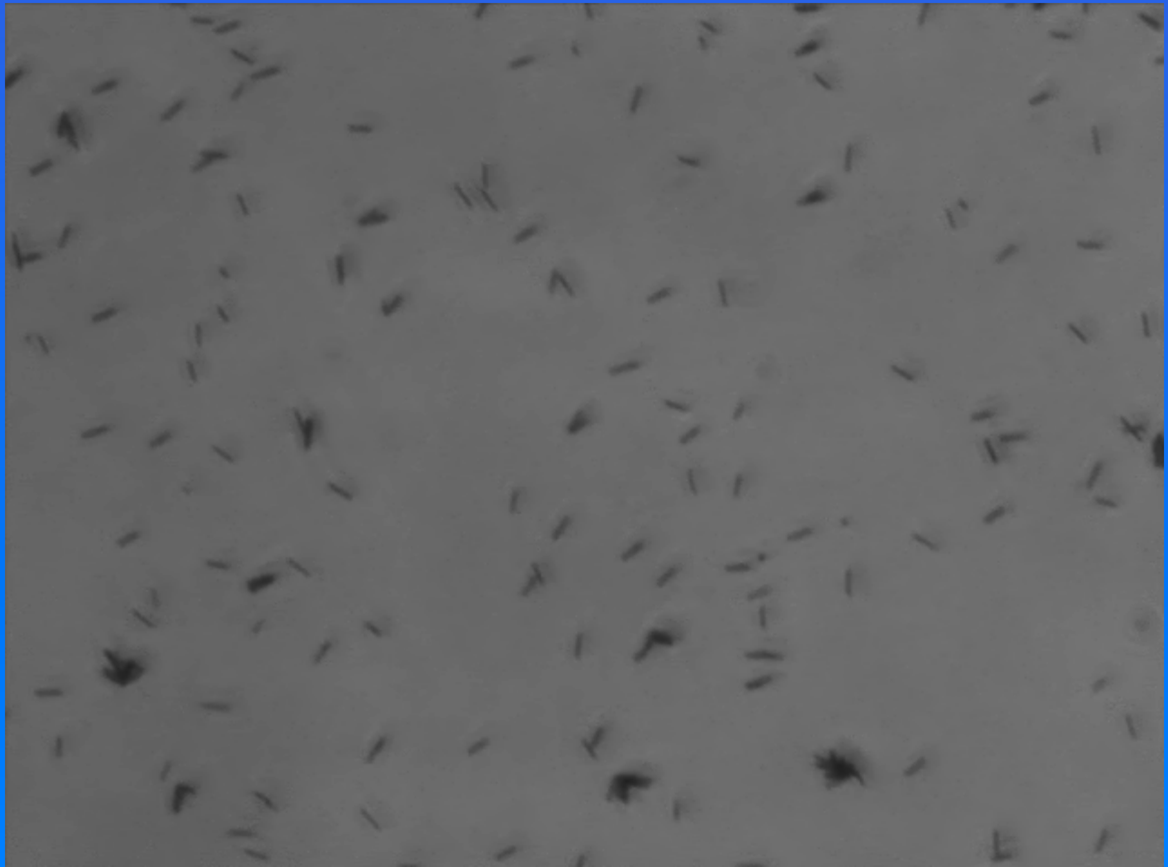
Deseigne, Dauchot, Chate, PRL 2010

nanofabrication: micron-size AuPt rods swim in H_2O_2



AuPt & AuRu microrods are provided by Ayusman Sen and Tom Mallouk, PSU

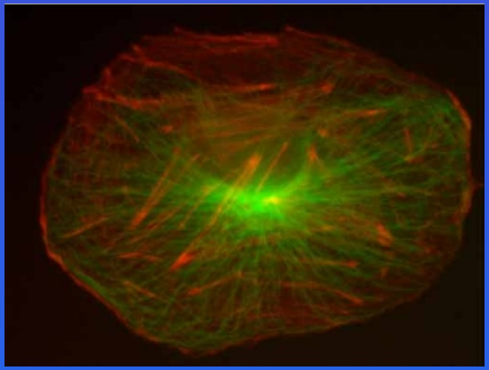
Movie: Argonne

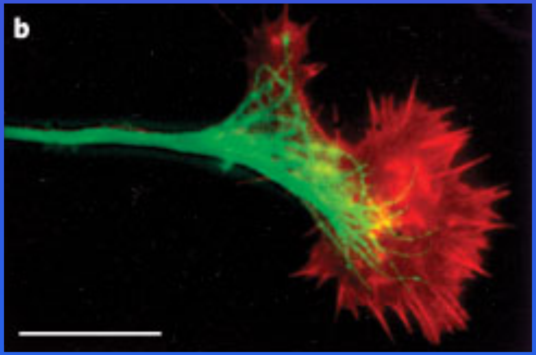


Cytoskeleton - components

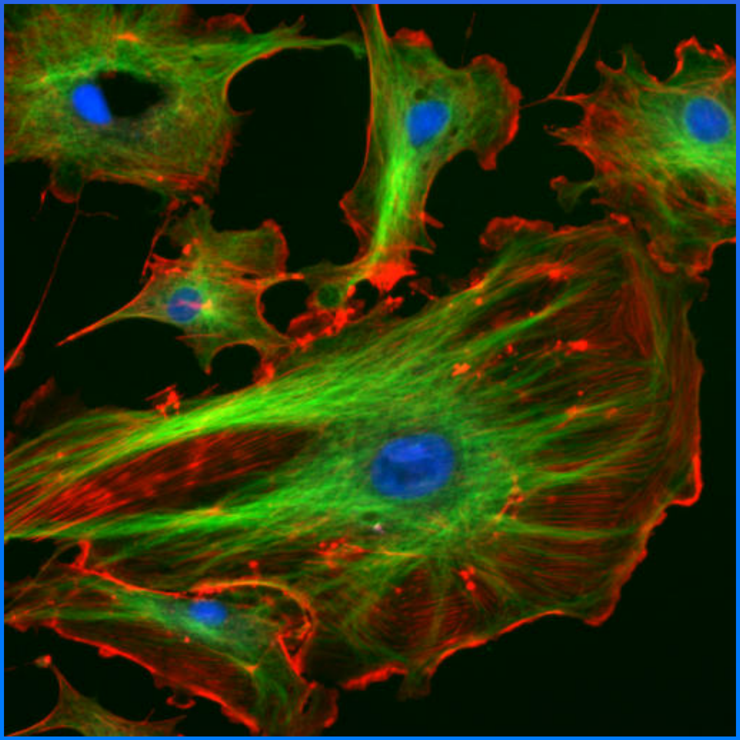
- *Actin (red)*

(1-20 μm, d=8 nm, semiflexible)



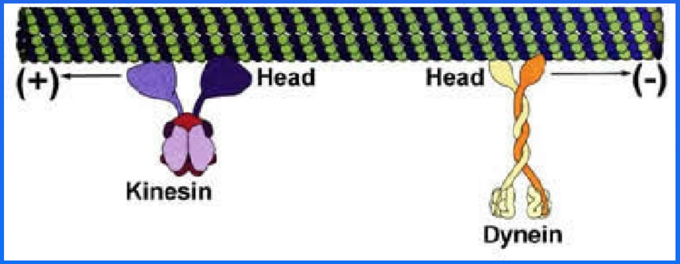


- *Microtubules (MTs, green)*
- *(1-20 mm, d=24 nm, rigid)*

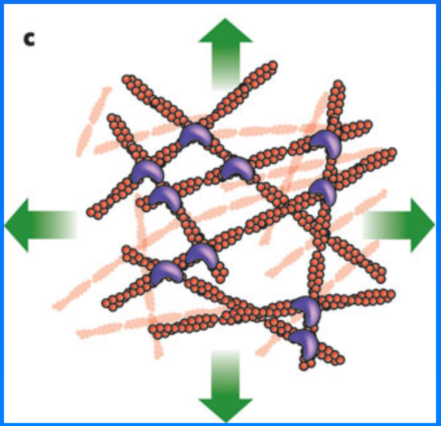


- *Motors*

(⟹ polarity)

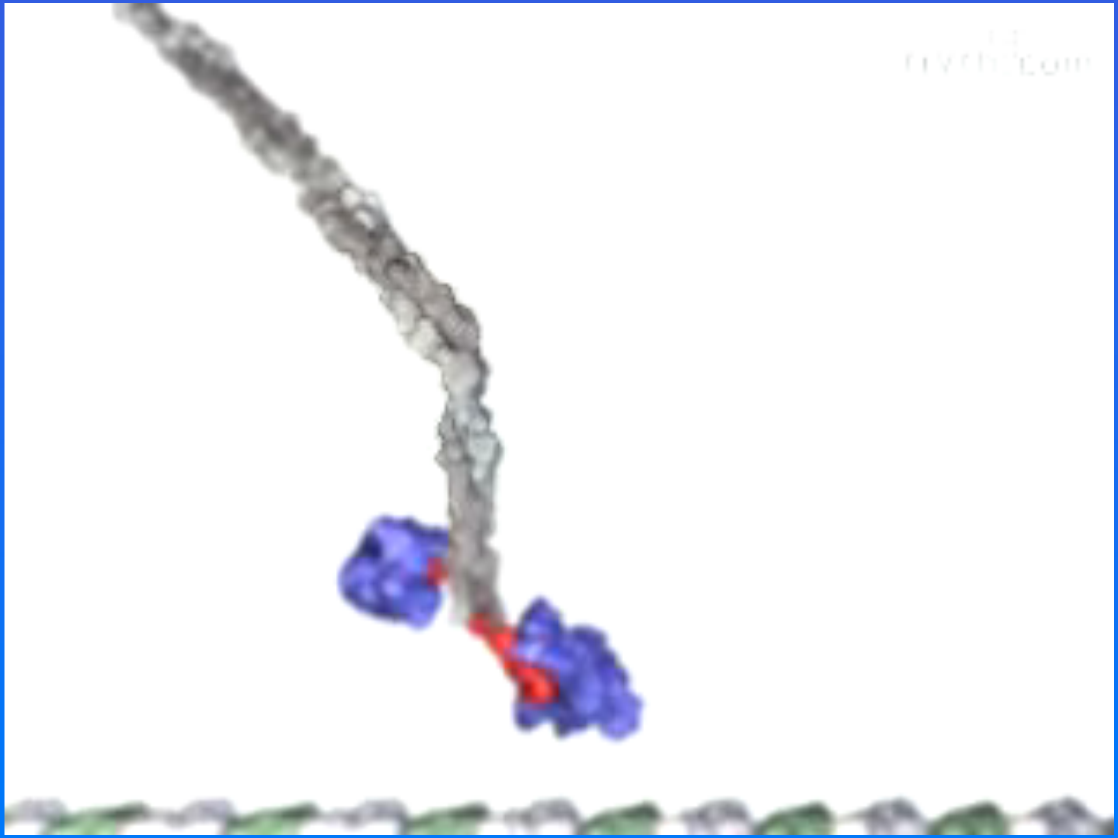


- *Crosslinks*

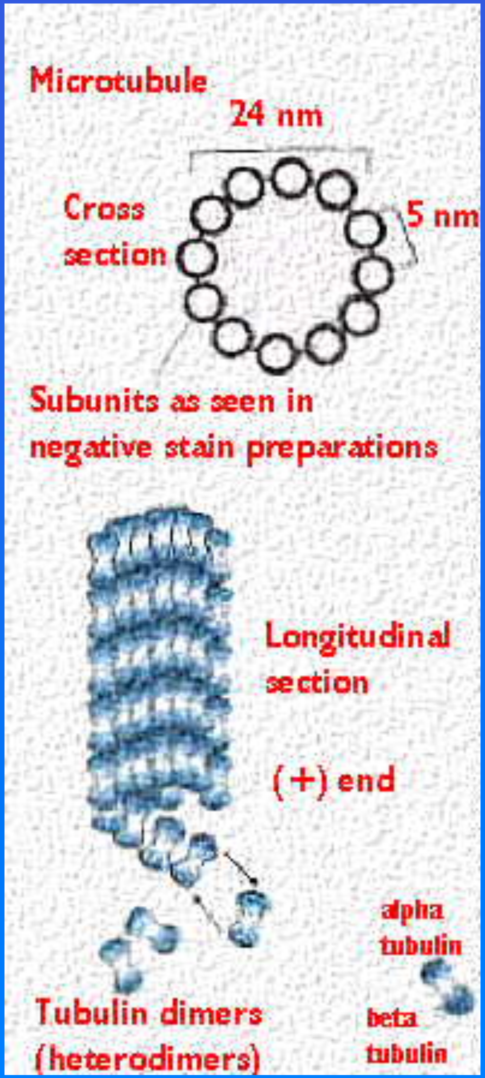


Molecular Motors

Kinesin motor converts ATP to ADP
and perform mechanical work

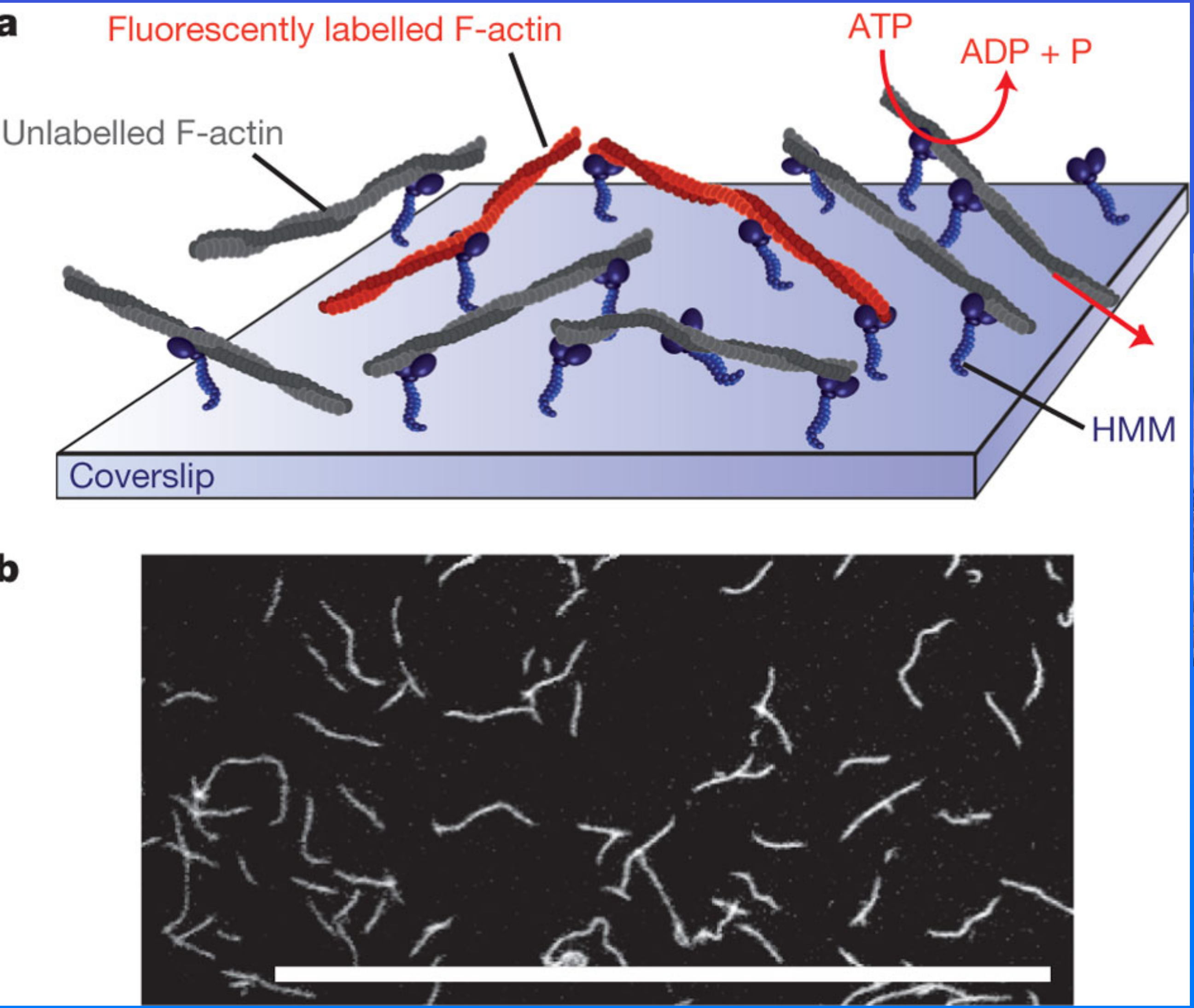


microtubules



Functions: muscle contraction, cargo transport,
cytoskeleton organization, cell division

In vitro: Actin-Myosin Motility Assay

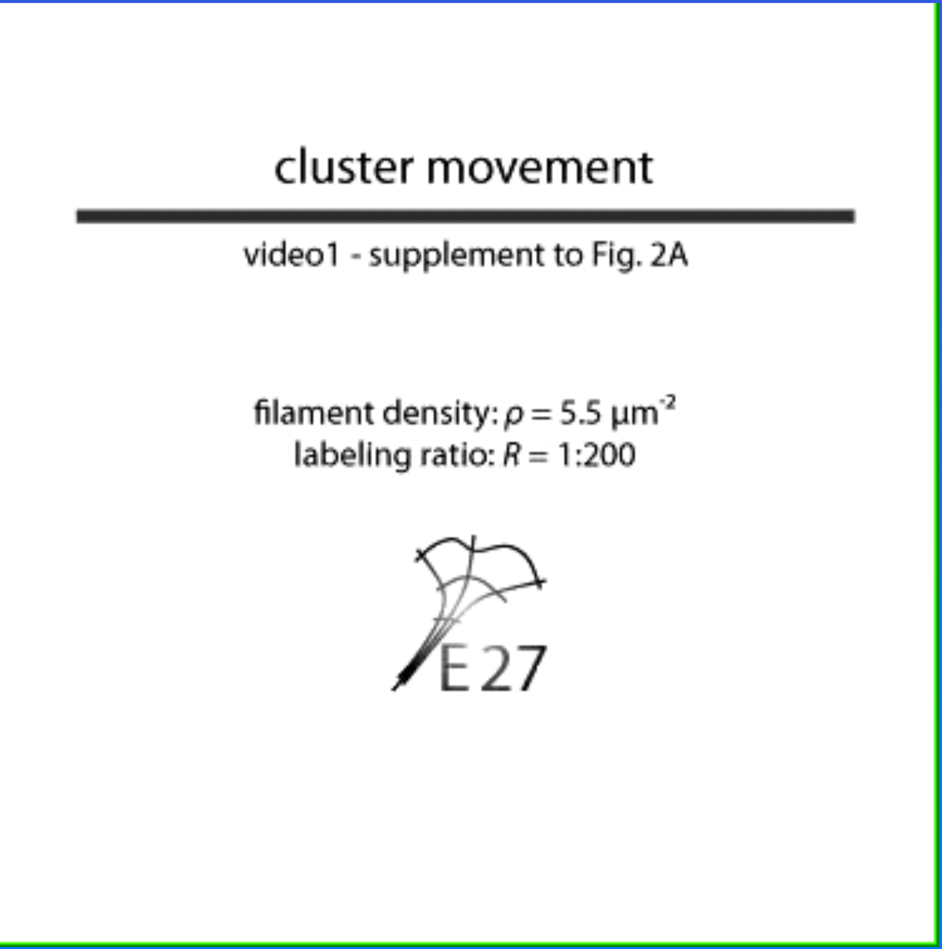


Crowd surfing

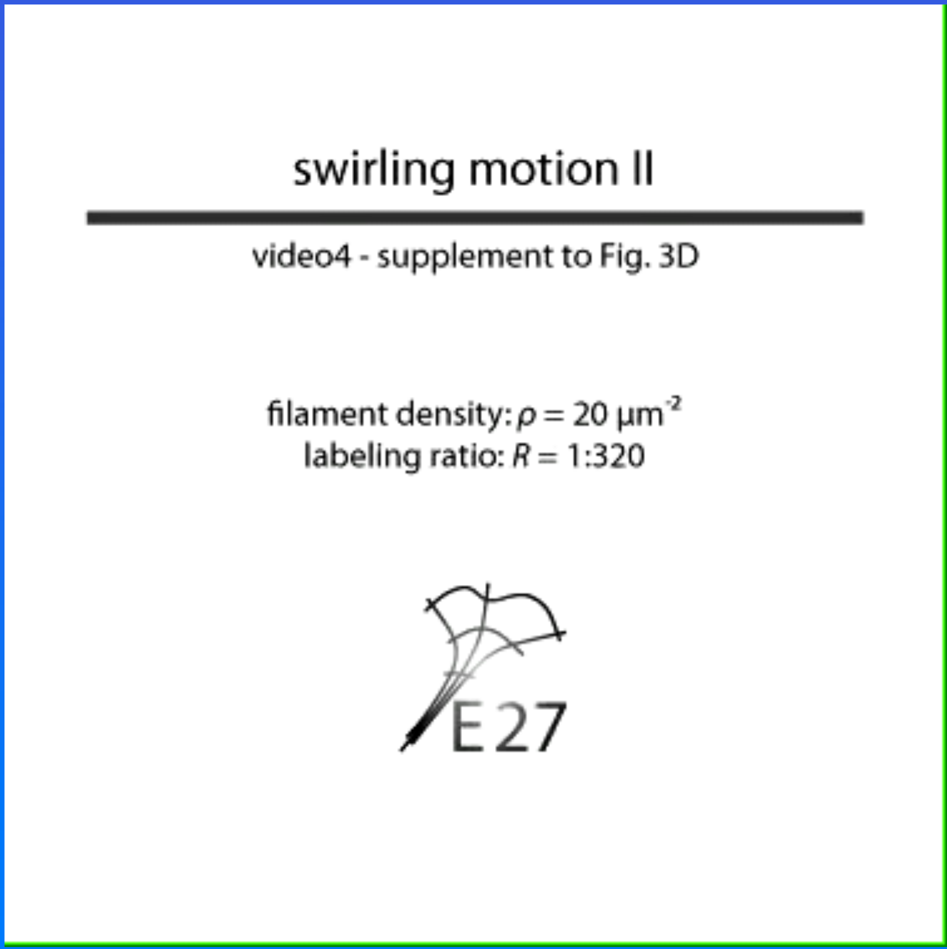
V Schaller et al. Nature 467, 73-77 (2010)

Moving Clusters and Swirls

moderate density



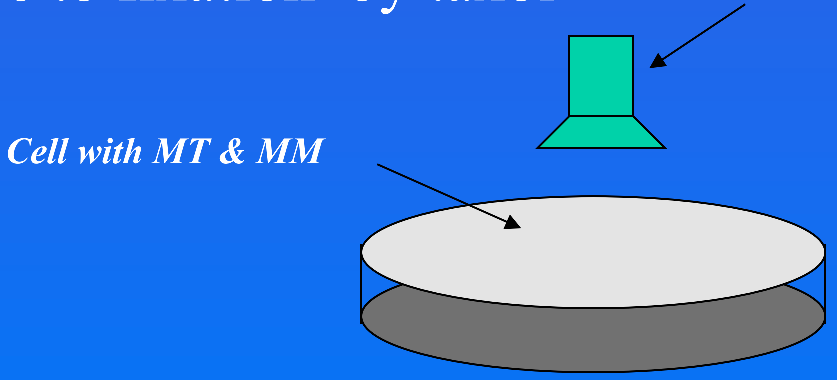
higher density



V Schaller et al. Nature 467, 73-77 (2010)

in-vitro Self-Assembly of MT and MM

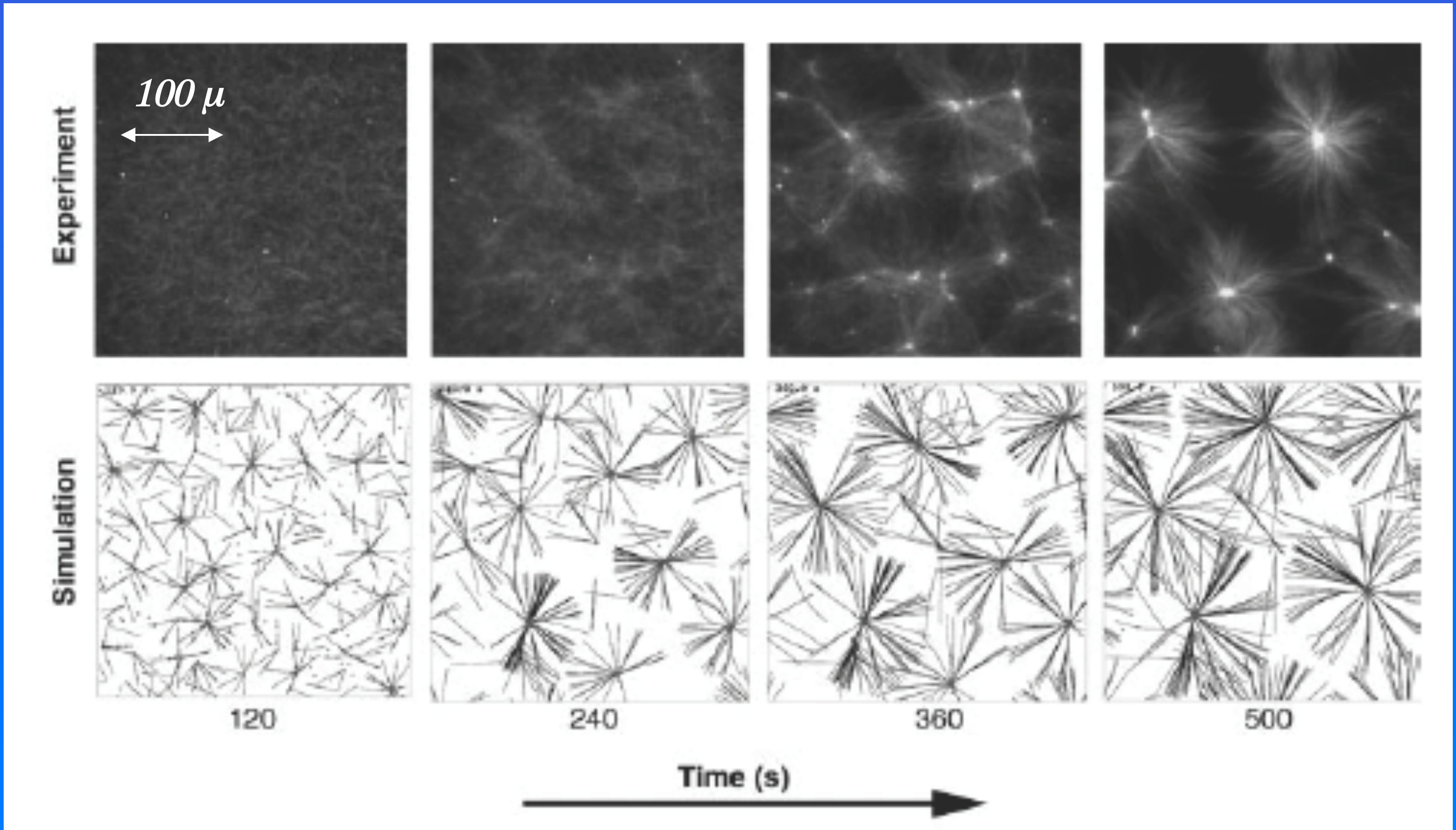
- Simplified system with only few purified components
- Experiments performed in 2D glass container: diameter 100 μm, height 5μm
- Controlled tubulin/motor concentrations and fixed temperature
- MT have fixed length 5μm due to fixation by taxol



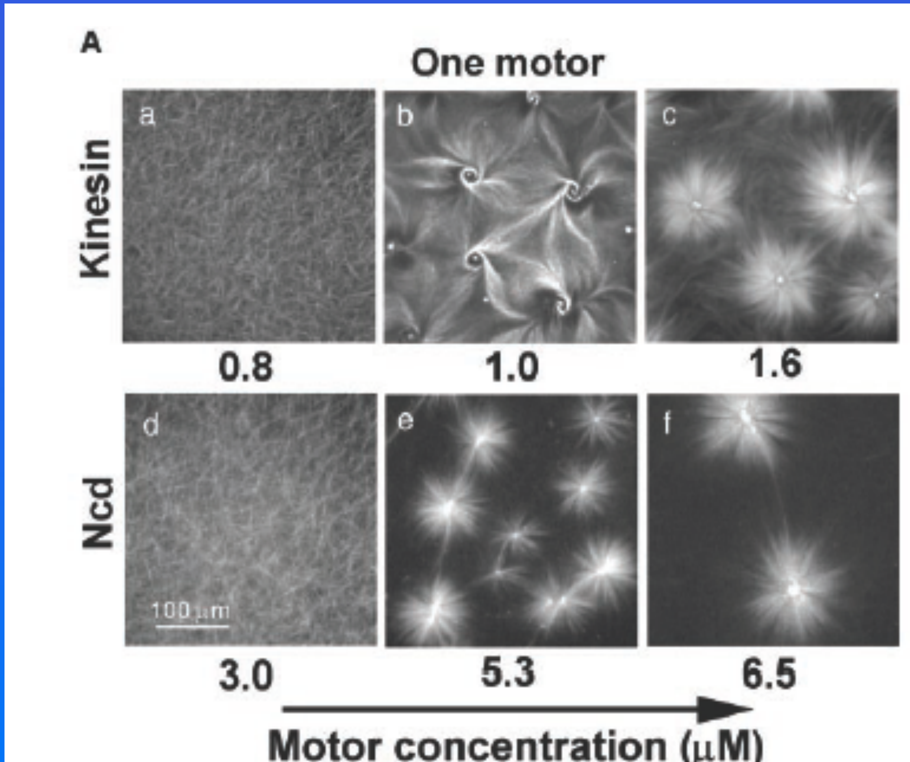
F. Nedelec, T. Surrey, A. Maggs, S. Leibler,
Self-Organization of Microtubules and Motors, Nature, 389 (1997)
T. Surray, F. Nedelec, S. Leibler & E. Karsenti,
Physical Properties Determining Self-Organization of Motors & Microtubules, Science, 292 (2001)

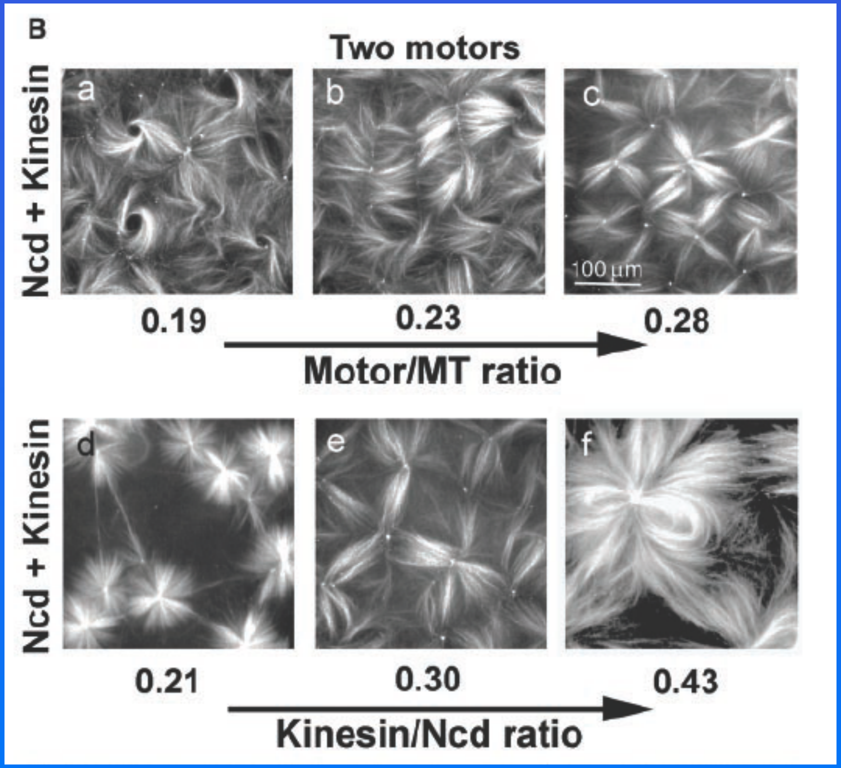
Patterns in MM-MT mixtures

Formation of asters, large kinesin concentration (scale 100 m)



Vortex – Aster Transitions



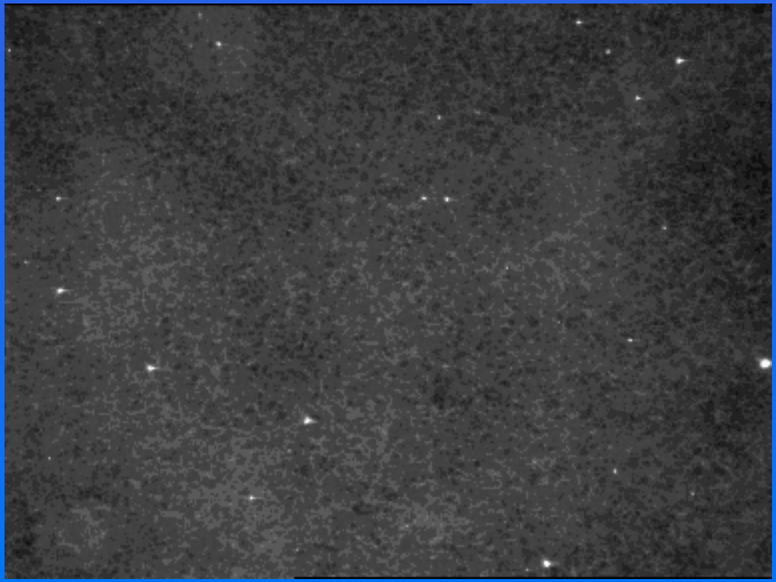


Ncd – gluththione-S-transferase-nonclaret disjunctional fusion protein

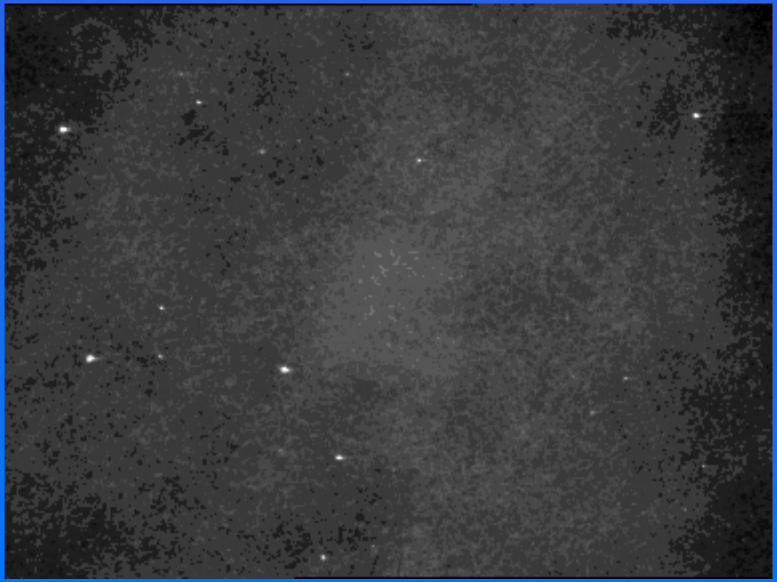
Ncd walks in opposite direction to kinesin

Dynamics of Aster/Vortex Formation

Kinesin



Ncd



Rotating Vortex

Kinesin

Summary of Experimental Results

- 2D mixture of MM & MT exhibits pattern formation
- Kinesin: vortices for low density of MM and asters for higher density
- Ncd: only asters are observed for all MM densities
- For very high MM density asters disappear and bundles are formed

New experiments: onset of spontaneous motion

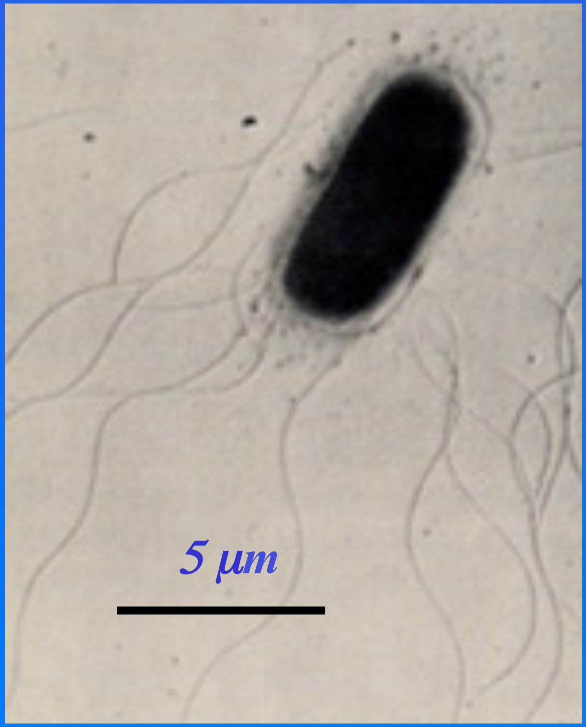
- Short microtubules
- Crowding agents
- High concentration
- Nematic ordering
- Topologic defects

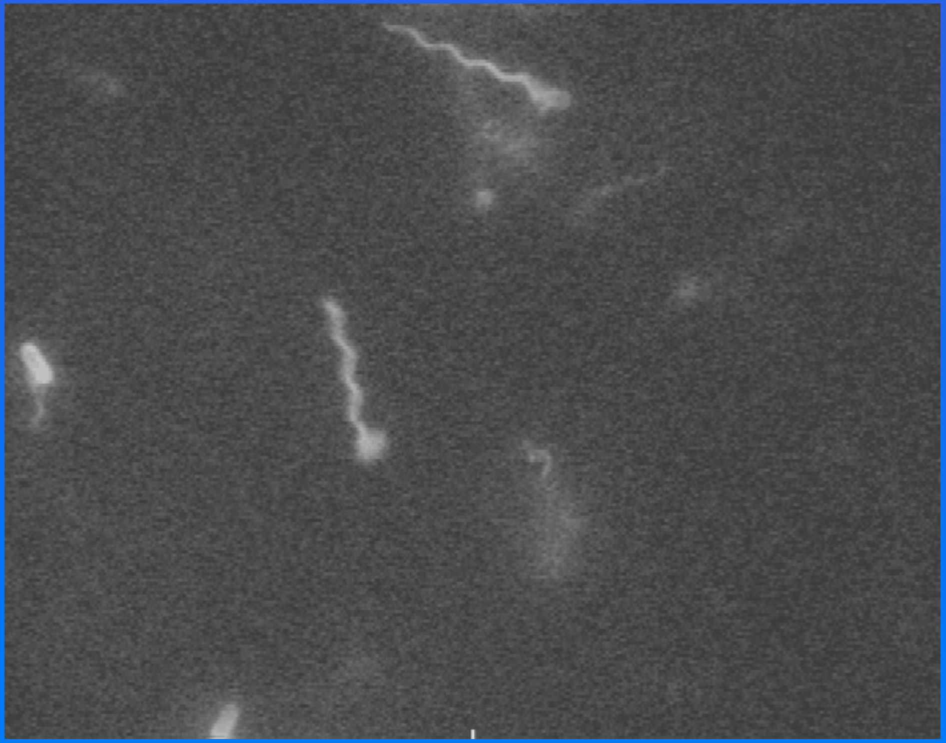
Active 2D nematic
Low curvature interface
60X mag
15μm bar

Sanchez et al, Nature, 2012

Self-Propelled BioParticles

- swimming aerobic bacteria *Bacillus Subtilis*
- length 5 μm, speed 20 μm/sec, Re=10^{-4}
- collective flows up to 100 μm/sec
- need Oxygen (oxygentaxis)





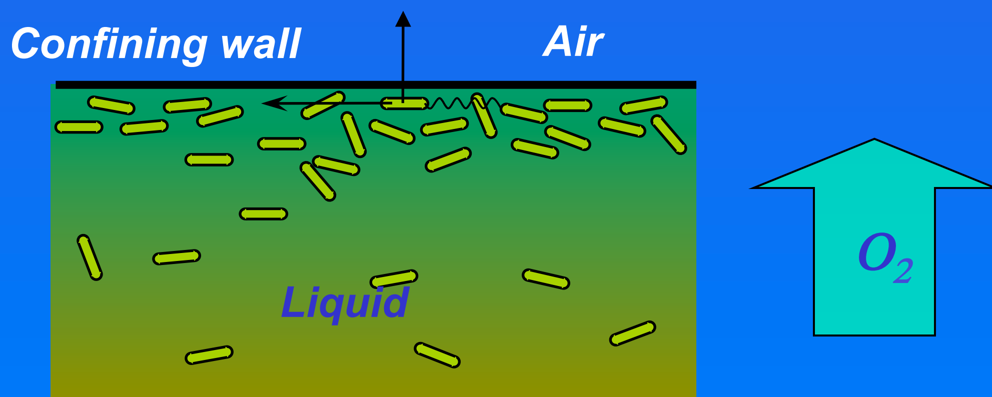
Turner, Ryu, and Berg (E. coli)

Bacillus subtilis primary behaviors

Top view

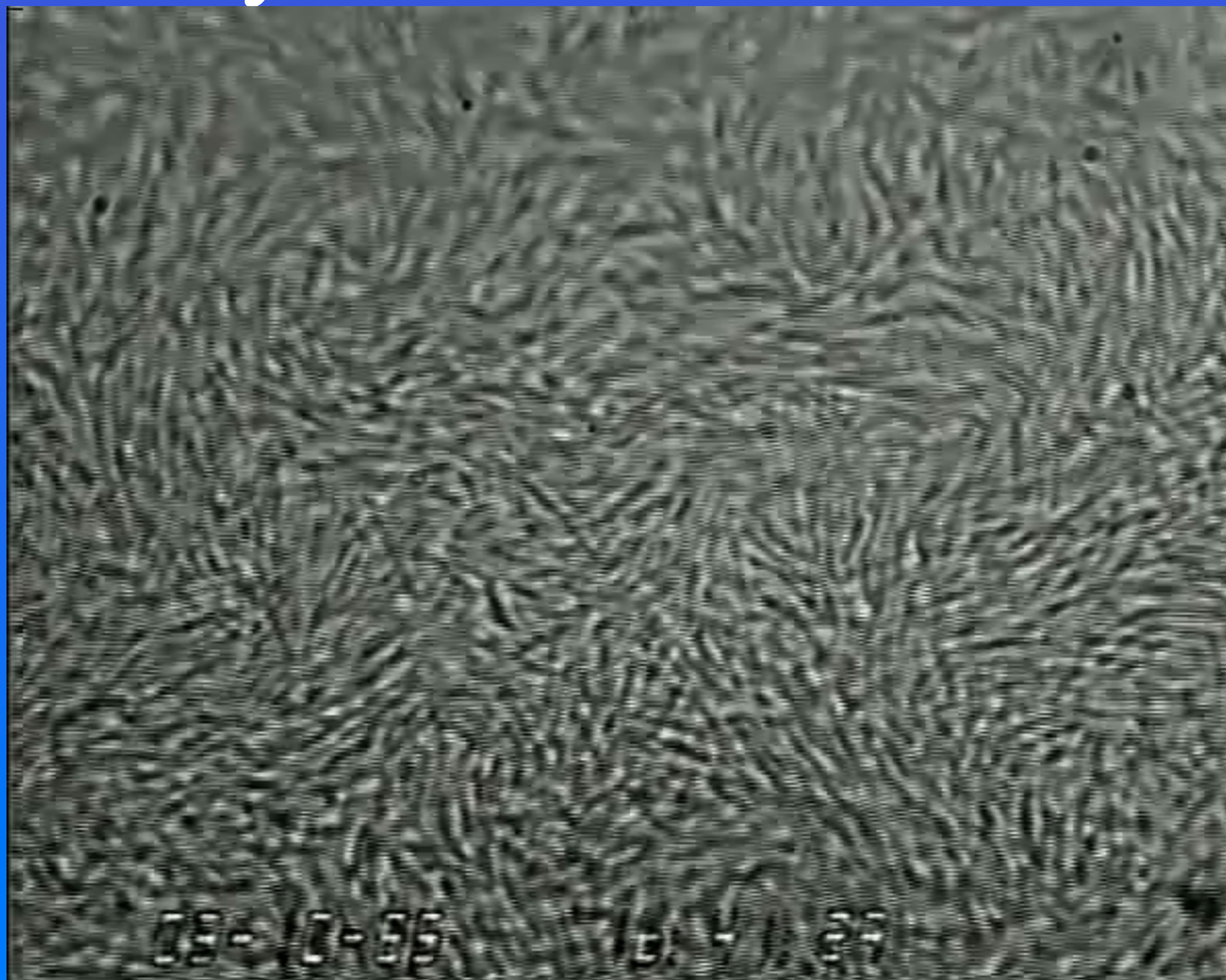
- *Excellent swimmers*
- *No tumbling*

Side view



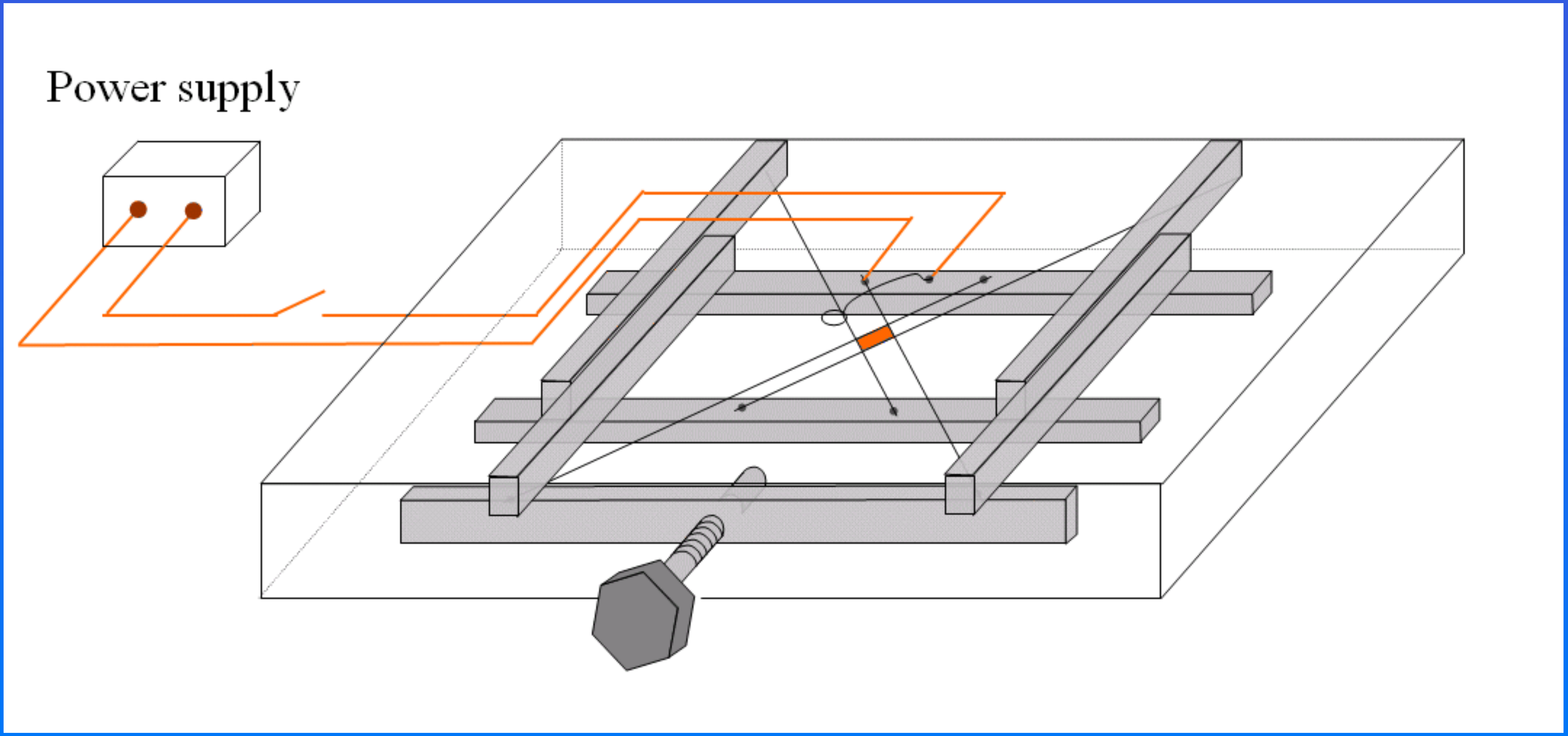
Concentration of bacteria near the surface due to gradient of dissolved Oxygen

Bacterial (or active) Turbulence
Reynolds number 10^{-4}



Dombrowski, Goldstein, Kessler, et al PRL 2004

Schematics of Experimental Setup

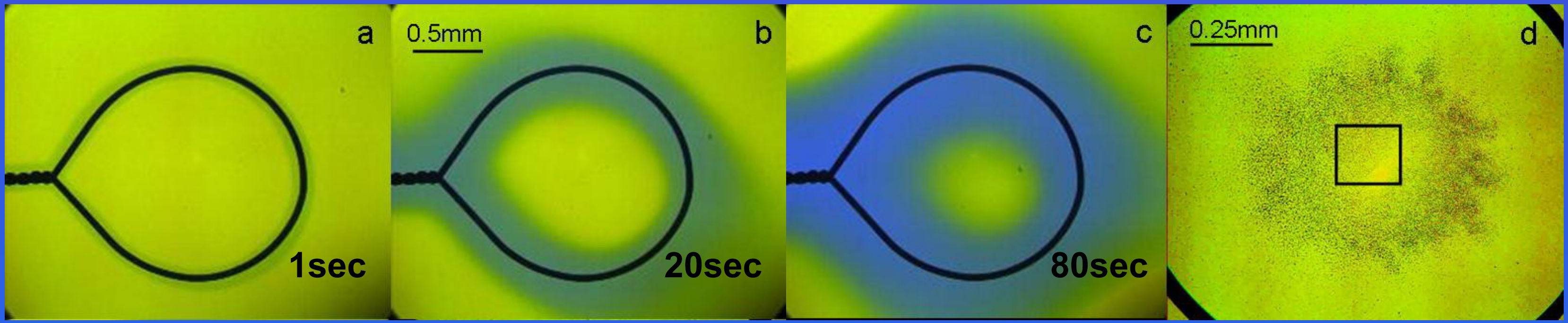


Thin free-standing film concept

Adjustable thickness

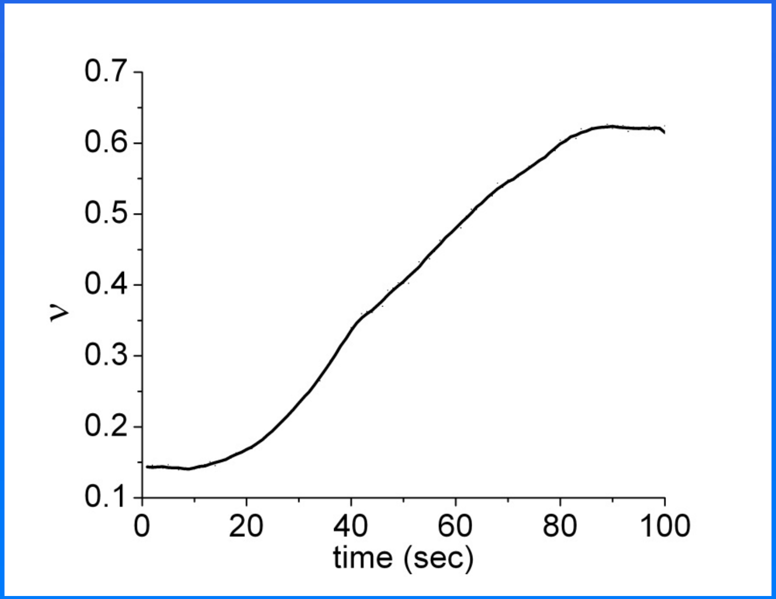
Adjustable concentration of bacteria

pH-Taxis & concentration of cells

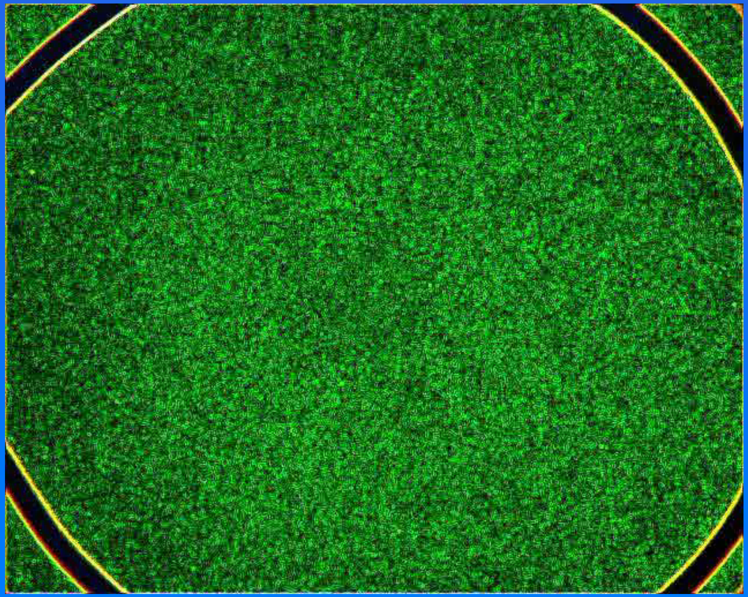


pH indicator (bromothynol blue) was added **field of view**

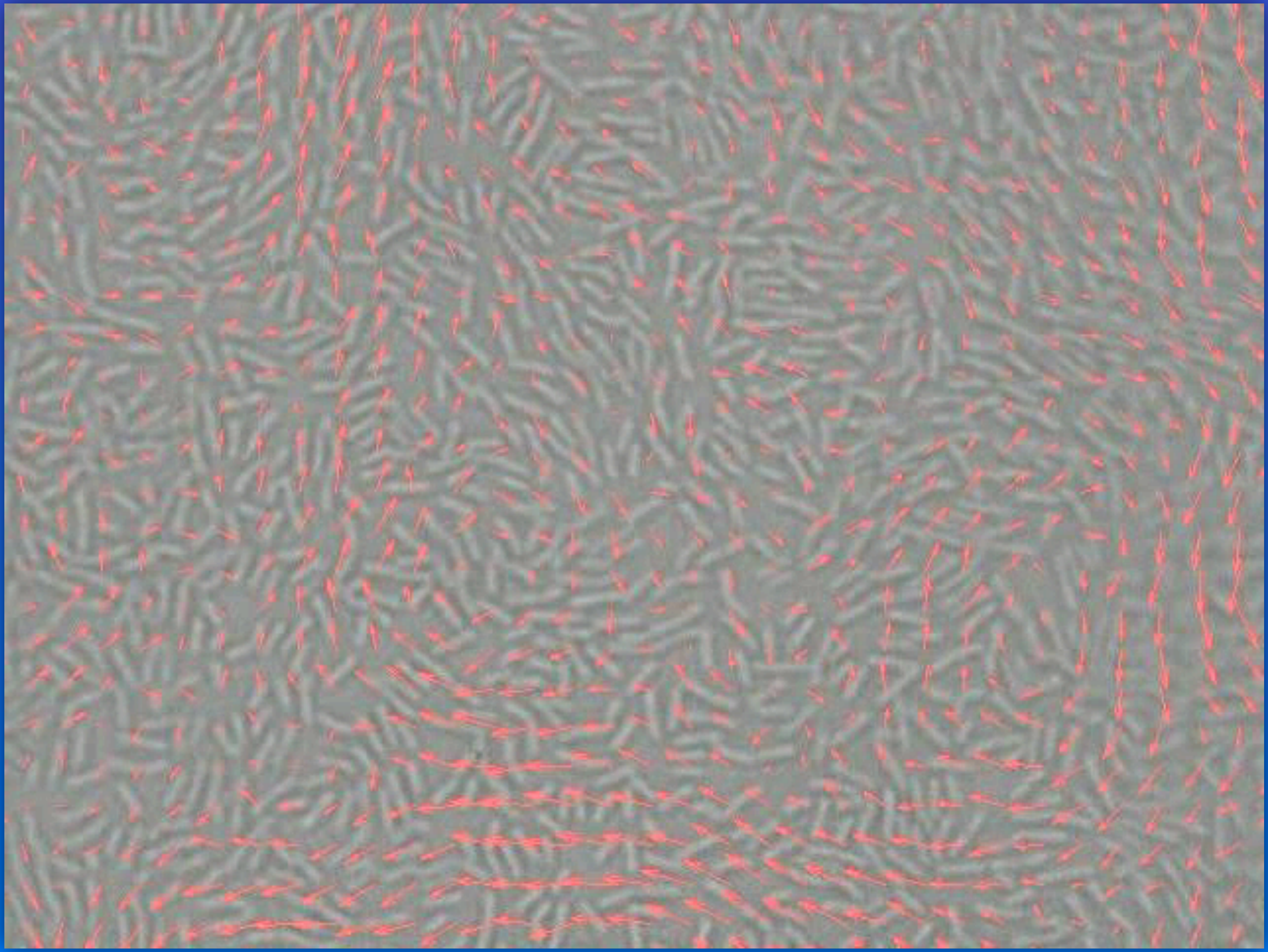
concentration vs. time



Bacteria crowd control



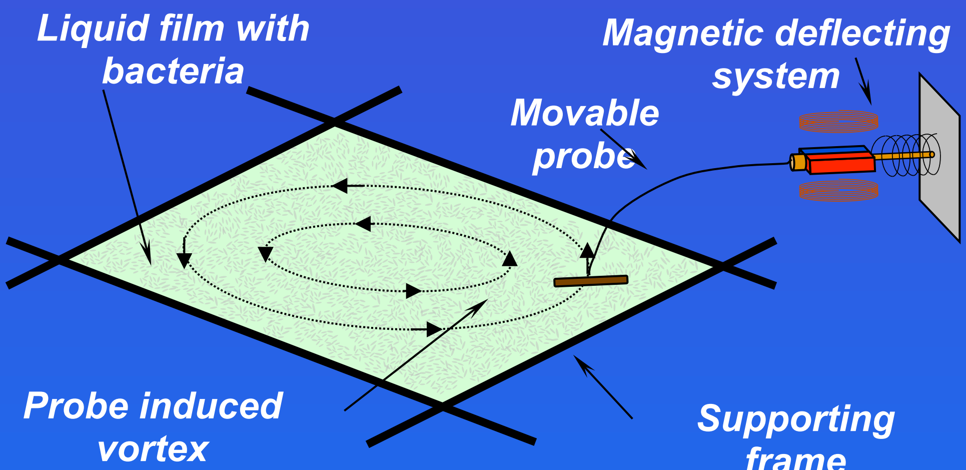
Bacterial Turbulence



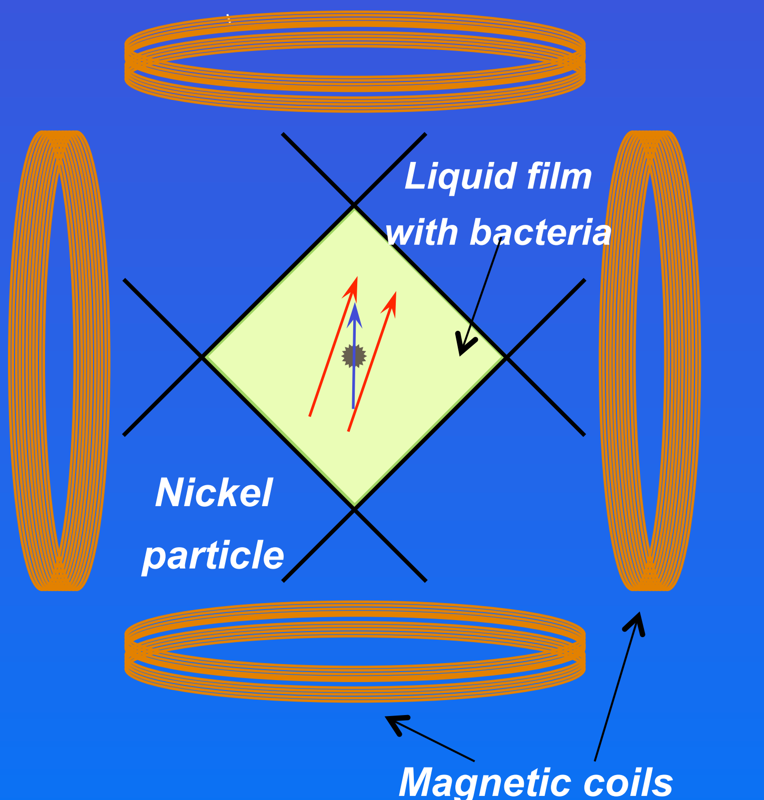
Sokolov, Goldstein, Kessler, I.A PRL (2007)

7-fold reduction of viscosity

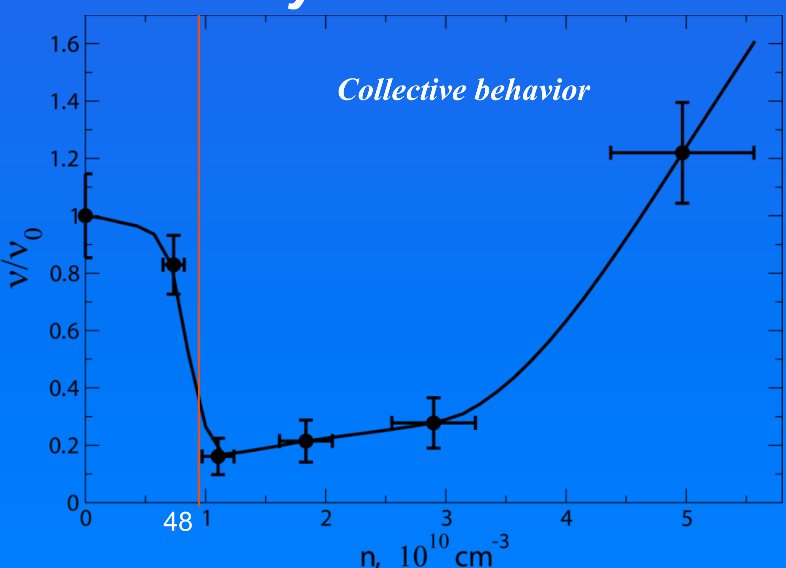
vortex probe micro-rheometer



rotational micro-rheometer



viscosity vs concentration

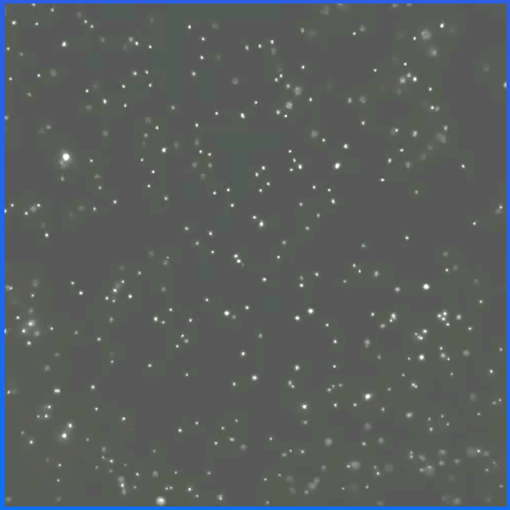


Sokolov & I.A, PRL 2009

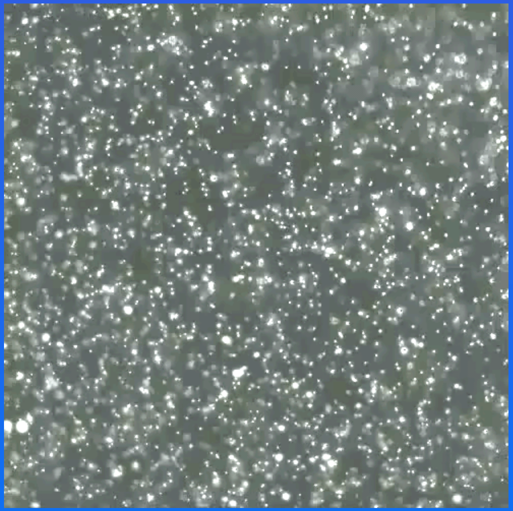
- viscosity is extracted from the vortex decay time
- viscosity is extracted from the magnetic torque
- viscosity vs concentration and swimming speed of bacteria

Novel Material Properties: Reduction of Viscosity

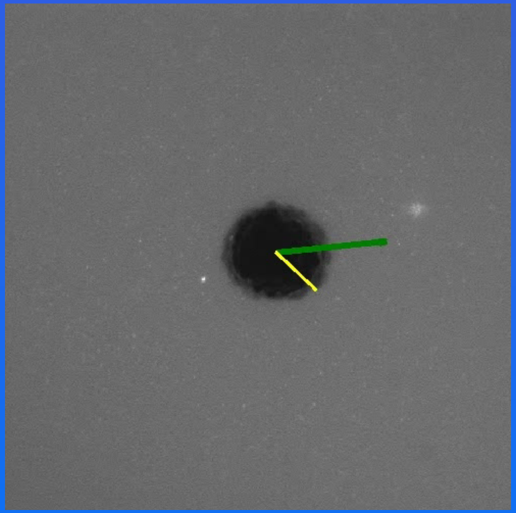
live bacteria



dead



rotational rheology



Machines Powered by Bacteria: Rectification of Chaotic Motion

Sokolov, Apodaca, Grzybowski, I.A, PNAS, December 2009

Lithographic Mask

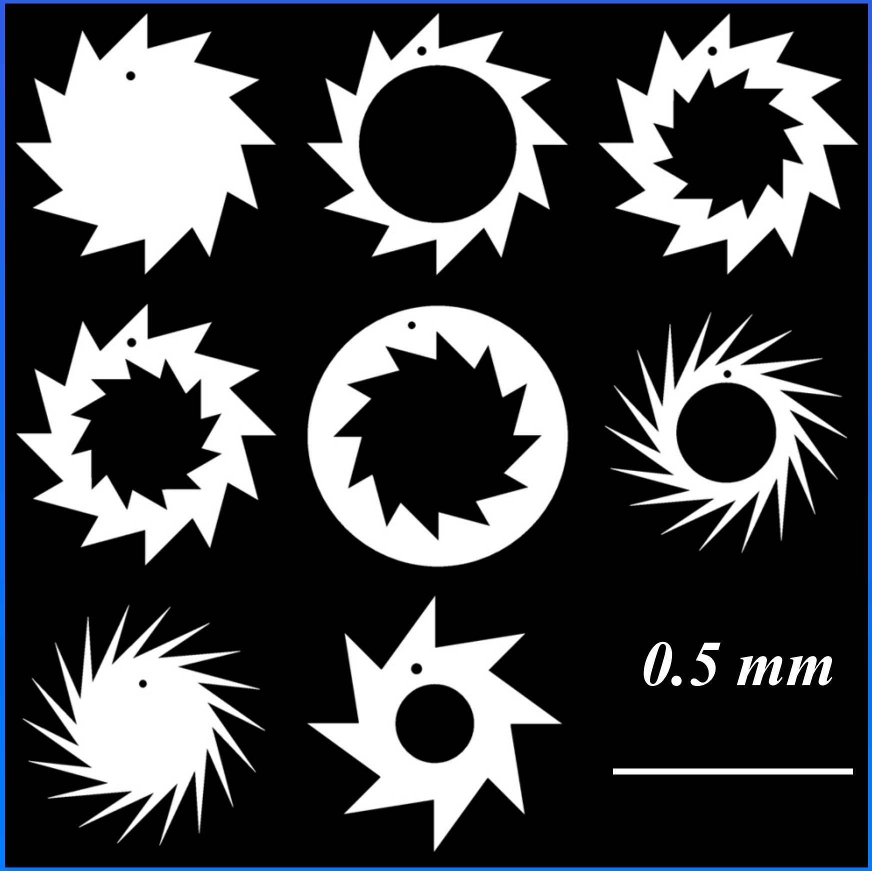
Size of gears: 350 μm, SU-8 photoresist

Photolithography technique

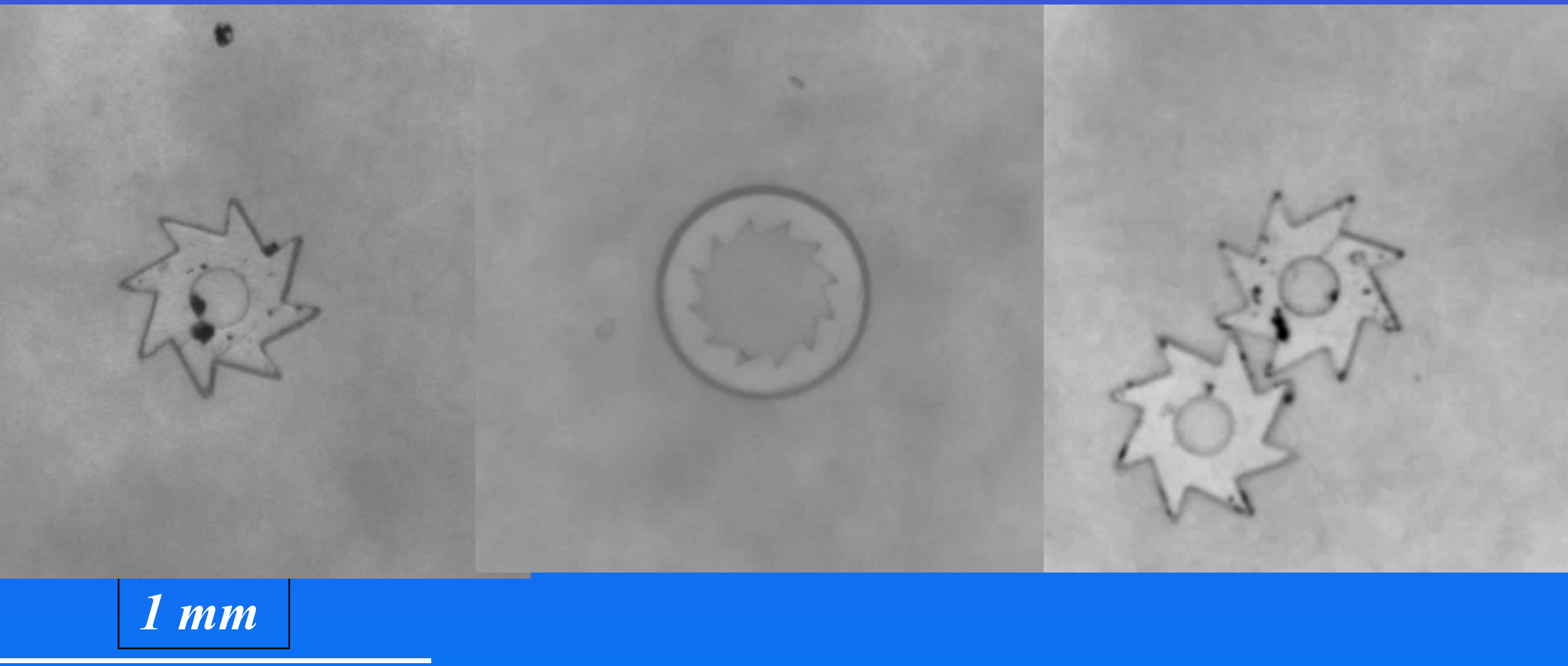
Mass of Gear ~10^6 mass of bacteria

Collaboration with Bartosz Grzybowski, Northwestern University

Featured in NY Times, Forbes, Wired, WDR, Sci American



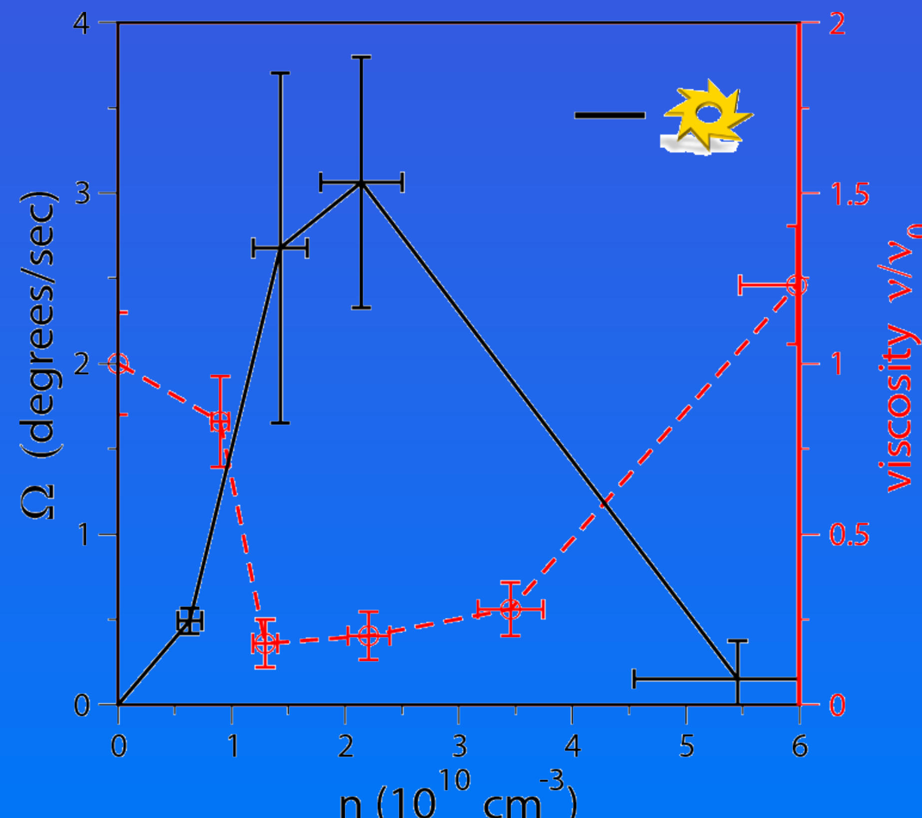
Gears Turned by Bacteria



- **1-2 rotations per minute**
- **Power about 1 femtowatt=10^{-15} Watt**
- **About 300 bacteria power the gear**

Control of Rotation

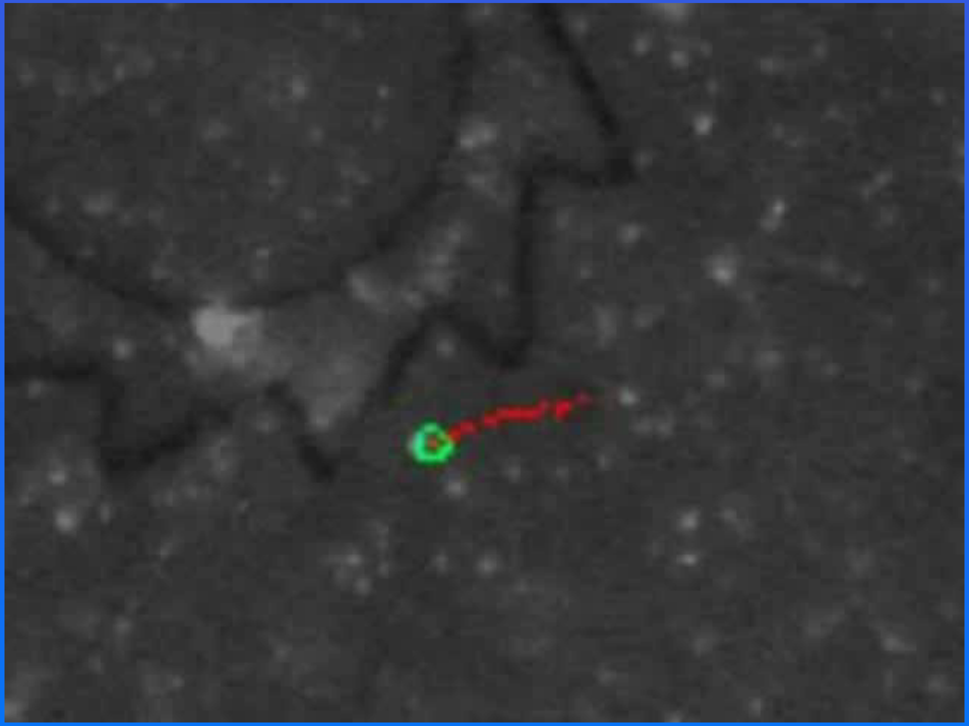
Rotation rate vs concentration

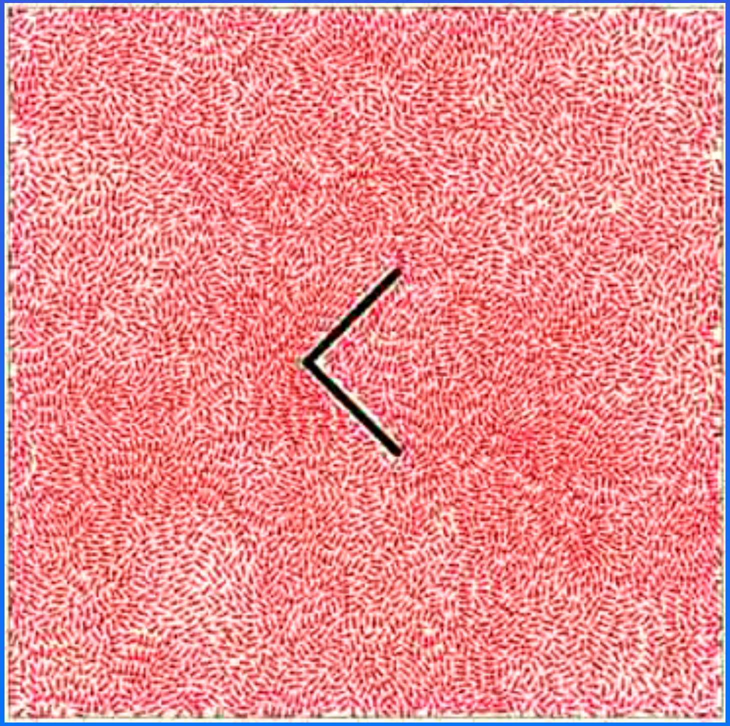


- **Rotation rate controlled by Oxygen/Nitrogen**
  - **Rotation rate depends on concentration**
- **Rotation enhanced by collective swimming**

Ratchet Mechanism of Rotation

Trajectory of fluorescent tracers

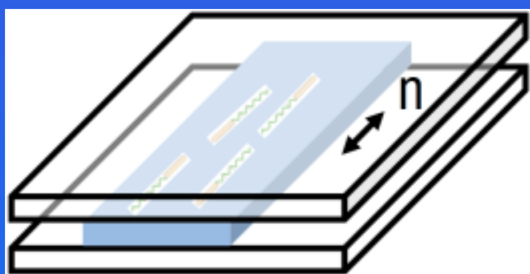




- **Bacteria slide along slanted edges**
- **Trapped in junctions formed by the teeth**
- **Simulations of Kaiser et al, PRL 2014**

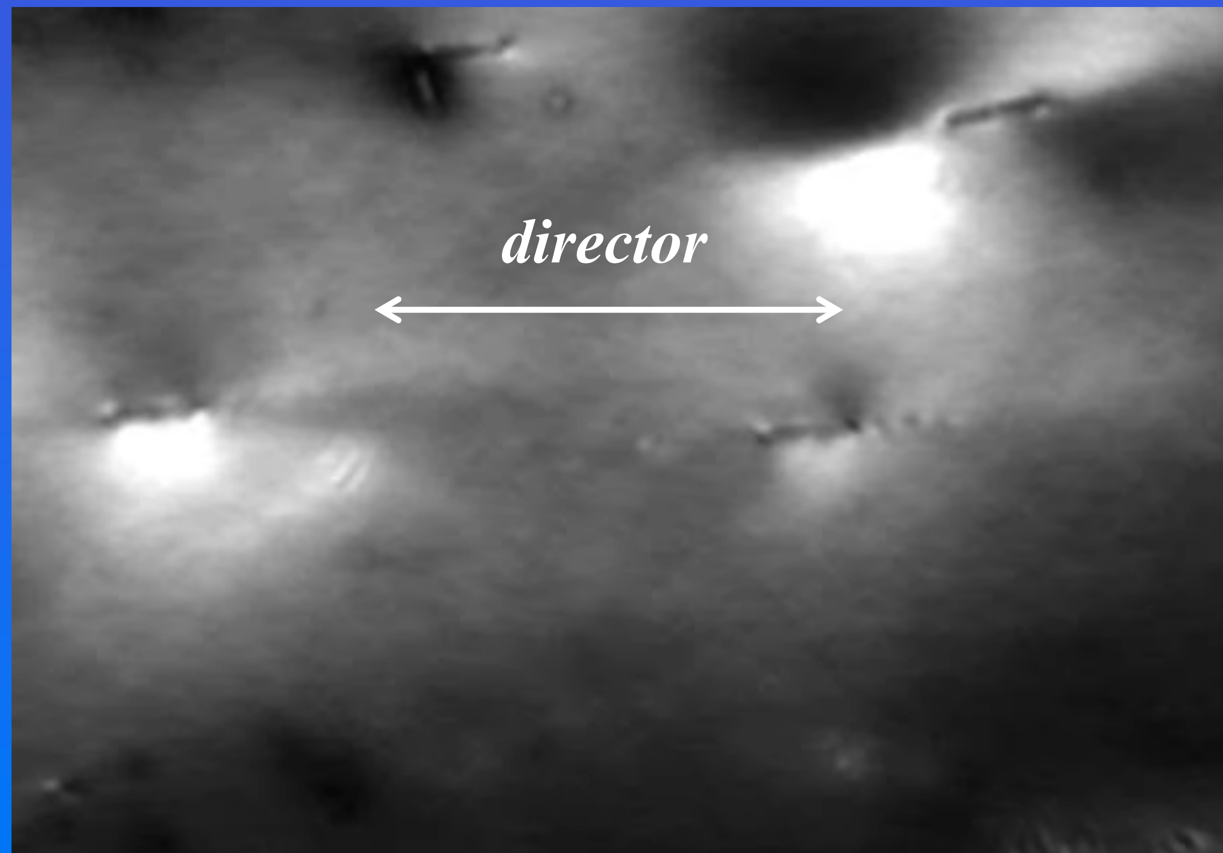
Bacteria follow director of the chromonic LC in a cell with strong planar anchoring

flat glass cell



Thickness h

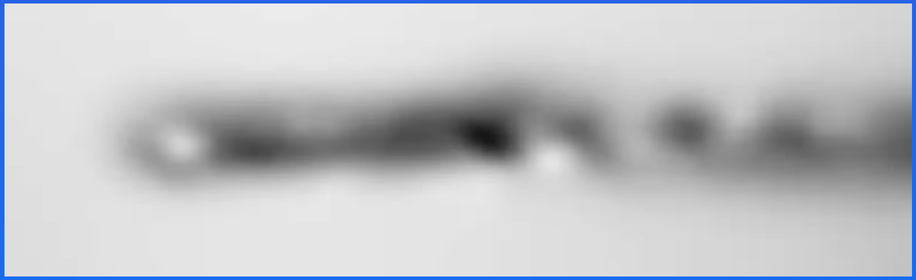
= 5-10 mm

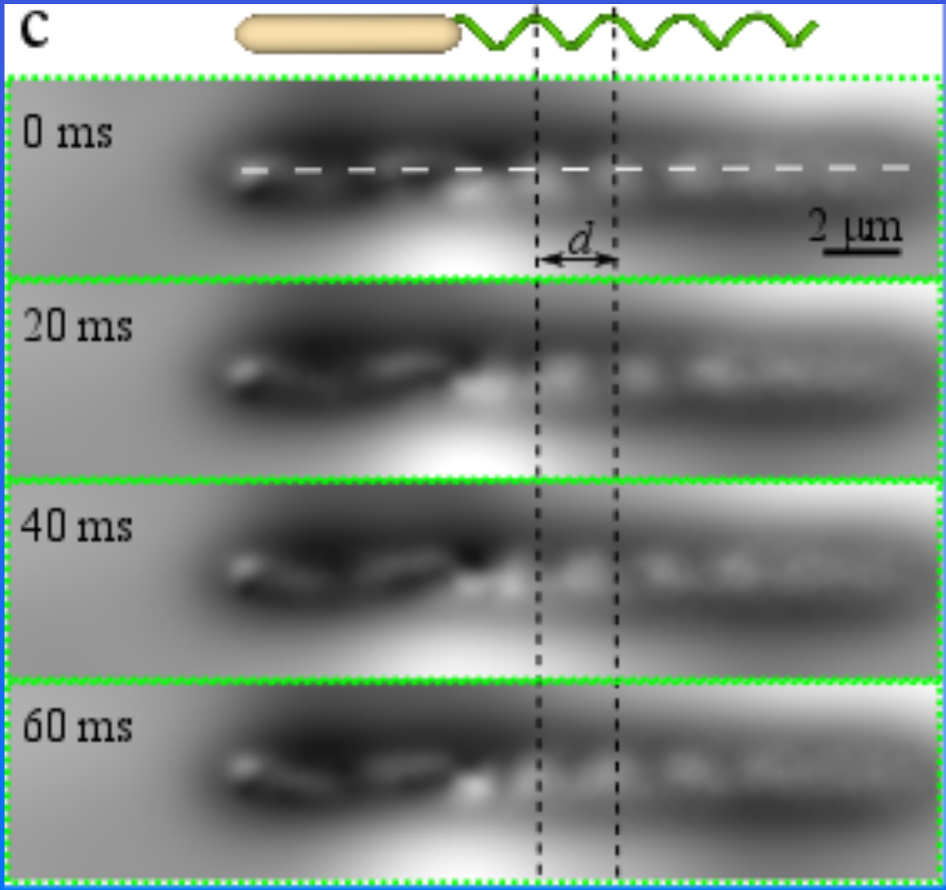


Zhou, Sokolov, Lavrentovich, IA, PNAS 2014

Zoom on individual bacterium

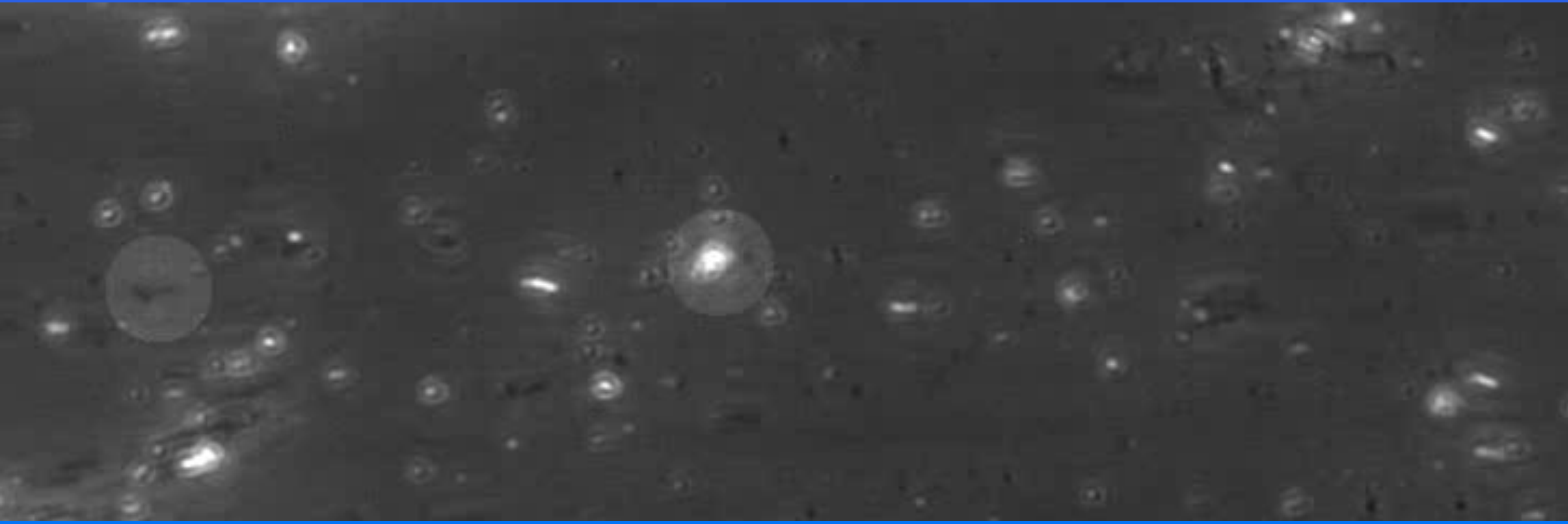
direct optical visualization
of the 24 nm flagella!





Tracer-bacterium interaction: cargo transport

Evidence for the long-range interaction

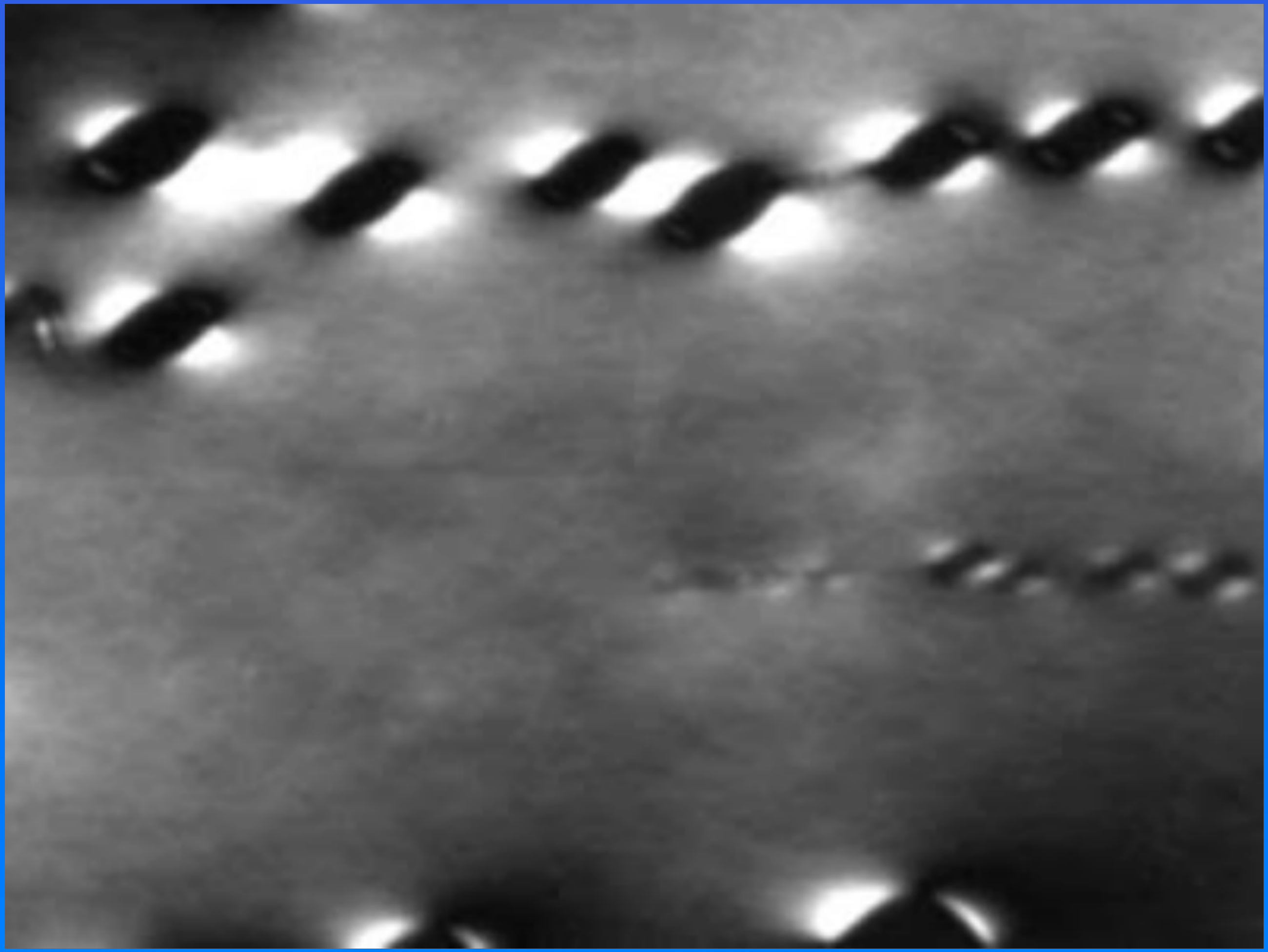


Sokolov, Zhou, Lavrentovich, IA PRE 2015

Living LC in the biphasic domain

higher temperature – nematic/isotropic phases co-exist

bacteria melt LC and nucleate tactoids – cloud chamber



Collective Effects: Formation of Stripes

scale depends on concentration, amount of oxygen

Active Turbulence in LC