Pattern Formation in Model Active Systems

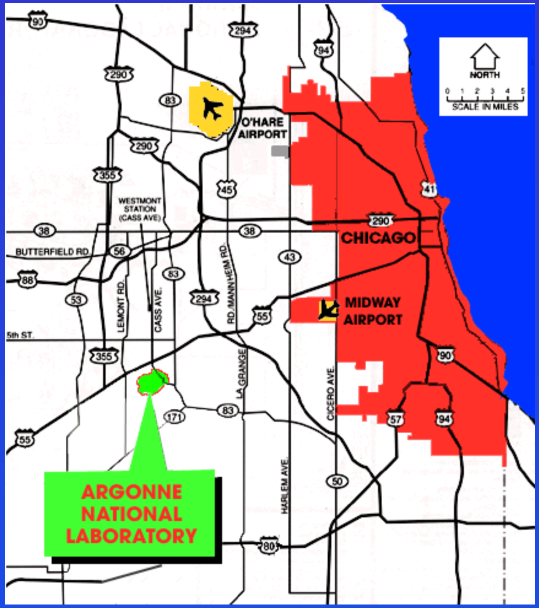
Igor Aronson

Argonne National Laboratory

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

- Tomorrow: simple kinetic theory for inelastic rods, application to microtubules/motors systems
- Then: models of collective swimming, viscosity reduction

Where in the World is Argonne?



World-Class Science

Unique Scientific Facilities

Free and Abundant Parking

25 min from Downtown Chicago

White Deer

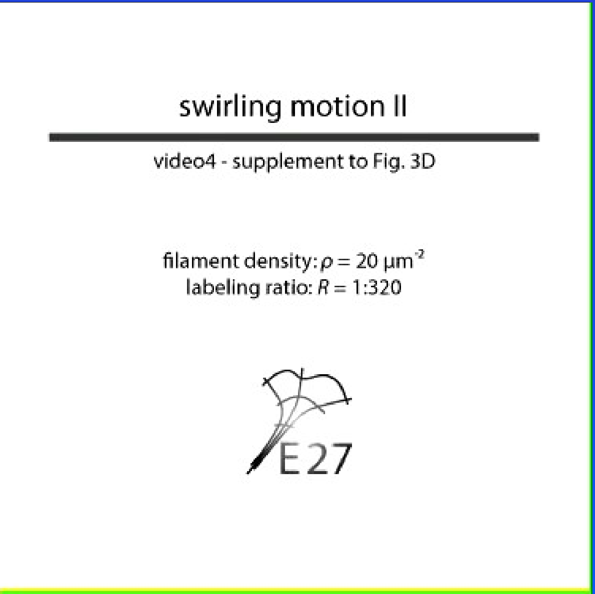
Energy Sciences Building

Stephen Chu

Collective Behavior in Living and Inanimate Matter

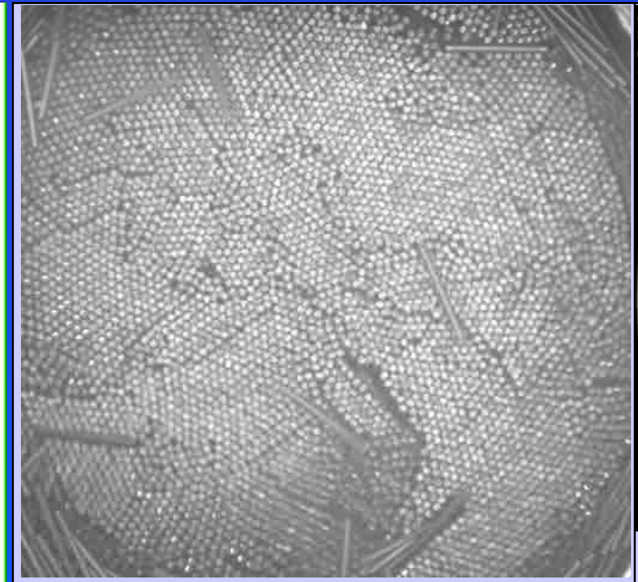
- **simple interactions – complex emergent behavior**
- **different mechanisms – similar patterns**

swirling actin



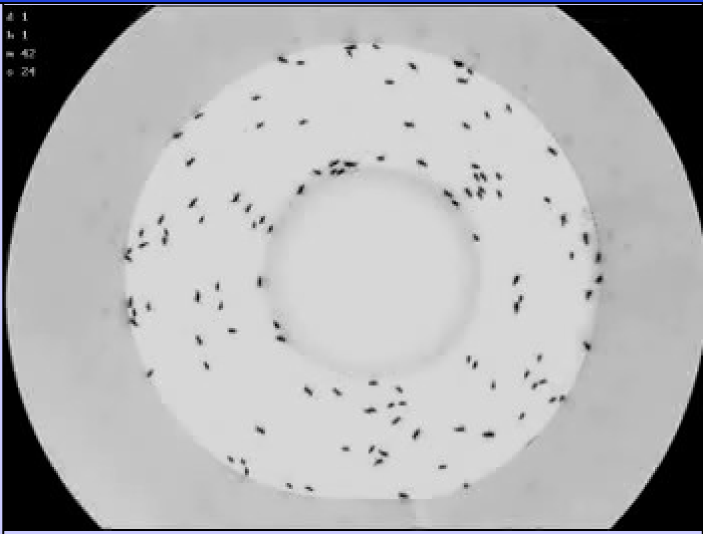
Schaller et al, Nature 2010

granular rods



Blair, Kudrolli, 2003

swarming hungry locusts

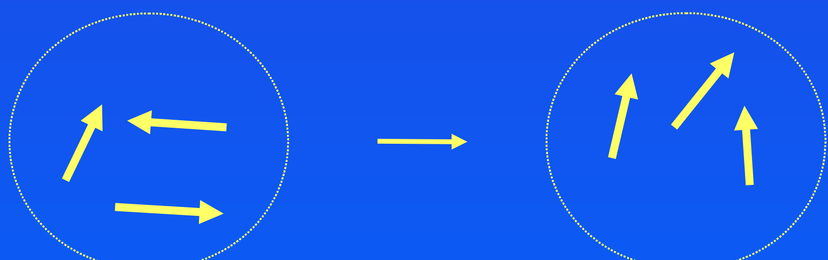


I. Cousin et al, Science, 2005

Vicsek Model: A Major Theoretical Milestone

- **Point particles (*boids*) 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**

1. Polar orienting interaction in a noisy environment



2. Streaming: motion along the polar direction

- **More complicated continuum hydrodynamic models (Tu, Toner, Ramaswamy)**

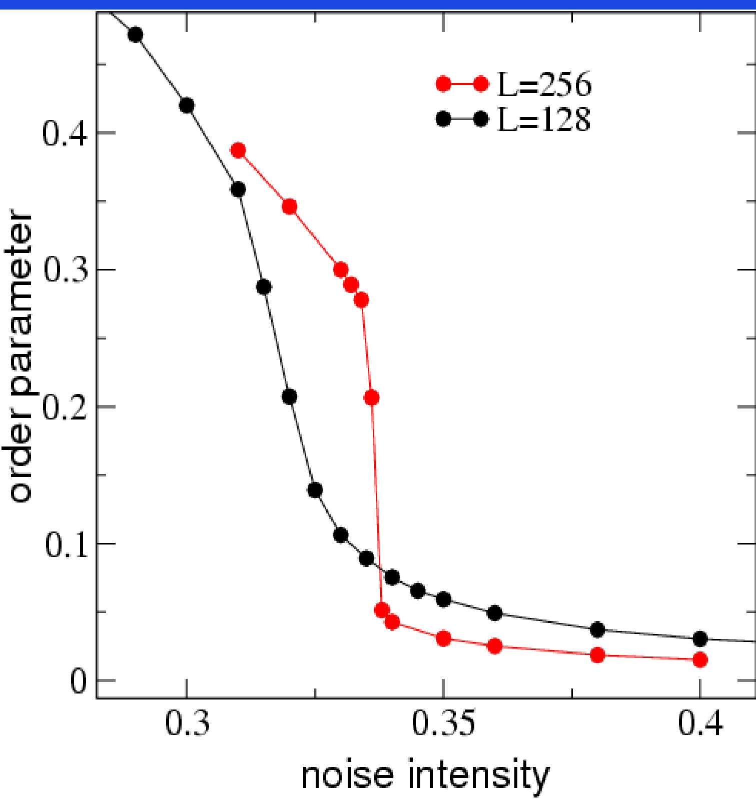
Simulations of Vicsek model

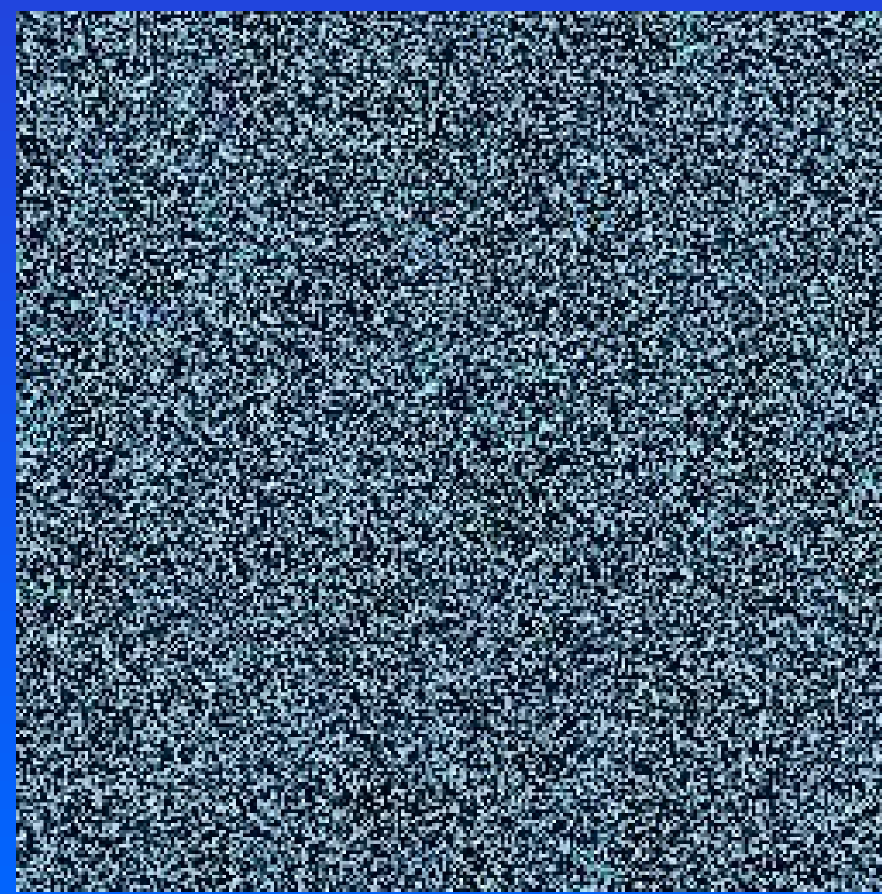
Chate and Gregoire,PRL 2004

Order parameter:
(similar to magnetization)

1,000,000 boids

at large size,
discontinuous transition





Fundamental Issues (Physicist Point of View)

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

Relation between collective behavior and the mechanisms of self-propulsion

Modeling of emergent collective behavior in the lab

Applications for dynamic self-assembly/materials design

Active Systems are Very Complex

Focus on simple yet non-trivial systems such as in vivo cytoskeletal networks, bacterial suspensions

Fundamental interactions are simple and well-characterized

Interactions are mostly of the “physical nature”: inelastic collisions, self-propulsion, hydrodynamic entrainment, vs chemotaxis, signaling etc

Derive continuum description from elementary interaction roles and connect observed patterns with experiment

Approach is mesoscopic and is complementary

Direct simulations of complex systems

Concept of Active Gels (extension of liquid crystal theory to active systems near thermodynamic equilibrium) by Prost, Joanny, Kruse, Julicher

Phenomenological theory by John Toner, Sriram Ramaswamy, Yuhai Tu

US DOE Materials Science and Engineering, Biomolecular Program

***Major thrust areas*: understanding, controlling, and building complex hierarchical structures by**

mimicking nature's self- and directed-assembly approaches

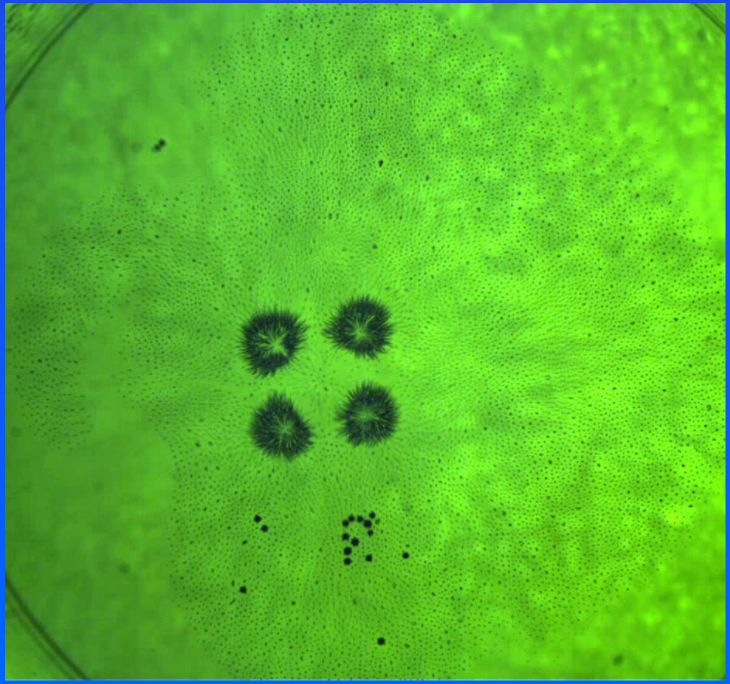
design and synthesis of environmentally adaptive, self-healing systems

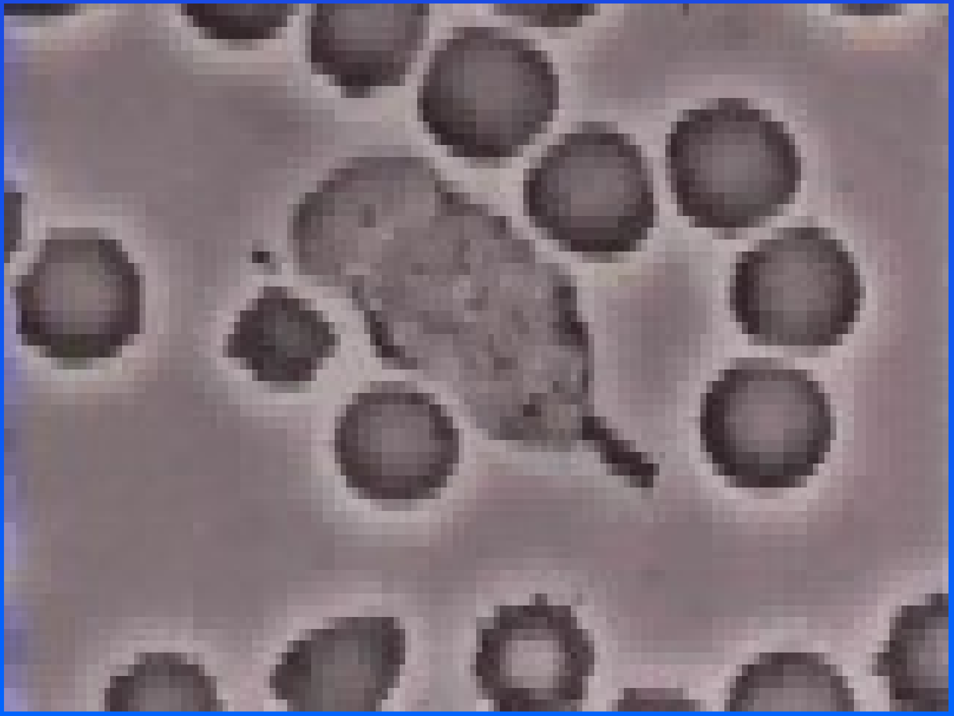
http://science.energy.gov/bes/mse/research-areas/biomolecular-mate

Active Systems – A Unique Opportunity for Materials Science

Design of active self-assembled structures with functionality not available under equilibrium conditions

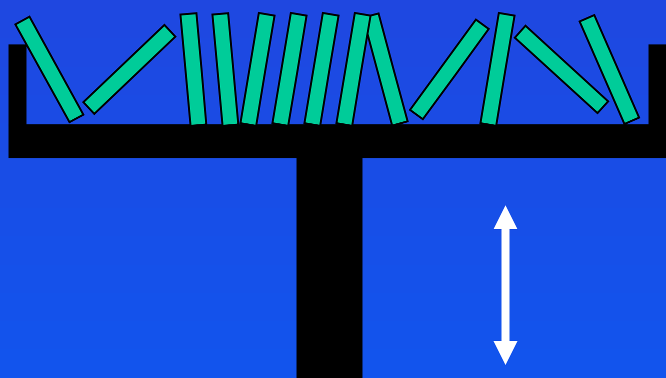
self-assembled colloidal robot





Blair-Neicu-Kudrolli experiment

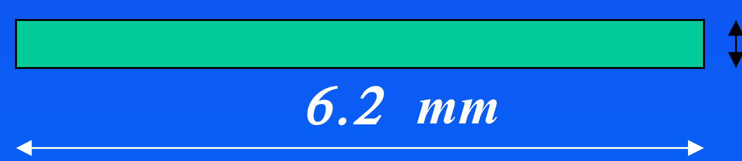
vibration of long rods



top view

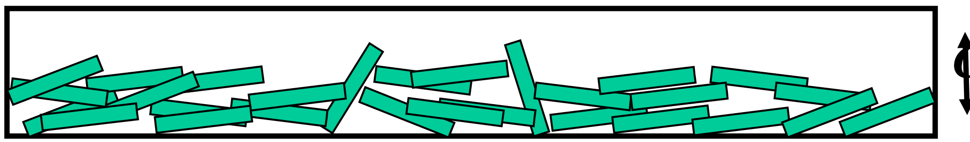
long Cu cylinders

# of particles 104

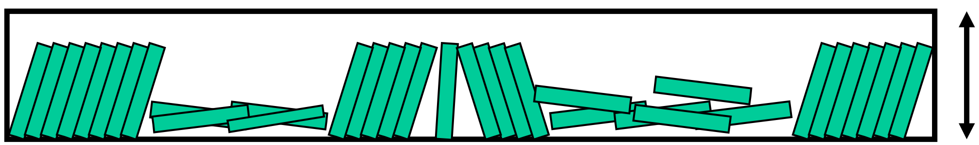


Phase transitions and vortices

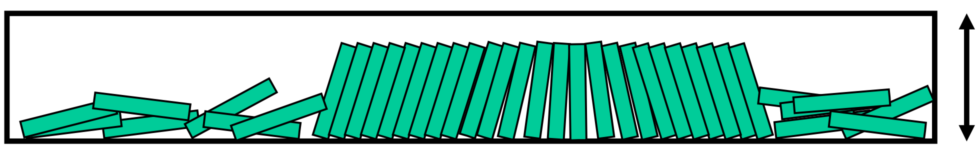
- *Weakly vibrated layer of rods*



- *Phase transition*



- *Coarsening*



- *Vortex motion*

Long-Term Evolution

Origin of Motion

Experiment

Simulations

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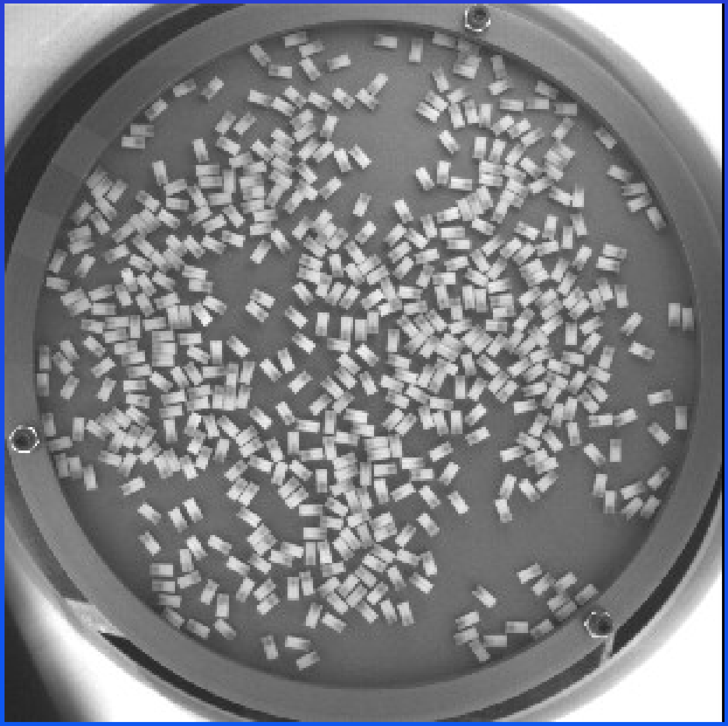
- ***Second level***
  - ***Third level***
    - ***Fourth level***
      - ***Fifth level***

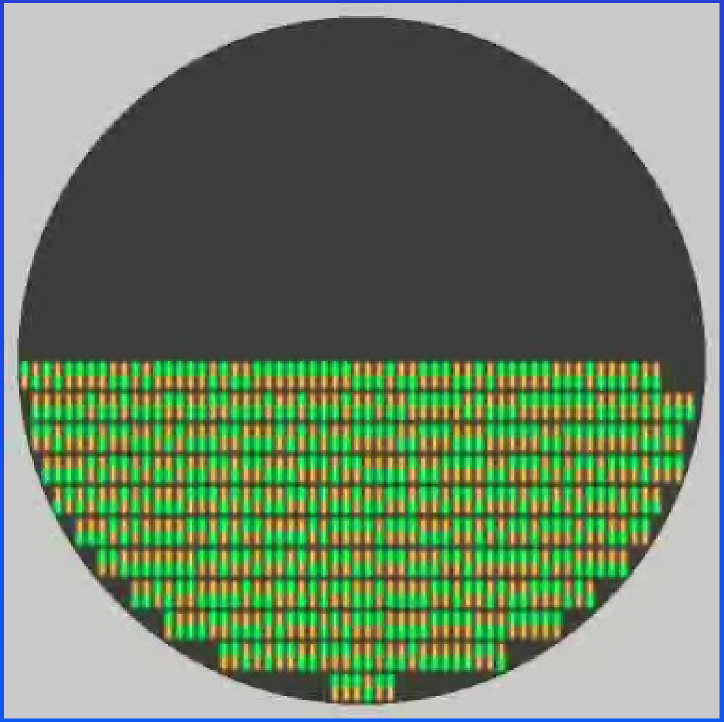
D Volfson, L Tsimring, A. Kudrolli

Swarming in Quasi-2D Experiments

Experiment, 500 asymmetric rods



Simulations, 500 rods

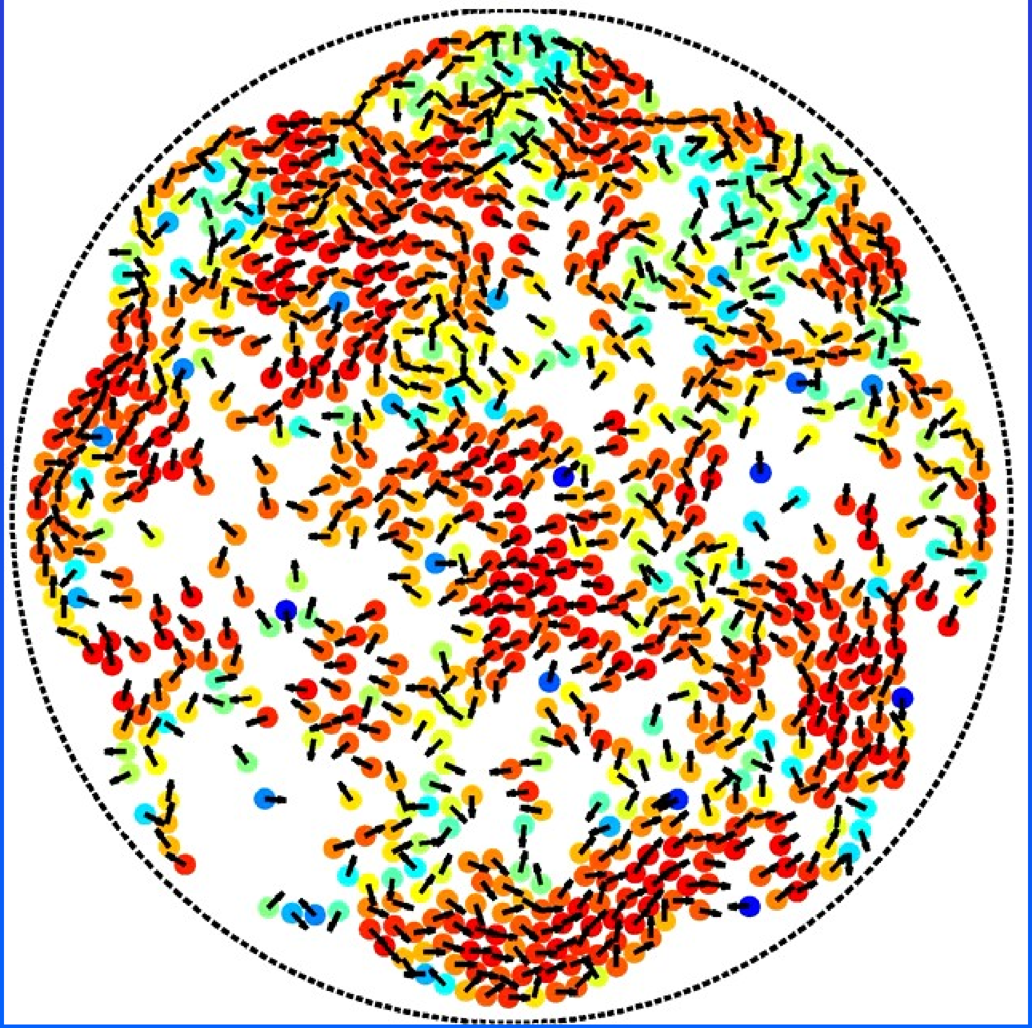


Lumay, D Volfson, L Tsimring, A. Kudrolli PRL 2008

Vibrated Polar Disks

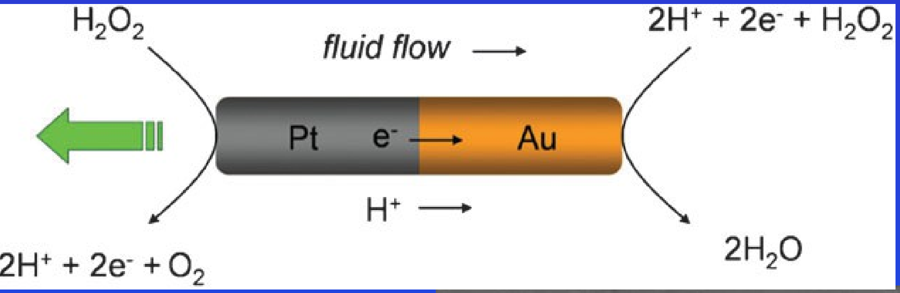
Experiment, 1000 asymmetric disks

re-injecting boundary conditions



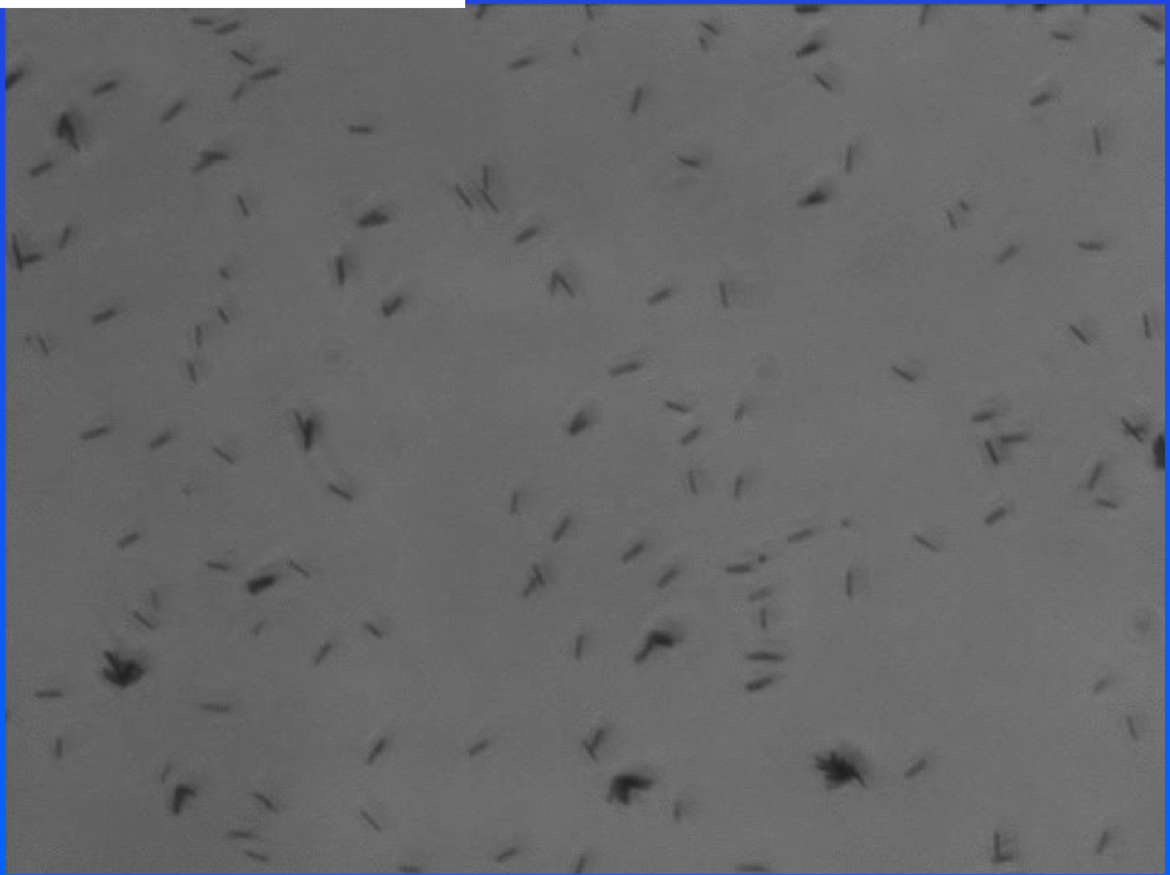
Deseigne, Dauchot, Chate, PRL 2010

Recruiting Nanofabrication: micron-size AuPt rods swim in H2O2

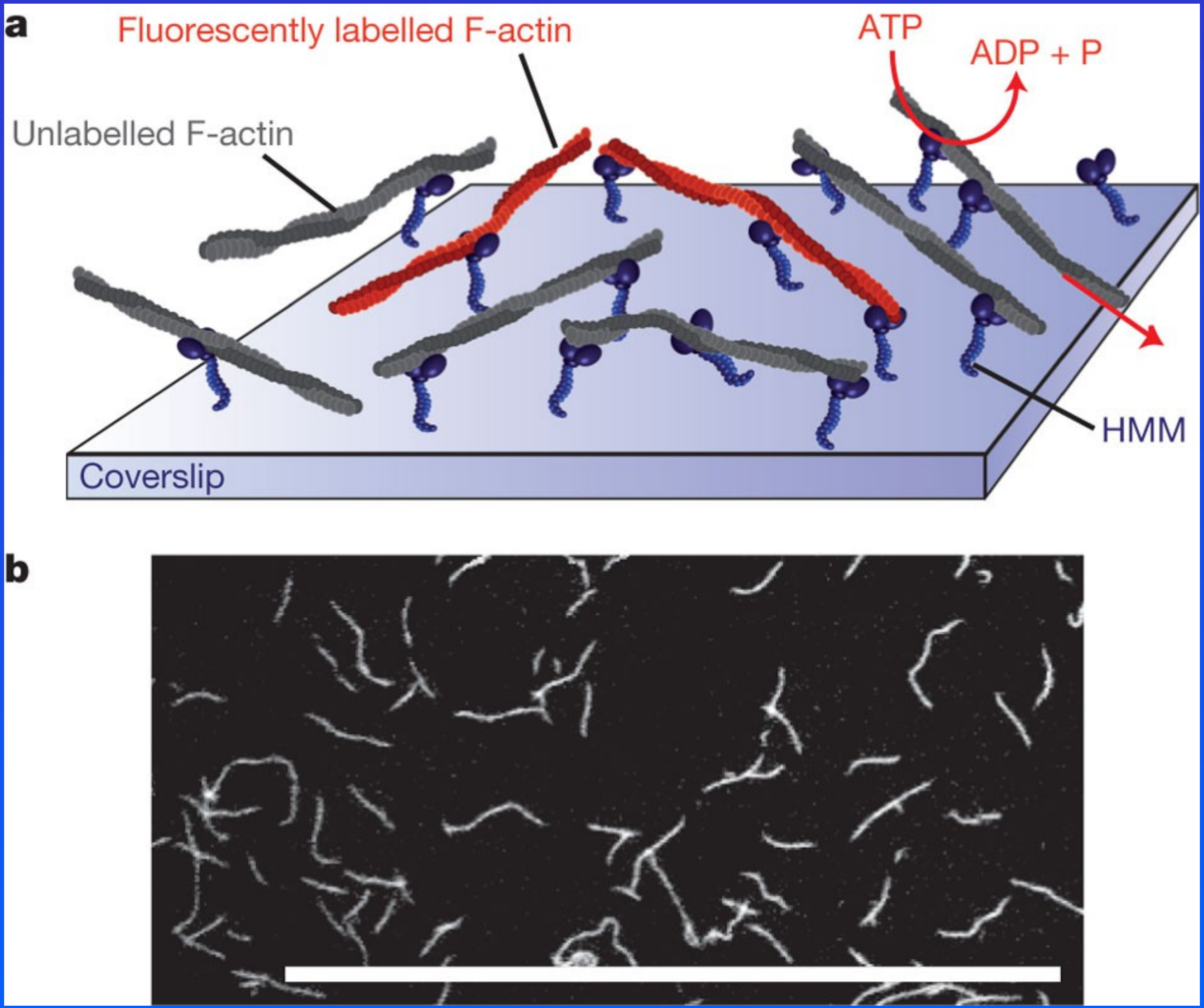


AuPt & AuRu microrods are provided by Ayusman Sen and Tom Mallouk, PSU

Movie: Argonne



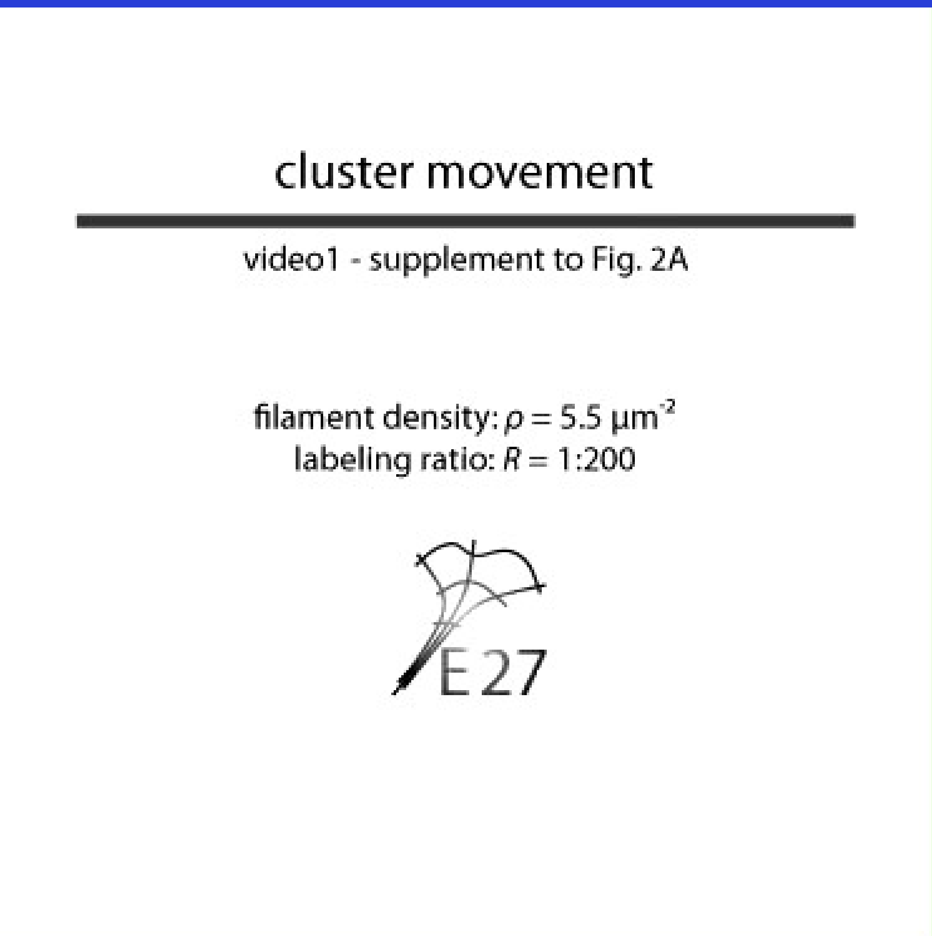
Actin-Myosin Motility Assay



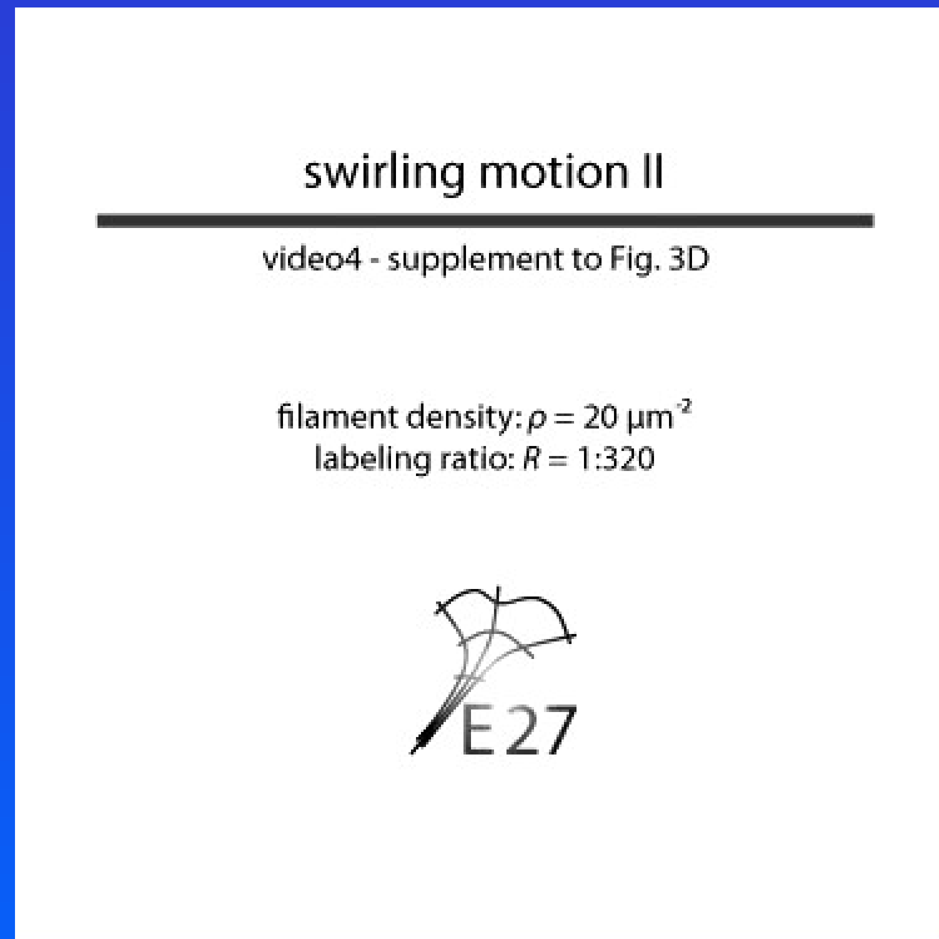
V Schaller et al. Nature 467, 73-77 (2010)

Moving Clusters and Swirls

moderate density



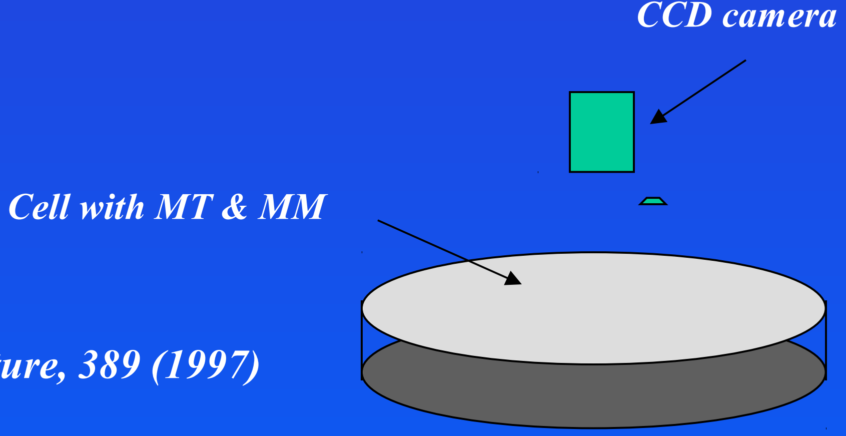
higher density



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

in-vitro Self-Assembly of MT and MM

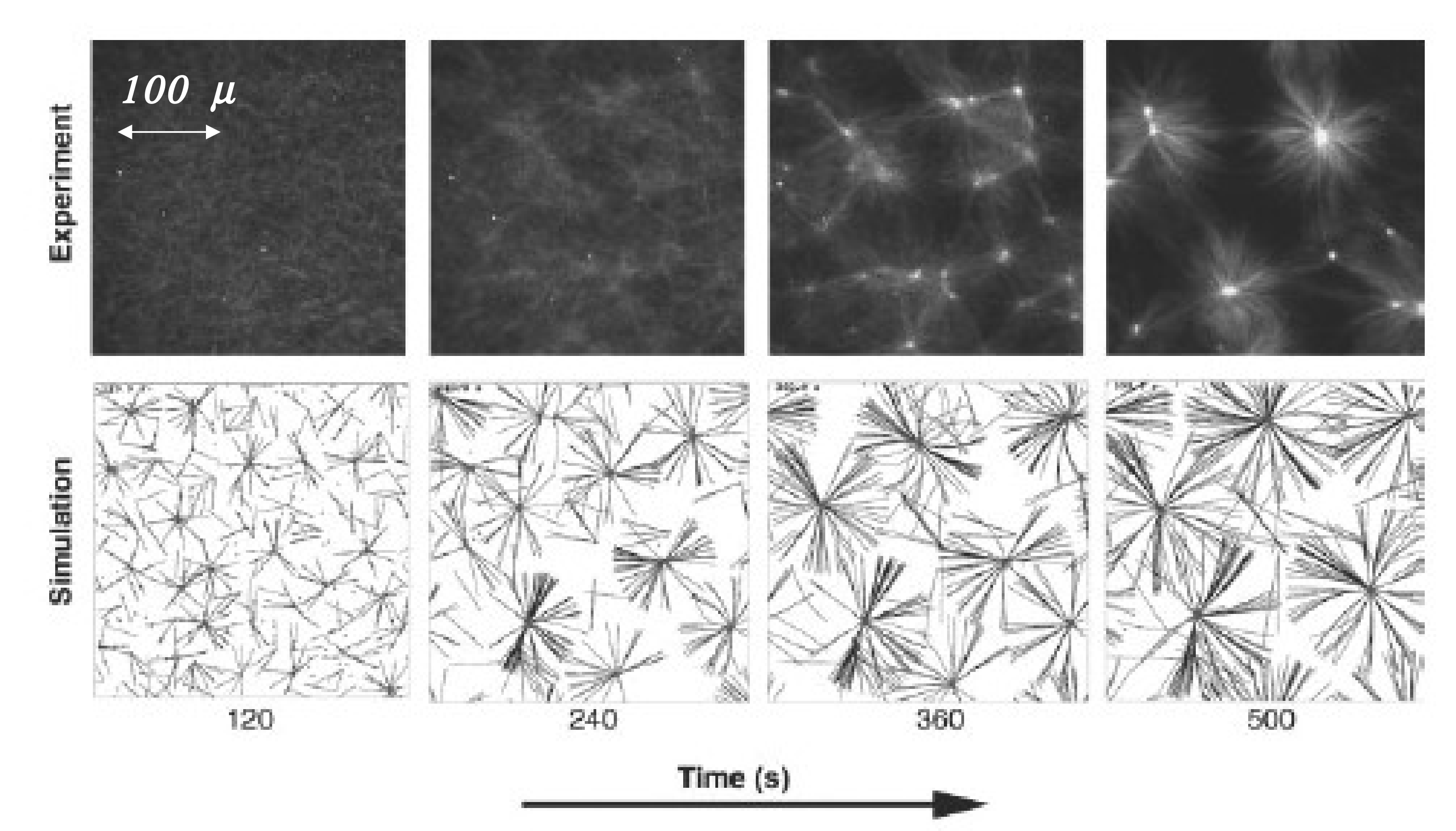
- ***Simplified system with only few purified components***
- ***Experiments performed in 2D glass container: diameter 100 µm, height 5µm***
- ***Controlled tubulin/motor concentrations and fixed temperature***
- ***MT have fixed length 5µm due to fixation by taxol***



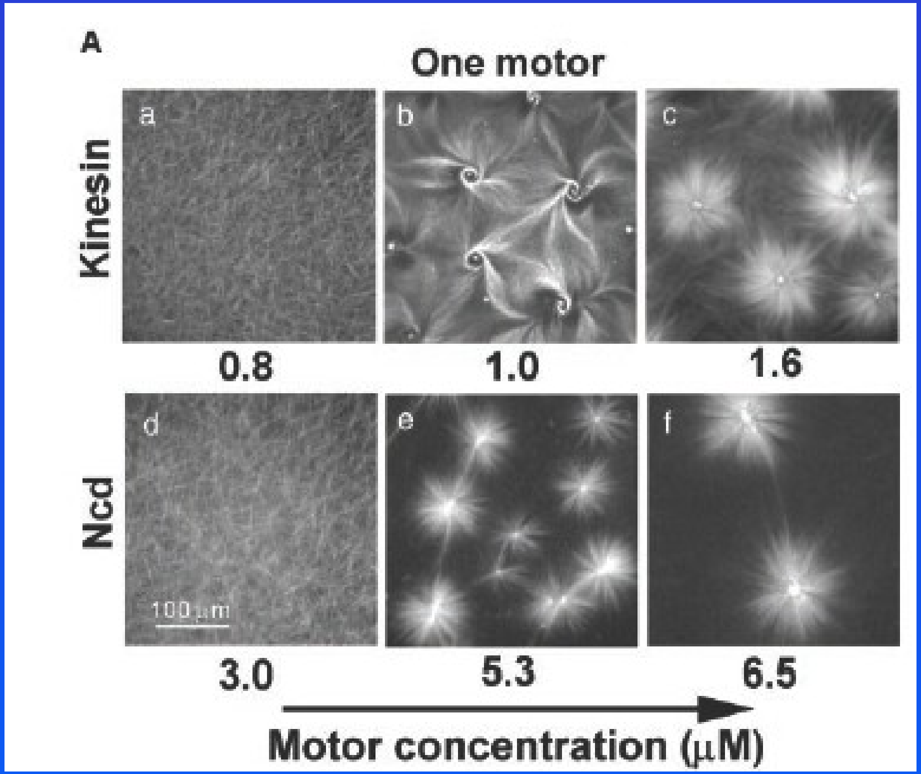
F. Nedelec, T. Surrey, A. Maggs, S. Leibler,
Self-Organization of Microtubules and Motors, Nature, 389 (1997)
T. Surray, F. Nedelec, S. Leibler & E. Karsenti,
Physical Properties Determining Self-Organization of Motors & Microtubules, Science, 292 (2001)

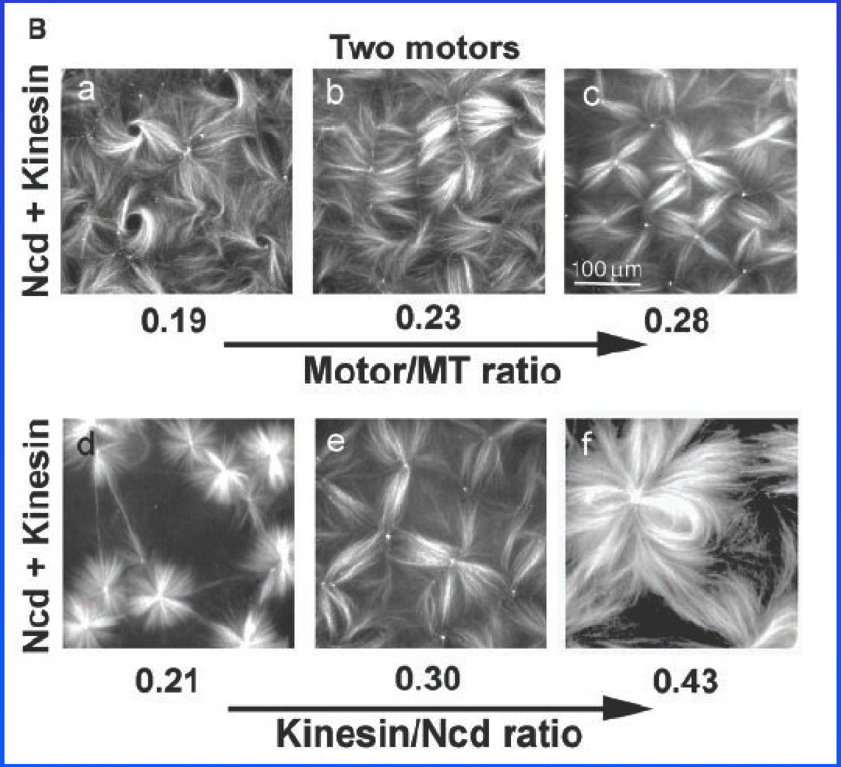
Patterns in MM-MT mixtures

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

Click to edit Master text styles

- *Second level*
  - *Third level*
    - *Fourth level*
      - *Fifth level*

Summary of Experimental Results

2D mixture of MM & MT exhibits pattern formation

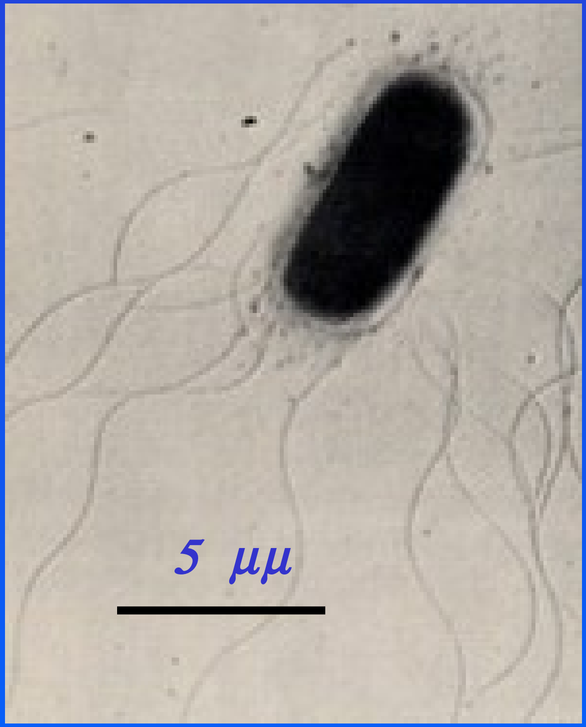
Kinesin: vortices for low density of MM and asters for higher density

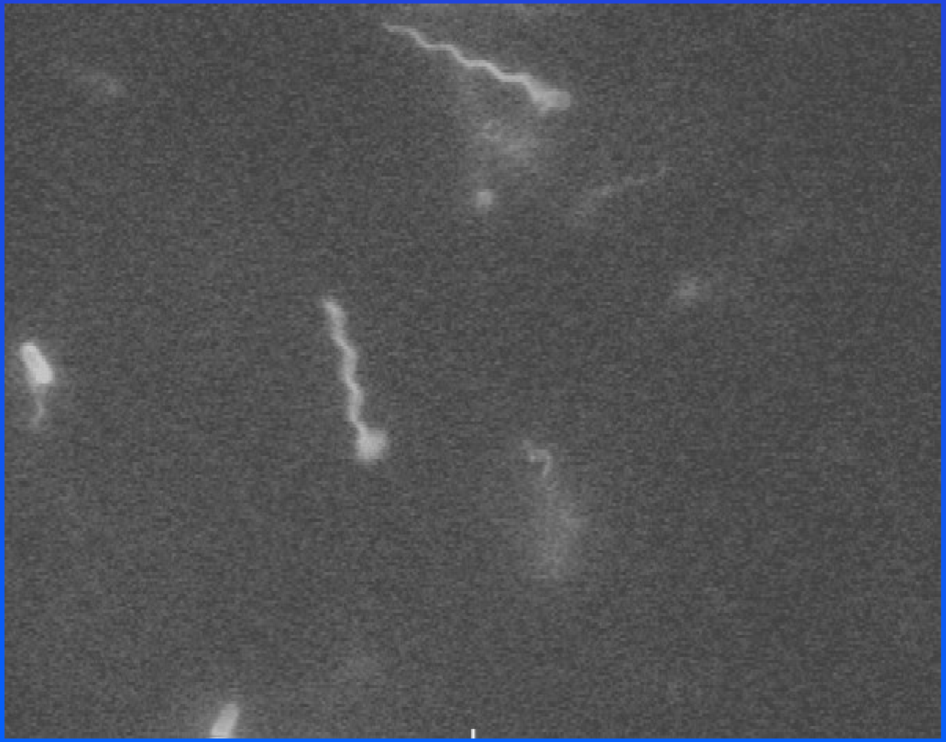
Ncd: only asters are observed for all MM densities

For very high MM density asters disappear and bundles are formed

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)

Swimming Algae

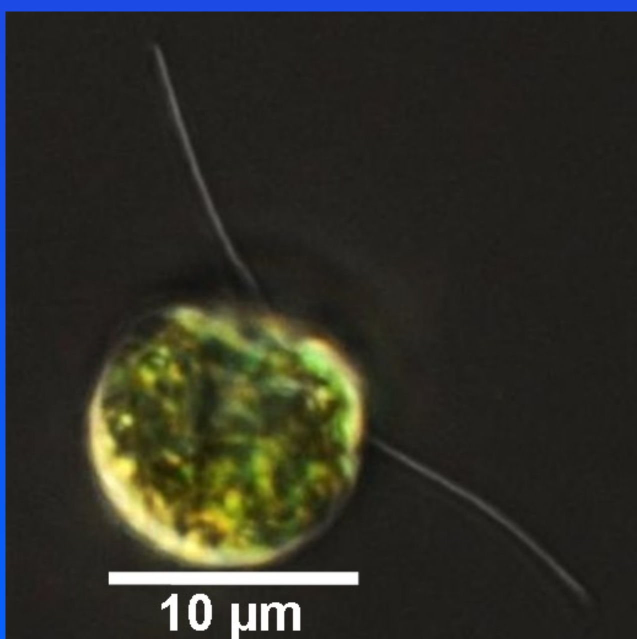
Eukaryotic Clamydomonas reinhardtii

Size: 10 mm, two flagella ~10 mm

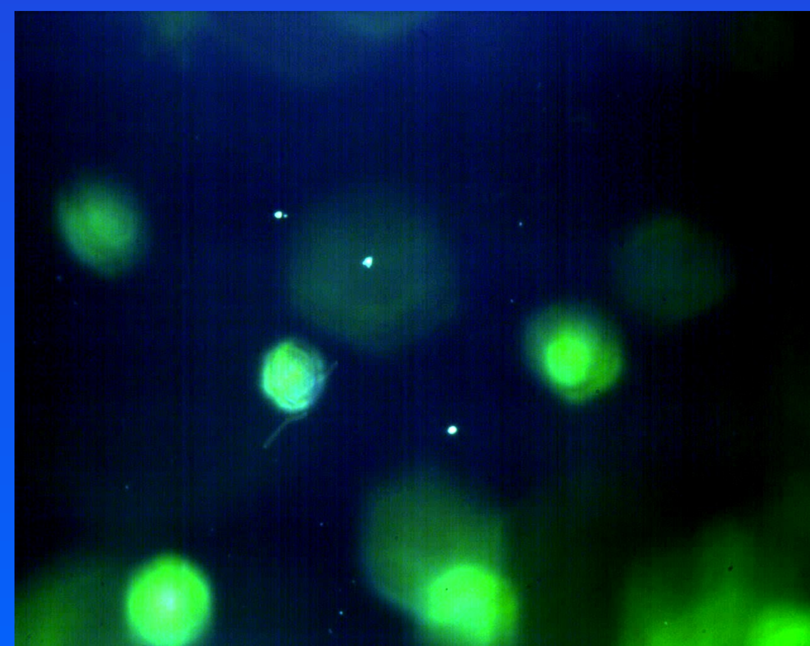
Swimming speed: 50-100 mm/sec

Highly asocial animals

Single Alga



Algae Suspension

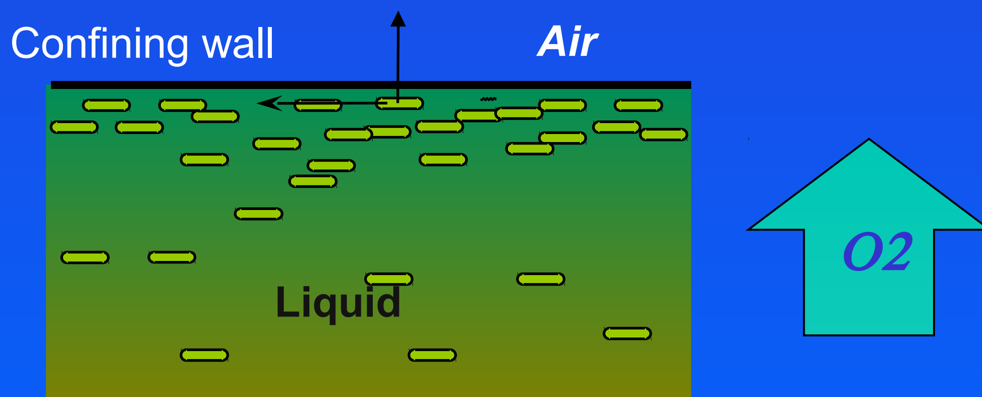


Bacillus subtilis primary behaviors

Top view

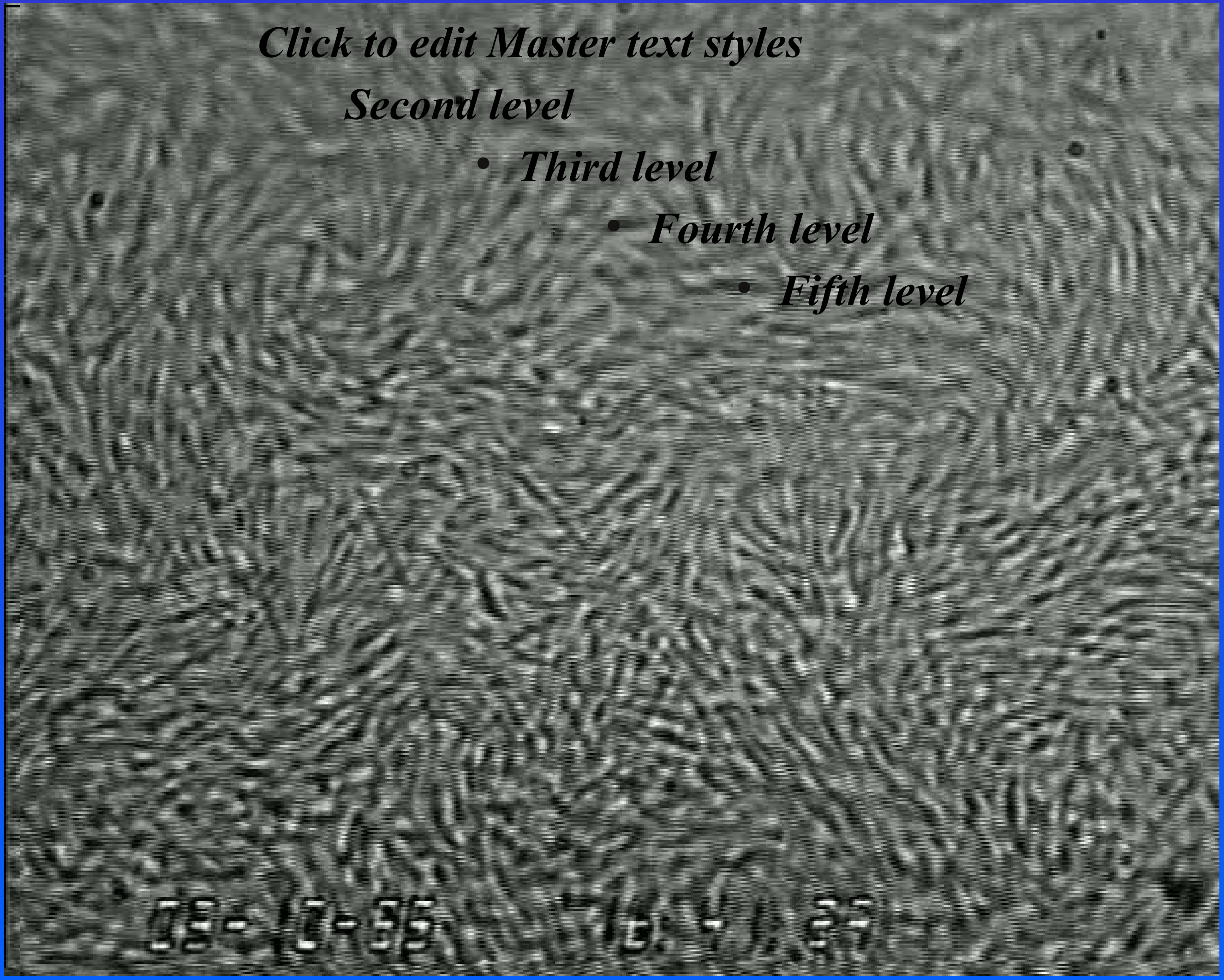
- *Excellent swimmers*
- *No tumbling*

Side view



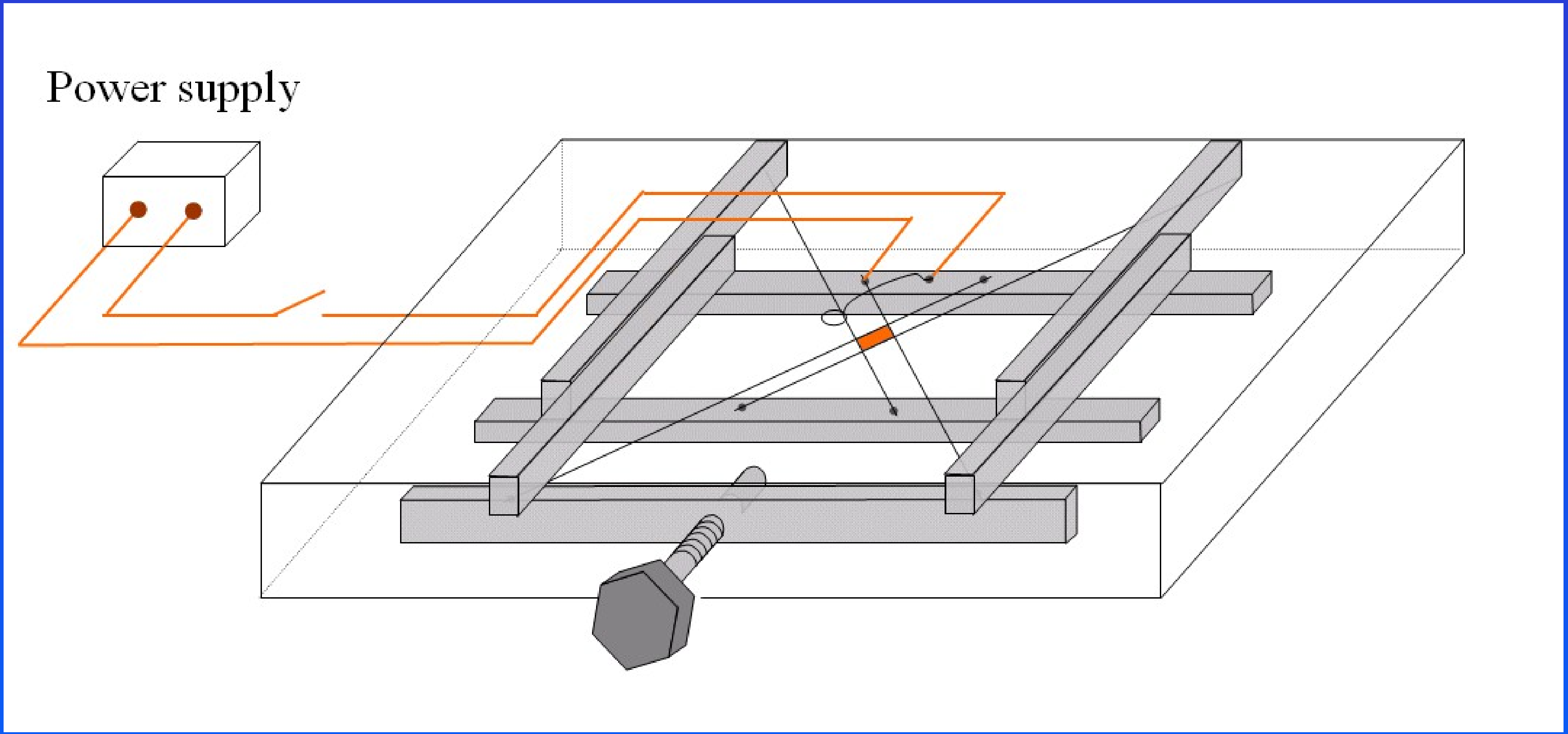
Concentration of bacteria near the surface due to gradient of dissolved Oxygen

Bacterial Turbulence



Goldstein, Kessler, et al PRL 2004

Schematics of Experimental Setup

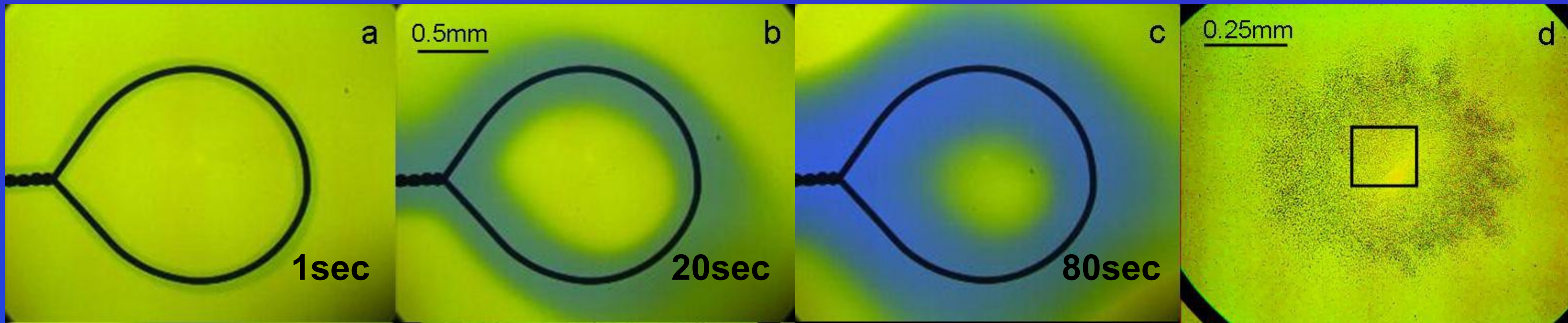


Thin free-standing film concept

Adjustable thickness

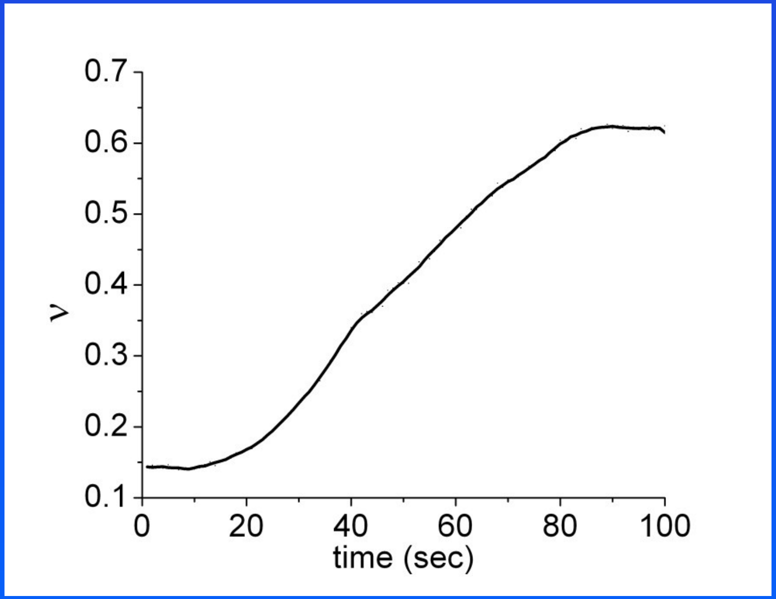
Adjustable concentration of bacteria

pH-Taxis & concentration of cells



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

concentration vs. time



Bacteria crowd control

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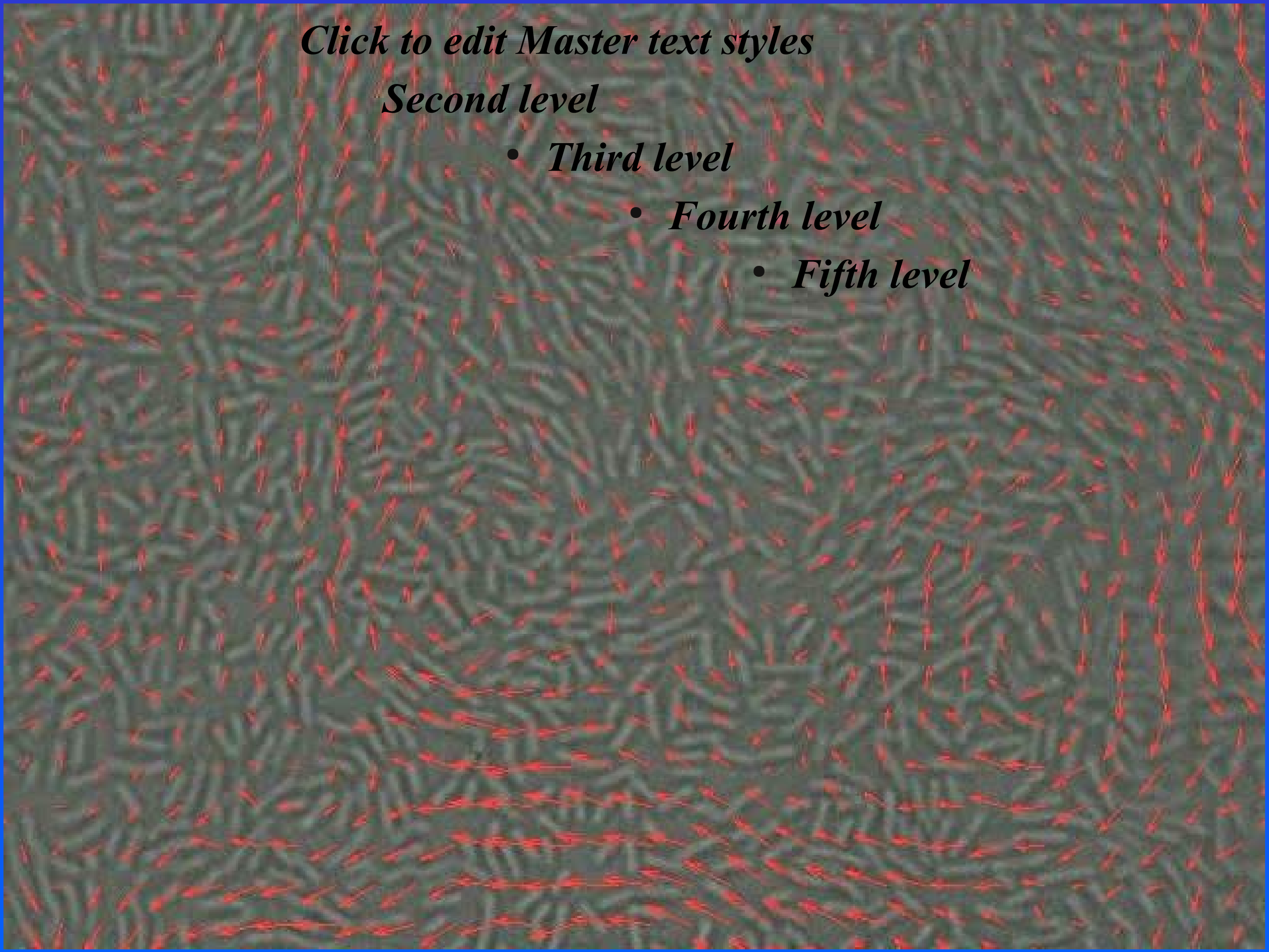
  - *Third level*
    - *Fourth level*
      - *Fifth level*

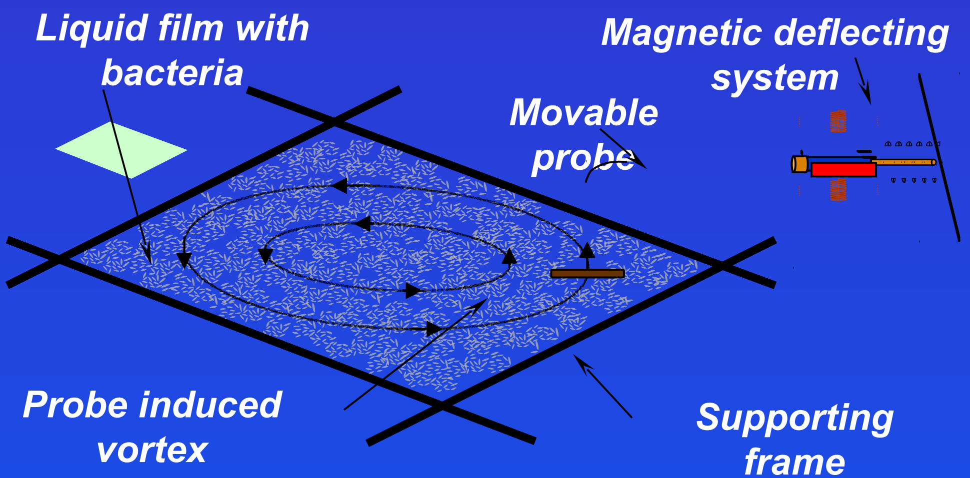
Bacterial Turbulence



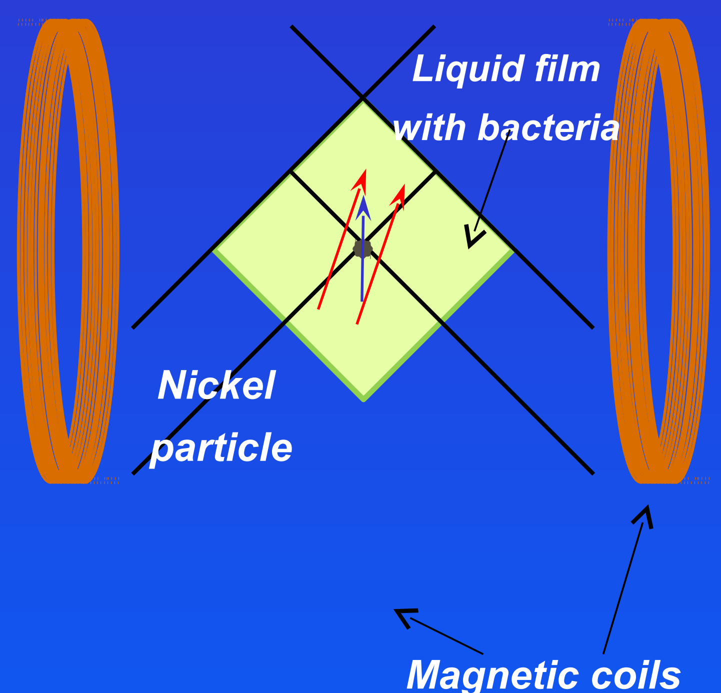
Sokolov, Goldstein, Kessler, I.A PRL (2007)

7-fold reduction of viscosity

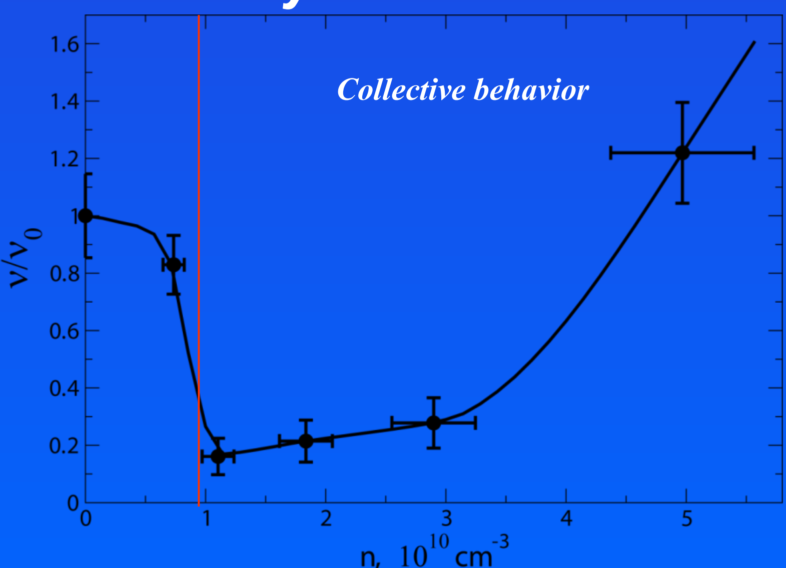
vortex probe micro-rheometer



rotational micro-rheometer



viscosity vs concentration



Sokolov & I.A, PRL 2009

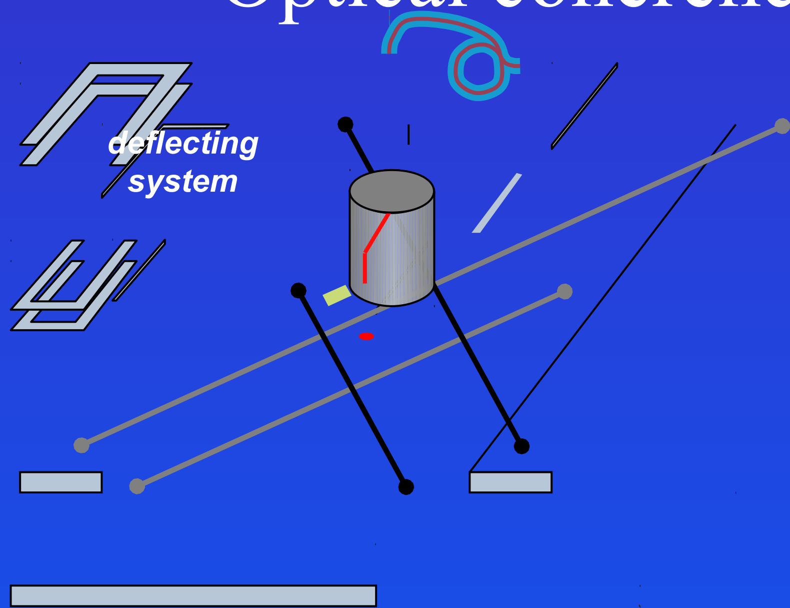
viscosity is extracted from the vortex decay time

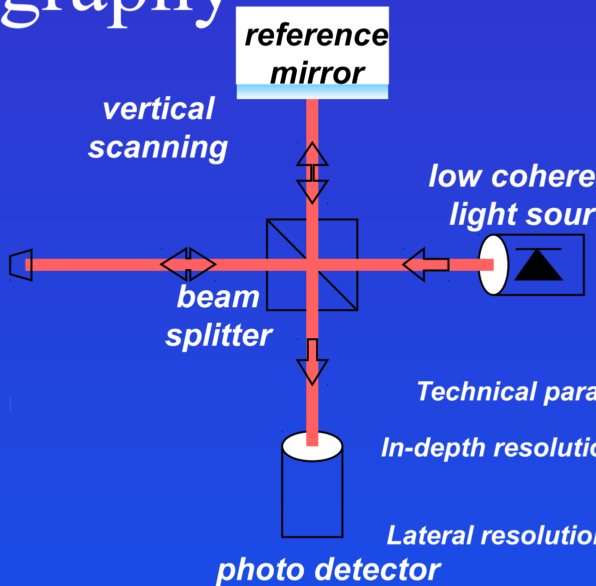
viscosity is extracted from the magnetic torque

viscosity vs concentration and swimming speed of bacteria

Mixing and self-diffusivity in bacterial suspensions

Optical coherence tomography



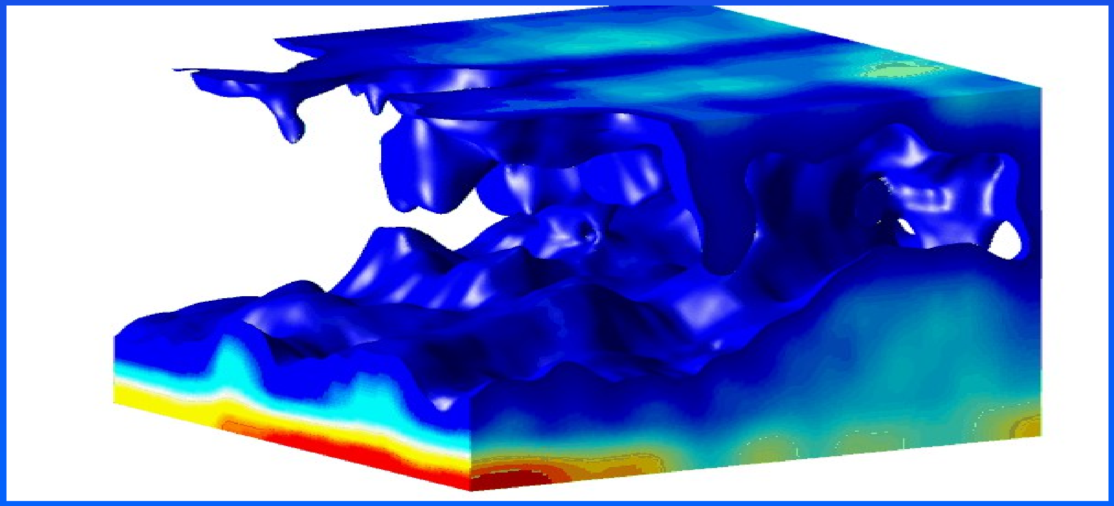


Technical parameters

In-depth resolution = 15μm

Lateral resolution = 25μm

3D concentration distribution



collective swimming enhances mixing by a factor of 10

confinement reduces mixing rates

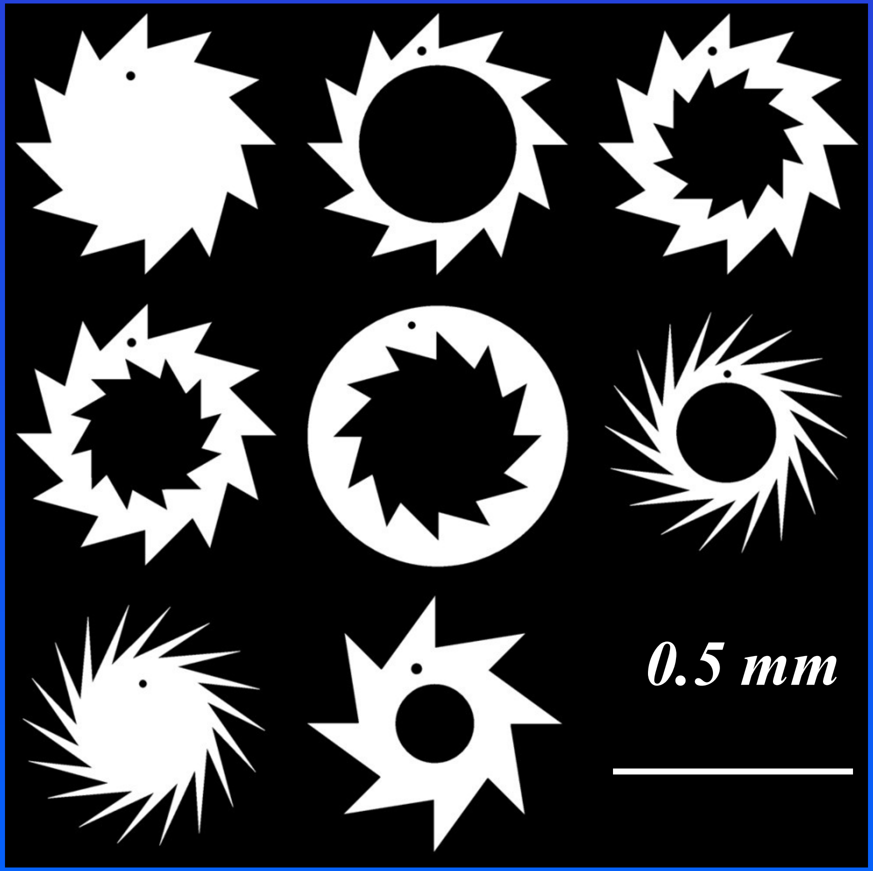
nontrivial 3D patterns result in enhanced transport

Sokolov, Feldstein, Goldstein, I.A, PRE 2009

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

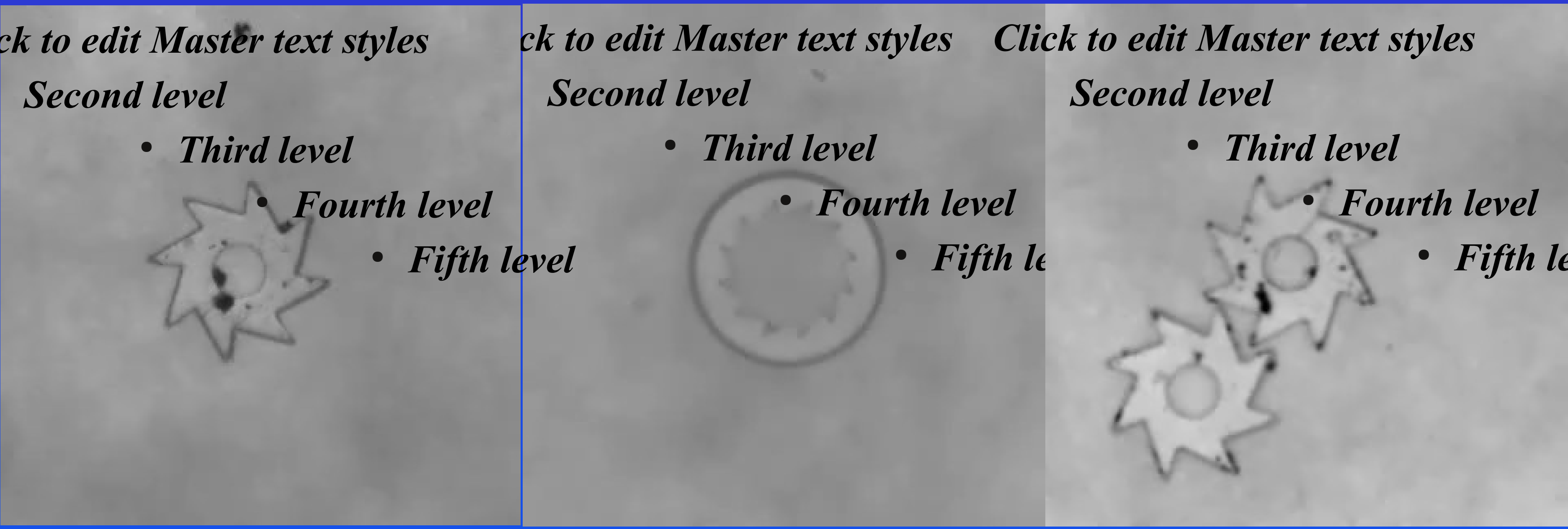
Photolithography technique

Mass of Gear ~106 mass of bacteria

Collaboration with Bartosz Grzybowski, Northwestern University

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

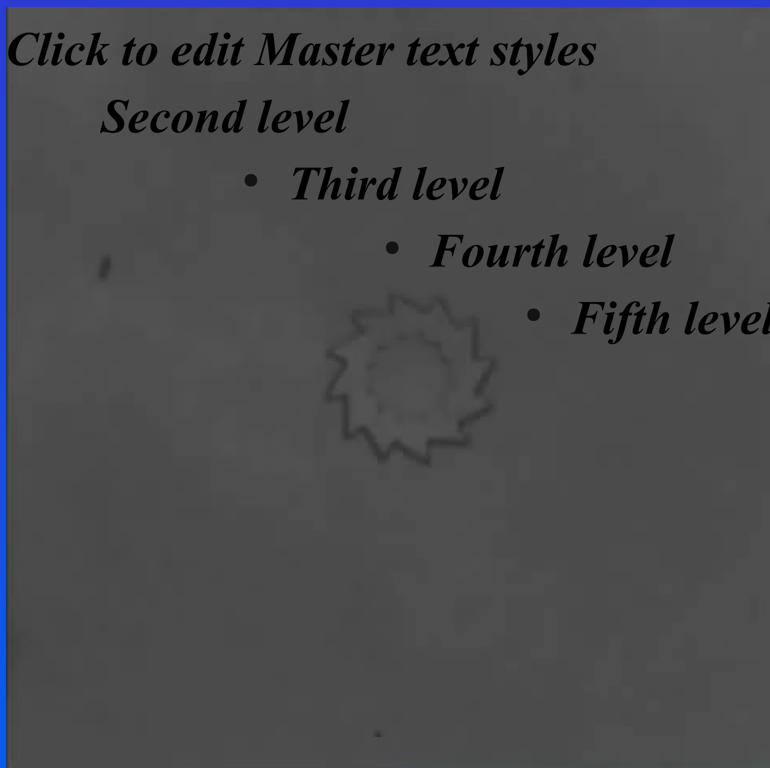
Gears Turned by Bacteria



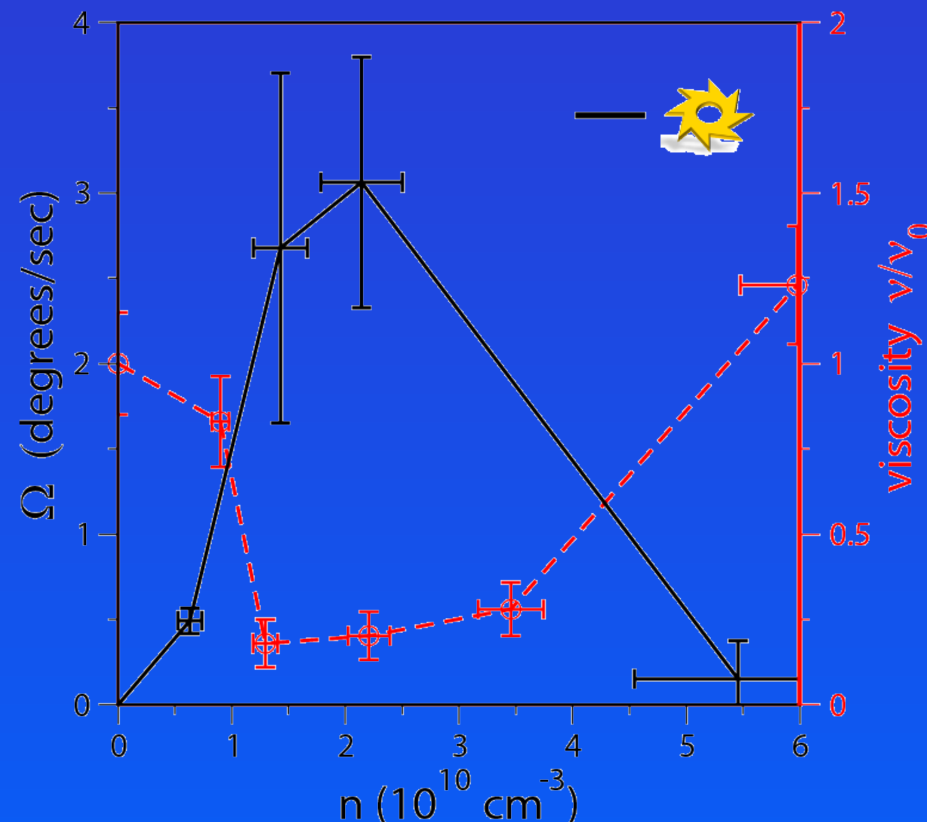
1 mm

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

Control of Rotation



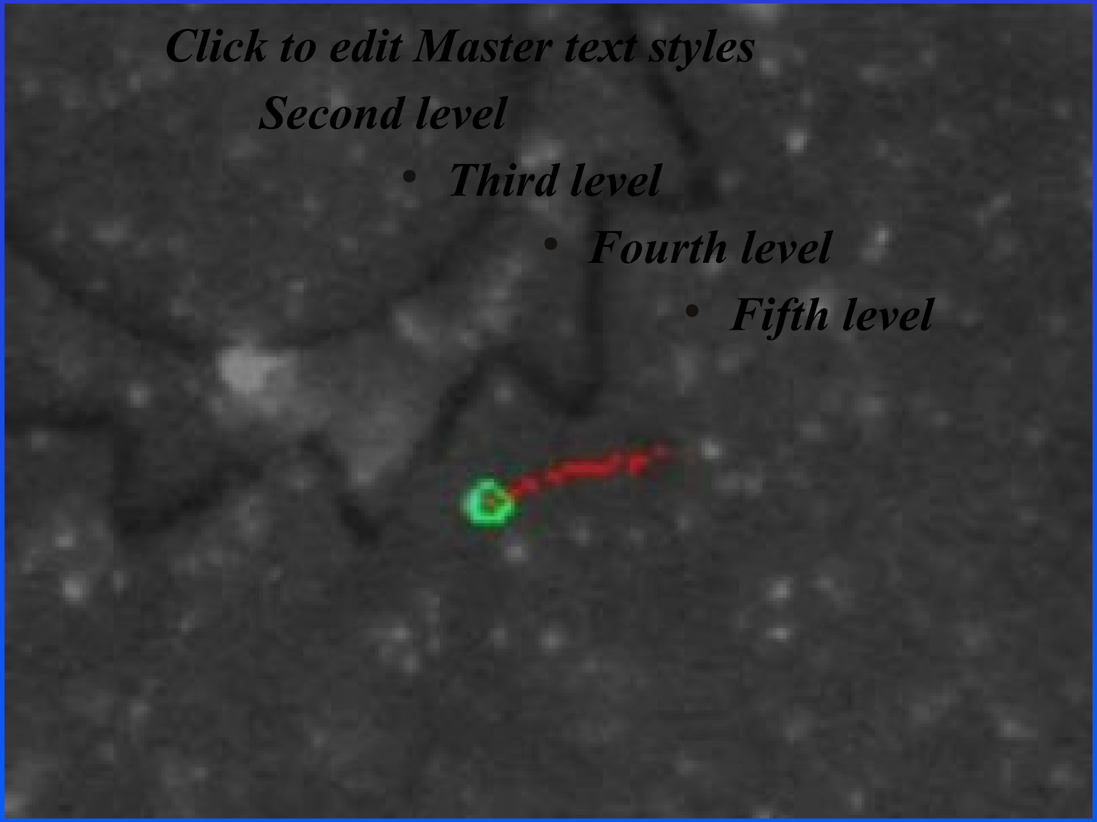
Rotation rate vs concentration



- **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**
- **Consistent with simulations by Angelini et al, PRL 2008**