Collective Dynamics in Suspensions of Swimmers

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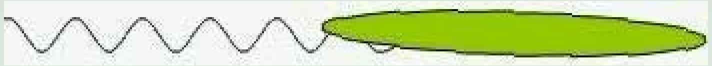
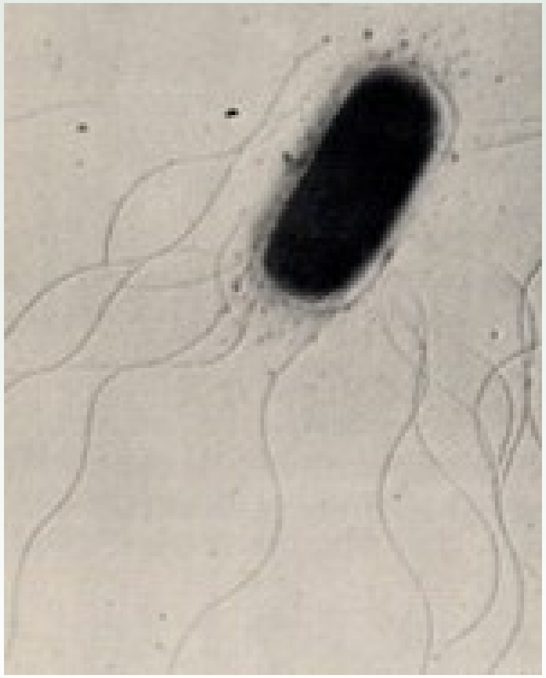
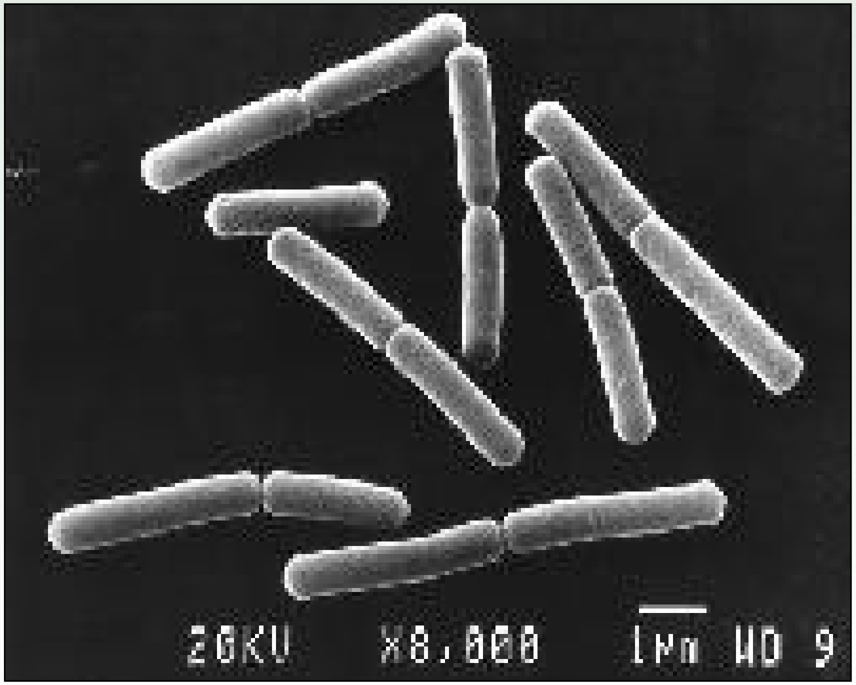
Supported by US Department of Energy

Self-Propelled BioParticles

swimming bacteria Bacillus Subtilis
length 5 μm, speed 20 μm/sec
collective flows up to 100 μm/sec

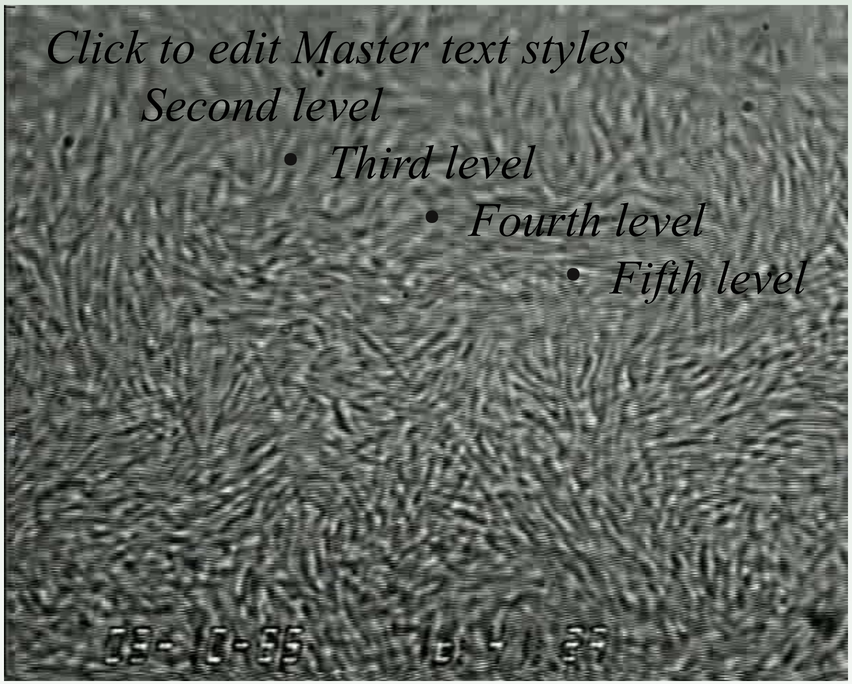


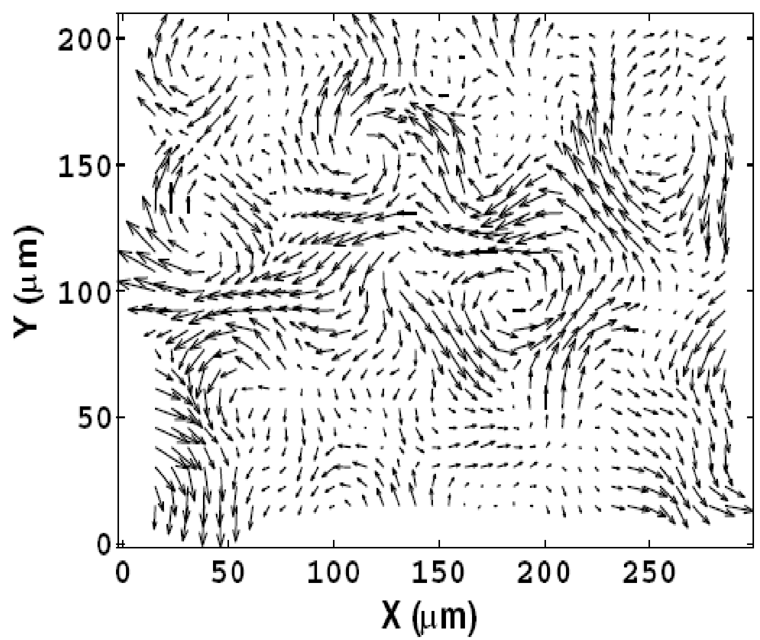




Large-Scale Coherence: “Flat” Sessile Drop

Bugs concentrate at the contact line

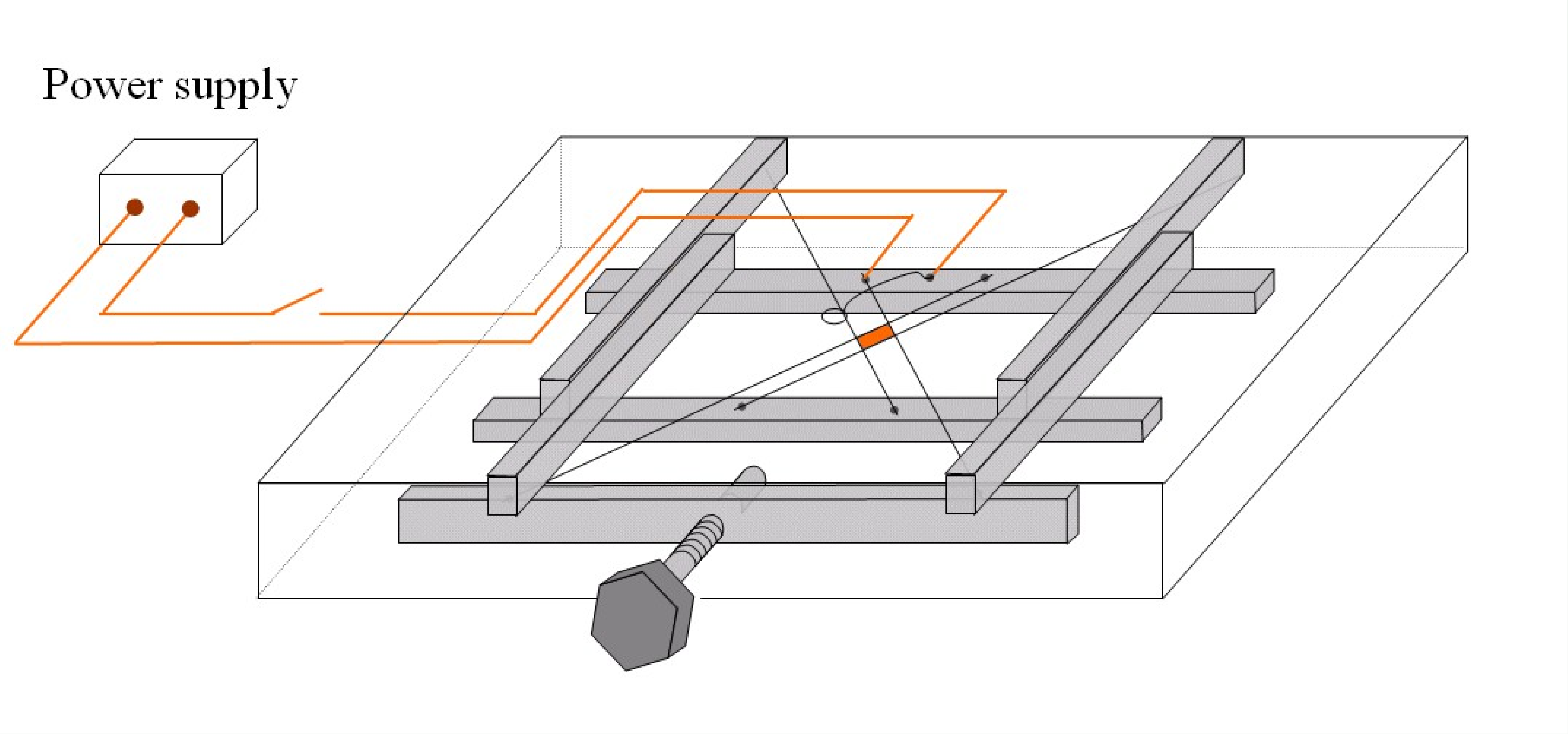




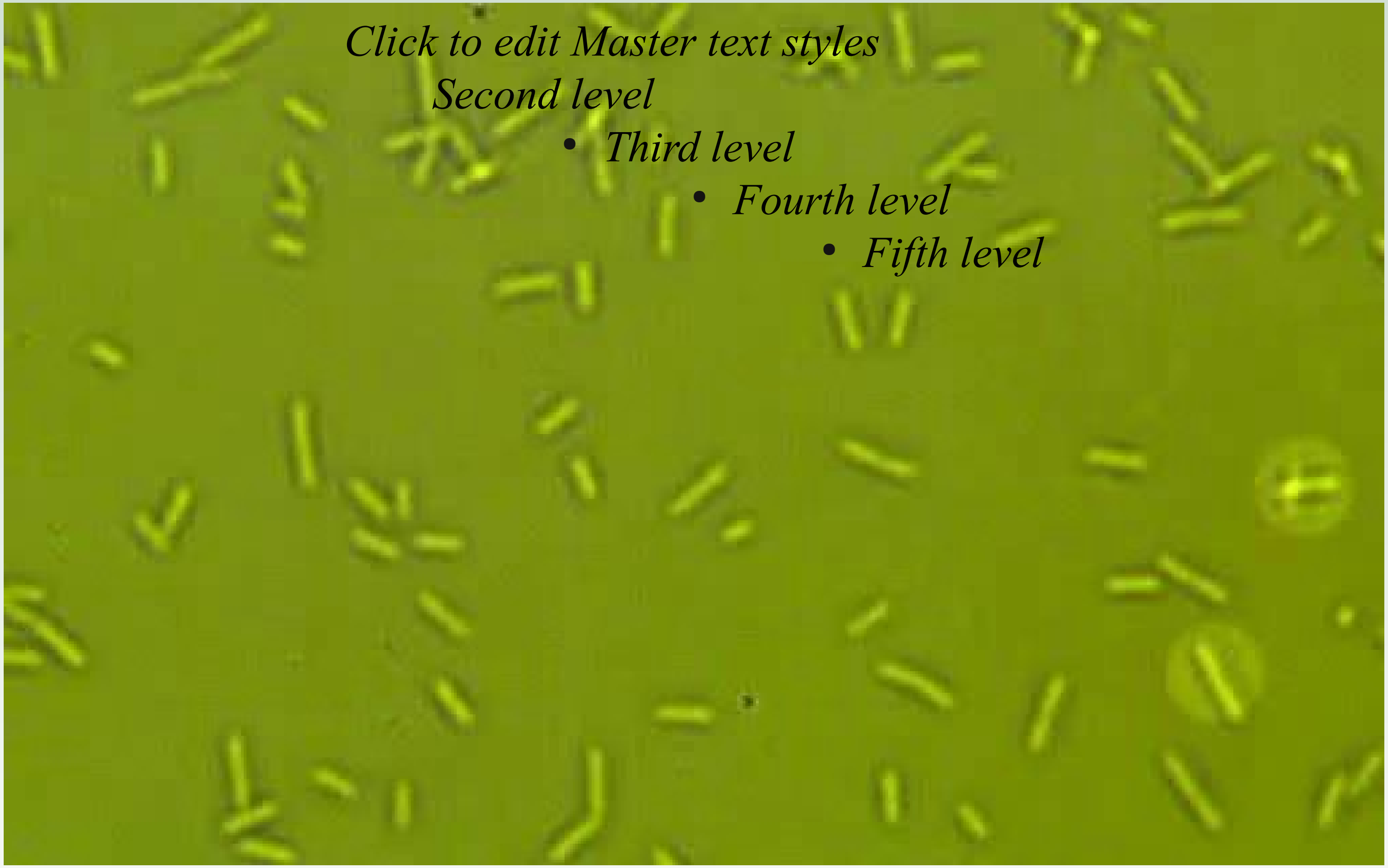
Dombrowski, Cisneros,Chatkaew, Goldstein, Kessler, PRL (2004)

Schematics of Experimental Setup

Concept: Andrey Sokolov, ANL



Inelastic collisions between bacteria



Click to edit Master text styles
- *Second level*
  - *Third level*
    - *Fourth level*
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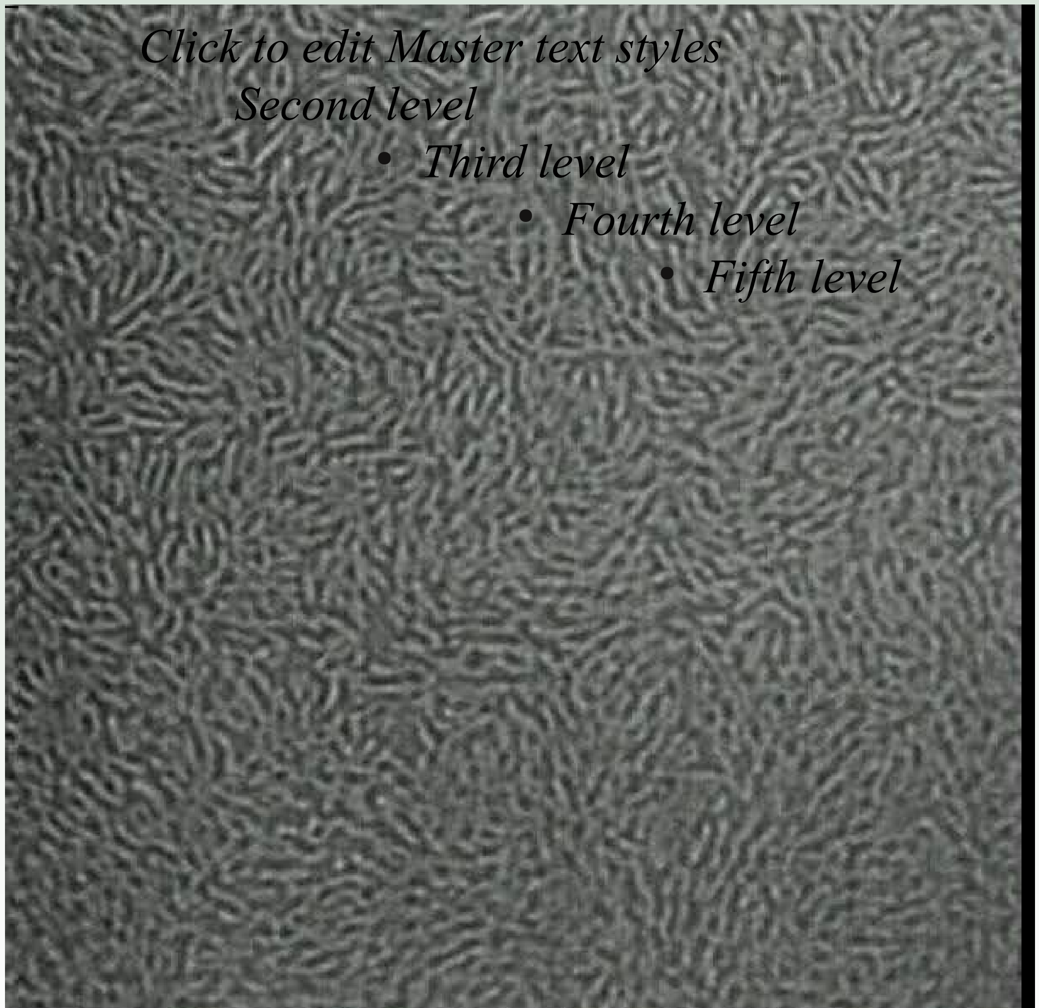
Andrey Sokolov & Igor Aranson, ANL
Ray Goldstein & John Kessler, U Arizona

Collective swimming transition



- *Click to edit Master text styles*
  - *Second level*
    - *Third level*
      - *Fourth level*
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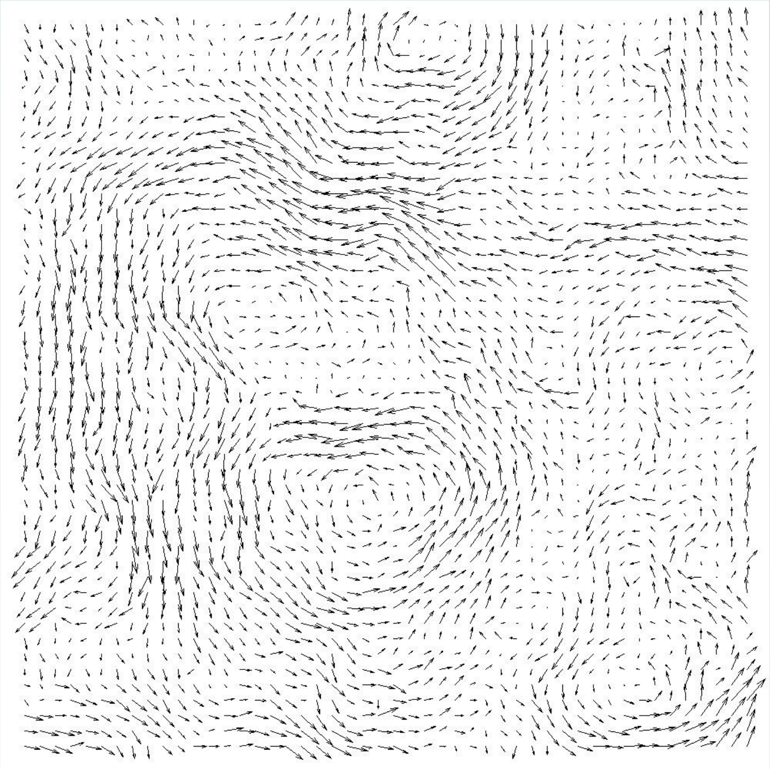
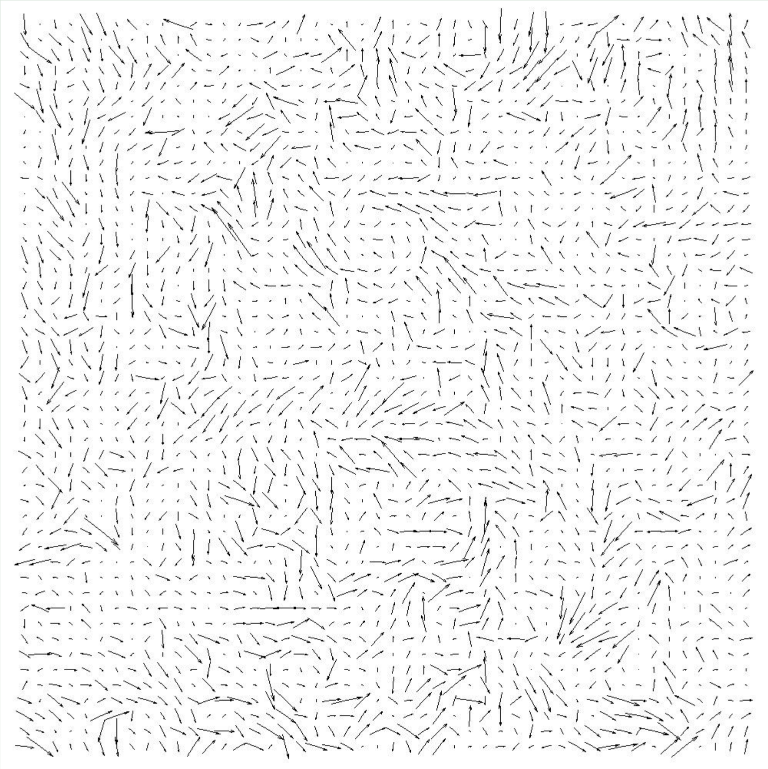
Velocity-Orientation Correlation Lost

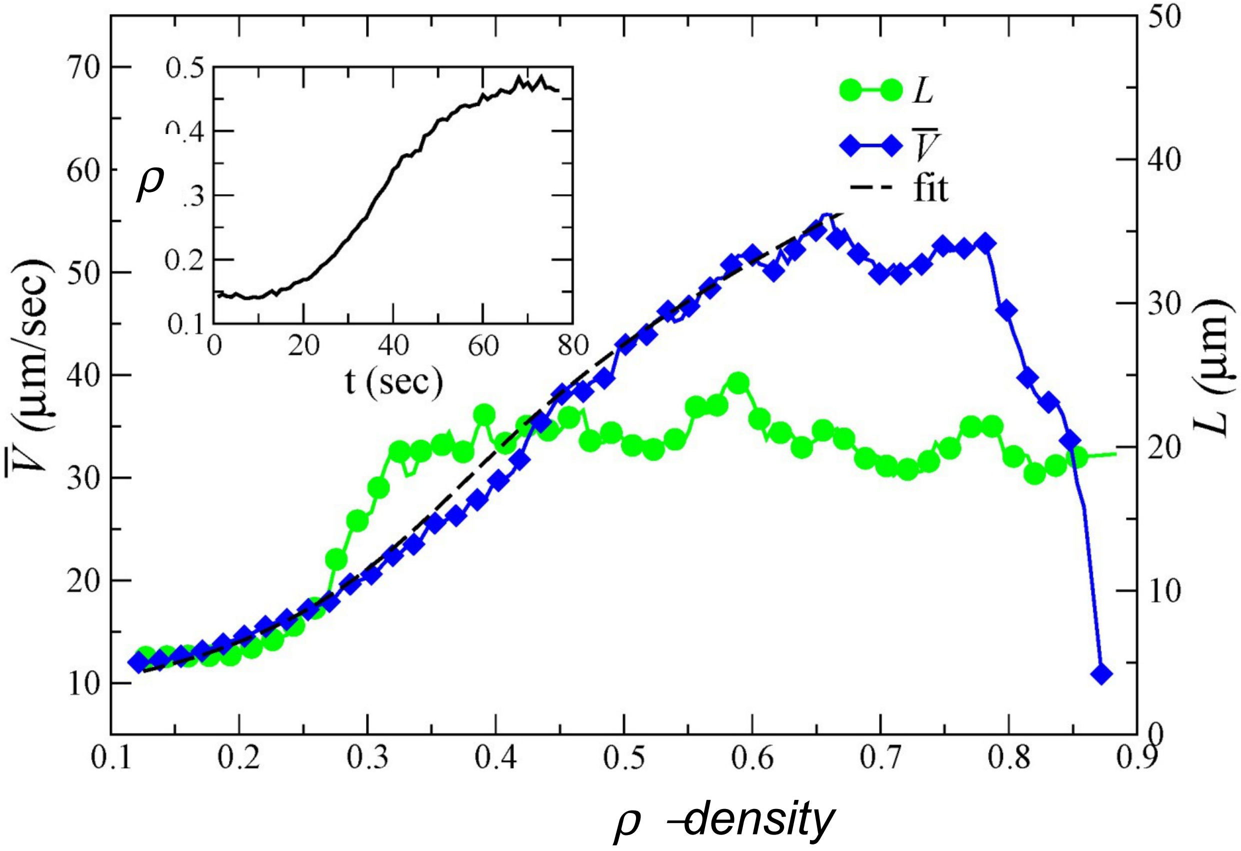
*Velocity Field **V***



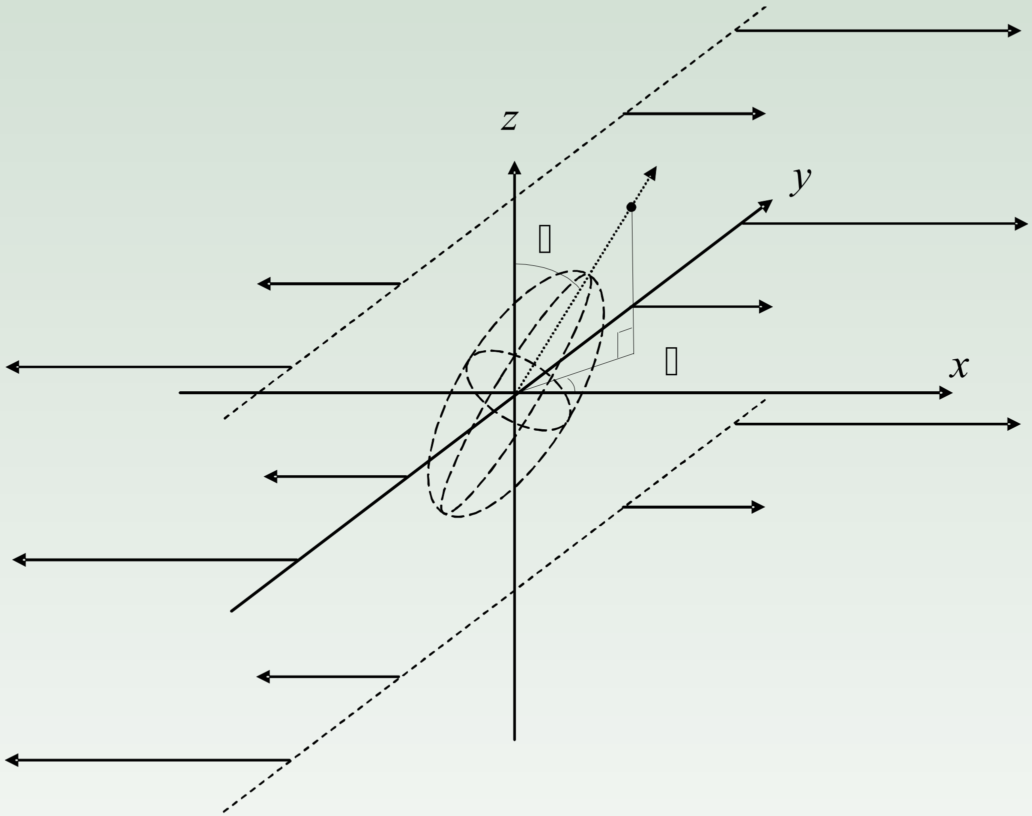
Orientation Field $\boldsymbol{\tau}$



Transition to Collective Swimming



Single particles (Jeffery orbits): Slender body in viscous fluid

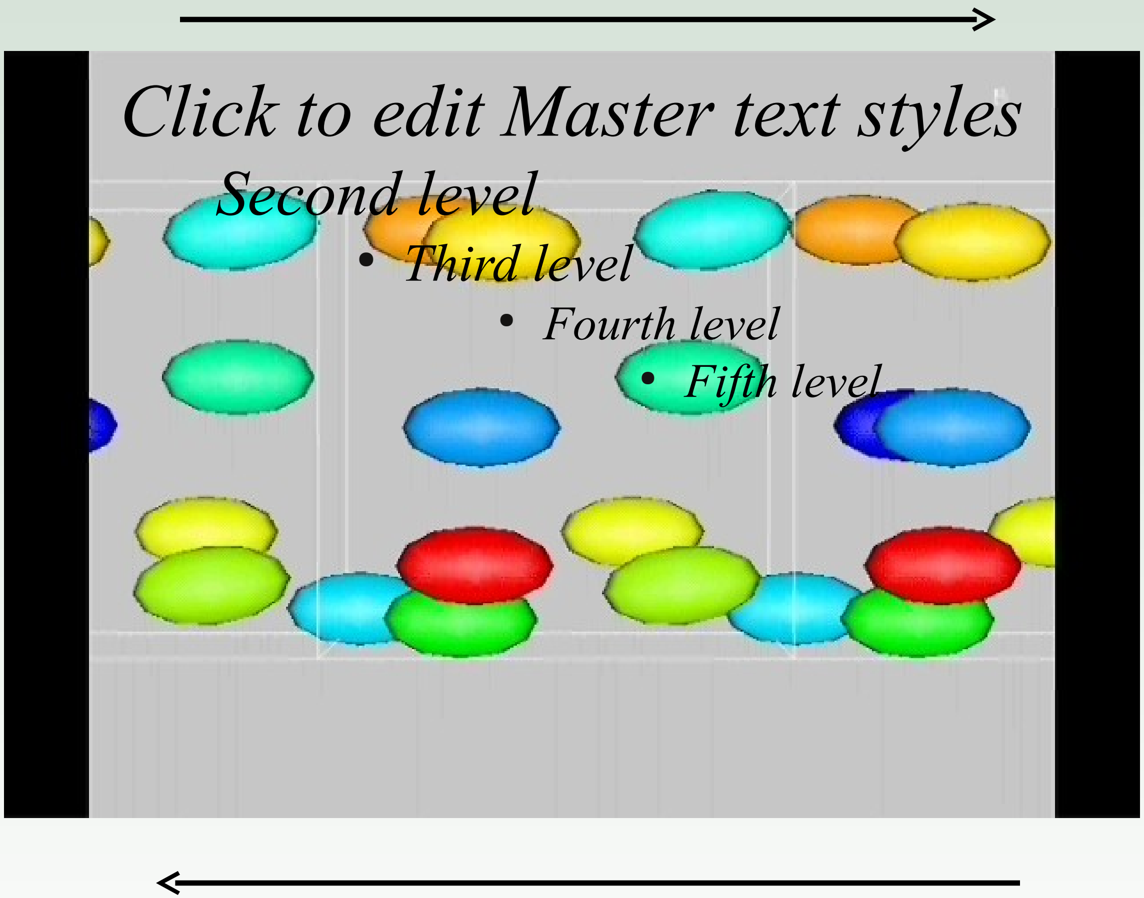


- **Planar shear flow: v=(*0,γy,0*) , γ strain rate, or pure shear**
- α,β **– polar angles**

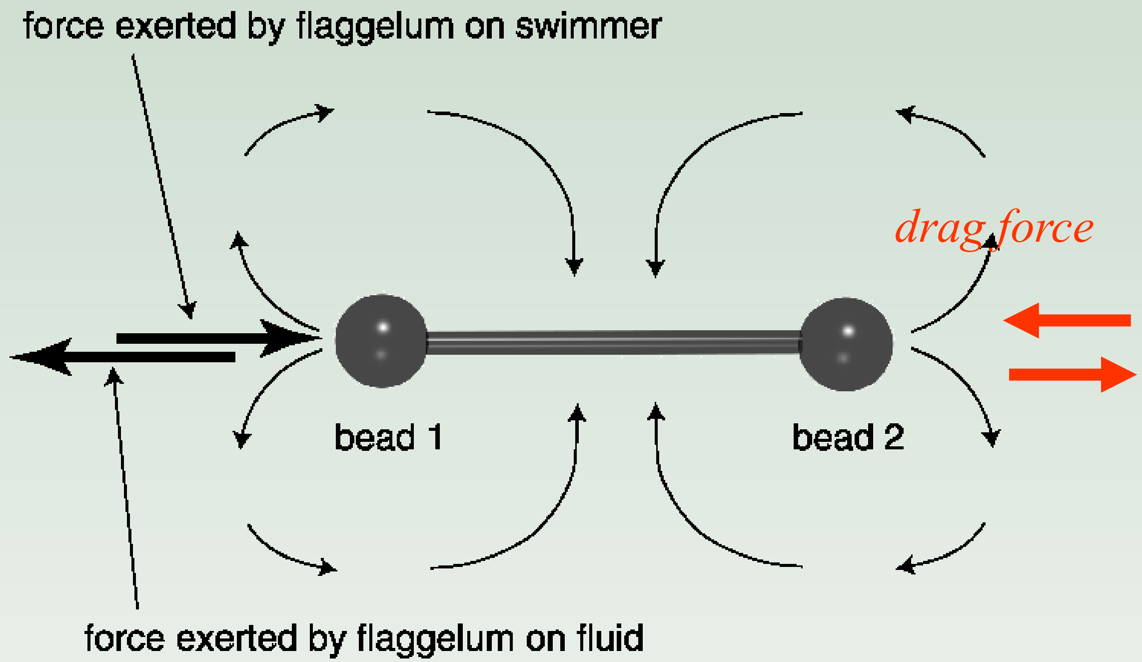
Slender body dynamics in shear flow

Kim and Karilla, Microhydrodynamics, 2005

Illustration of Jeffery orbits, planar shear flow



Velocity field: Bacteria are force dipoles



- **Bacteria are low Reynolds number creatures: Re=V L/n~10-4**
- **Bacteria motion is overdamped: no acceleration, zero net force**
- **Bacterium acts as a force dipole: force of self-propulsion and force opposing drag act on water in opposite directions**

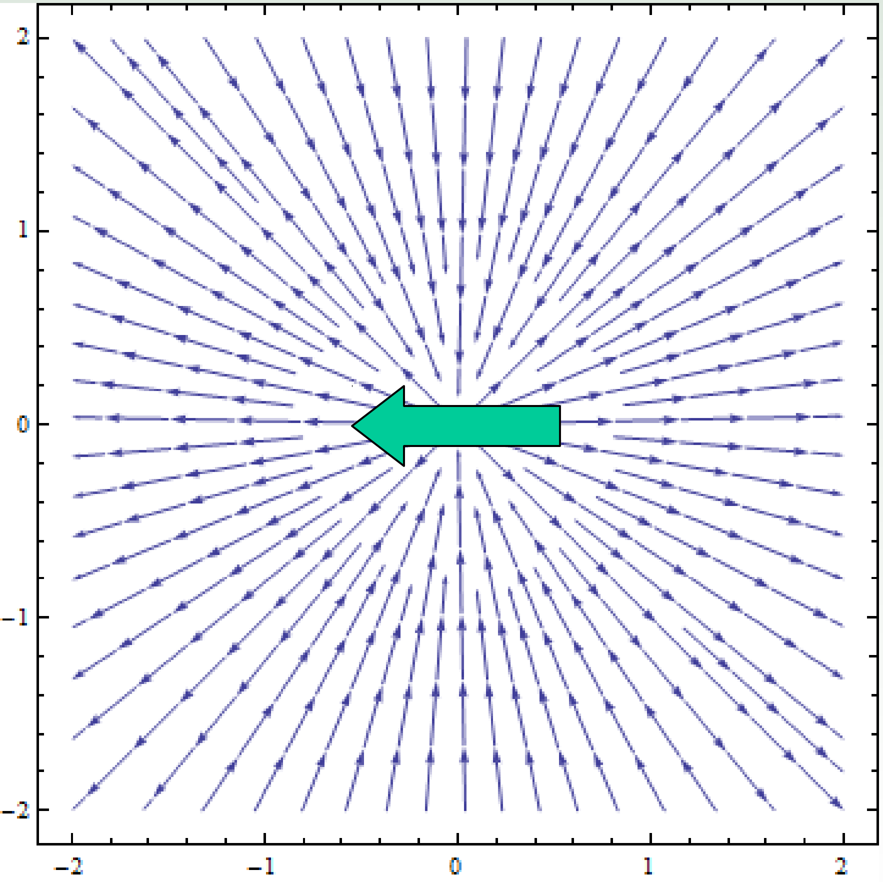
Michael Graham et al, PRL 2005

velocity of point monopole in 3D (stokeslet)

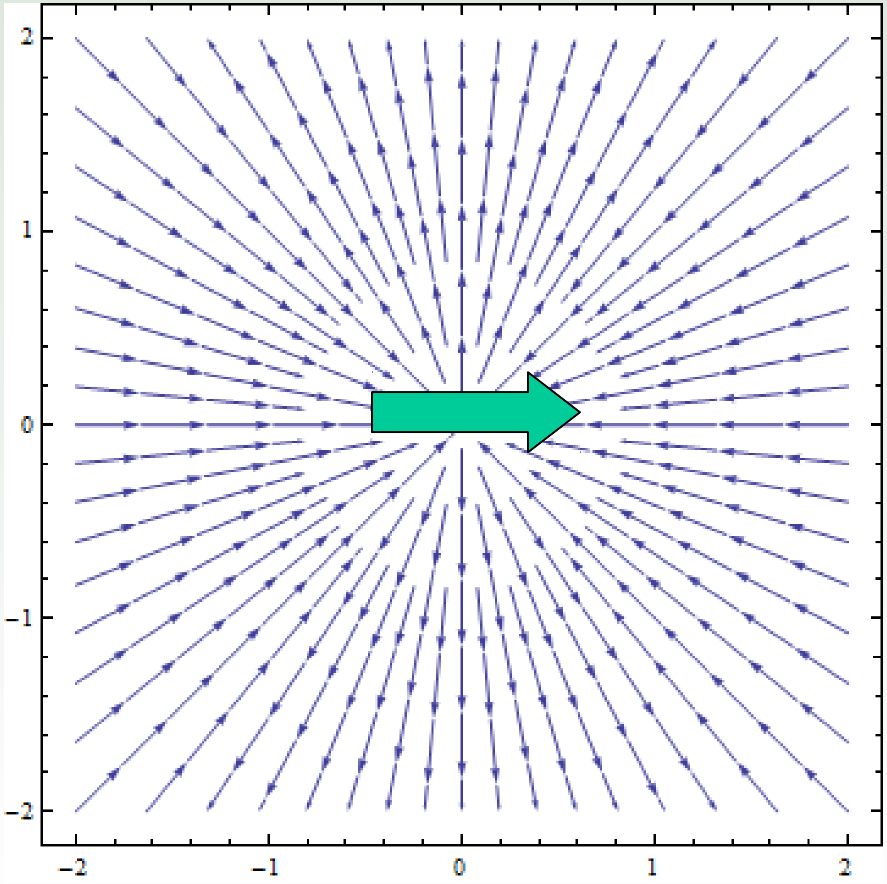
velocity of point dipole $u0$ in 3D (stresslet)

velocity fields of pushers and pullers

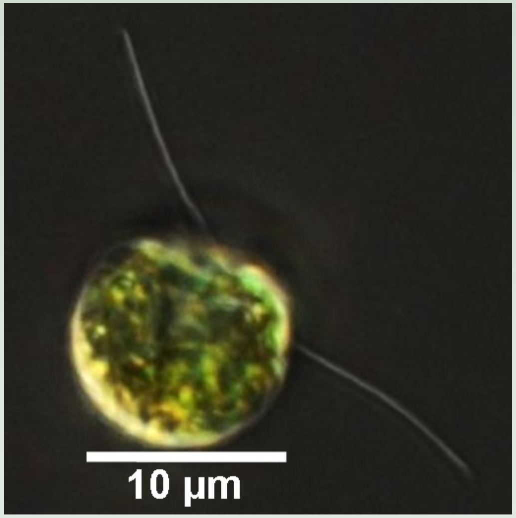
u0<0 – pushers (bacteria)

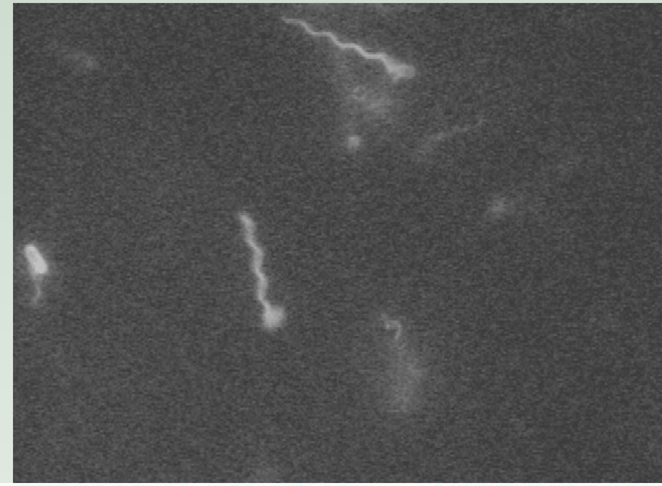


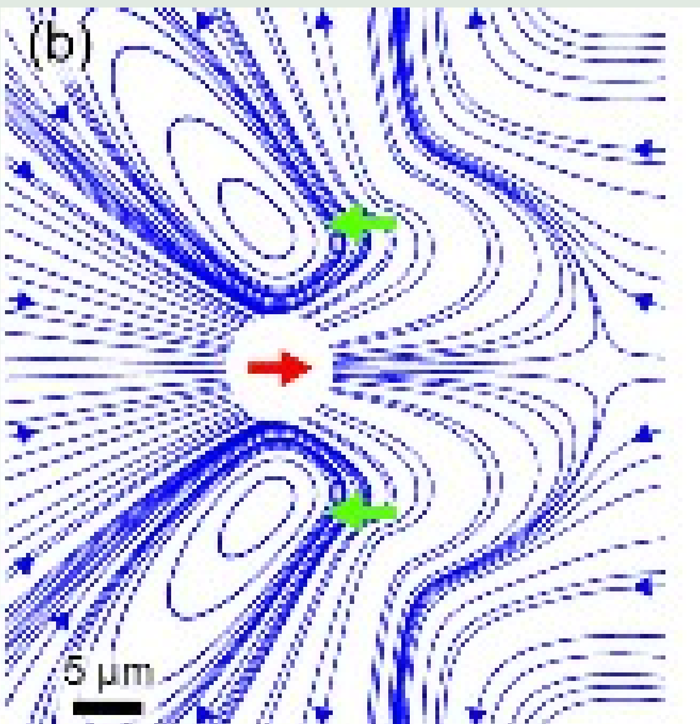
u0>0 – pullers (algae)

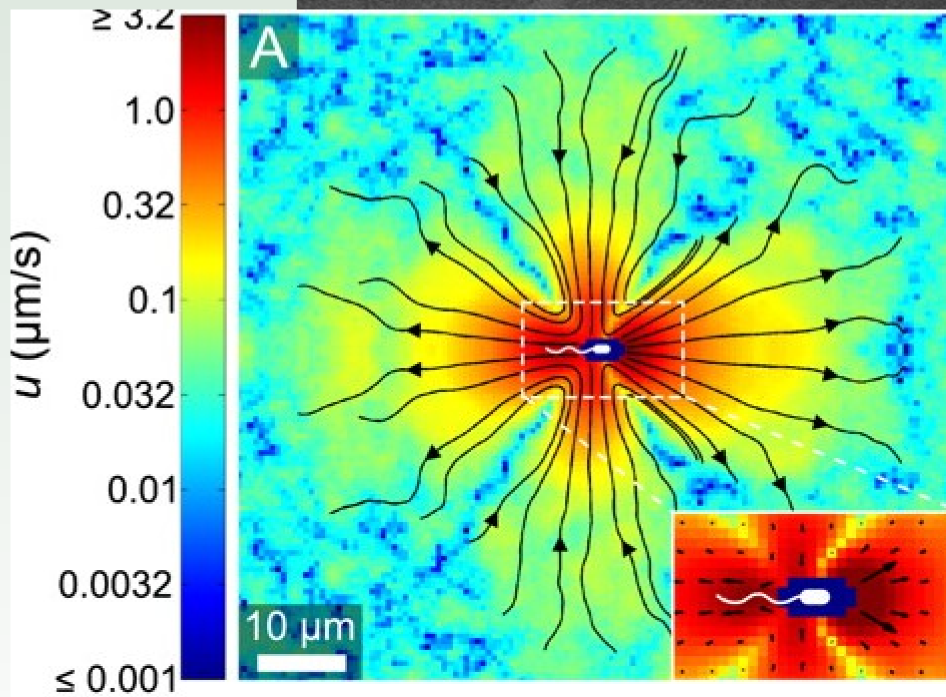


algae *bacteria*









Drescher et al, PRL 2010, PNAS 2011

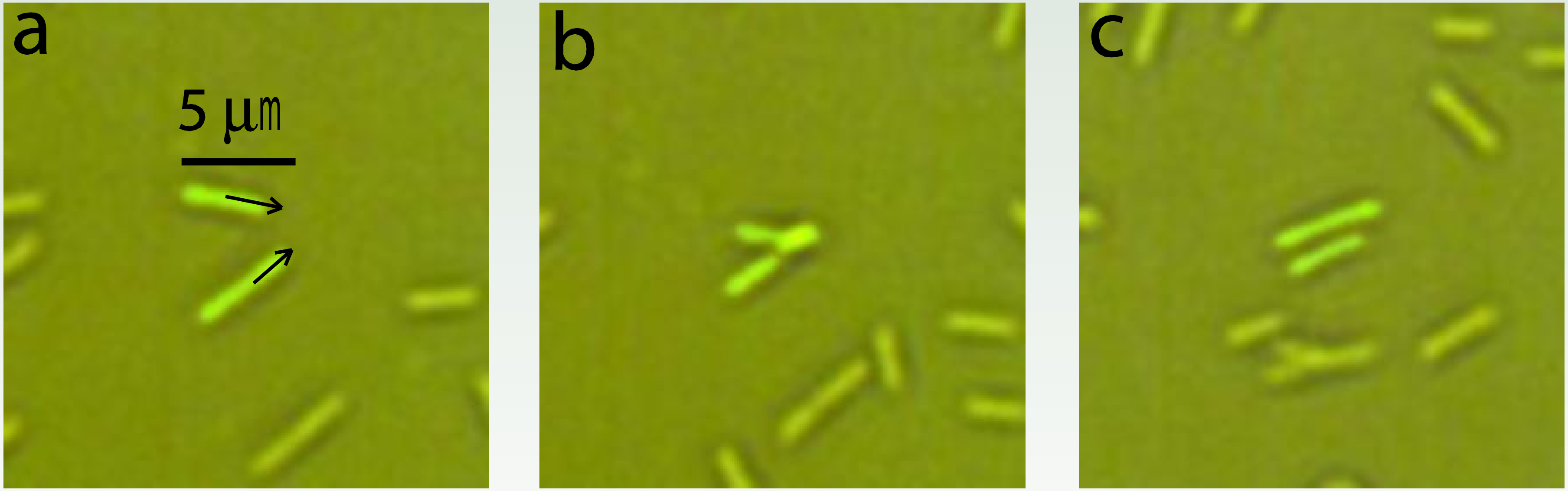
Theoretical Model

Microscopic interaction rules:

-self-propulsion; hydrodynamically-induced inelastic collision

-flow advection; direction realignment in shear flow

Inelastic collision of two bacteria



Spatial Localization of Interaction

W- interaction kernel, interaction between rods decay with the distance
Dij,Dr -translational and rotational diffusion of rods
v0 - propulsion velocity
v,*Ω – hydrodynamic velocity and vorticity*
E – strain rate tensor

$$\begin{aligned}\partial_t P \quad &+ \quad \nabla \cdot [(v_0 \mathbf{n} + \mathbf{v})\, P] + \frac{1}{2}\Omega \partial_\phi P = D_r \partial_\phi^2 P + \partial_i D_{ij} \partial_j P + \iint d\mathbf{r_1} d\mathbf{r}_2 \int_{-\pi}^{\pi} d\phi_2 \\ &\times \quad W(\mathbf{r}_1, \mathbf{r}_2) P(\mathbf{r_1}, \phi_1) P(\mathbf{r_2}, \phi_2) \left[\delta\left(\bar{\mathbf{r}} - \mathbf{r}, \bar{\phi} - \phi\right) - \delta\left(\mathbf{r}_2 - \mathbf{r}, \phi_2 - \phi\right)\right] - \gamma \left(\mathbf{E} \cdot \mathbf{n} \cdot \frac{\partial P}{\partial \mathbf{n}}\right) \quad .\end{aligned}$$

The Diffusion Matrix in Kirkwood Approximation

l – length of the rod, *d*- diameter, ηs – viscosity of solvent

Theoretical Model

Microscopic interaction rules:

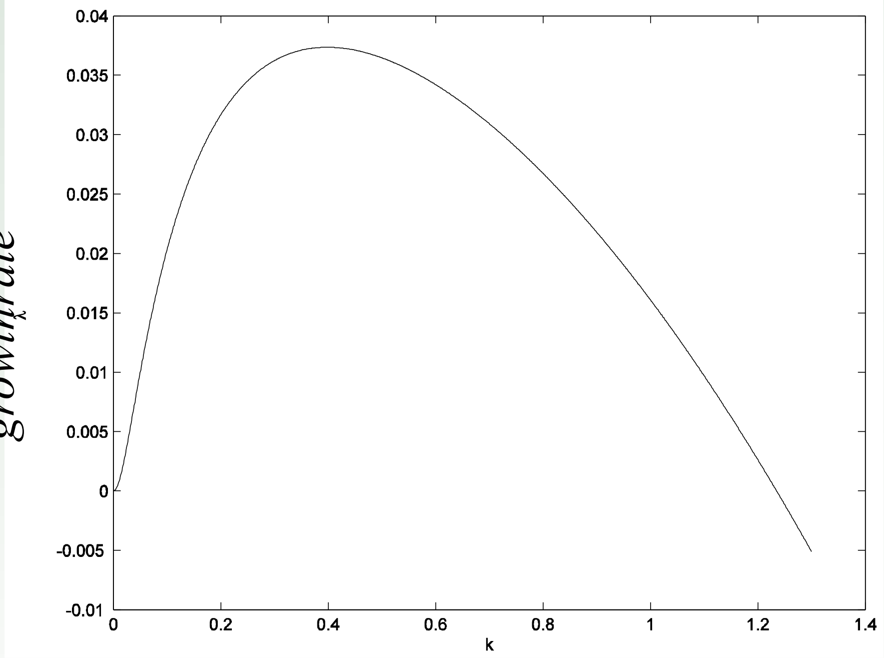
-self-propulsion; hydrodynamically-induced inelastic collision

-flow advection; direction realignment in shear flow

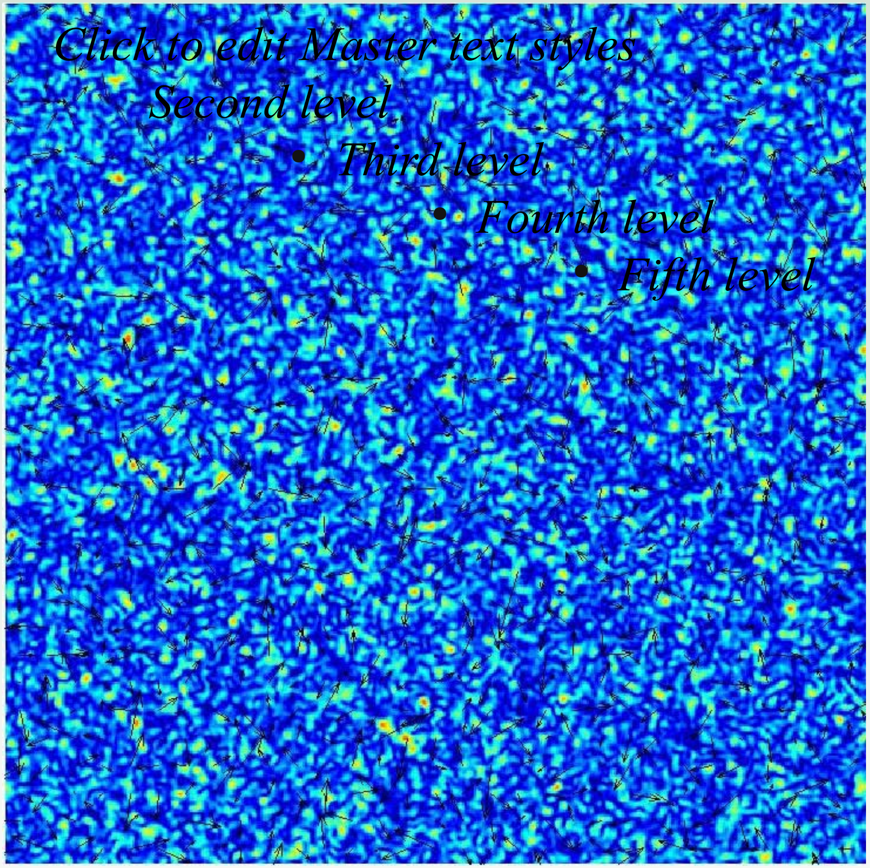
Results of Modeling

·*Instability of uniform flow*
·*Mechanism: coupling between self-propulsion and shear-induced alignment*

growthrate

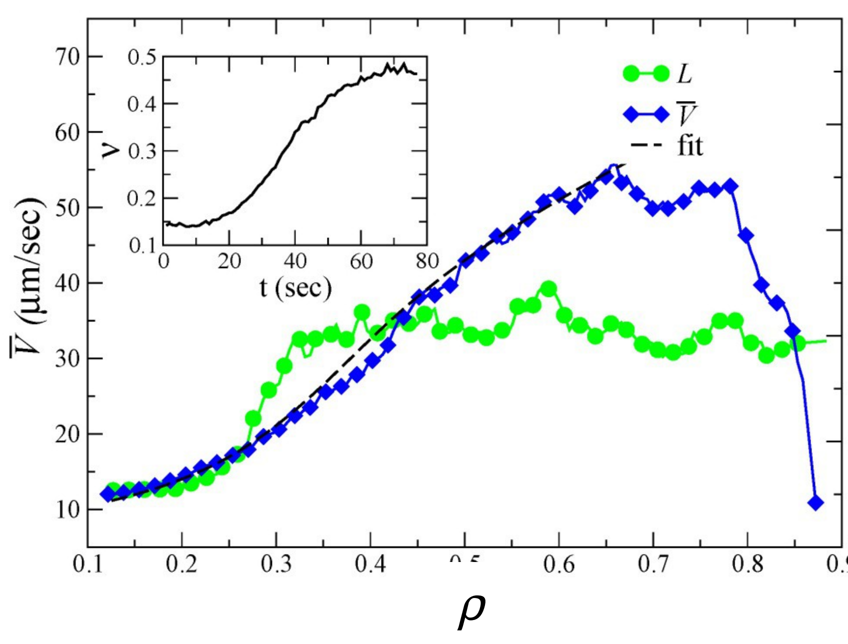


wavenumber

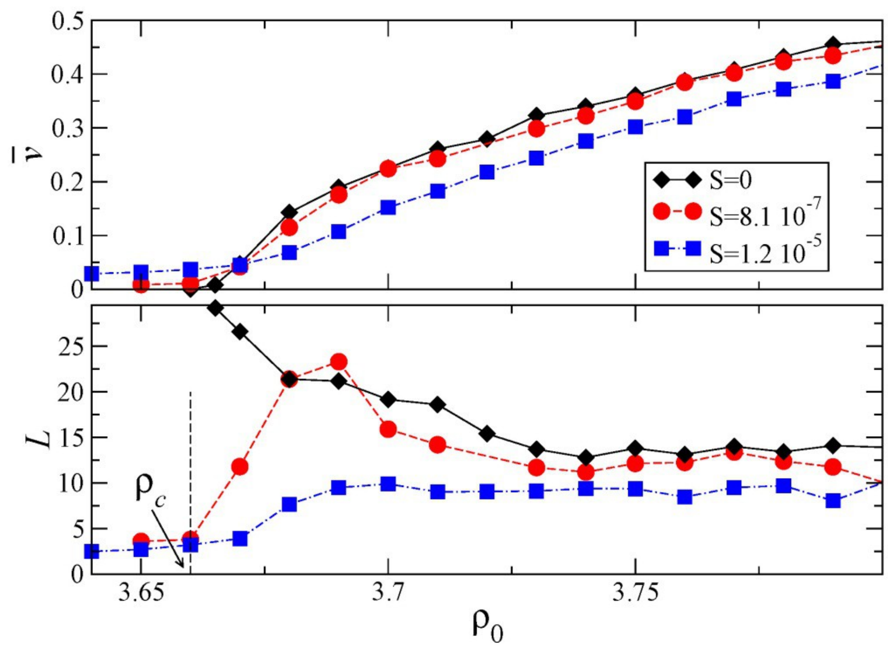


Experiment and Theory

Experiment



Theory



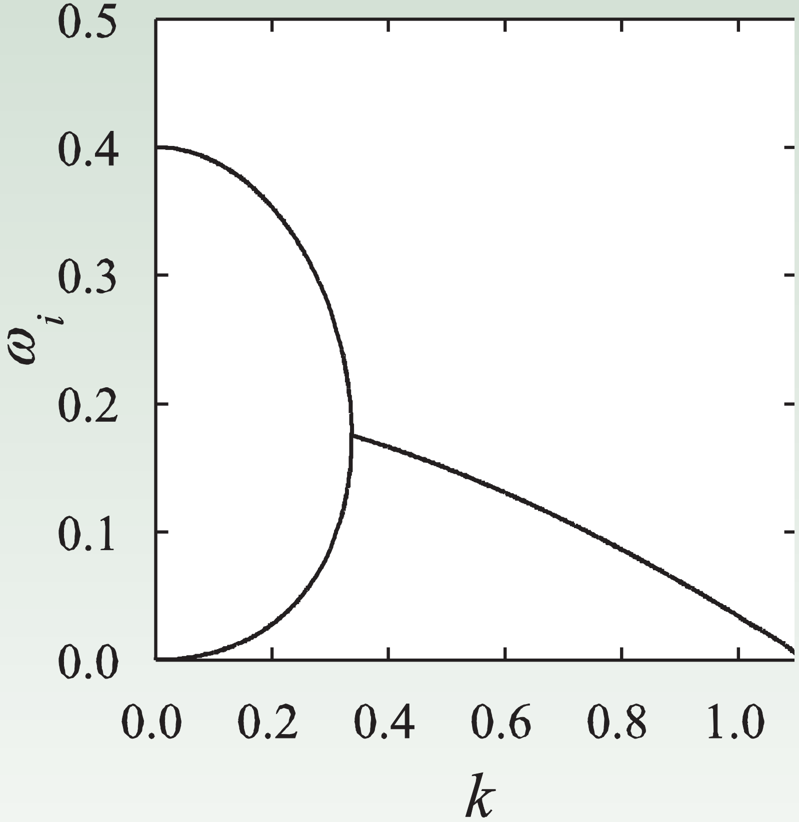
Mean-Field Hydrodynamic Theory Saintillan & Shelley

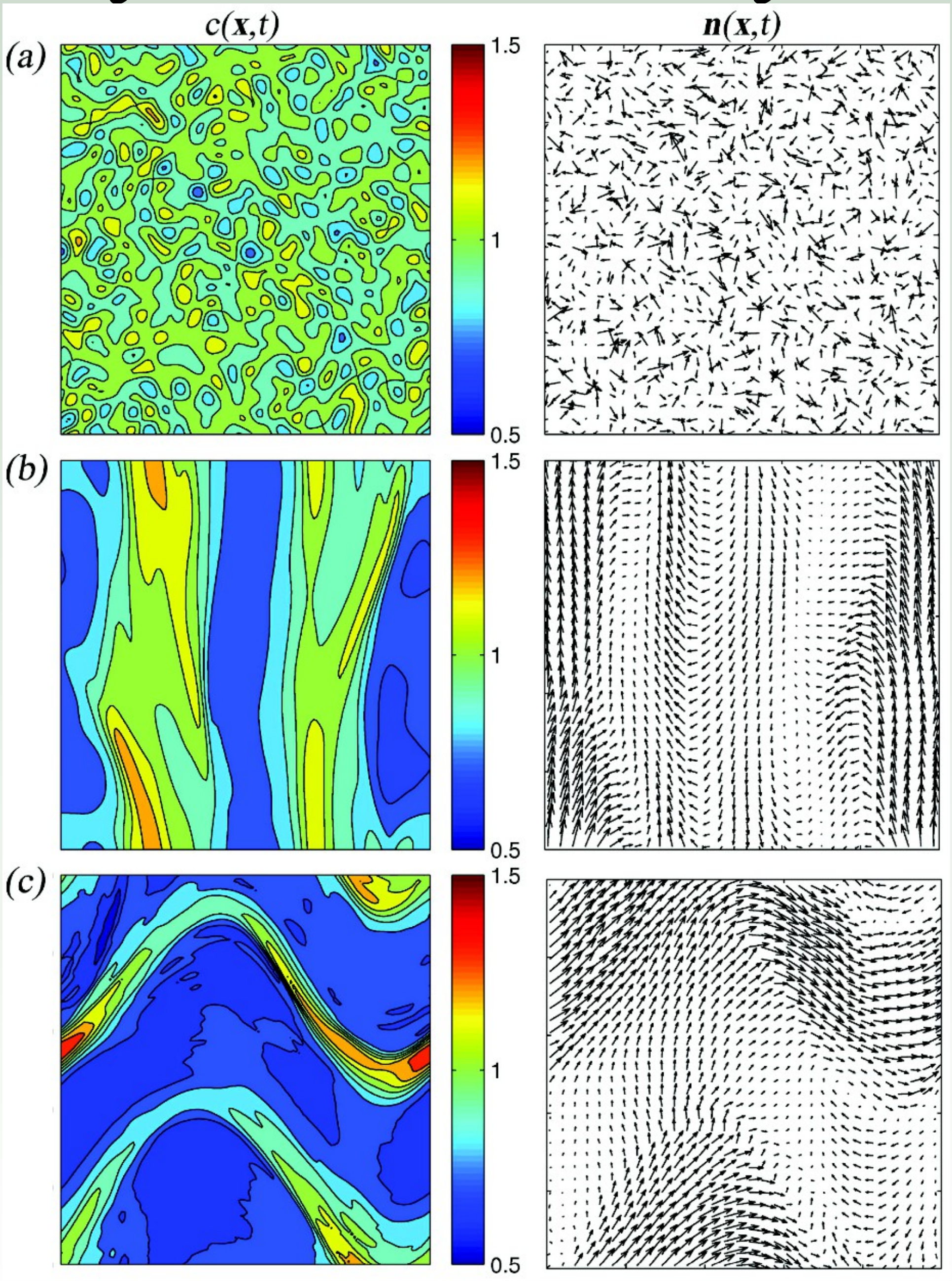
Kinetic equation for probability distribution

Saintillan and Shelley, PRL 2008

Meanfield Hydrodynamic Theory

Linear growth rate

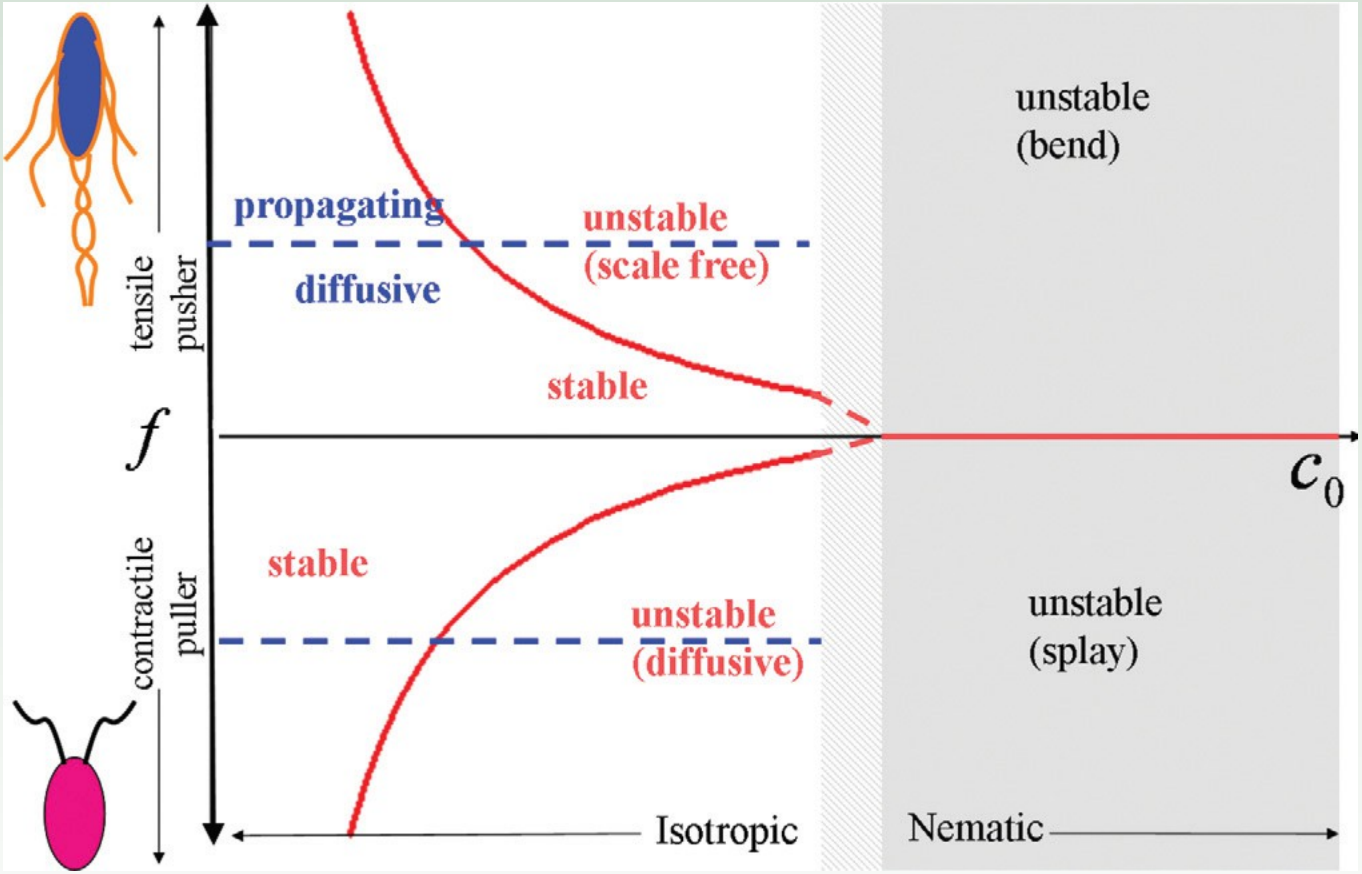




Saintillan and Shelley, PRL 2008

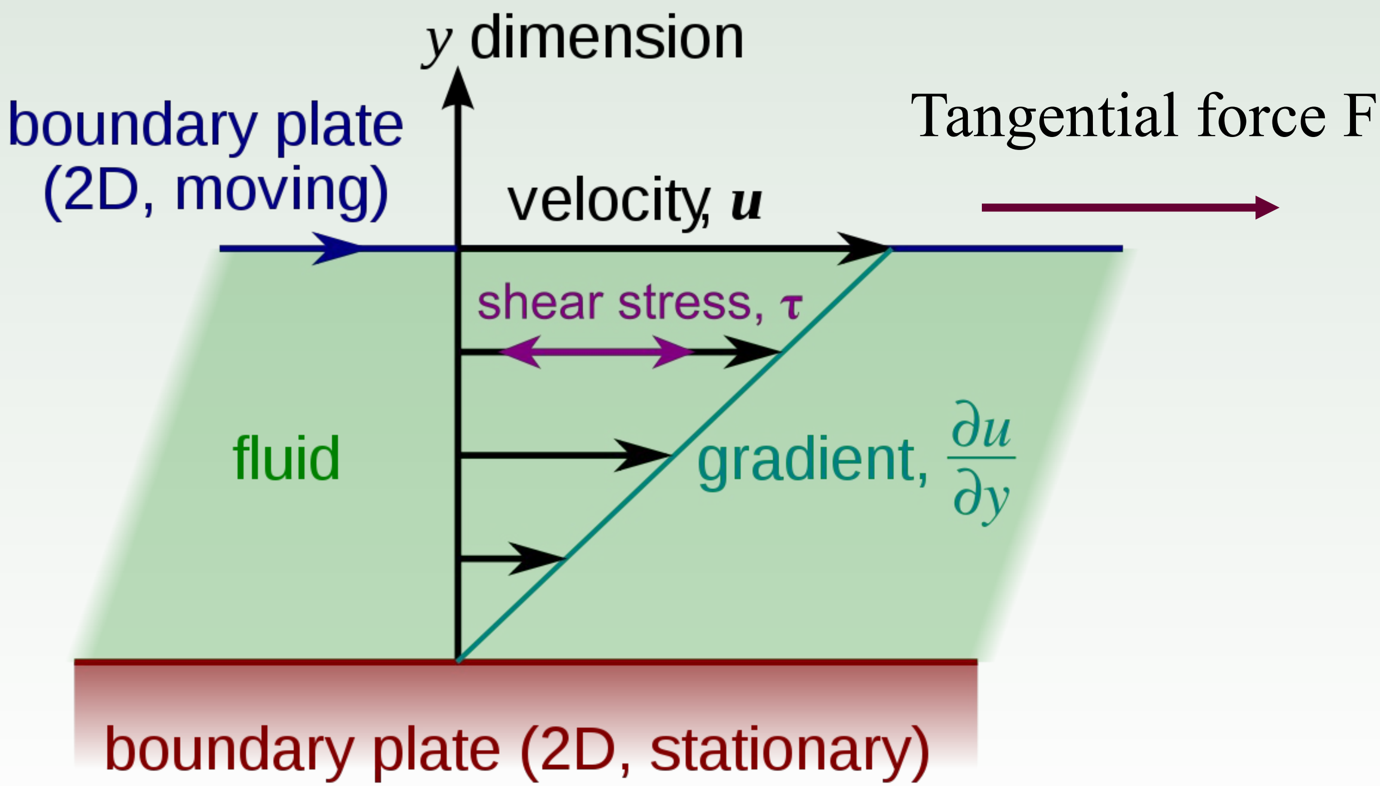
Hydrodynamic Coarse-Grained Theory

- *eqs for concentration, orientation, nematic tensor*
- *long-wave linear stability analysis*



Baskaran & Marchetti, PNAS 2009

Rheology: apparent viscosity



Viscosity of Passive Suspensions: (Albert) Einstein theory

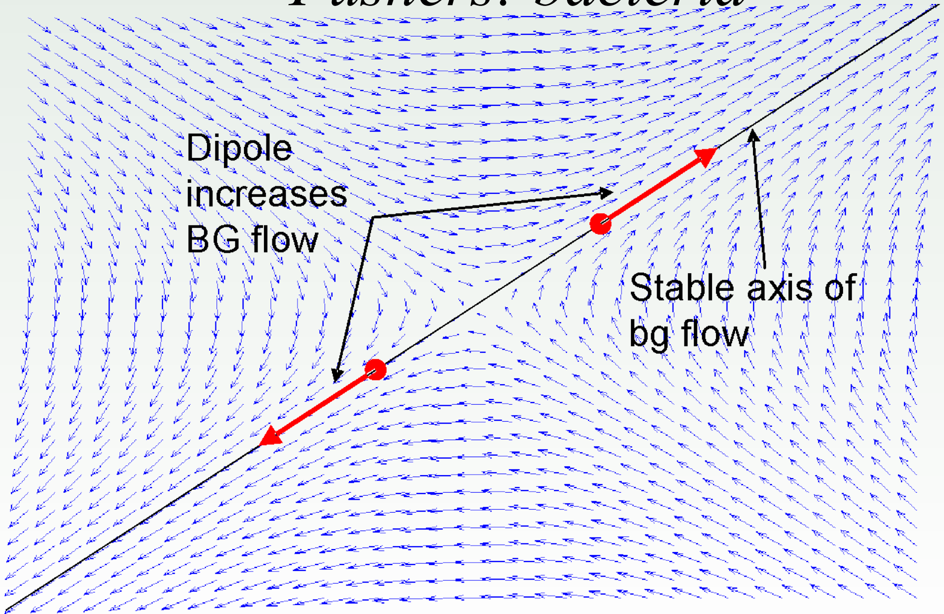
Dilute suspensions of impenetrable spheres, zero Reynolds number (Stokes limit)

$\eta 0$ – viscosity of the background fluid,
ϕ – volume fraction of spheres

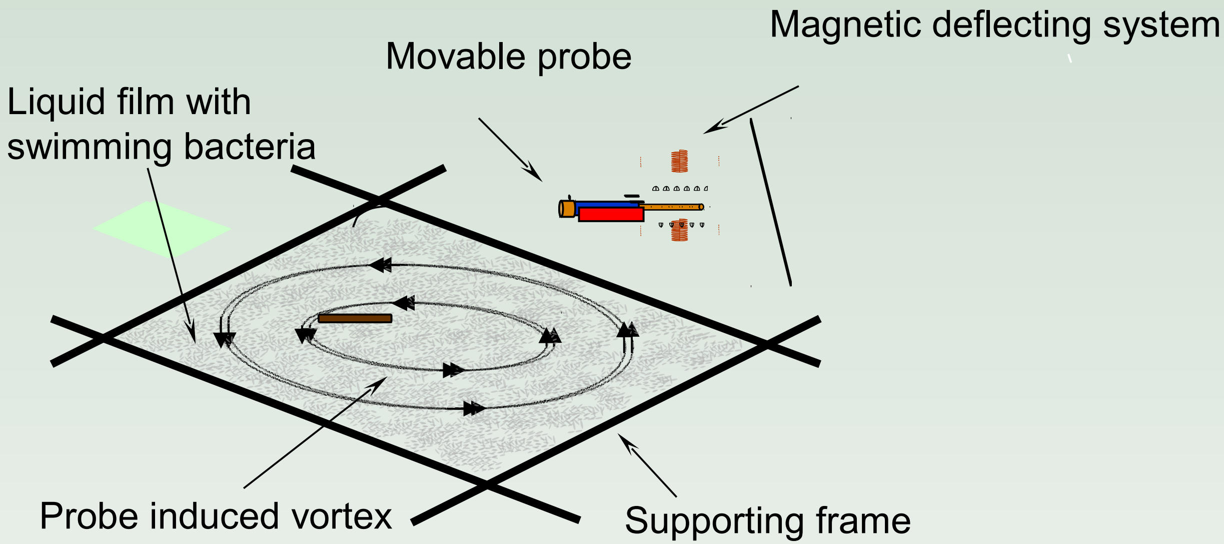
Self-propulsion and Viscosity

- **When dipole is aligned with flow, dipole increases rate of strain without changing forces at the boundary**
- **Non-spherical particles tend to align with stable axis of flow**
- **Increase of background (bg) flow, decrease of viscosity**
- **For passive suspensions and pullers , viscosity increases with concentration of inclusions**

Pushers: bacteria



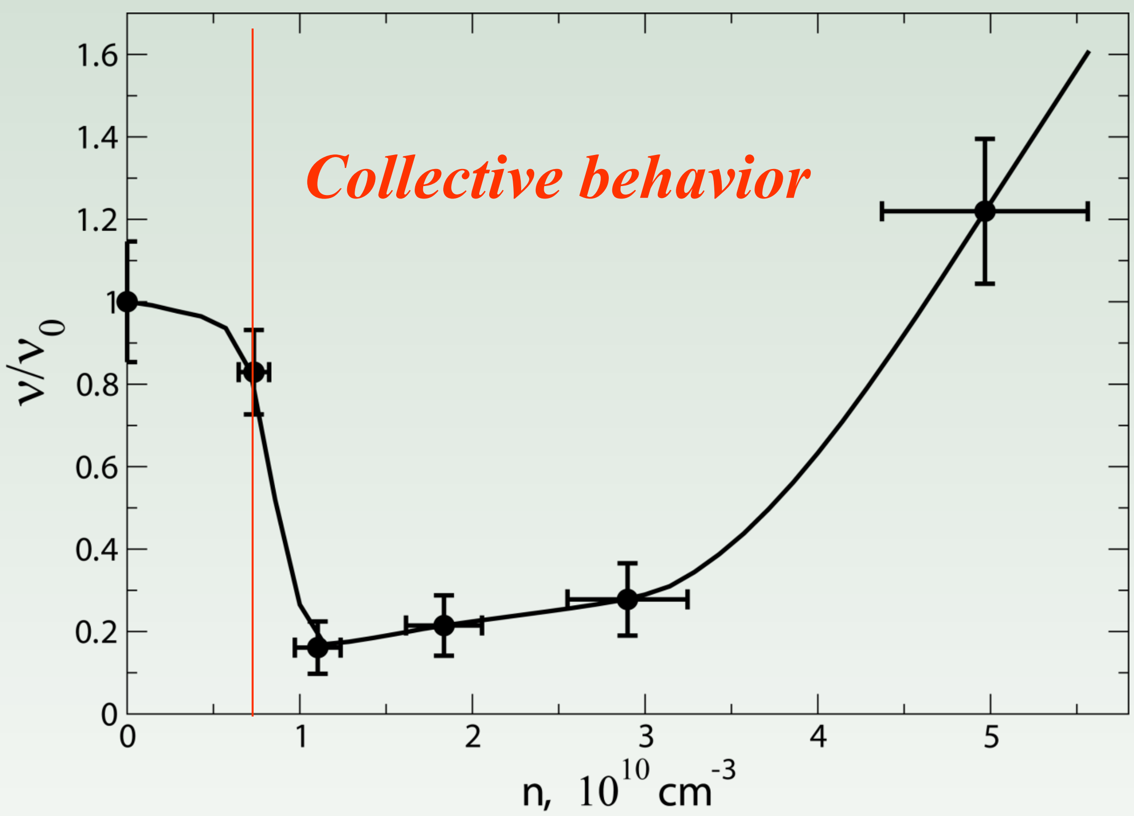
Probing Micro-Rheology of Active Suspensions
Experiment #1



Microrheology is studied in thin free-standing film geometry
Experiment performed in closed chamber in air and in Nitrogen
Control of activity: N2→no swimming, O2 →swimming
Viscosity is extracted from decay time (T) of a large vortex (L)

Sokolov & Aranson, PRL 2009 and also Physics World

Viscosity vs. Concentration



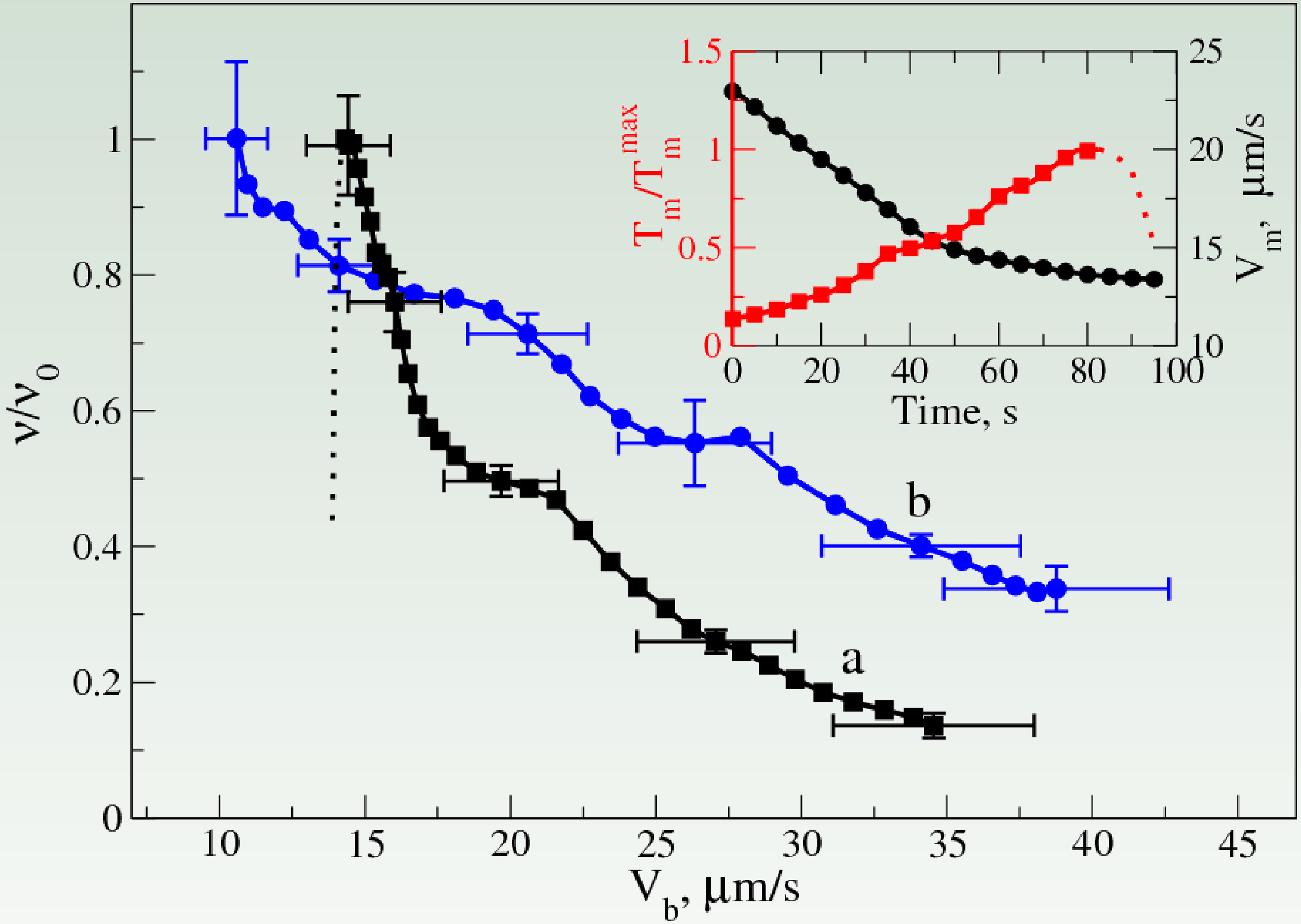
Assuming that the viscosity is spatially independent

Assuming that the viscosity is time-independent

viscosity:

Concentration: ***<u>10-20 times stationary growth conditions</u>***

Viscosity vs Swimming Speed



a) n=1.8·1010 cm-3

b) n=1010 cm-3

Slender body dynamics in shear flow

Effective Viscosity via Dissipation Rate

Stress Tensor for Dipoles

Particles rotation: Jeffery orbits

- Ω and – vorticity and rate of strain of the background flow
- $\xi\alpha,\beta$ fluctuations (tumbling) with the strength D

$\alpha = \Omega t$ for $\varepsilon < < 1$ – pure rotation

$B \sim (b2-a2)/(a2+b2)$, a,b - semiaxis

Linear Fokker-Planck Equation

$P(\alpha,\beta)$ – *probability distribution function for bacteria orientations*
κ – *angular velocity vector*

Leal & Hinch, JFM 1971

Bulk Stress

Contribution due to passive spheroid (Kim & Karilla, 1991)
Contribution due to tumbling (noise) (Leal & Hinch, 1971)
Contribution due to self-propulsion (Haines et al, PRE 2009)
K, YH – resistance functions (depend on aspect ratio and position of flagella)

$$\begin{aligned}\Sigma_{ij} =& 2\eta E_{ij} + \frac{5b}{a}\phi\eta \int_{S^2} \Lambda_{ijkl} P^{\infty} dS E_{kl} \\ & + 3\eta\phi Y^H \frac{b}{a} \int_{S^2} (\epsilon_{ikl} d_j + \epsilon_{jkl} d_i) d_l (\Omega_k - \omega_k^D - \omega^R) P^{\infty} dS \\ & + \frac{1}{16\pi b^2}\phi K \int_{S^2} (\delta_{ij} - 3 d_i d_j) P^{\infty} dS + \mathcal{O}(\phi^2),\end{aligned}$$

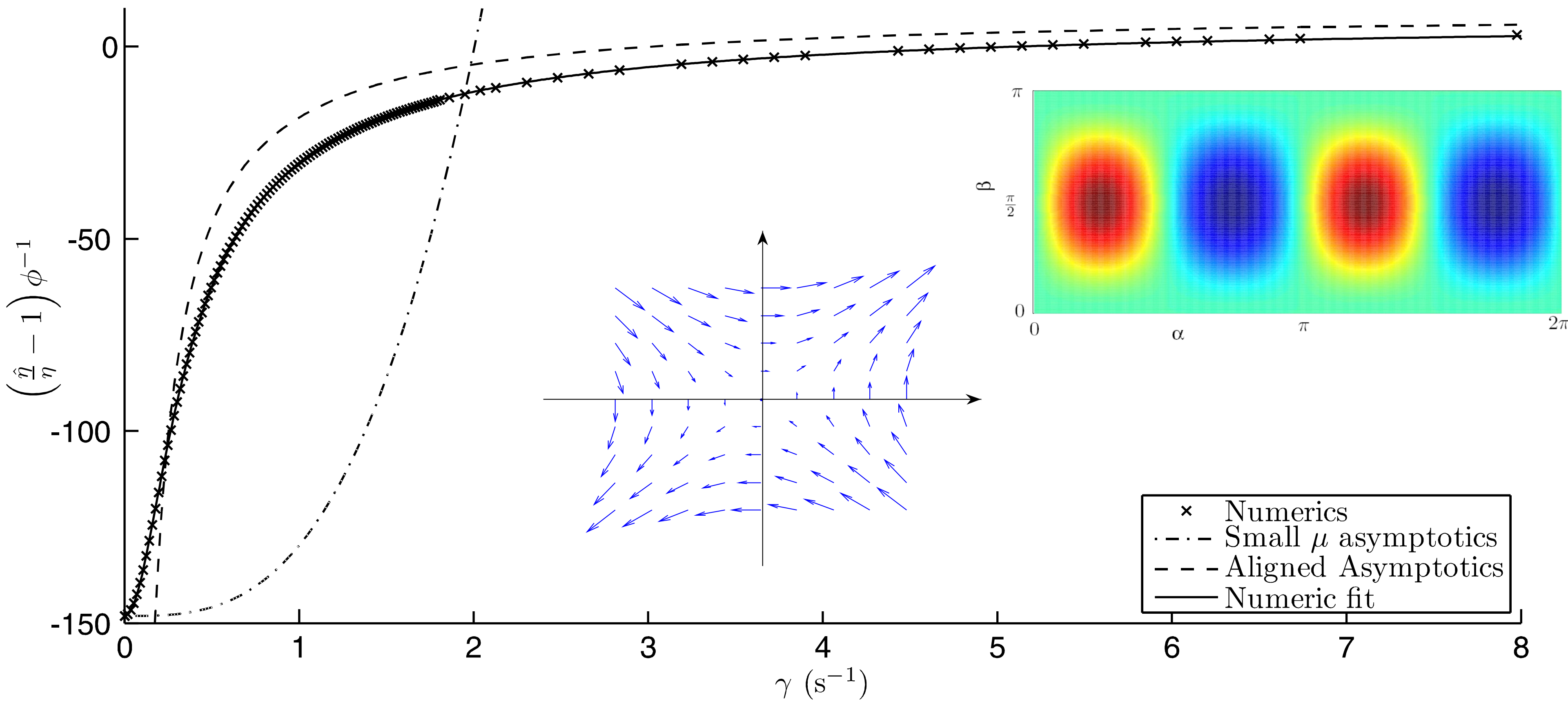
Effective Viscosity in 3D (almost spheres, $B \to 0$)

- *V0* – swimming speed, *F* -propulsion force
- small fluctuations limit (*D* <<   ) is singular
- Decrease of viscosity due to swimming (for pushers, $\lambda>0$)
- Also strain rate $\to 0$ limit is singular limit

Haines et al, 2009; Saintillan 2010

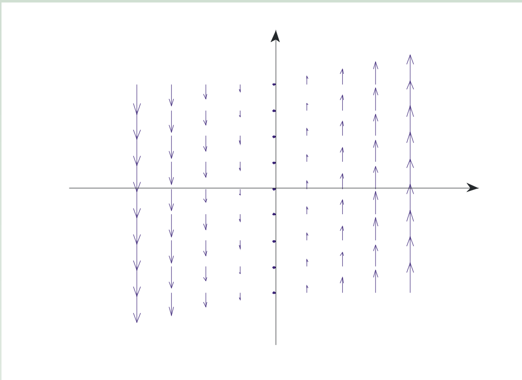
Flow without Vorticity

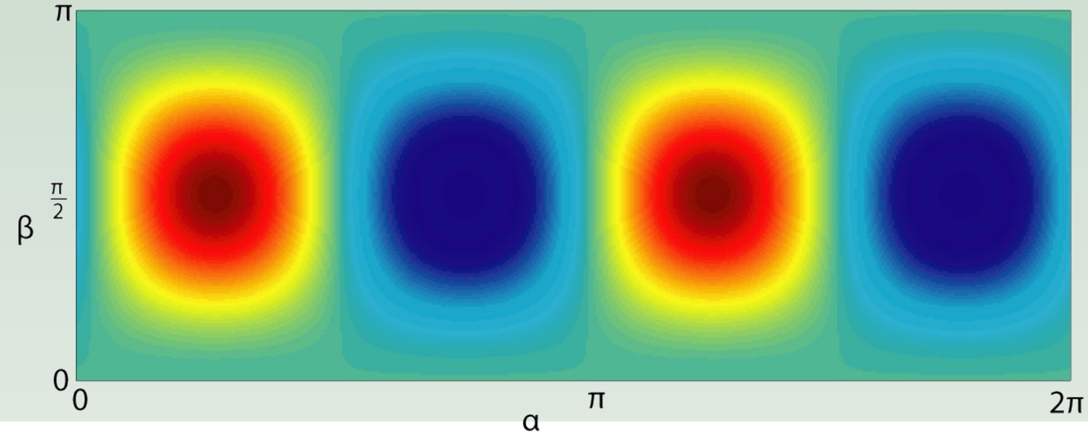
Negative contribution to viscosity for small stain rates

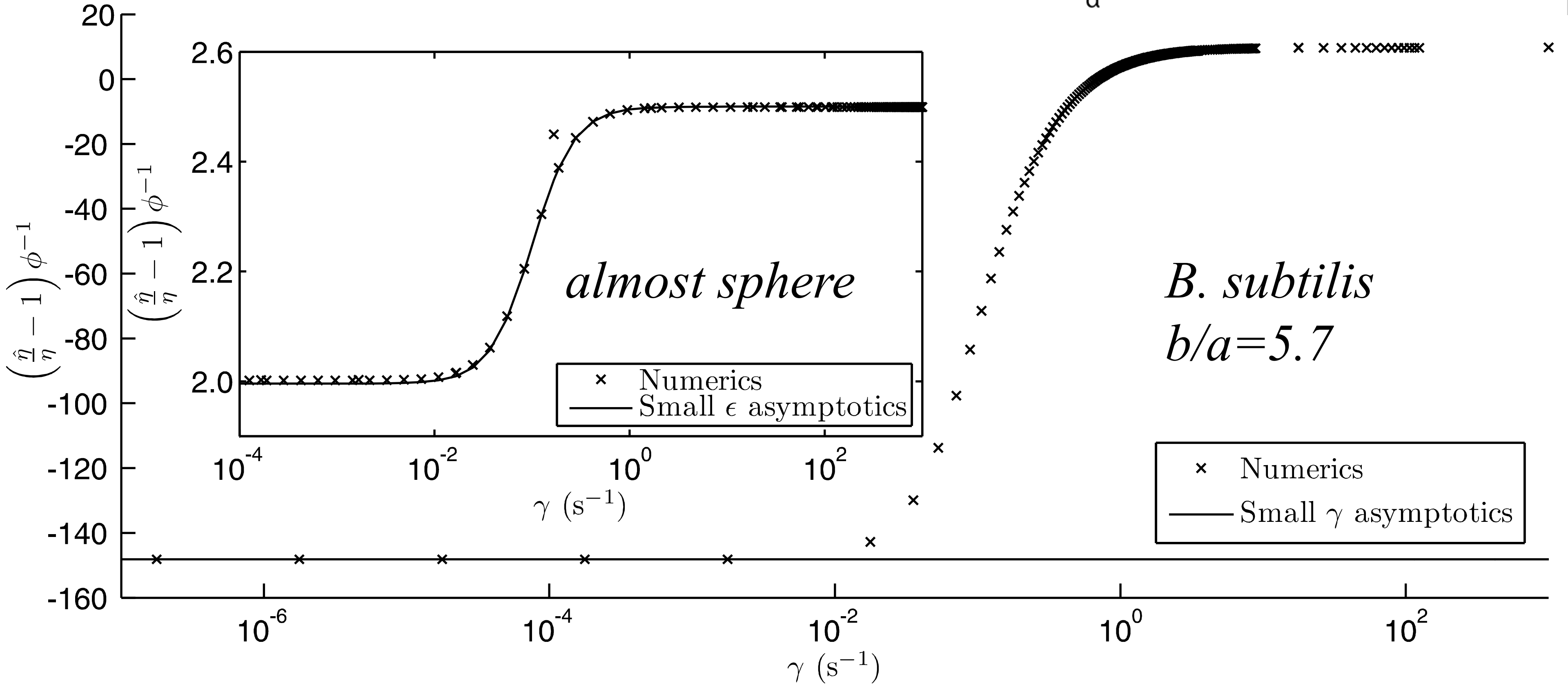


μ~ εγ/D<<1 – weak tendency to align; μ>>1 – strong alignment

Planar Shear Flow







Counter-Intuitive Conclusion:

No viscosity reduction without tumbling for planar shear flow

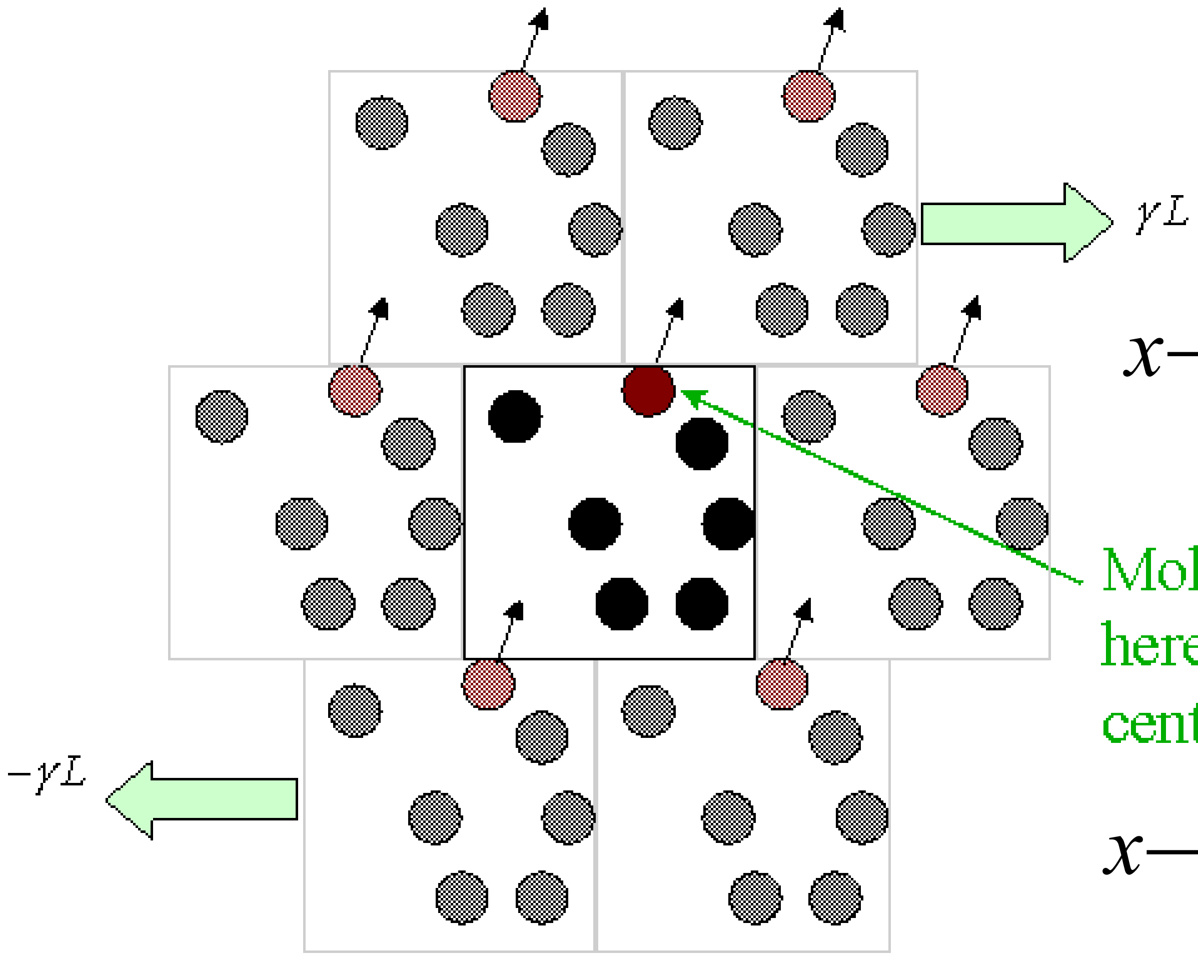
However, experiments show almost no tumbling for Bacillus subtilis

Simulations

Bacteria are modeled by swimming point dipoles
No tumbling
Short-range repulsion to account for finite particle size
3D simulation domain
Lee-Edwards boundary conditions in the direction of shear
>100,000 particles
Simulations are implemented on GPU

Shawn Ryan, Penn State Univ, 2010

Lees-Edwards Boundary Conditions



$$\gamma = \frac{dv_x}{dy}$$

$$x \rightarrow x + \gamma L t$$

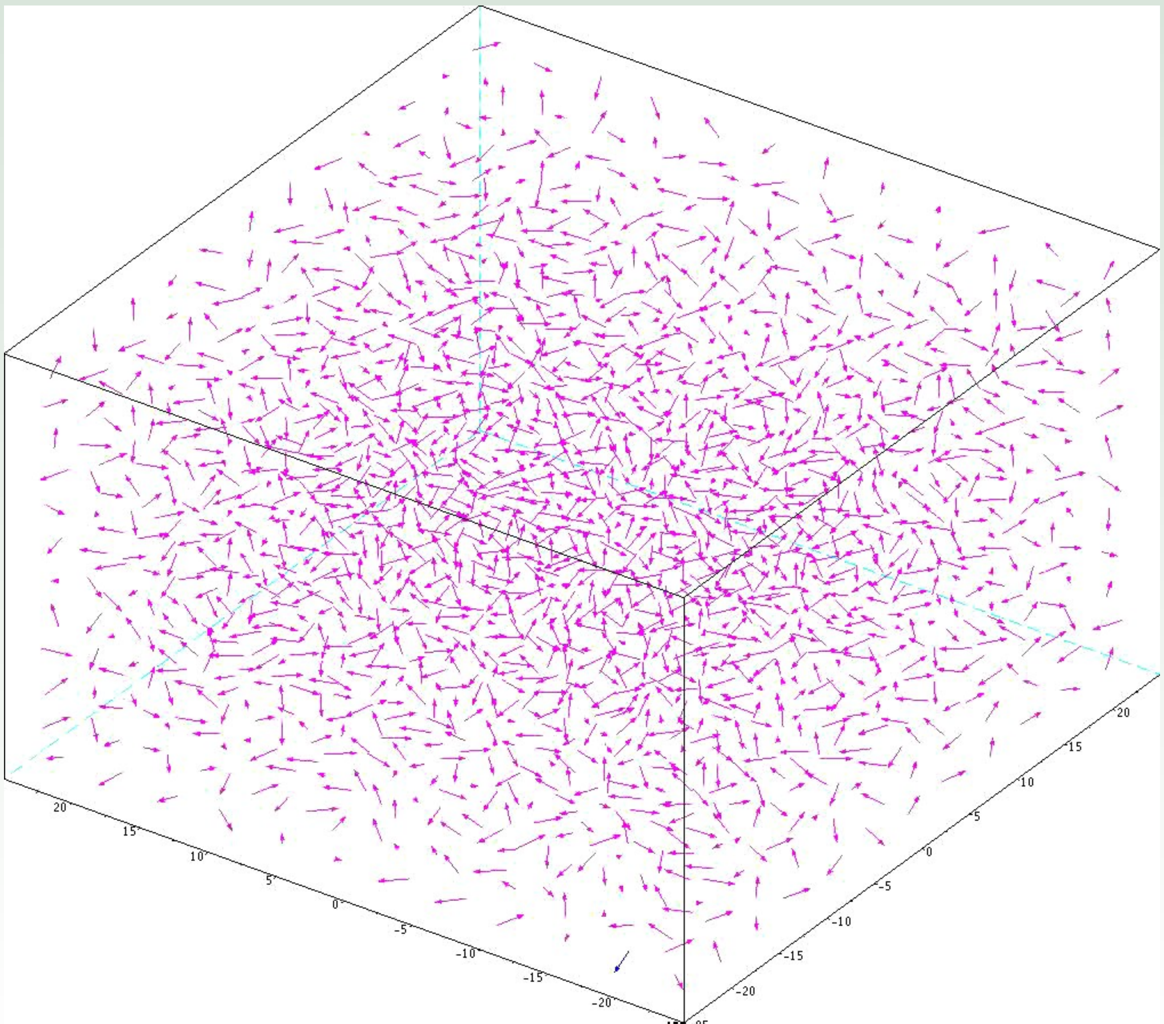
Molecule exiting here, in middle of central cell

$$x \rightarrow x - \gamma L t$$

Equations

Typical simulation

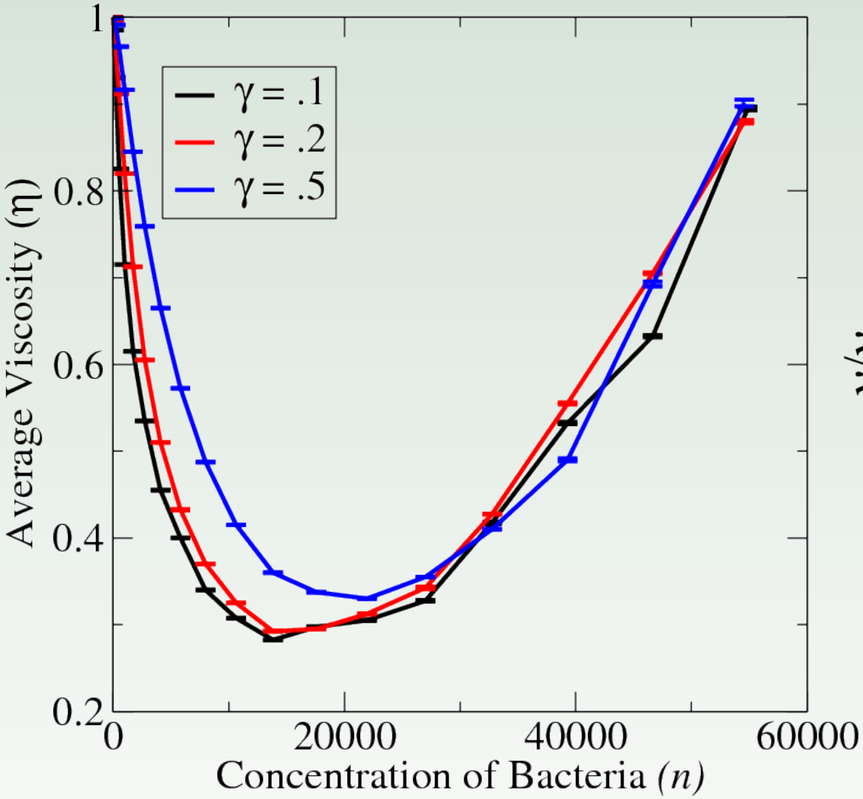
Full 3D, up to 483 particles
Fermi GTX480 GPU, 2-3 hours
Range of velocities, concentrations, strains



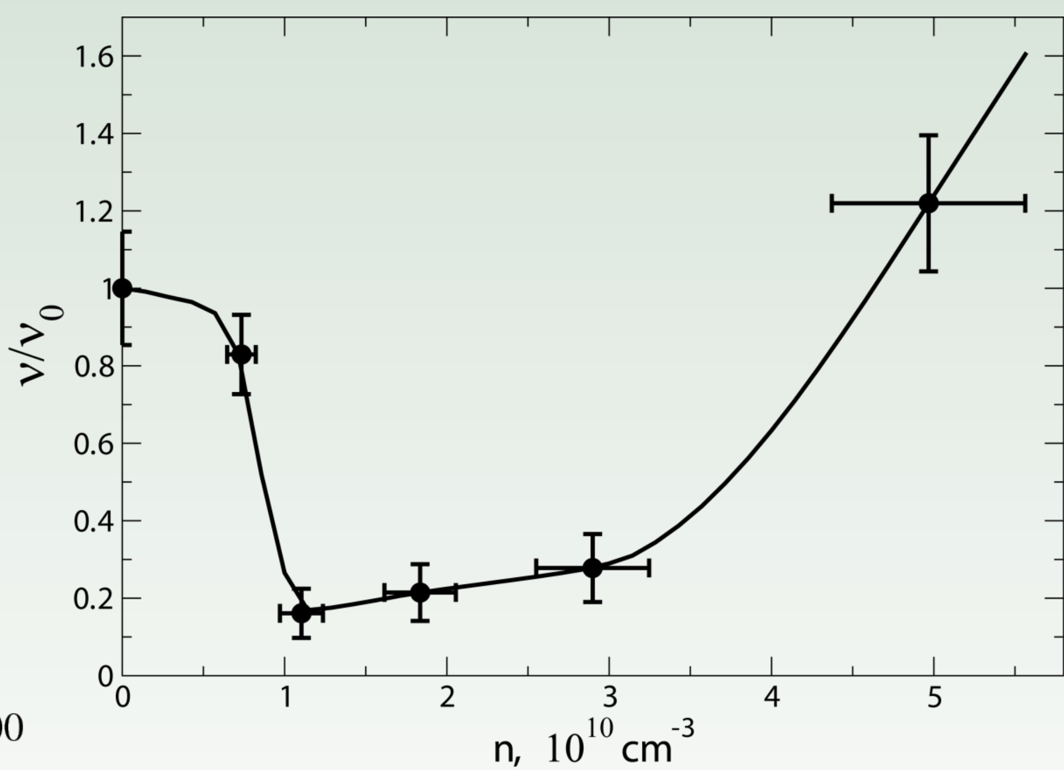
Stress Tensor

Viscosity vs Concentration

Simulations

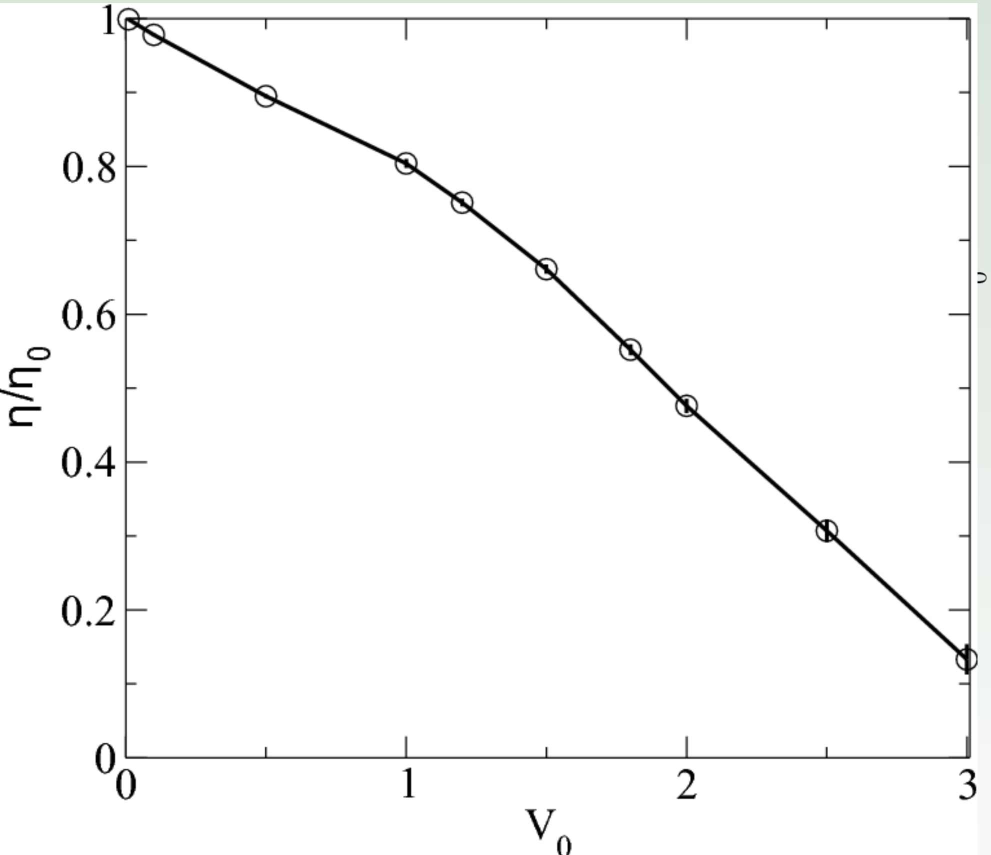


Experiment



Viscosity vs Swimming Speed

Simulations



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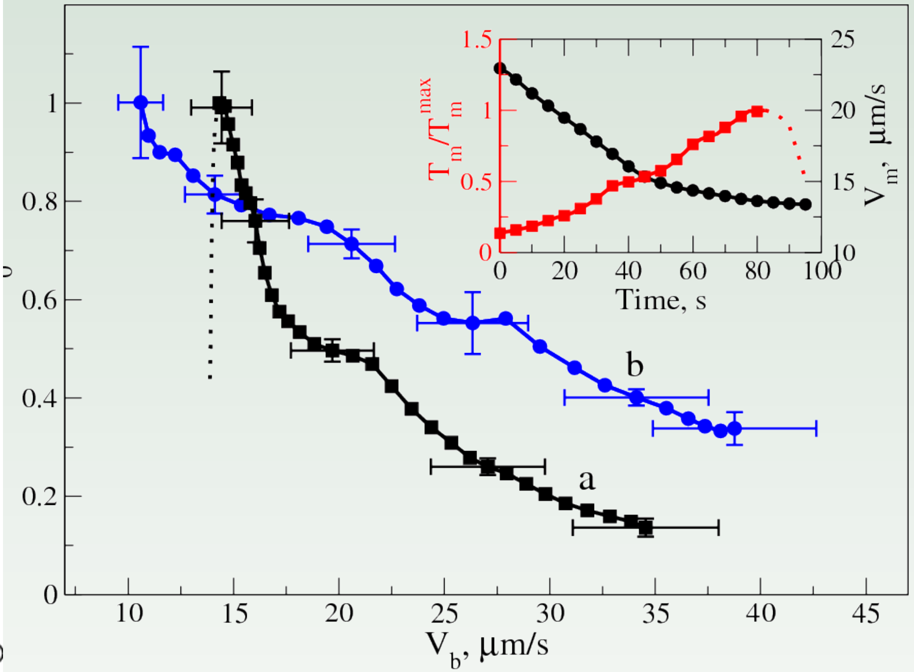
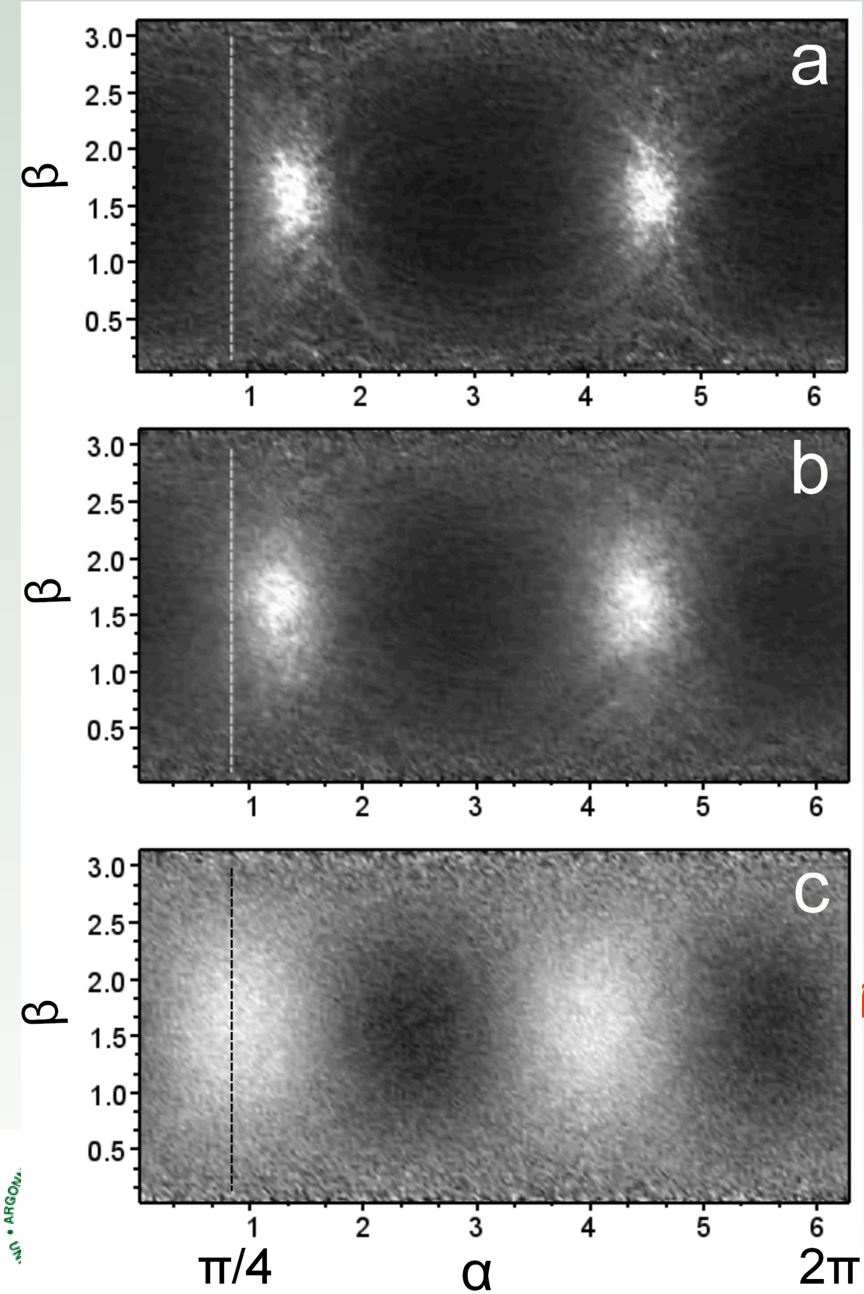


a) n=1.8·1010 cm-3

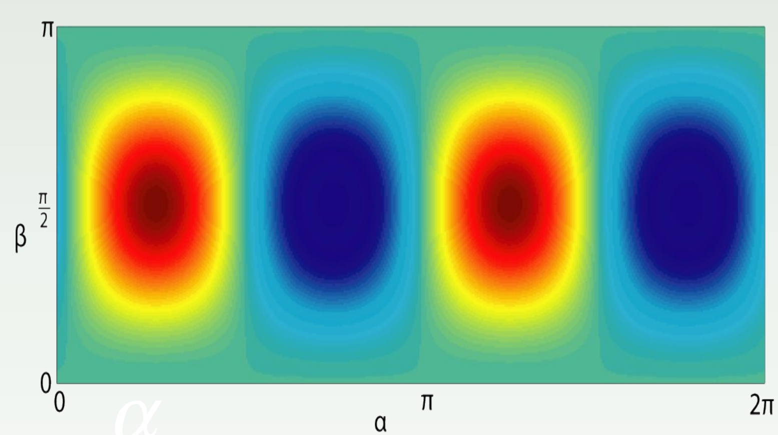
b) n=1010 cm-3

Orientation Distribution Functions P(α,β)



low concentration, max at π/2

Dilute limit with tumbling



high concentration, max at π/4

Analytical Results

Conclusions

Equations are derived from microscopic interaction rules
Reasonable agreement with experiment
Applications for biological and non-biological systems:

- *bacterial colonies*
- *cytoskeleton dynamics*
- *self-propelled particles (vibrated rods, etc)*