

Computational Soft Matter Physics

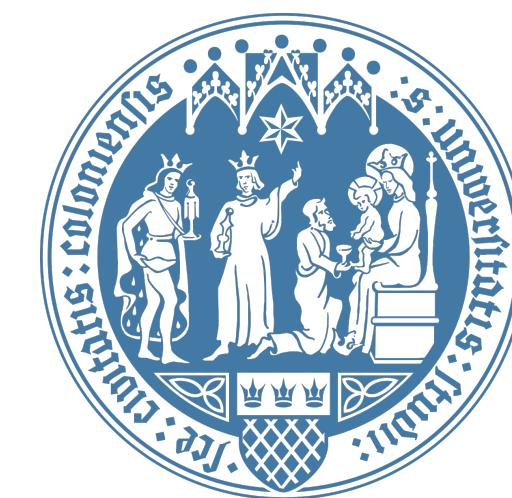
Prof. Dr. Gerhard Gompper; PD Dr. Dmitry Fedosov; PD Dr. Marisol Ripoll

Institute of Biological Information Processing (IBI)
Theoretical Physics of Living Matter (IBI-5/IAS-2)
Forschungszentrum Jülich

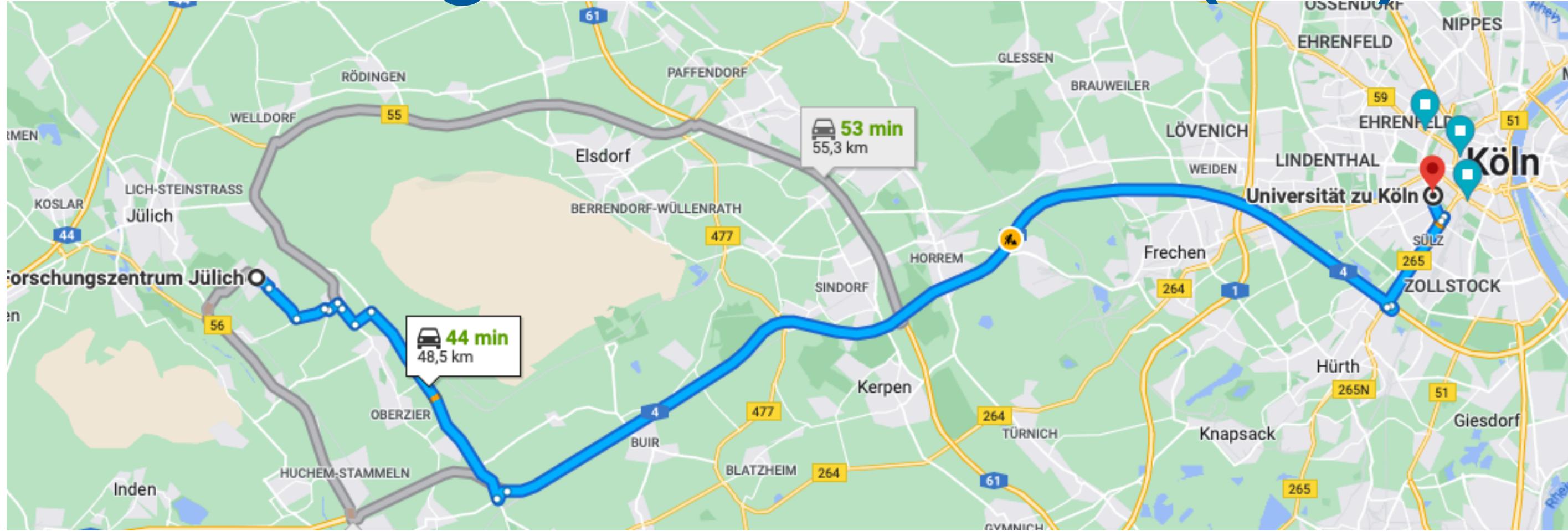
Universität zu Köln, Forchungszentrum Jülich, April 2023

Mitglied der Helmholtz-Gemeinschaft

Marisol Ripoll, 4 April 2023



Forschungszentrum Jülich (FZJ)



- Founded December 1956
- Helmholtz Association
- Employees: ~ 6800





Forschungszentrum Jülich (FZJ)

Mitglied der Helmholtz-Gemeinschaft



Computational Soft Matter Physics

Theory class

Practical exercises class

Tuesdays 10:00-11:30

Tuesdays 11:45-12:30

Lectures:



Gerhard Gompper



Dmitry Fedosov



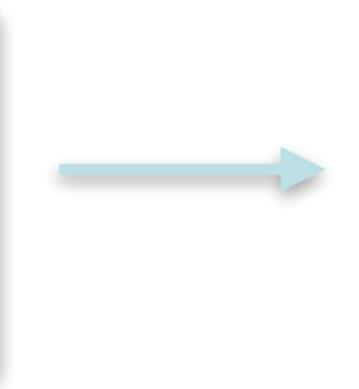
Marisol Ripoll



Computational Soft Matter Physics

Theory class

Practical exercises class



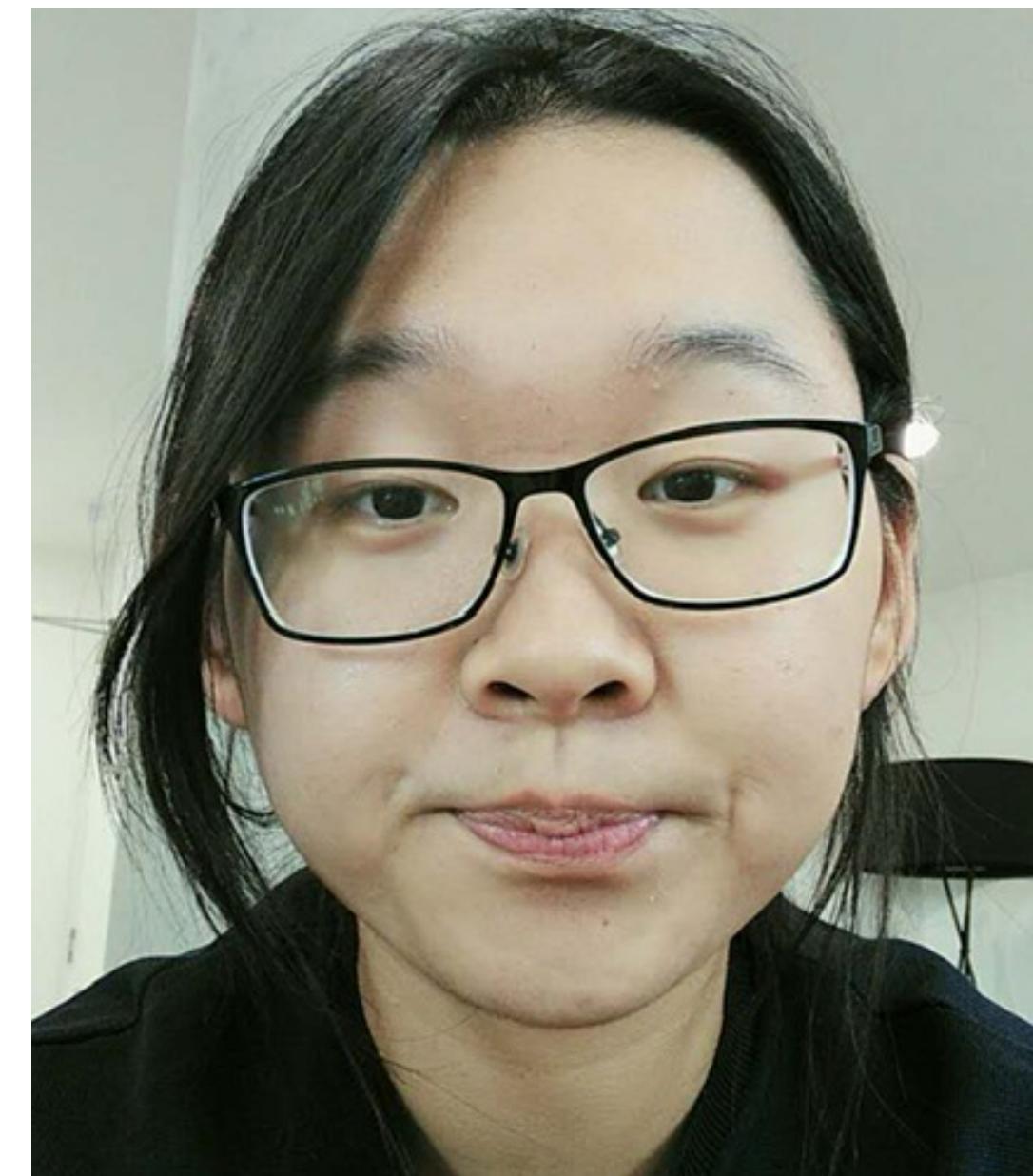
Tuesdays 10:00-11:30

Tuesdays 11:45-12:30

Exercises:



Florian Overberg

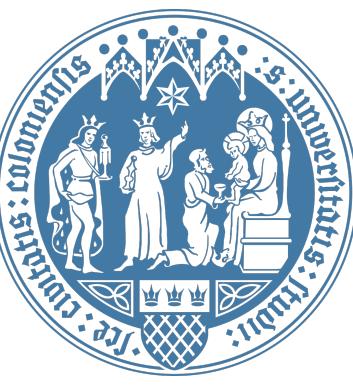


Bohan Zhang



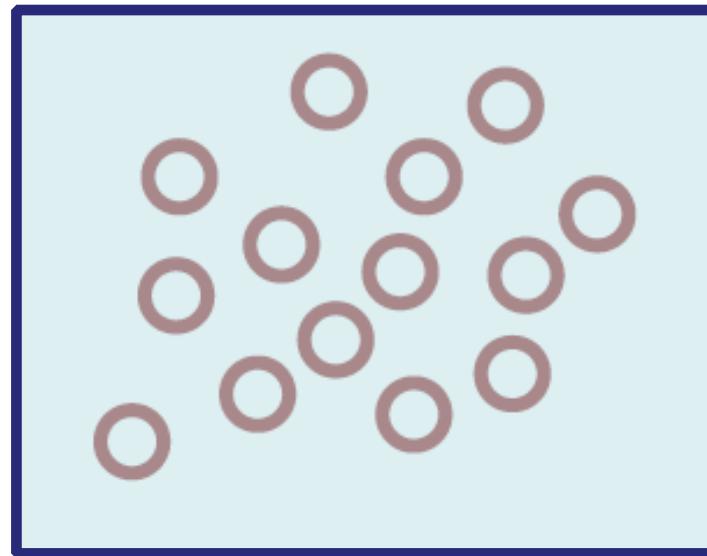
Alper Topuz

Chapter 1: Introduction

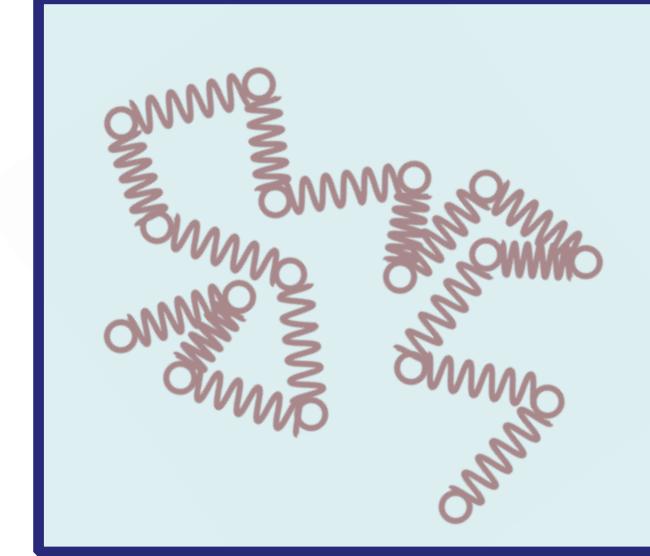


1.1.) Systems: Soft Matter

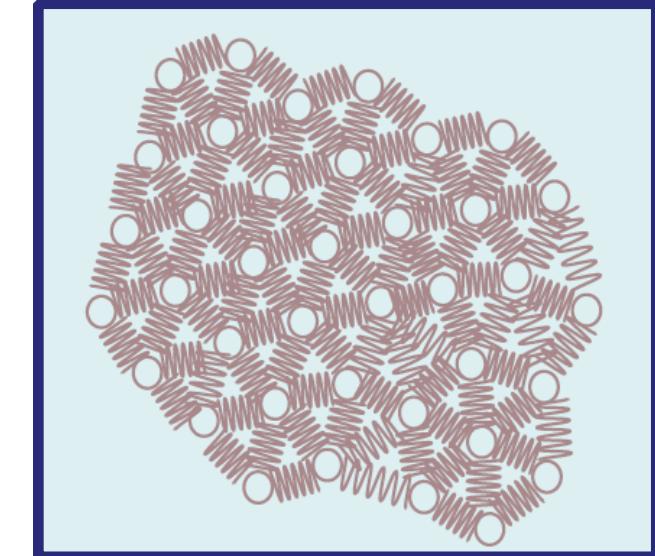
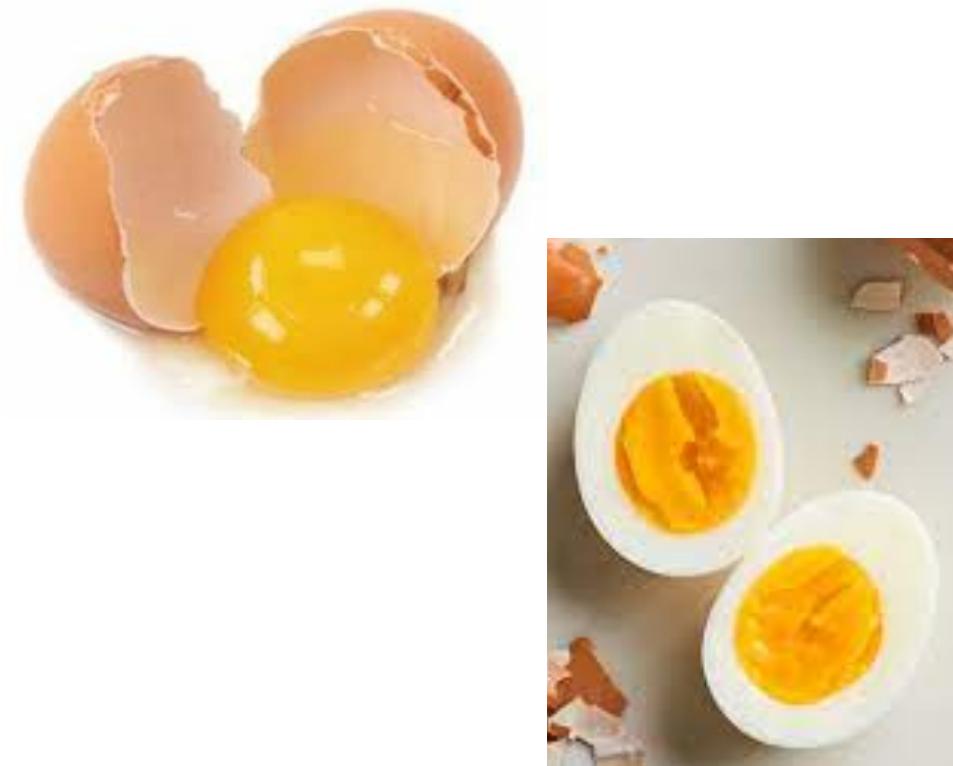
- Colloidal suspensions: small solid particles in solution
- Polymer solutions and polymer melts: long flexible chain-like macromolecules in a solvent
- Membranes: deformable and fluctuating surfaces in a solvent
- Interfaces: surfaces separating two coexisting phases



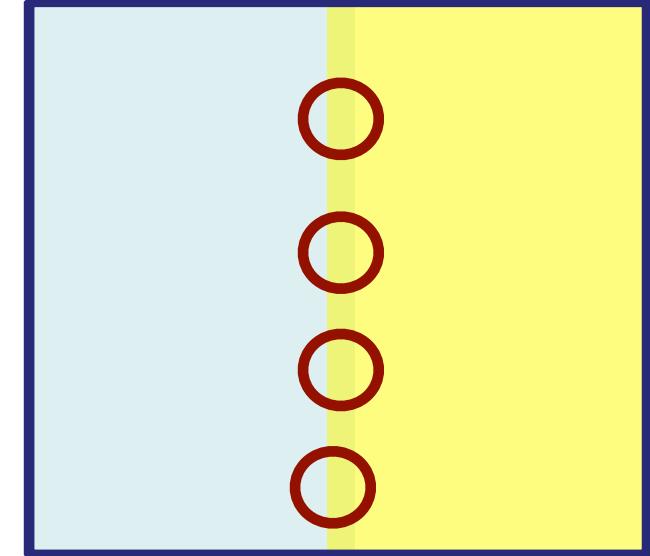
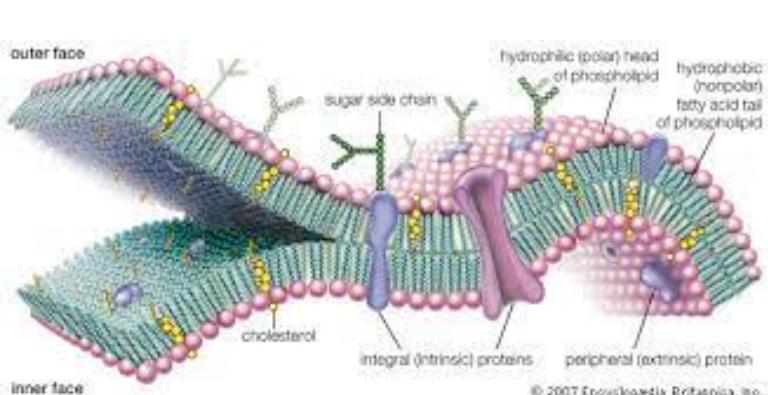
Colloids



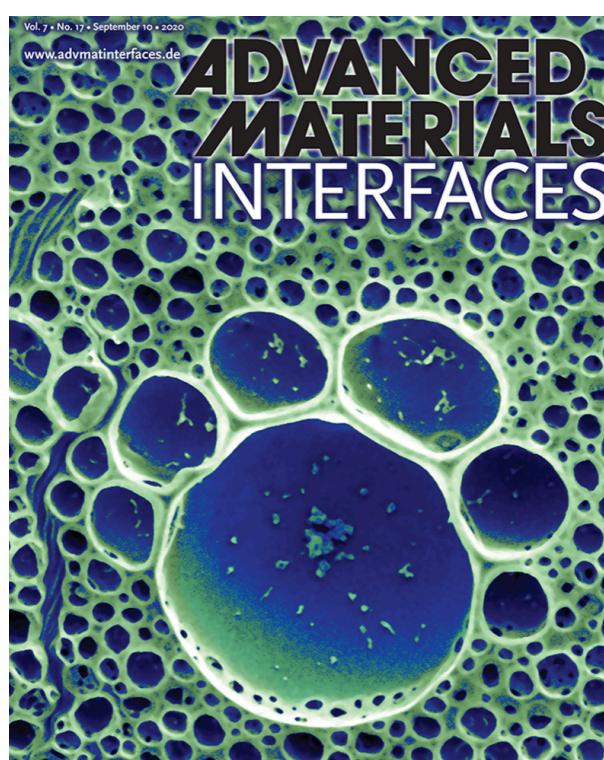
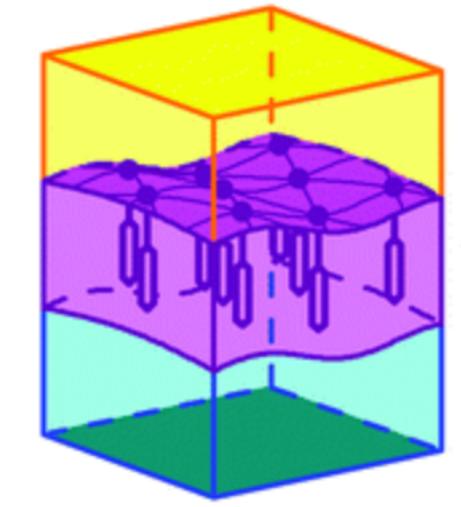
Polymers



Membranes

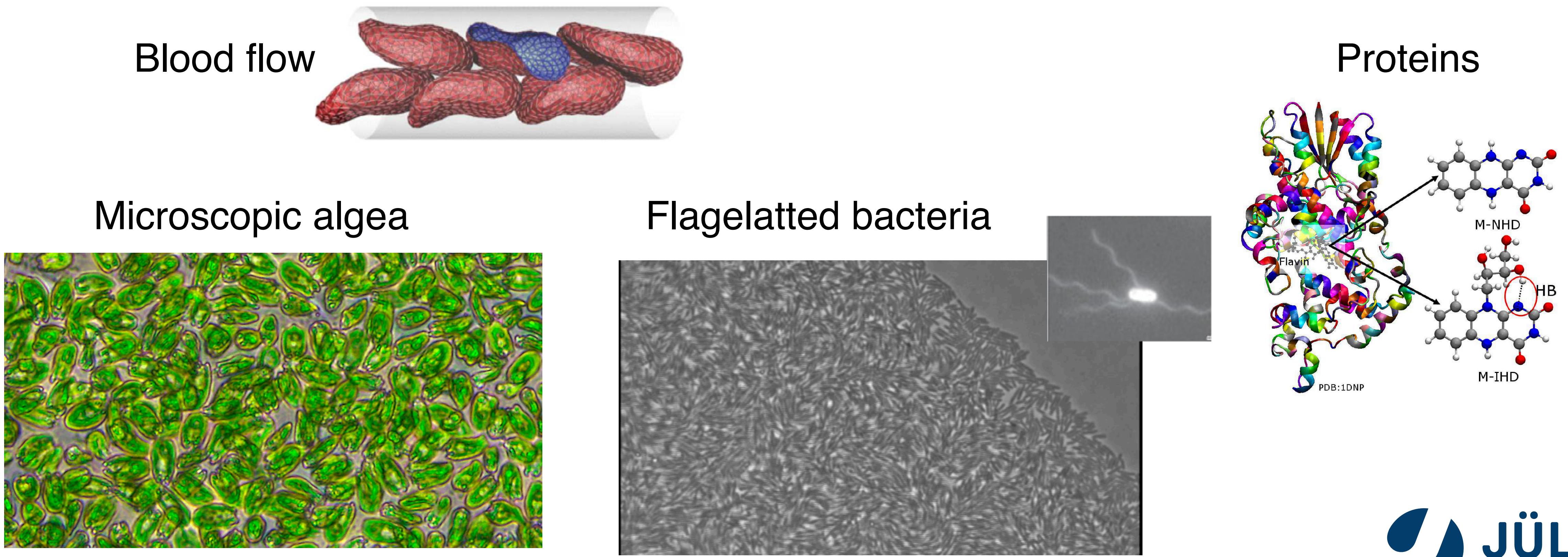


Interfaces





- Non-equilibrium systems: fluid flows, heat flow, flood flow,....
- Active matter: moving microscopic constituent which drive the system out of equilibrium (microalgae, bacteria, cytoskeleton, ...)
- Living matter: proteins, cell function, tissue growth, genetic networks, ...





1.2.): Computational Physics: General considerations

Physics as a modern and quantitative science is nowadays characterized by an interplay of:

Experiments \longleftrightarrow Theory

In theory numerical mathematical methods are common...

for example:

- Linear algebra
- Interpolation
- Integration
- Solution of differential equations



- These traditional methods:
 - treat „easy“ mathematical questions
 - are affected by numerical errors
 - provide columns of numbers
- An alternative approach has been developed in the last 7 decades

These are computer programs that can carry out symbolic operations,
the so-called **Computer-Algebra**
- Advantages:
 - results exact or with smaller errors
 - functional interrelations (larger complexity)
- Another completely different approach, that provides a detailed understanding of complex systems the with help of numerical procedures are:

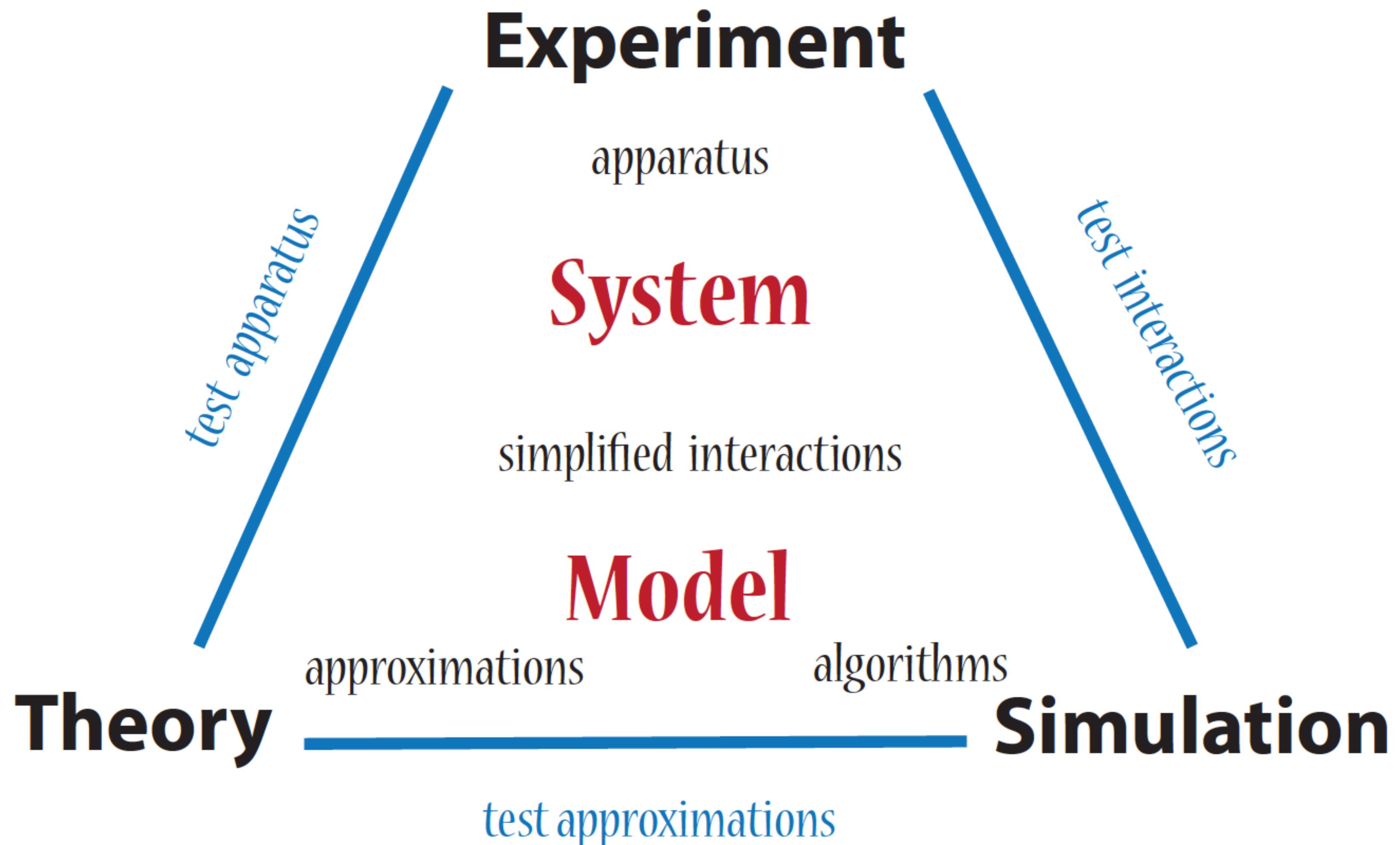
Computer-simulations



Computer-simulations

- Computer simulations are frequently referred as „numerical experiments“
- Essential ideas :
 - to track the dynamics of microscopic degrees of freedom
 - macroscopic properties are obtained from the average of the many microscopic motions
- Advantages:
 - for small enough systems, the results are in principle exact
 - microscopic and macroscopic information is easily accessible
 - there are very few restrictions about the number of components, nor about the type, range, and number of interactions to be considered

Why do we need computer simulations ?





Types of computer-simulations:

i) Close-to-experiment simulations

Idea: to consider a model that accounts for a real system with as much detail as possible

Example: Protein in a lipid membrane

Advantage: Microscopic information which experimentally is very difficult (or impossible) to obtain is now easily accessible

ii) Close-to-theory simulations

Idea: to consider a strongly simplified model which is the starting point of a theoretical calculation

Example: Ising model

Advantage: In simulations no further approximations are necessary, so that testing of the theoretical description is possible without additional complications that occur when comparing with experiment due to simplified modelling



- Computer-simulations and computer-algebra are now employed in all areas of natural and engineering sciences
- General advantages:
 - Visualization:** Simulation data is specially well suited for visualization, thus providing insight and intuition into physical systems
 - Risk and cost reductions:** Ways of avoiding risky or expensive experiments might be provided, such as nuclear or large parameter searches
 - New perspectives:** Simulations provide a novel and independent view on the problem at hand suggesting new observables, models, or even experiments

In this course we will concentrate in the methods and application
for Physics of condensed matter



1.3.): Computer simulations methods for solids and fluids

i) Monte-Carlo

- Particle evolve with a fictitious random hopping motion
- Such motions are constructed such that the correct average thermodynamic values are provided
- The very first publication of a „computer experiment“ set the basis of all the Monte Carlo algorithms. And this was „only“ 70 years ago ..

THE JOURNAL OF CHEMICAL PHYSICS

VOLUME 21, NUMBER 6

JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*
(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

VI. CONCLUSION

The method of Monte Carlo integrations over configuration space seems to be a feasible approach to statistical mechanical problems which are as yet not analytically soluble. At least for a single-phase system a sample of several hundred particles seems sufficient. In the case of two-dimensional rigid spheres, runs made with 56 particles and with 224 particles agreed within statistical error. For a computing time of a few hours with presently available electronic computers, it seems possible to obtain the pressure for a given volume and temperature to an accuracy of a few percent.

In the case of two-dimensional rigid spheres our results are in agreement with the free volume approximation for $A/A_0 < 1.8$ and with a five-term virial expansion for $A/A_0 > 2.5$. There is no indication of a phase transition.

Work is now in progress for a system of particles with Lennard-Jones type interactions and for three-dimensional rigid spheres.



ii) Molecular Dynamics

- Solution of the Newton equations of motion for many interacting particles
- The possible length and time scales to be reproduced still varies largely, depending in what do we consider as a particle
- This is anyhow the most „microscopic“ method that we will treat here

iii) Brownian Dynamics

- Many relevant systems consider particles in solution
- Their dynamic properties are importantly influenced by the interaction with solvent molecules
 - ▶ Solvent details are not really relevant: no explicit solvent particles
 - ▶ Interaction with the solvent is considered with additional friction and random noise terms
 - ▶ For micrometer sized particles the inertia can be typically neglected (overdamped motion)



iv) Mesoscale hydrodynamics

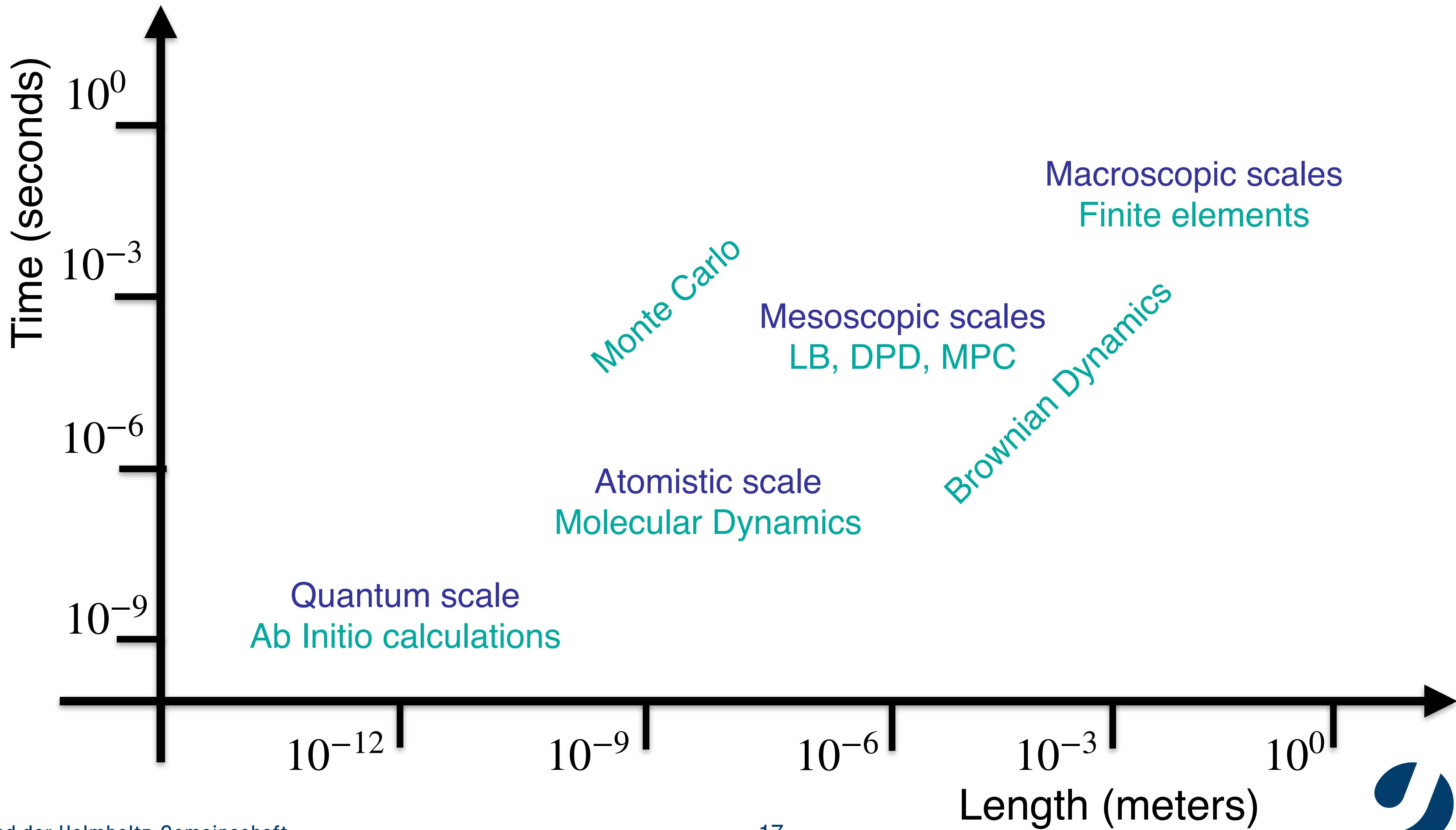
- Hydrodynamics refers to solvent mediated interactions among suspended particles
- Complex fluids (milk, blood,..) offer many examples where hydrodynamics is relevant, which does not require solvent details
- Approaches are used where the solvent is very strongly simplified, but where the conservation of mass and momentum is ensured
 - ◆ Lattice Boltzmann (1988)
 - ◆ Multiparticle Collision Dynamics (1999)
 - ◆ Dissipative Particle Dynamics (1992)
 - ◆

v) Machine learning data-driven techniques

- These are mathematical algorithms that use available data to build models
- The algorithms correct themselves using data as „training“, and being afterwards able to make predictions and/or decisions
- Many applications: search engines, face recognition,... and also soft matter systems



Computer simulations methods for solids and fluids

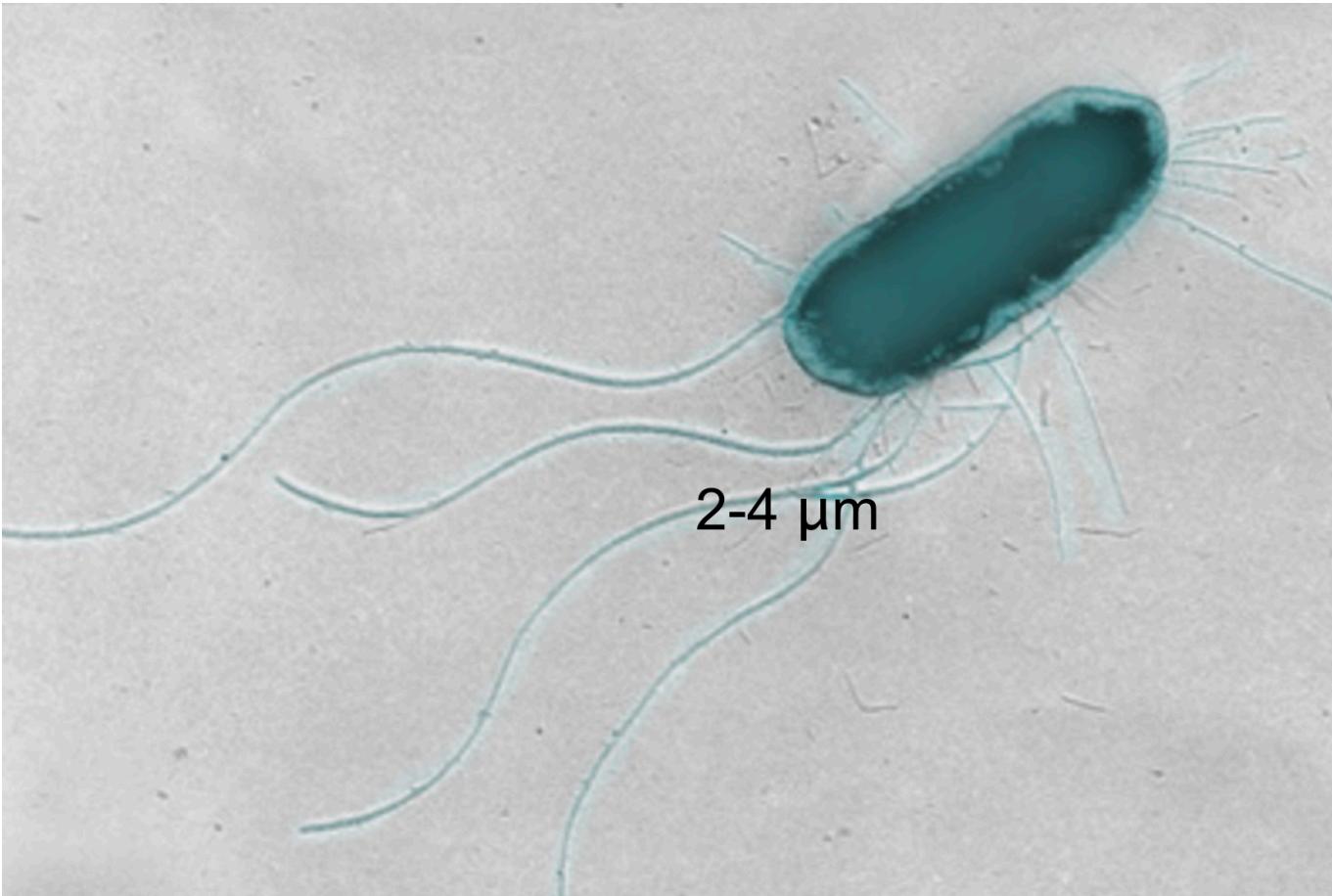




1.4.) Example of simulations in bio-soft matter systems

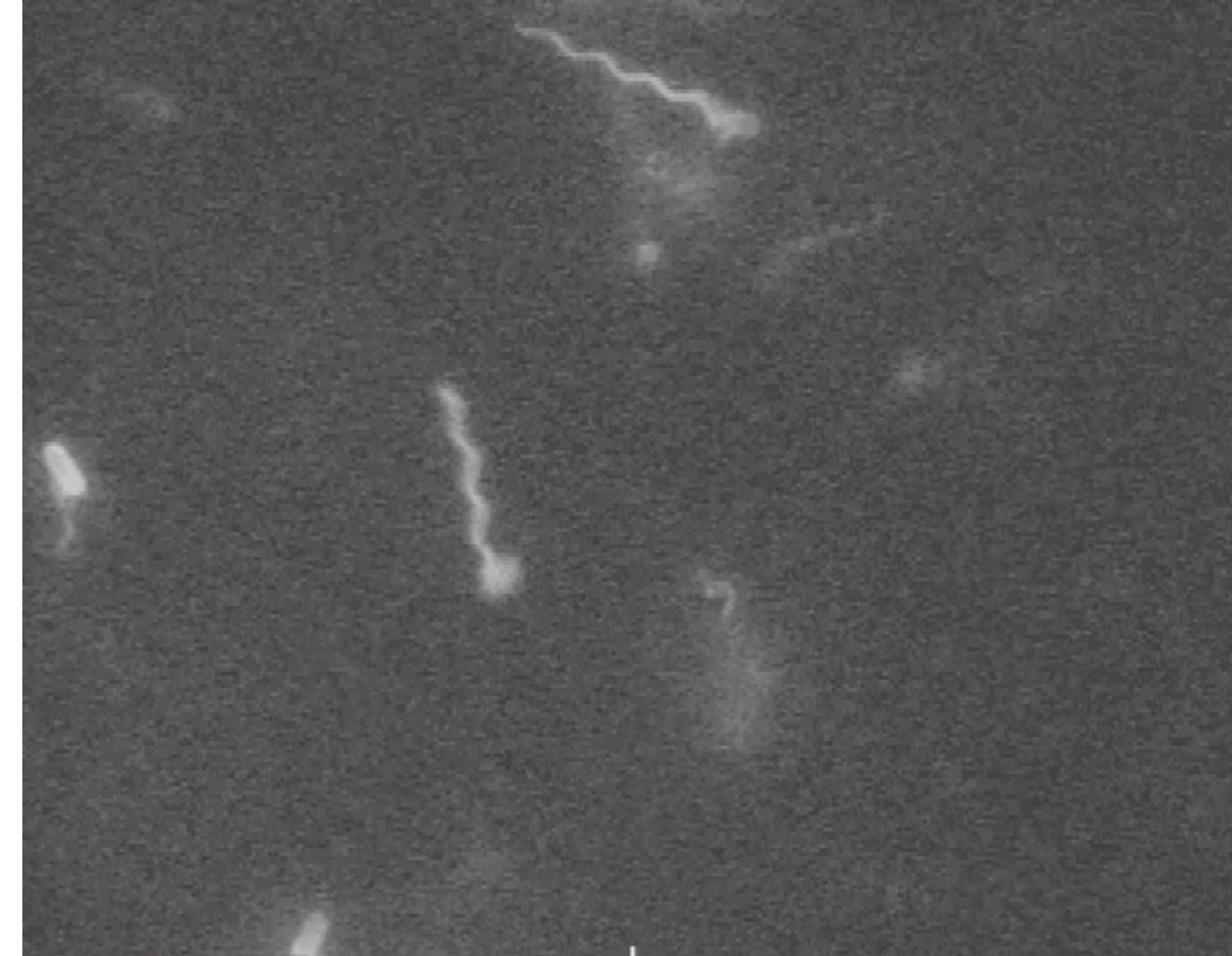
Swimming E-coli bacteria

- Movement task: Searching for food
- How can a bacterium swim?
 - By using helical flagella
 - Flagella rotate in a bundle or independently -
„Run and Tumble“

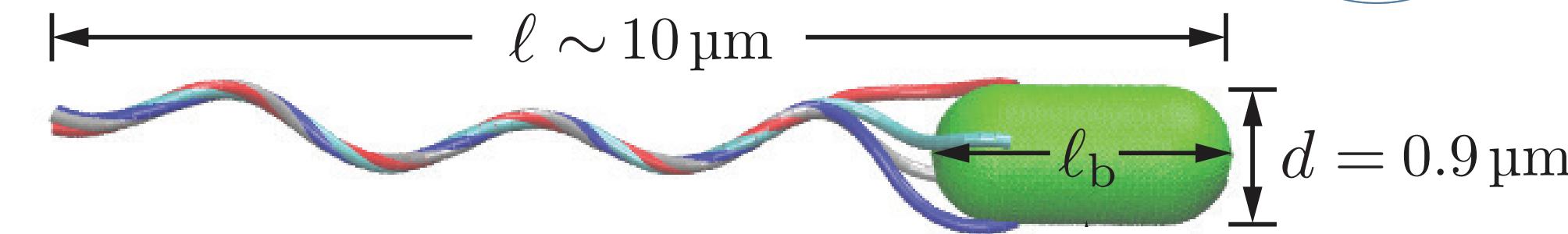


Escherichia coli

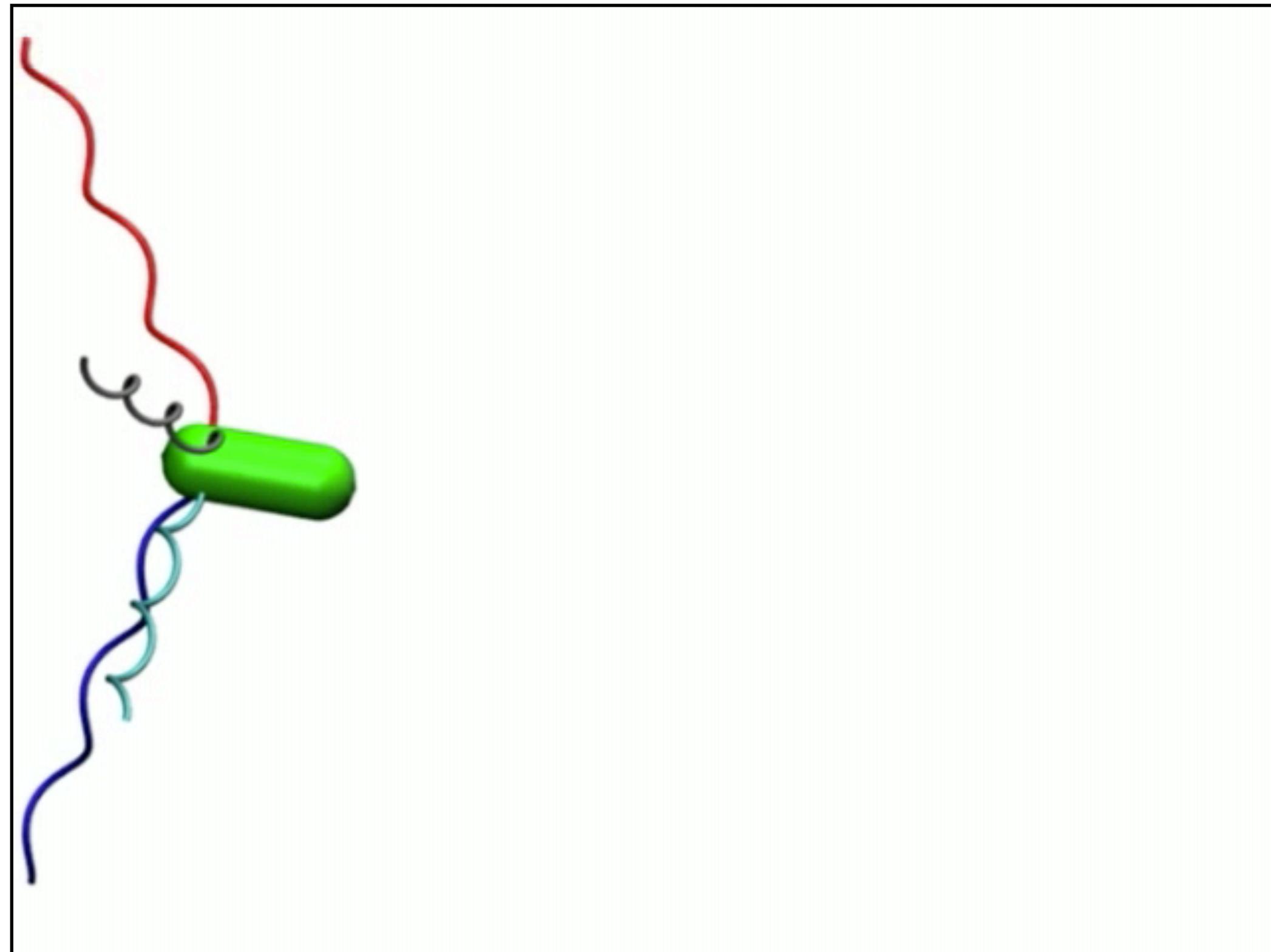
Experiments



http://www.rowland.harvard.edu/labs/bacteria/movies_ecoli.html



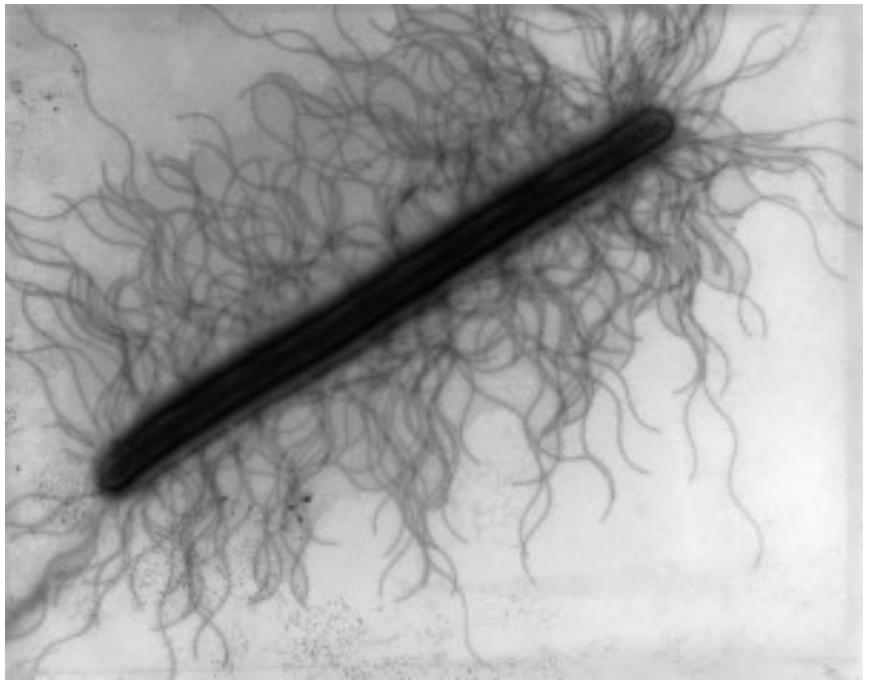
Simulations



Swimming with many flagella

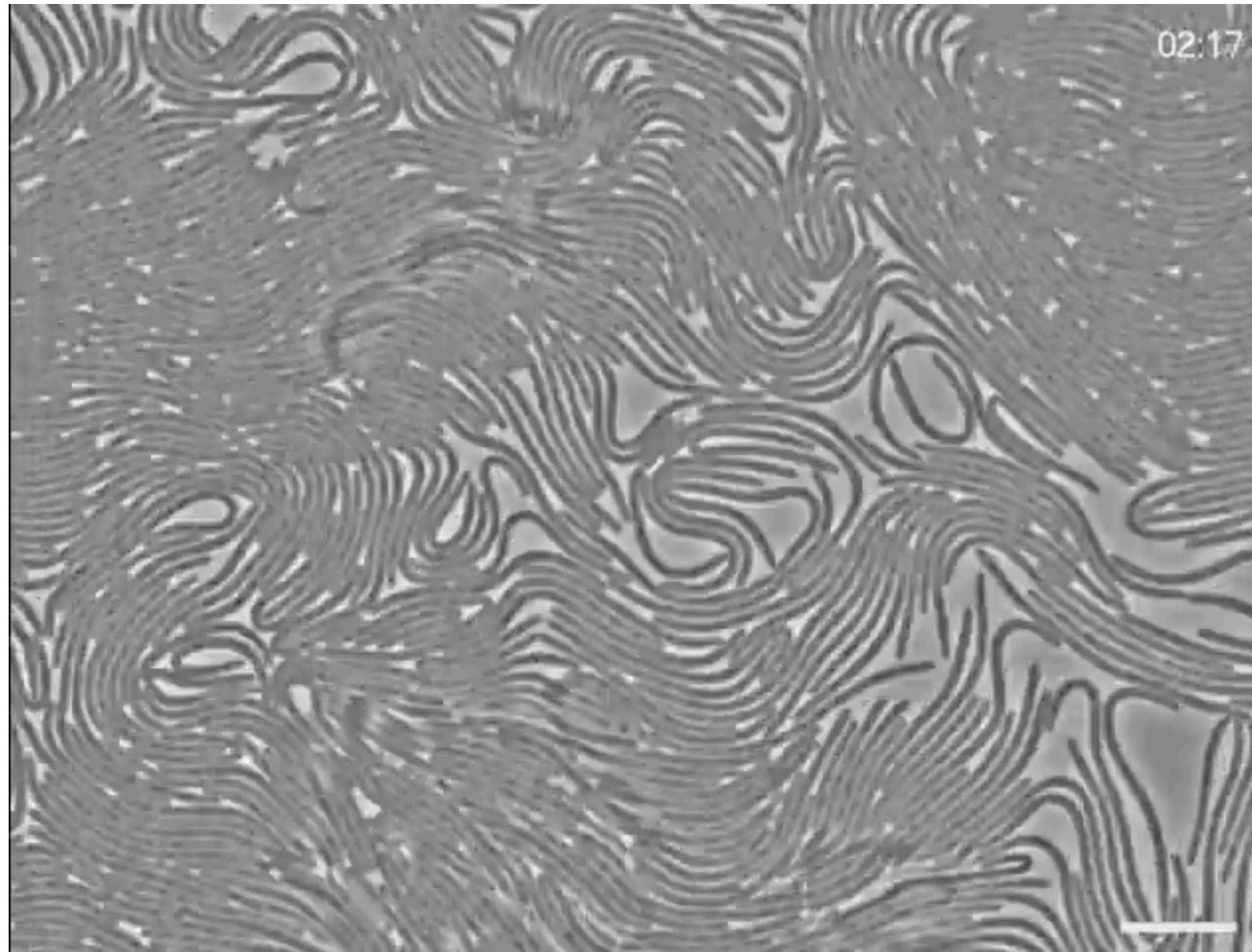


Proteus mirabilis bacteria



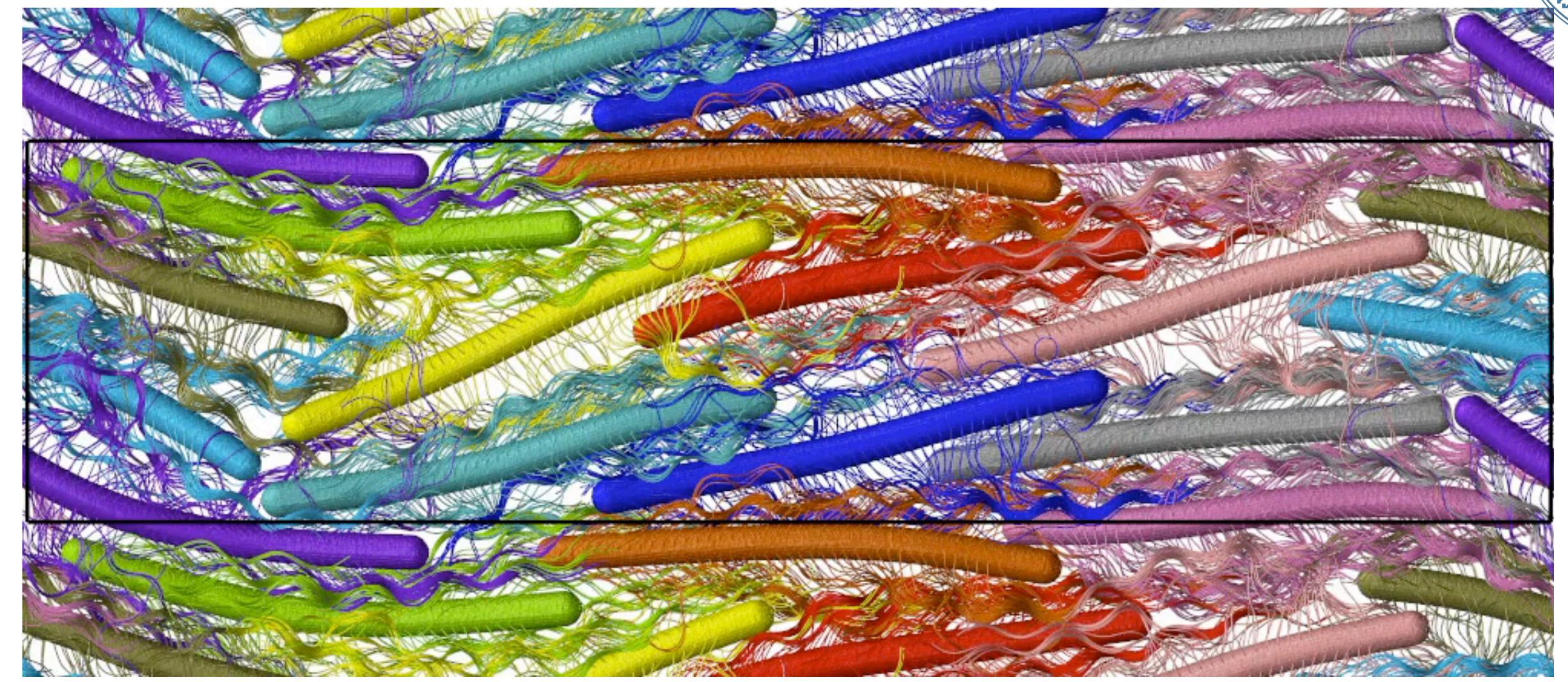
The bacteria only swim when they have neighbours

Experiment



Mitglied der Helmholtz-Gemeinschaft

Detailed simulation model



Simplified simulation model

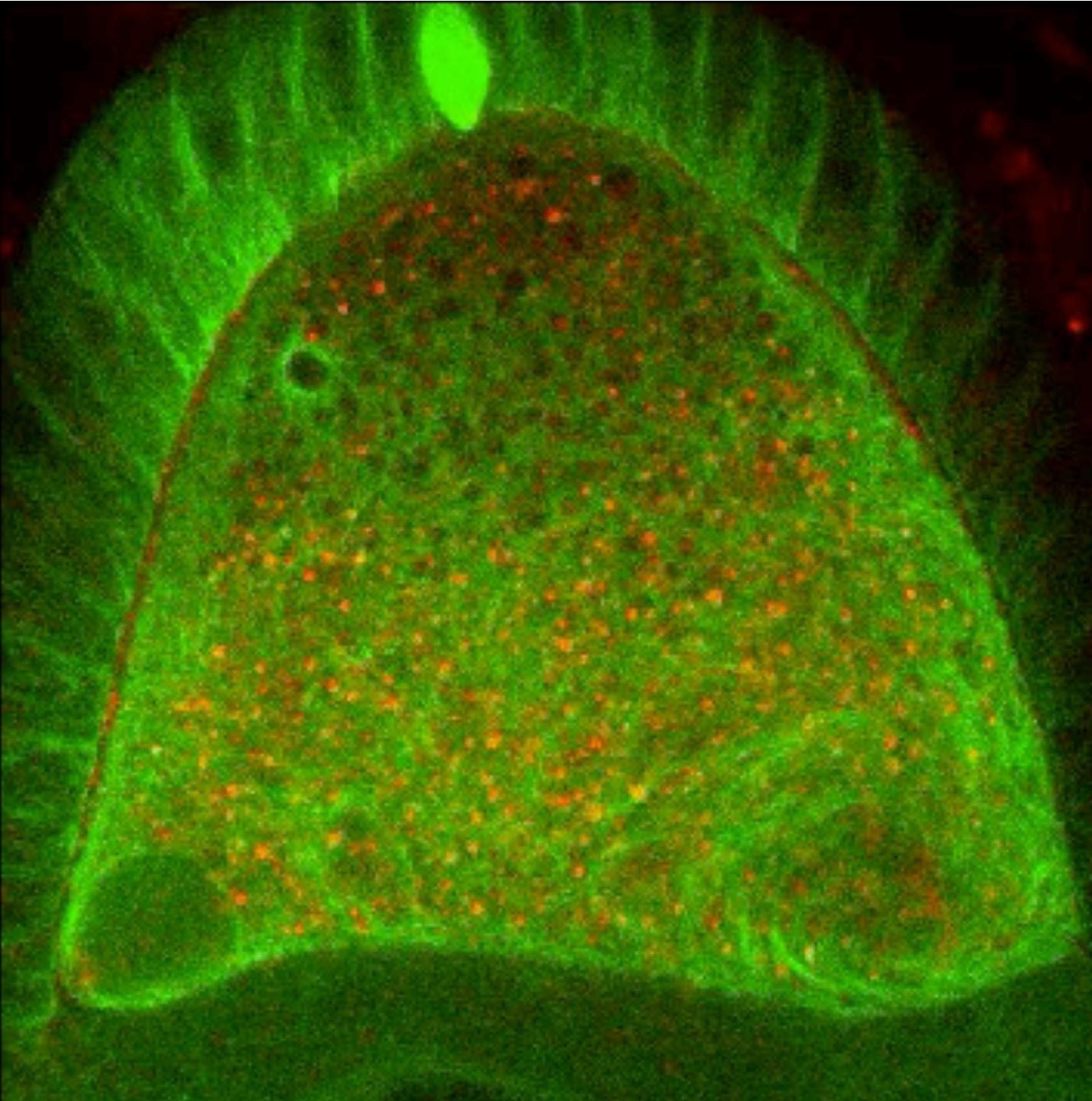




Filaments and molecular motors

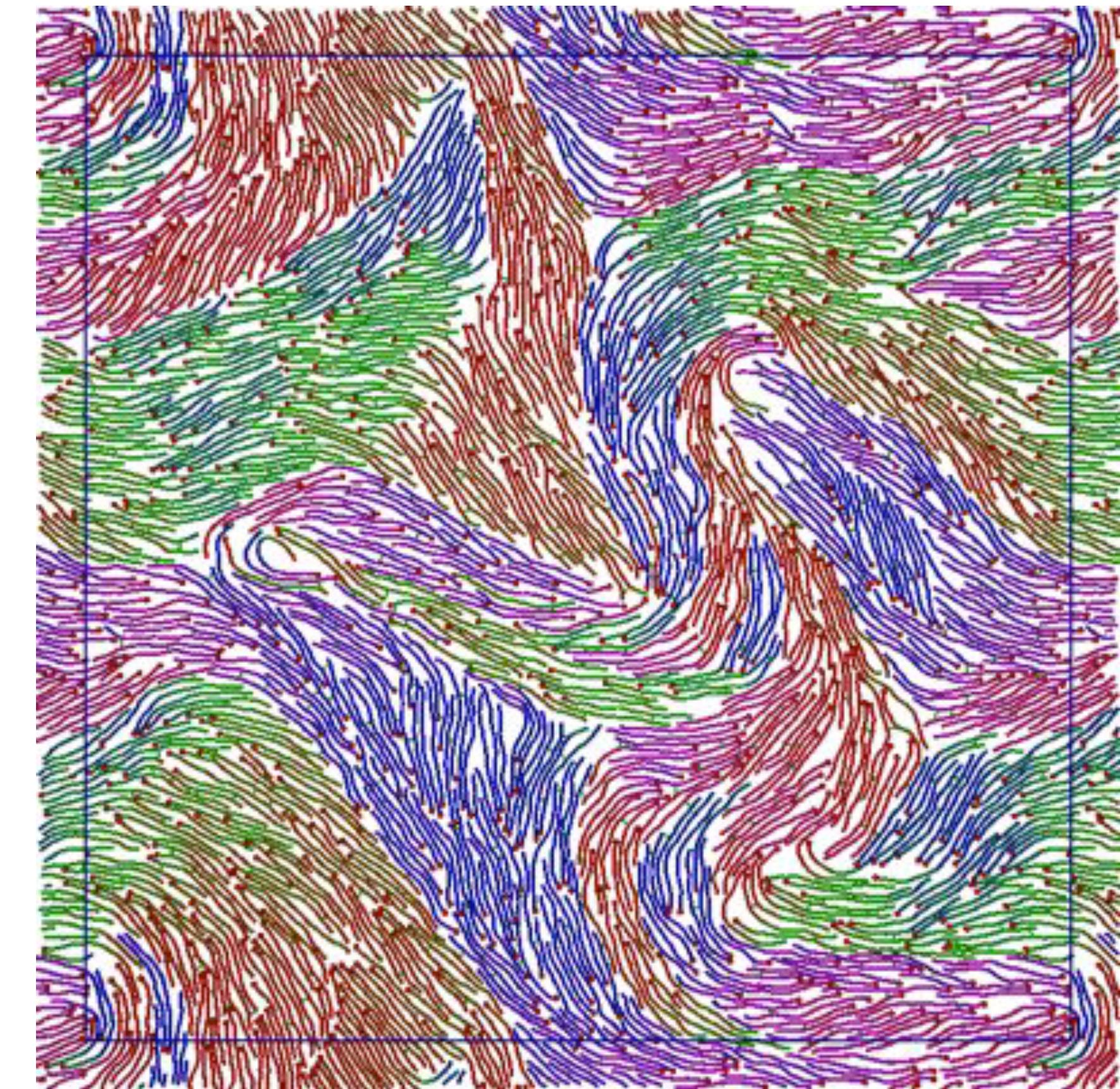
How does the motion occur the motion inside the cell ?

Experiment



Cytoplasmic flow in oocytes

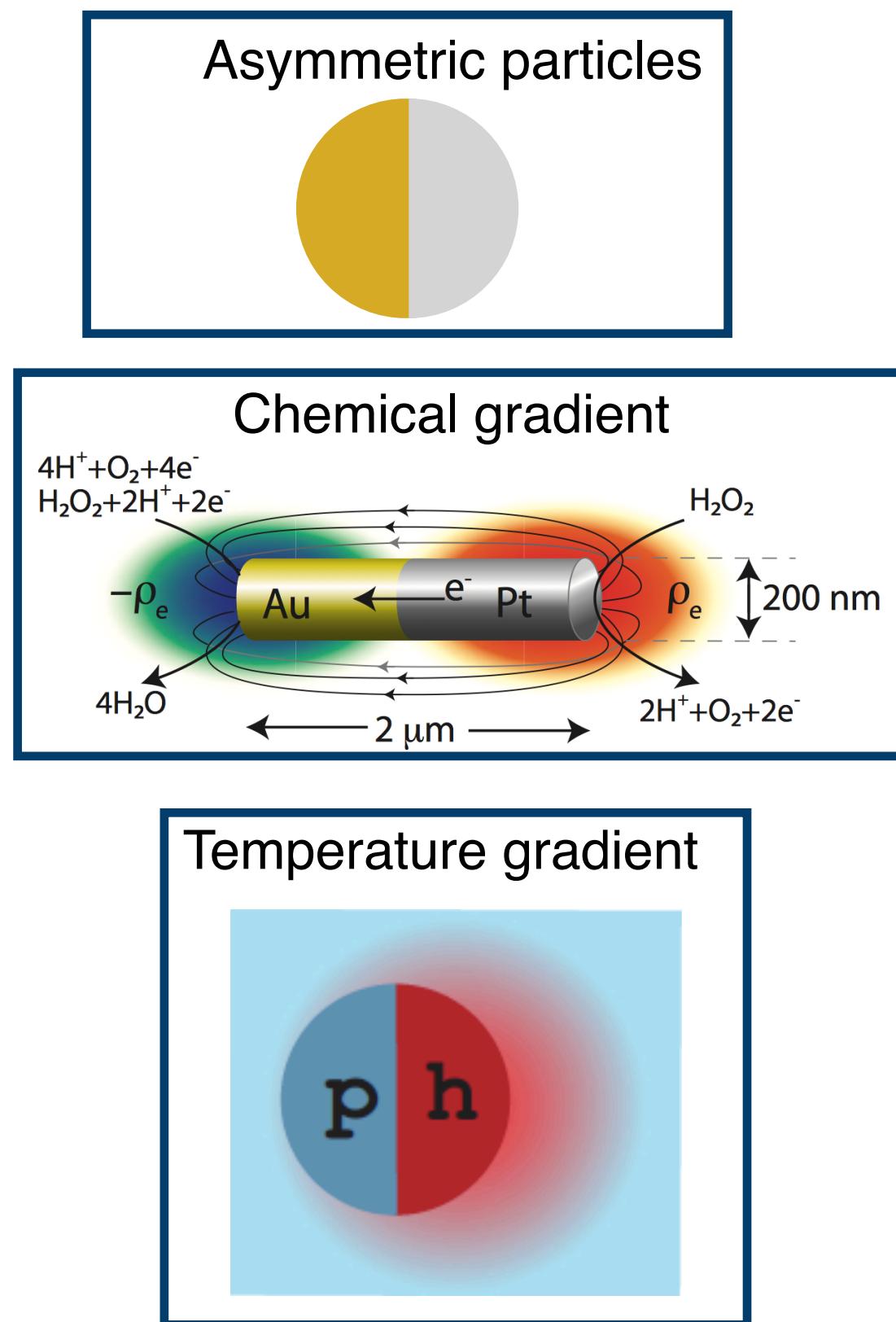
Simulation



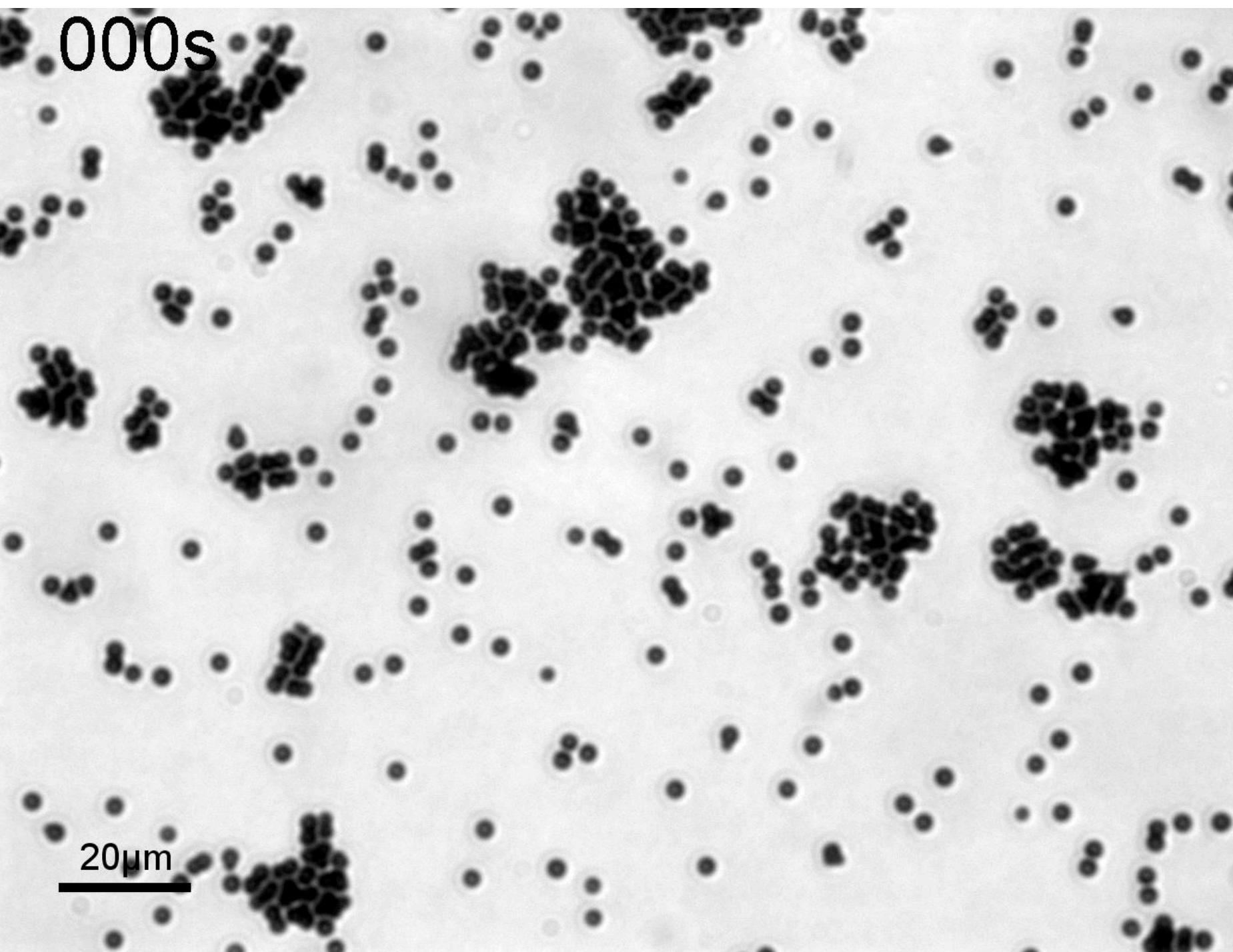
Filaments driven by molecular motors

Synthetic swimmers

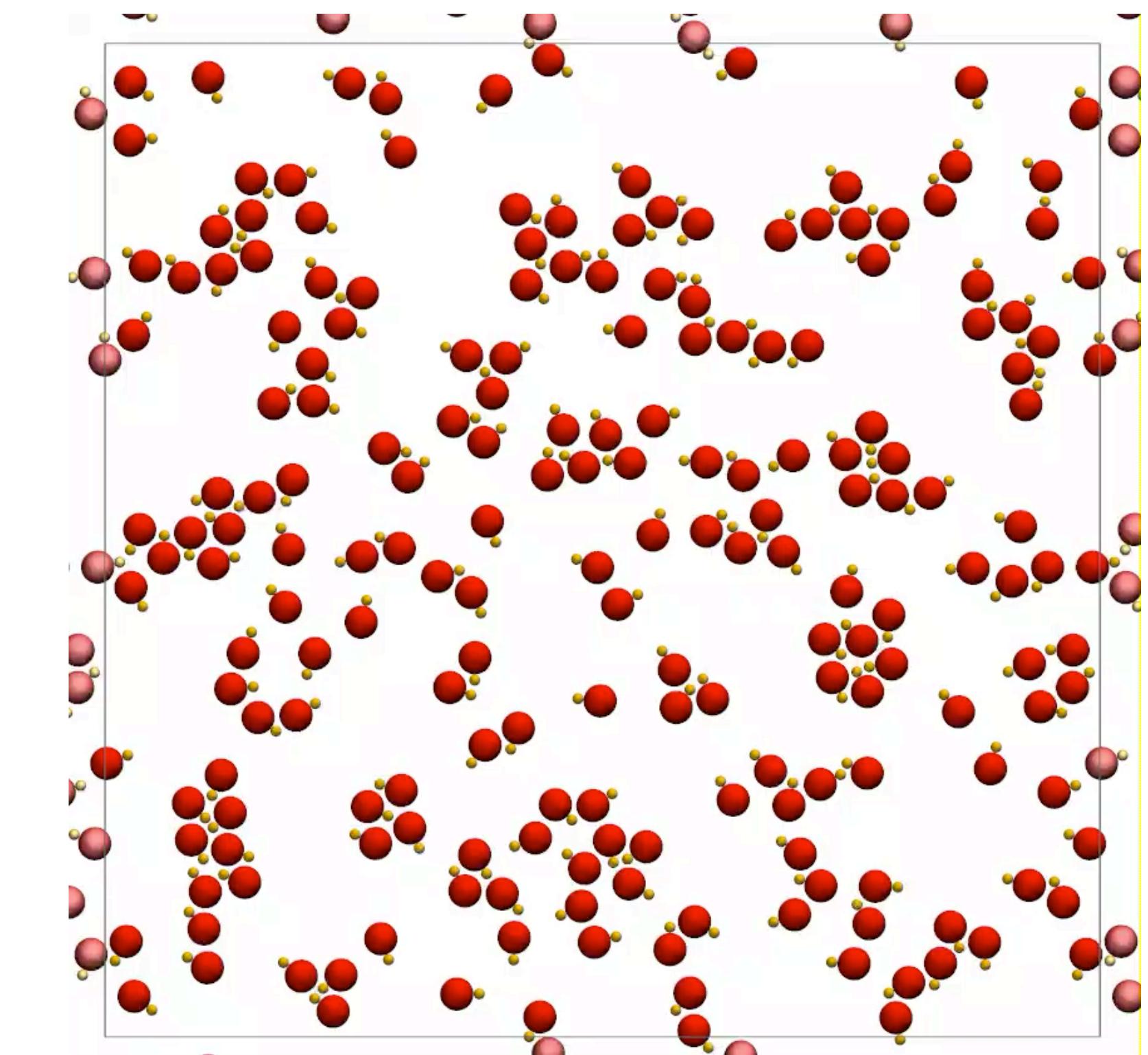
- How can floats be built?
- Why? New biomimetic/compatible materials and microfluidics



Experiment



Simulation



Theurkauff, Cottin-Bizonne, Palacci, Ybert, Bocquet (2012) *Phys. Rev. Lett.* **108** 268303



Practical exercises class

- You will have to write small computer programs related with the topics seen in class
- Some programming knowledge: C, C++, Python, ...
- Tutors will solve questions and check the exercises
- Slack already available: 23SS - Computational Soft Matter - UzK
(to get access, please send me an email: m.ripoll@fz-juelich.de)

→ Next week: no exercise but crash-introduction to [Python](#)

Thanks and... I see you next Tuesday, 11th April at 10:00