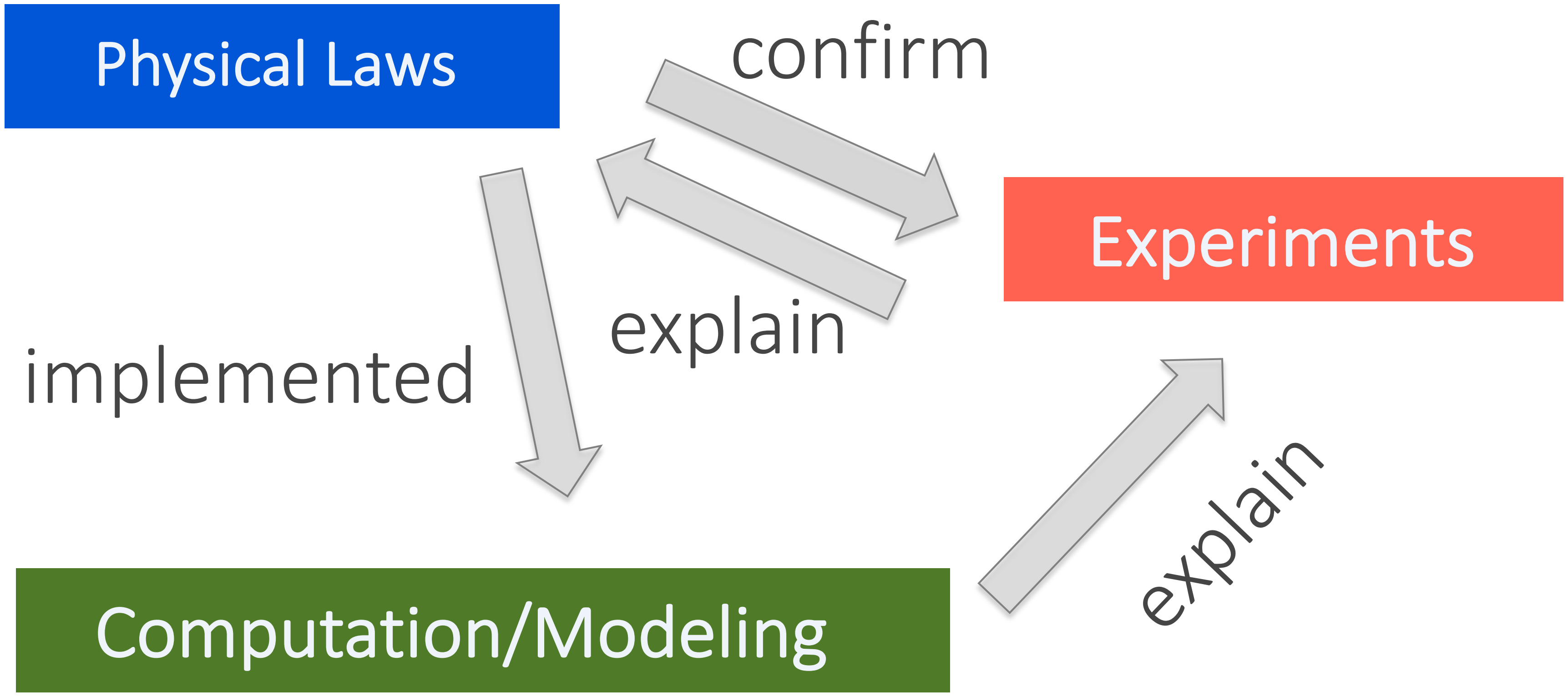
University of Stuttgart
Germany

INSTITUTE FOR COMPUTATIONAL PHYSICS

Research at the Institute for Computational Physics

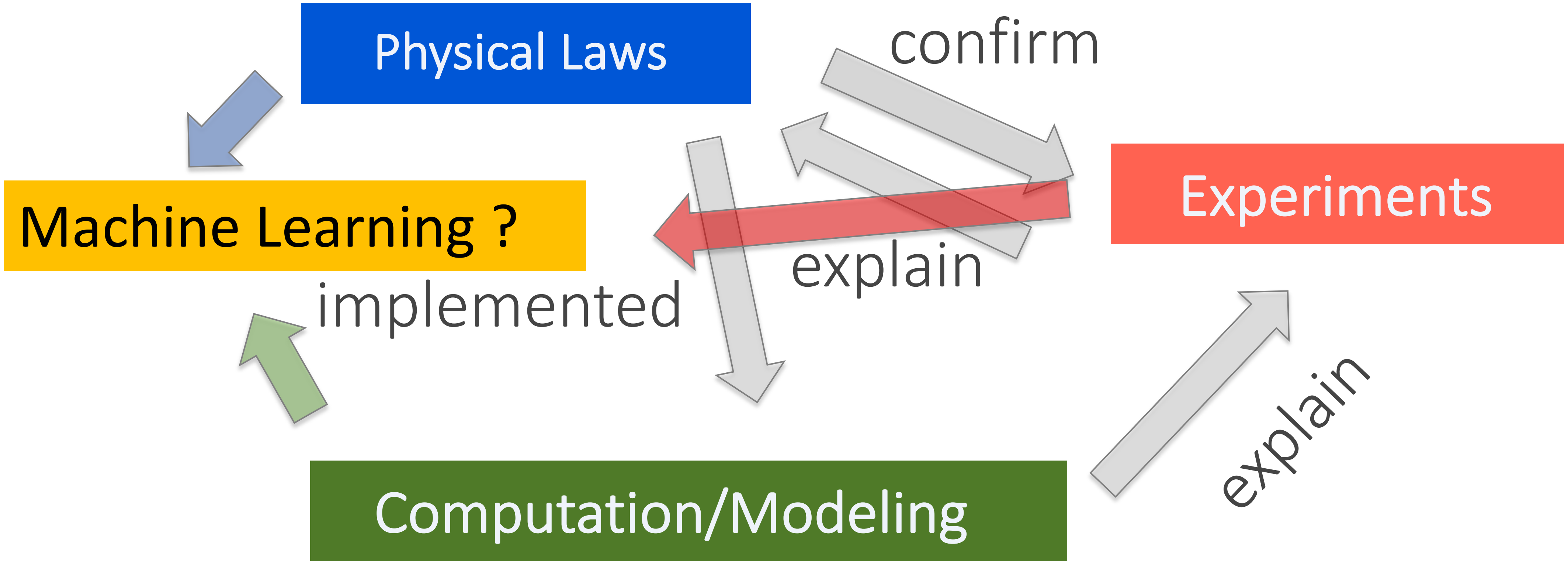
Christian Holm, Rudolf Weeber, Slavko Kondrat
Institut für Computerphysik, Universität Stuttgart, Allmandring 3
Stuttgart, Germany

The Way Physics works today…



Tool: scientific codes

The Way Physics works tomorrow…??



Tool: scientific codes

Institut for Computational Physics (ICP)

C. Holm (Director)
Theory and Simulations of Soft charged and dipolar matter
Machine Learning for Soft Matter

R. Weeber (permanent staff)
Magnetic Soft Matter, ESPResSo Software Suite

S. Kondrat (part time here permanent in Academy of Sciences, Warsaw):
Soft Matter Theory, Supercapacitor applications

S. Tovey (part time here Senior scientist at Quantum Brilliance):
ML in Physics

- Perform frontier research through high level publications
- Develop scientific computational tools and algorithms
- Education and teaching in theoretical and computational physics

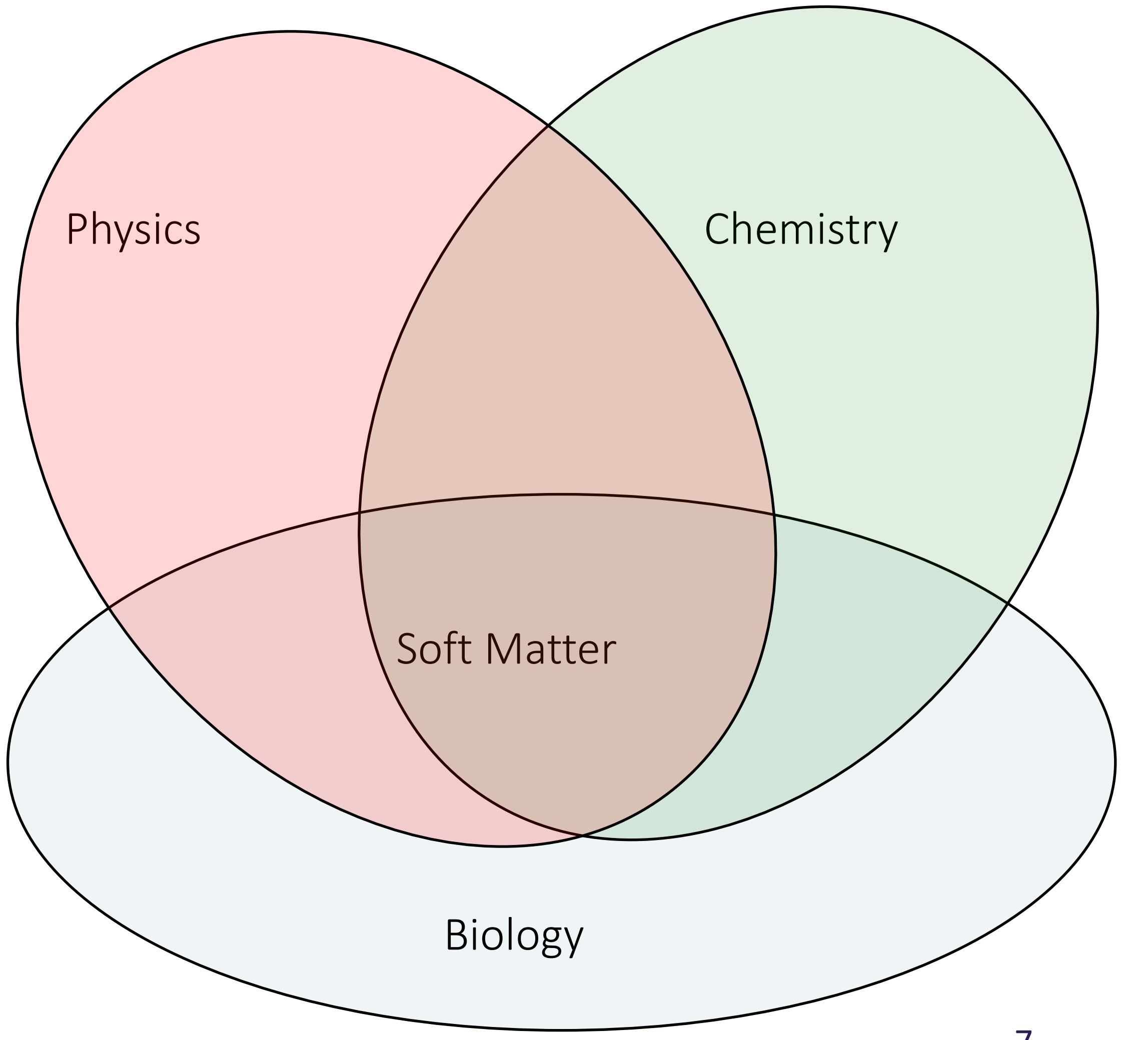
Soft Matter Physics.....

....and why is it interesting?

What is Soft Matter?

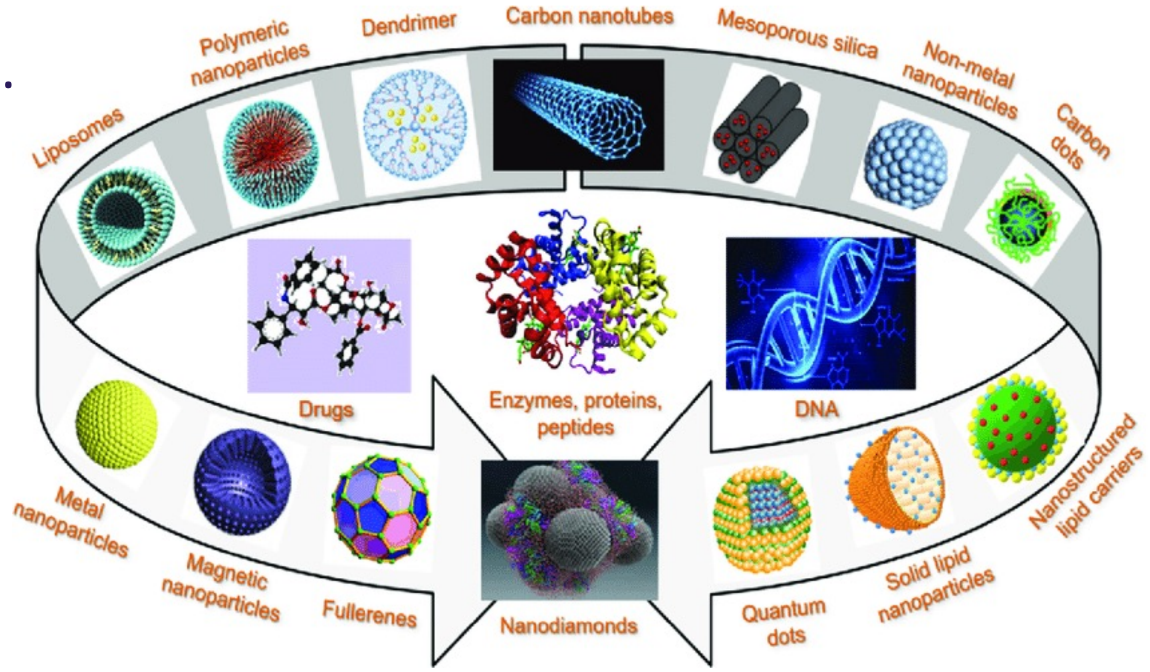
Definition of Soft Matter

Wikipedia: Soft matter is a sub-field of condensed matter comprising a variety of physical states that are easily deformed by thermal stresses or thermal fluctuations.

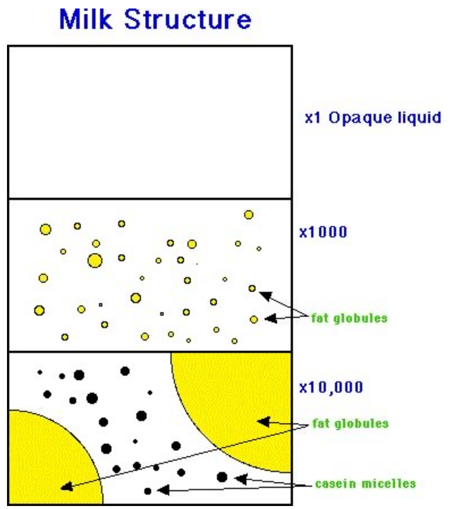


What is Soft Matter?

- Colloidal systems: milk, mayonnaise, paints, cosmetics…
- “Simple” plastics: joghurt cups, many car parts, CDs, …
- Gummy bears, gels, rubber, low fat food,
- Fibers (z.B. Goretex, Nylon)…
- Membranes: cell walls, artificial tissue, vesicles…
- Many parts of the cell, cytoskeleton, nucleus
- Most biomolecules (RNA, DNA, proteins, amino-acids)
- Liquid crystals, magnetic gels and fluids (MSM)
- Many applications: smart materials (actuators, sensors, photonic crystals), biotechnology, biomedicine (hyperthermia, drug targeting, cell separation techniques), energy materials, model systems for statistical physics

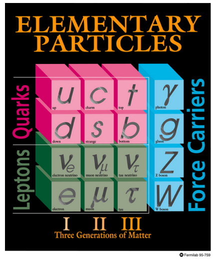


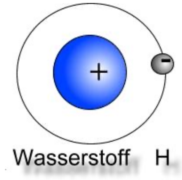
R. Kanwar et al., *Green Nanotechnology-Driven Drug Delivery Assemblies*, ACS Omega, 2019, doi:10.1021/acsomega.9b00304



Length Scales of Soft Matter

1 fm 1pm 1 Å 1nm 10 µm 1mm 1m 1km 10^3km 10^6parsec

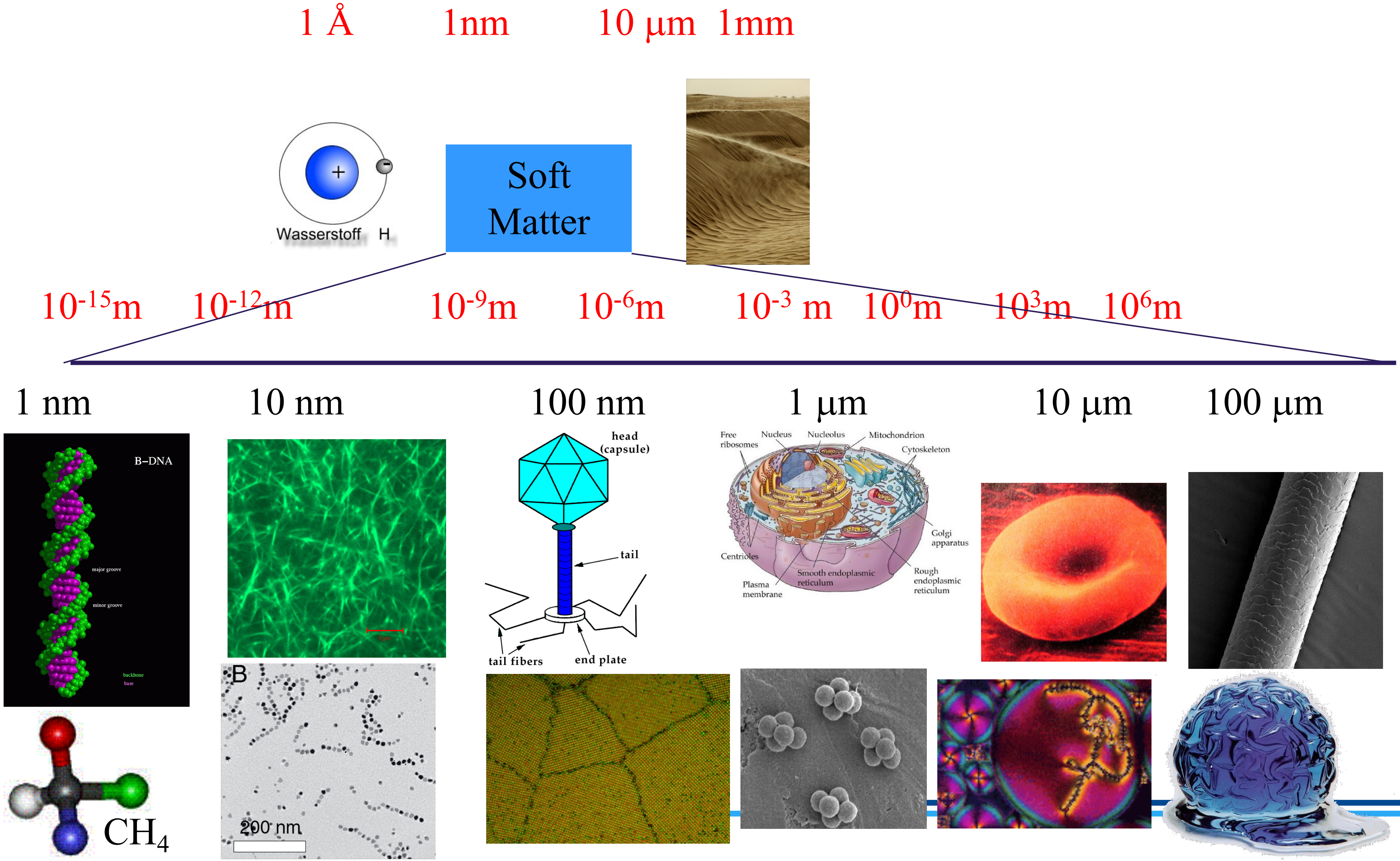




Soft Matter

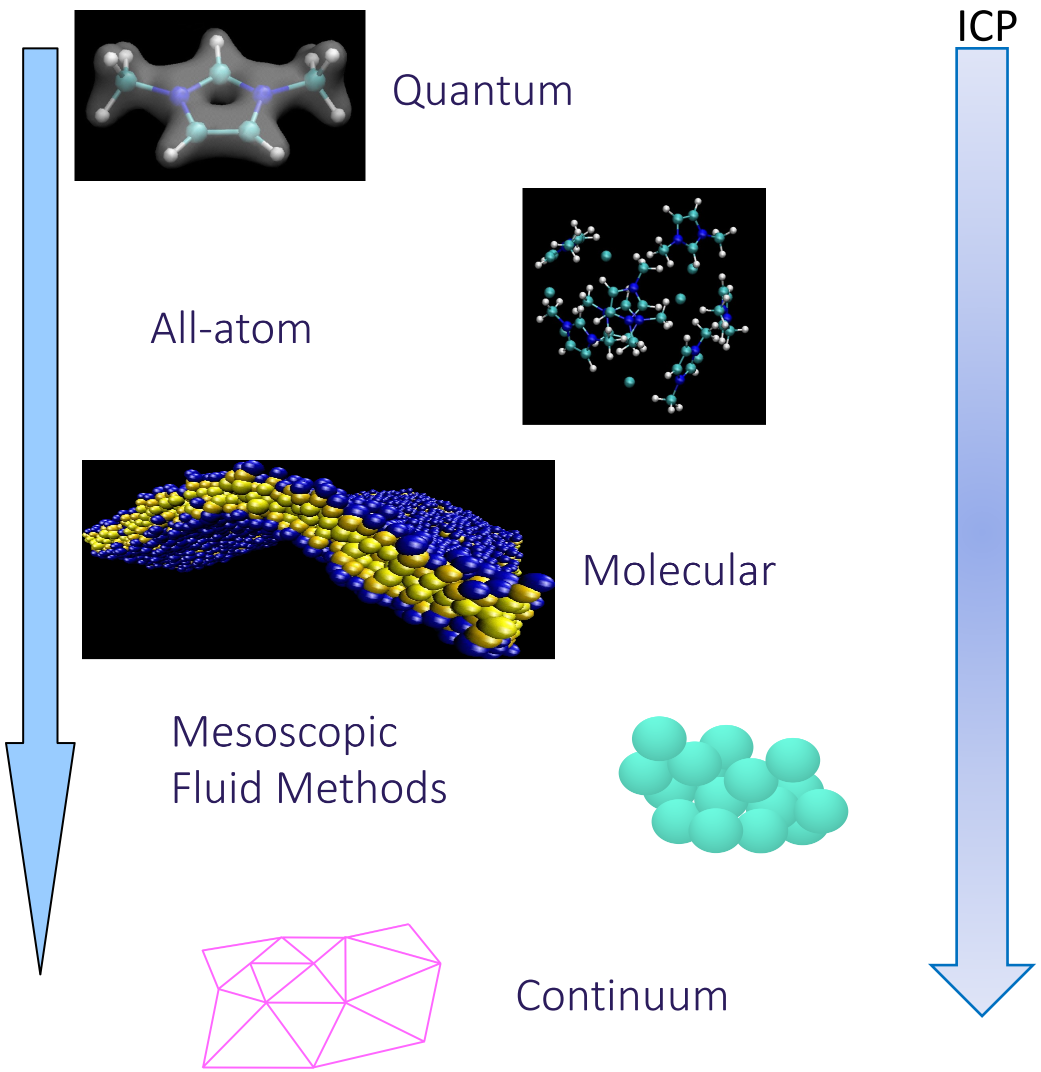
10^{-15}m 10^{-12}m 10^{-9}m 10^{-6}m 10^{-3} m 10^0m 10^3m 10^6m

Length Scales of Soft Matter



Coarse-graining for Soft Matter Systems

- A model consists of a number of ***degrees of freedom*** (e.g. atomic positions: translation) and the "***interactions***" between them.
- <u>*Coarse-graining*</u>*:*
  - reduce the number of degrees of freedom by keeping only the "important" degrees of freedom,
  - use "effective" interactions
- Classical first step: Atoms and Interactions (*all-atom* or *atomistic*)
- Further coarse-graining is often needed and useful
- For Soft Matter we are often on the molecular and mesoscopic level



Members of Various Research Consortia

SFB 1313 "Interface-Driven Multi-Field Processes in Porous Media – Flow, Transport and Deformation"

SFB 1333 “Molecular Heterogeneous Catalysis in Confined Geometries"

FOR 2811: Adaptive Polymer Gels with Model-Network Structure

Cluster of Excellence
EXC 2075

EuroHPC Centre of Excellence

Nanopore technology for the molecular diagnostics of the future

[CECAM Node Soft Matter and Statistical Mechanics (SMSM)]()

Current Research Fields

Computational Methods and Algorithms

- **ESPResSo (parallel MD package)**
- Lattice-Boltzmann for coarse-grained hydrodynamics
- Reaction-Diffusion systems (FEM) for Catalysis
- ML strategies for developing better FF for MD
- ML assisted Coarse-graining strategies
- Understand Neural Network learning strategy
- QML or ML for physics applications

Biophysical Problems

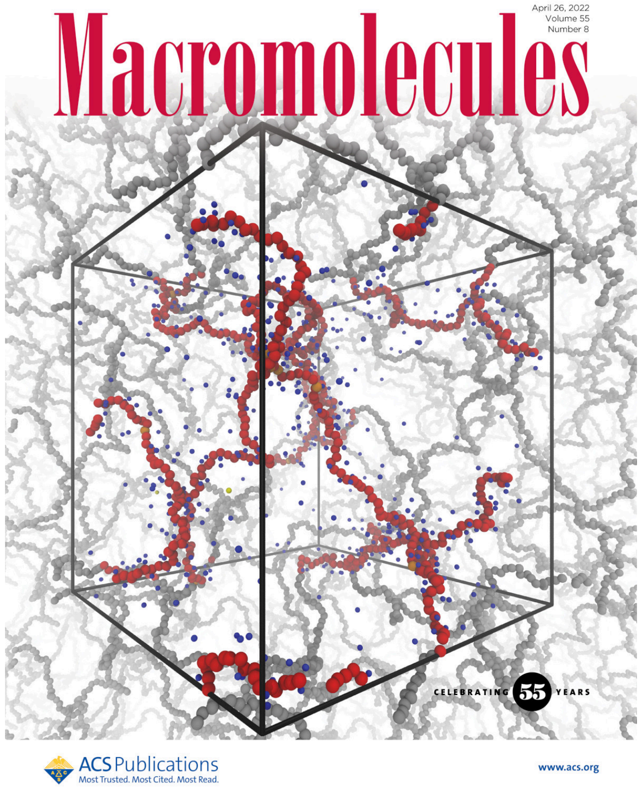
- Macromolecular complexes
- Nanopore sequencing and separation techniques
- Targeted drug delivery
- Properties of peptides and DNA

Soft Matter Problems

- Better Batteries (Electrodes, Fluids)
- Active Matter and SPPs
- Charged macromolecules
- Hydrogels
- Magnetic colloids and ferrogels
- Transport properties of ions and charged macromolecules in porous media

ESPResSo school
2025 at the ICP

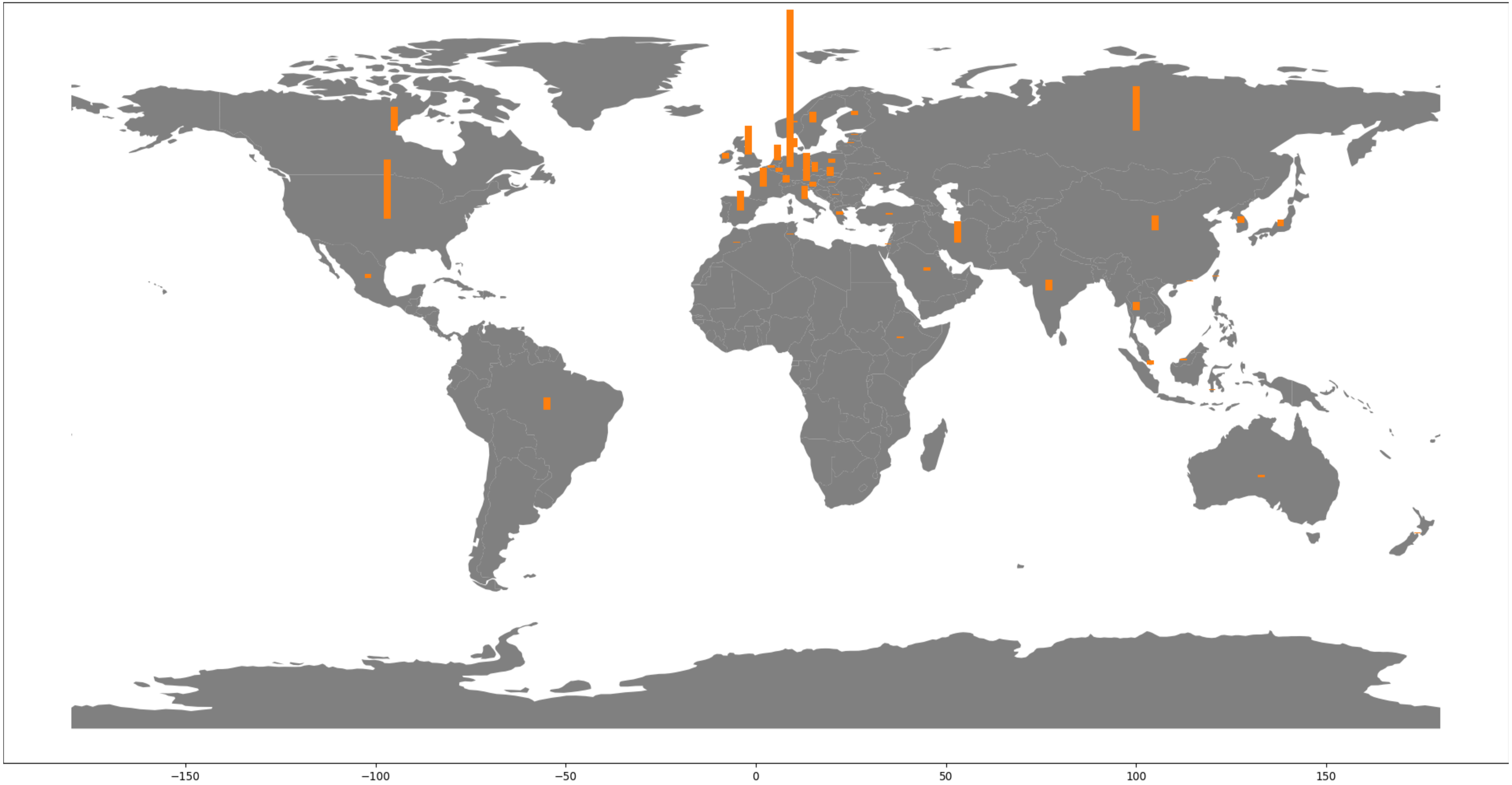
www.espressomd.org



ESPResSo is a highly versatile software package for performing and analyzing scientific **Molecular Dynamics** many-particle simulations of **coarse-grained** atomistic or bead-spring models as they are used in **soft matter research** in physics, chemistry and molecular biology. It can be used to simulate systems such as polymers, liquid crystals, colloids, polyelectrolytes, ferrofluids and biological systems, for example DNA and lipid membranes.

Talk to Rudolf Weeber weeber@icp
or Jean-Noel Grad jgrad@icp

World Map of ESPResSo Users

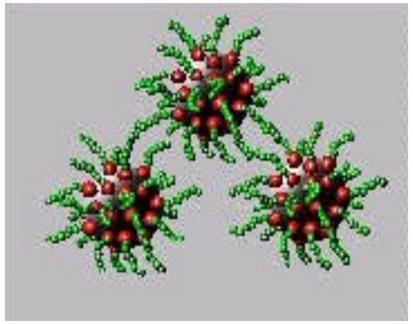


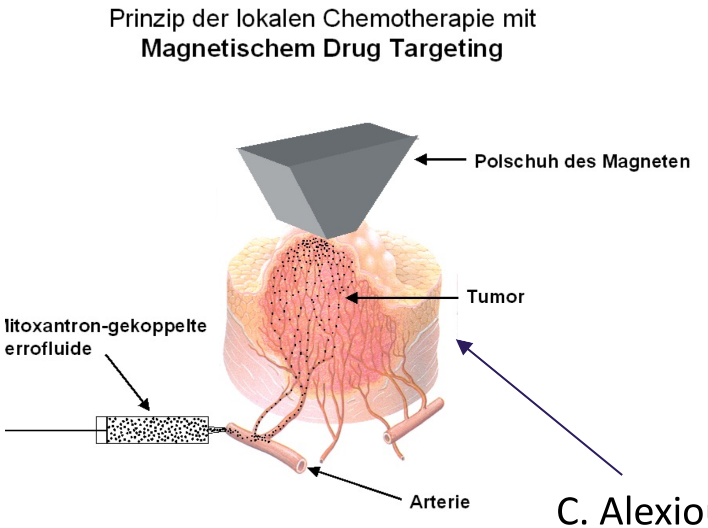
Magnetic Soft Matter

- **Magnetic particles suspended in a carrier**:
- **Ferrofluids**: live in a liquid carrier
- **Ferrogels**: have a gel as carrier
- The investigated magnetic nanoparticles:

size ~ 10 nm

single ferromagnetic domain with a permanent dipole moment (superparamagnetic)





C. Alexiou (HNO- Klinikum Erlangen)

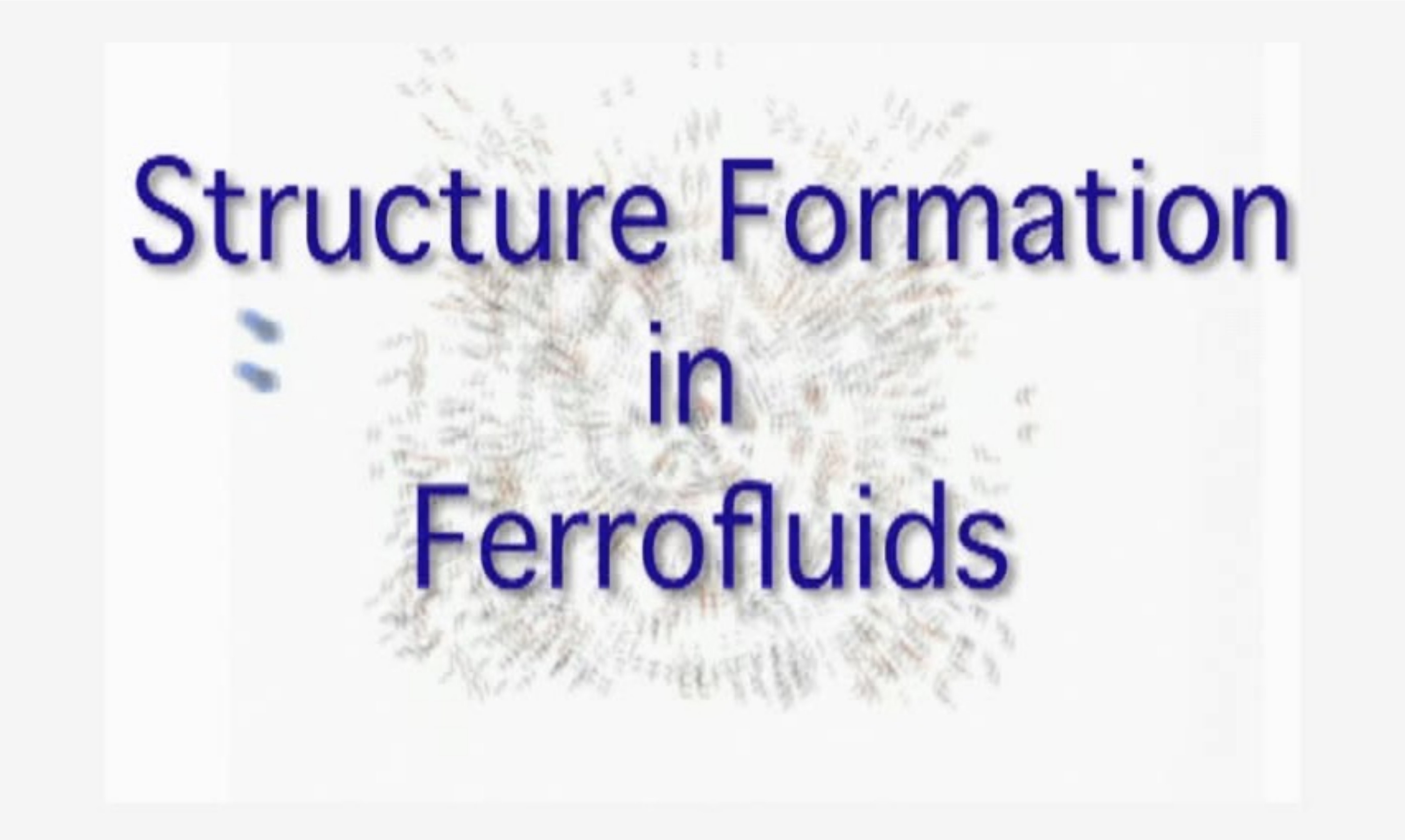
Applications:

mechanical (*sealing of rotating shafts*);

thermal (*cooling of loud speakers*);

medical (*cancer treatment, hyper-thermia, magnetic cell separation)*

Ferrofluids can be influenced via magnetic fields



Magnetic Gels

- Hydrogels are polymer networks swollen by a carrier fluid
- Magnetic gels additionally contain magnetic nanoparticles
- Using an external field, the shape and elasticity can be controlled

Magnetic gels

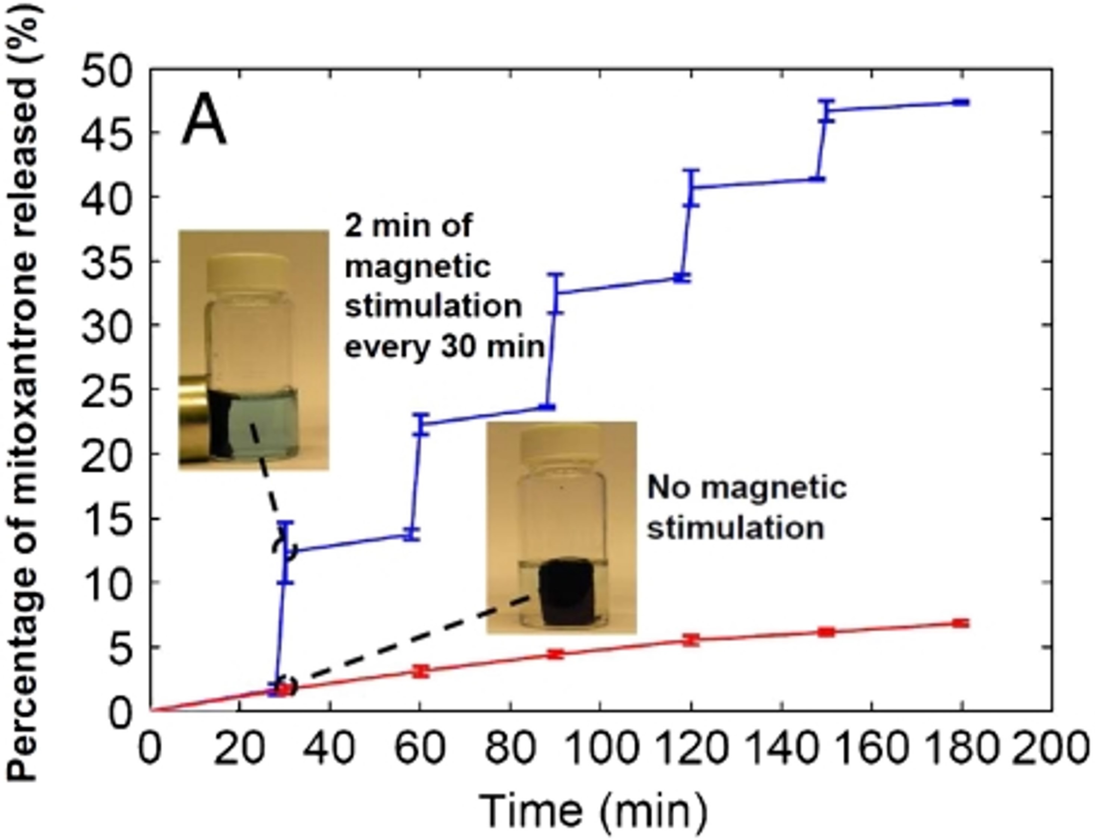
Shape-Programable Magneto-Active Elastomers Composites
for Curve and Biomimetic Behavior Imitation

Supporting Movie 2

Biomimetic Deformation Behavior of MAEs Composite
Mimicking Wing-Flapping of Birds

Gong, Yang, Lin, Qian, Li, Li, Chen, Jia. Soft Matter, 2021

Drug Release From Magnetic Gels



- It is possible to enclose a drug within the magnetic gel
- Using an external field, the release of the drug can be controlled

Zhao, Kim, Cezar, Huebsch, Lee, Bouhadir, Mooney. PNAS USA, 2011

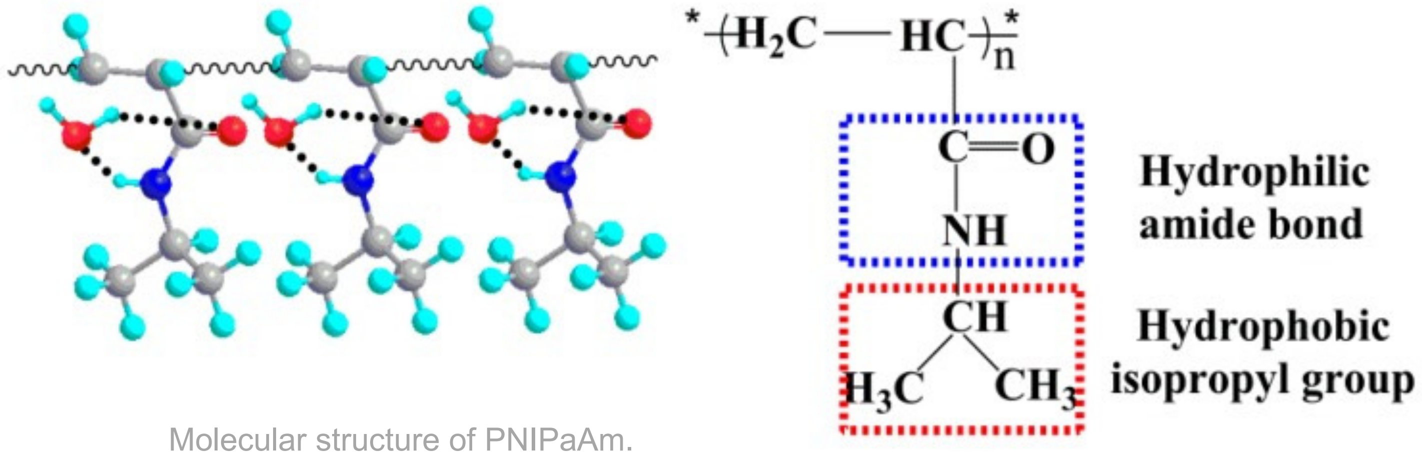
Possible Thesis Topics

- Model the loading and release of drugs from magnetic gels
- Understanding the influence of inhomogeneities in the network on experimentally observable properties

Coarse-graining and Machine-learned Potentials

Creating a Coarse-grained Model for Thermo-reversible Polymers

- Some polymers change their properties drastically with temperature
- For example, PNIPaAm collapses when driven over the lower critical solution temperature
- This can be modelled using atomistic simulations, but they are costly
- In the thesis, an approximate coarse-grained model should be generated which allows simulating bigger systems



Molecular structure of PNIPaAm.
Yang L, Fan X, Zhang J, Ju J. Polymers (Basel), 2020

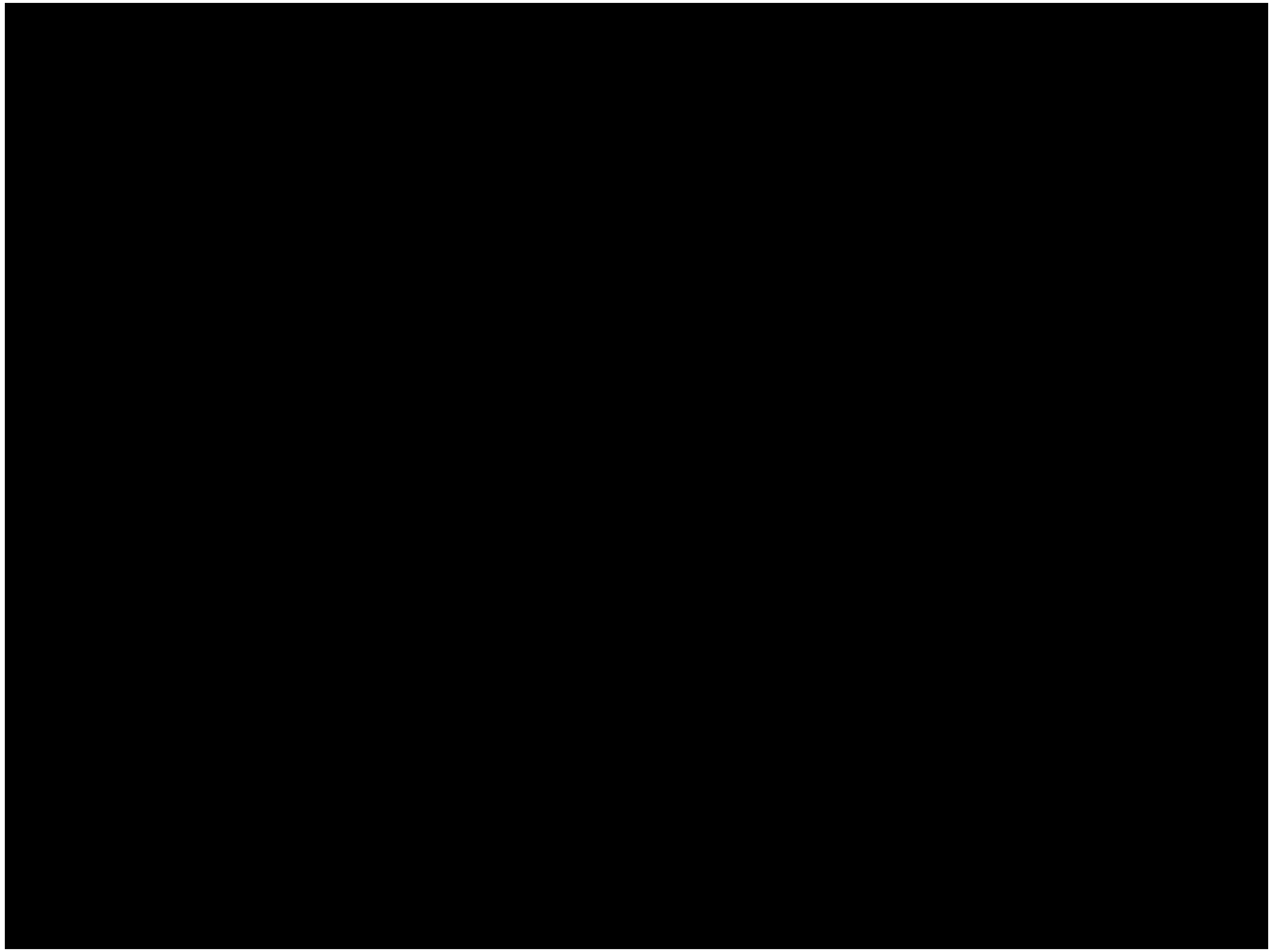
Viscoelastic Fluids

Viscoelasticity

Viscoelastic materials combine properties of a fluid and a solid:

- They are viscous like fluids: stress proportional to shear rate
- But also elastic like solids: stress proportional to shear amplitude

Viscoelasticity



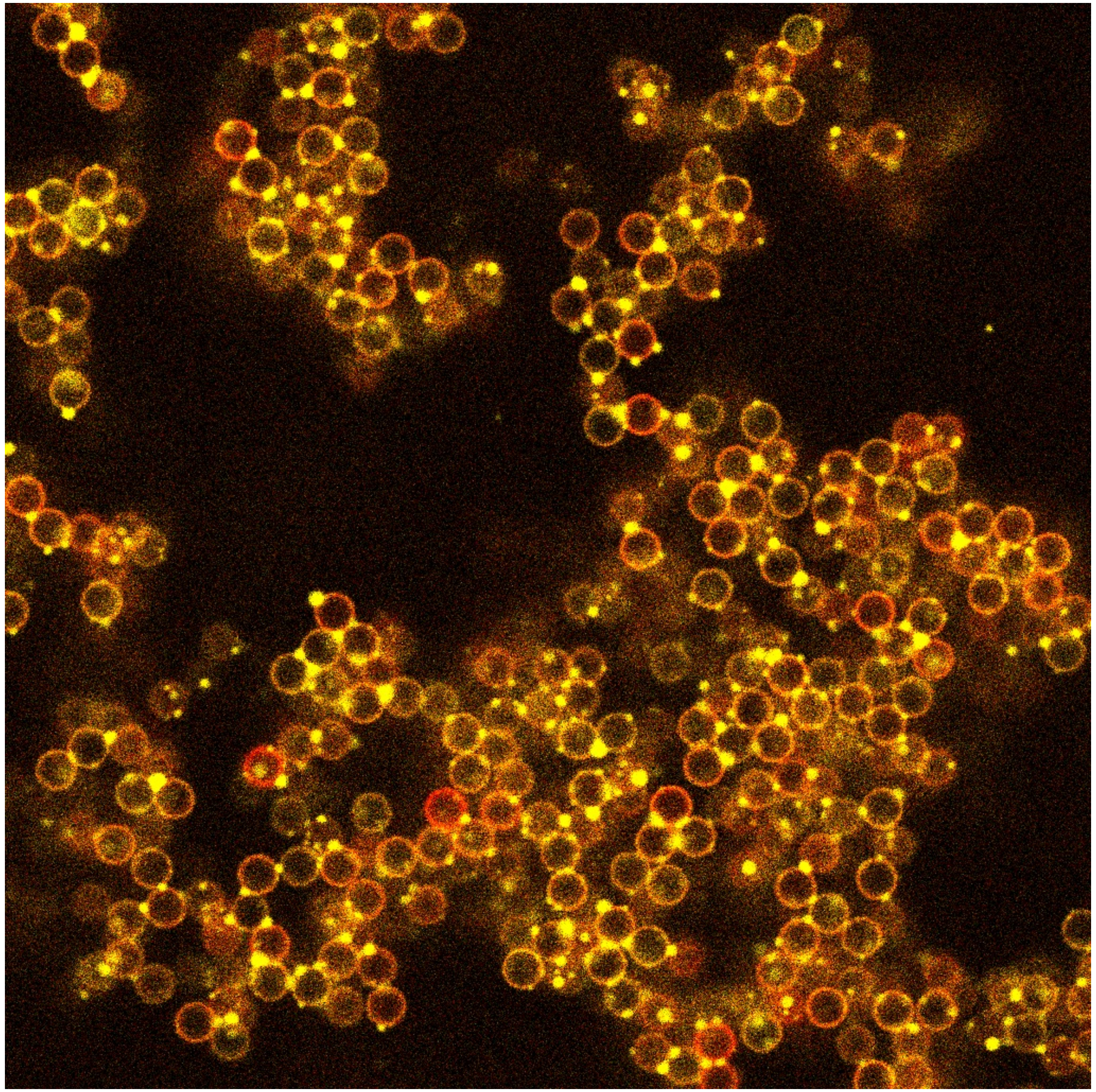
psidot, 14.07.2007. “The Barus Effect“, YouTube.

Viscoelasticity with Thermal Fluctuations

- Goal of the project is to extend an existing solver for a viscoelastic fluid to thermal fluctuations
- We will use this to look at self-propelled particles in viscoelastic media
- The project has a significant analytical component

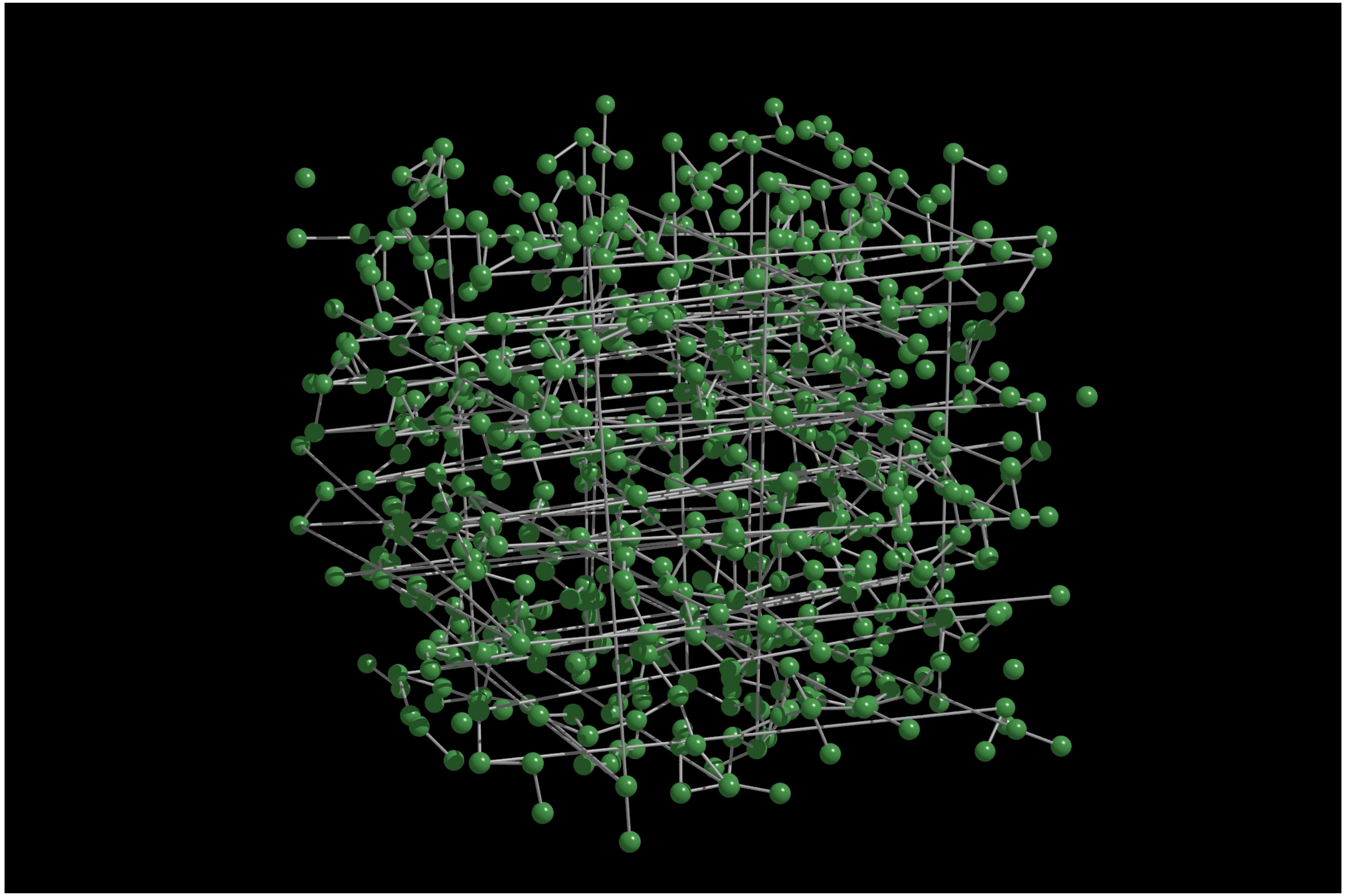
Capillary Suspensions

Capillary Suspensions



- A small amount of imissible fluid is added to a colloidal suspension
- It forms capillary bridges between the colloidal particles, forming a network
- The suspension becomes highly viscoelastic

Capillary Suspensions

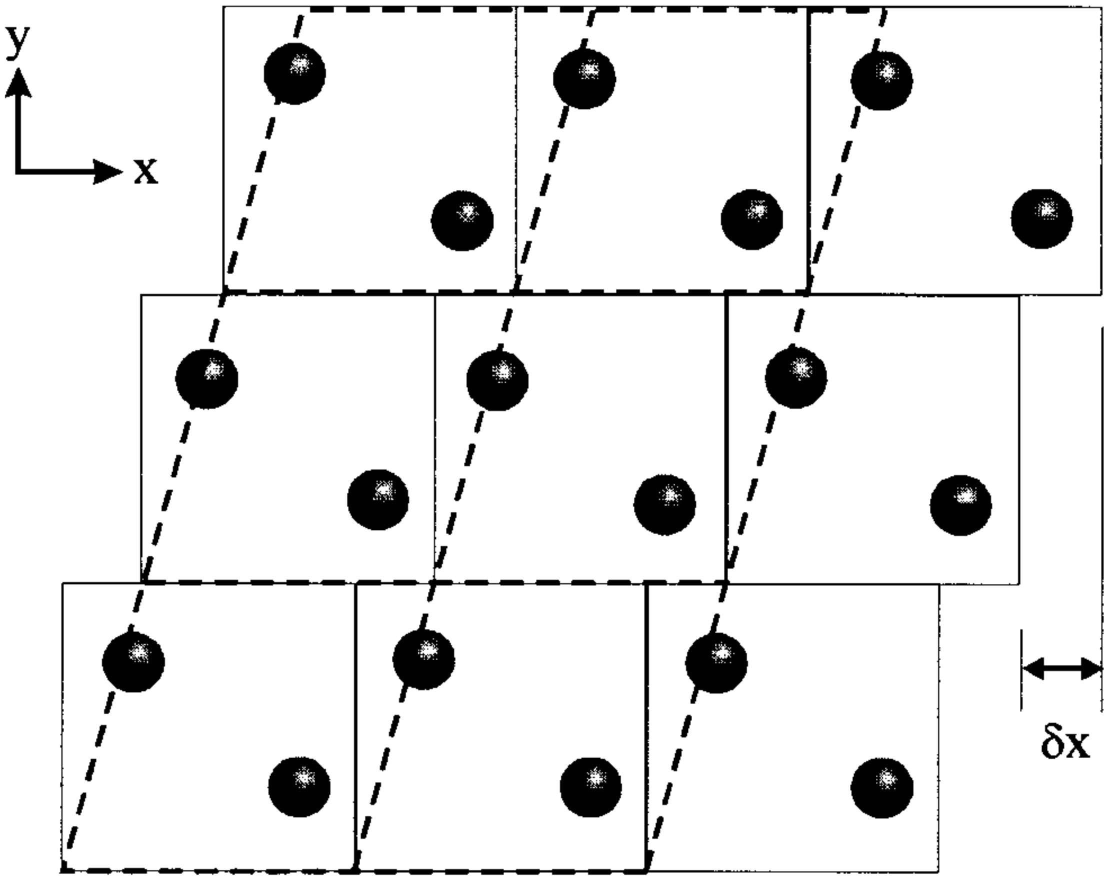


System under oscillatory shear.

- In the project, we will study the break-up of this network under shear

Electrostatics Under Shear

Electrostatics Under Shear

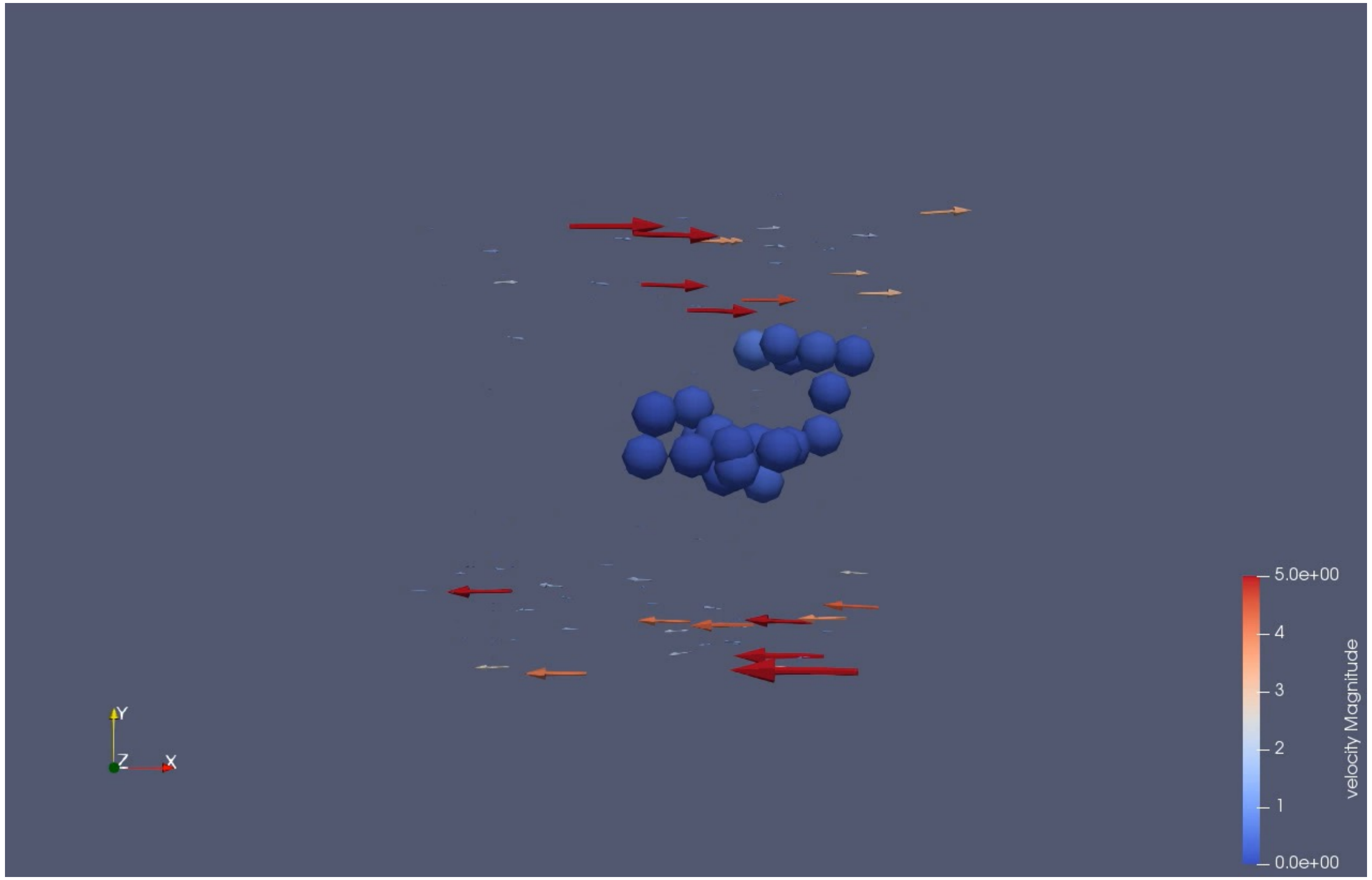


- The flow properties of a system are studied by applying shear in a viscosimeter and measuring the resulting stress
- We can do this in simulations using Lees-Edwards boundary conditions
- In the project, the P3M electrostatics solver will be extended to support this

Wheeler et al. 2010

Electrostatics Under Shear

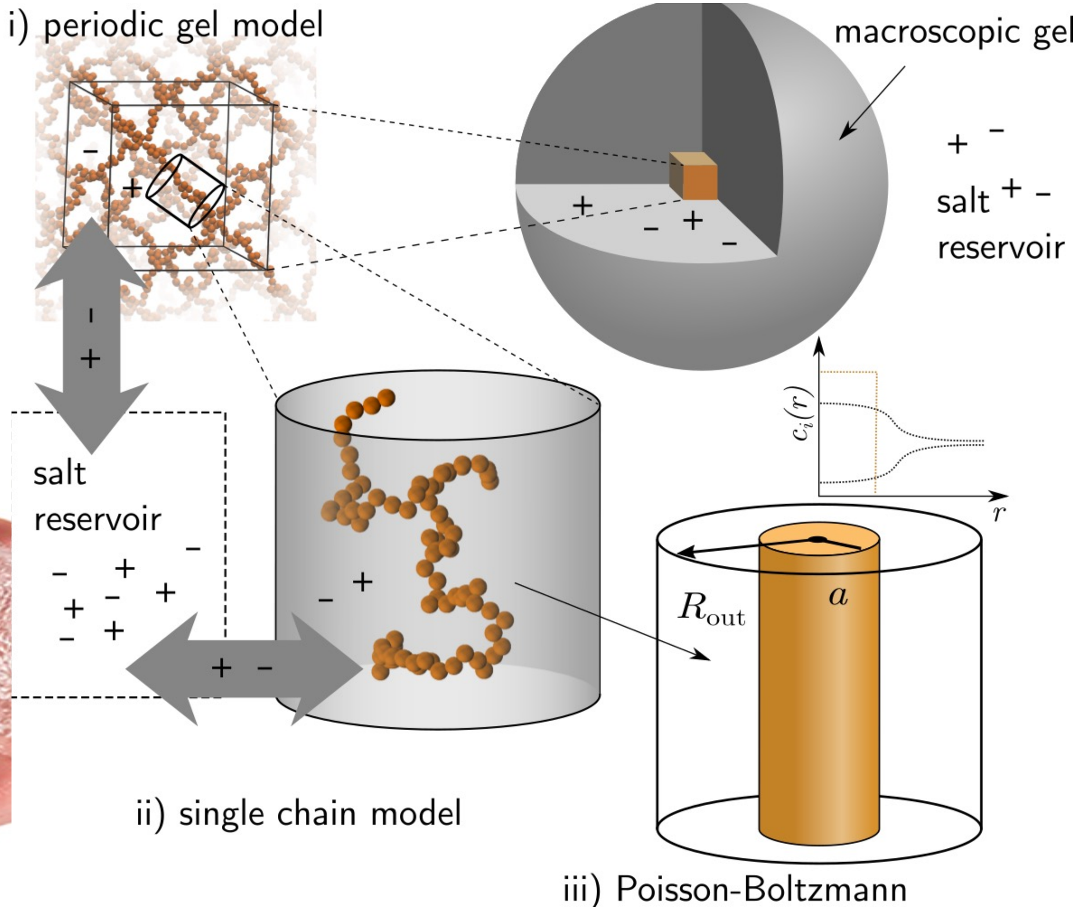
- We will then explore, how a polyelectrolyte suspension behaves under shear



Polymer in a shear flow.

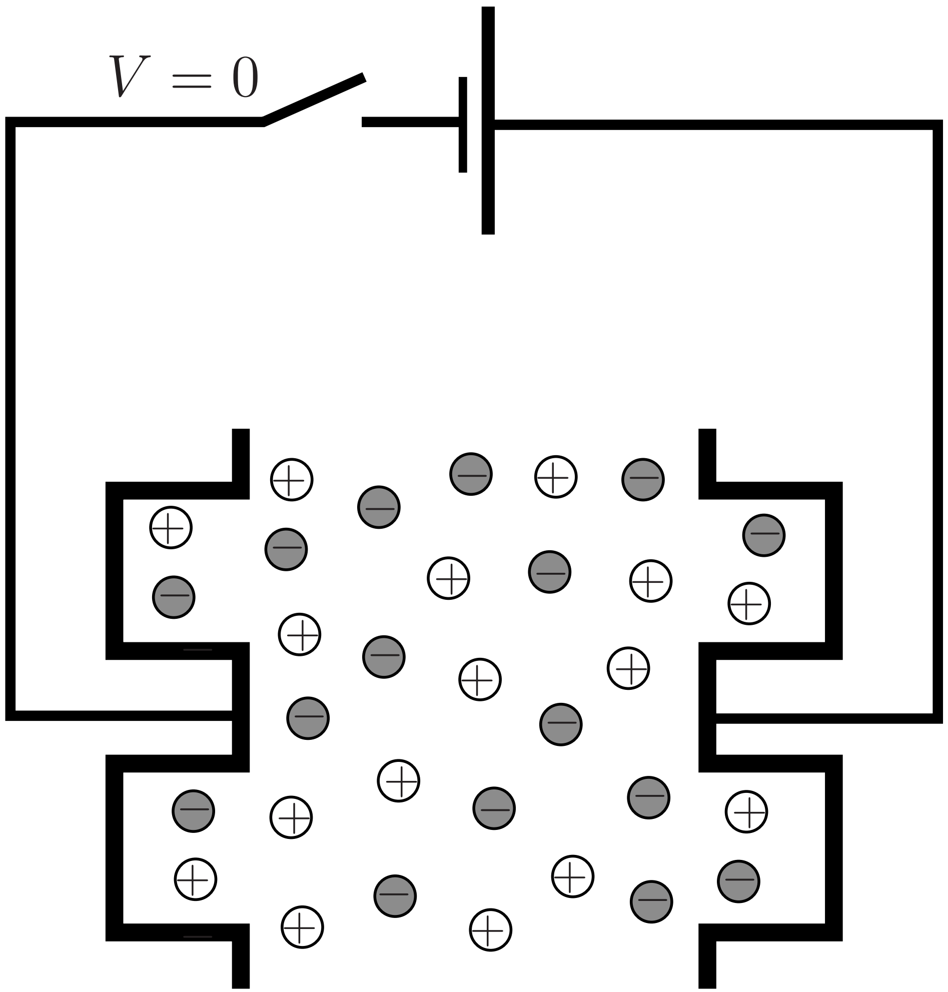
Hydrogels: Smart Funtional Materials

Modeling Approaches for Hydrogels on Different Levels

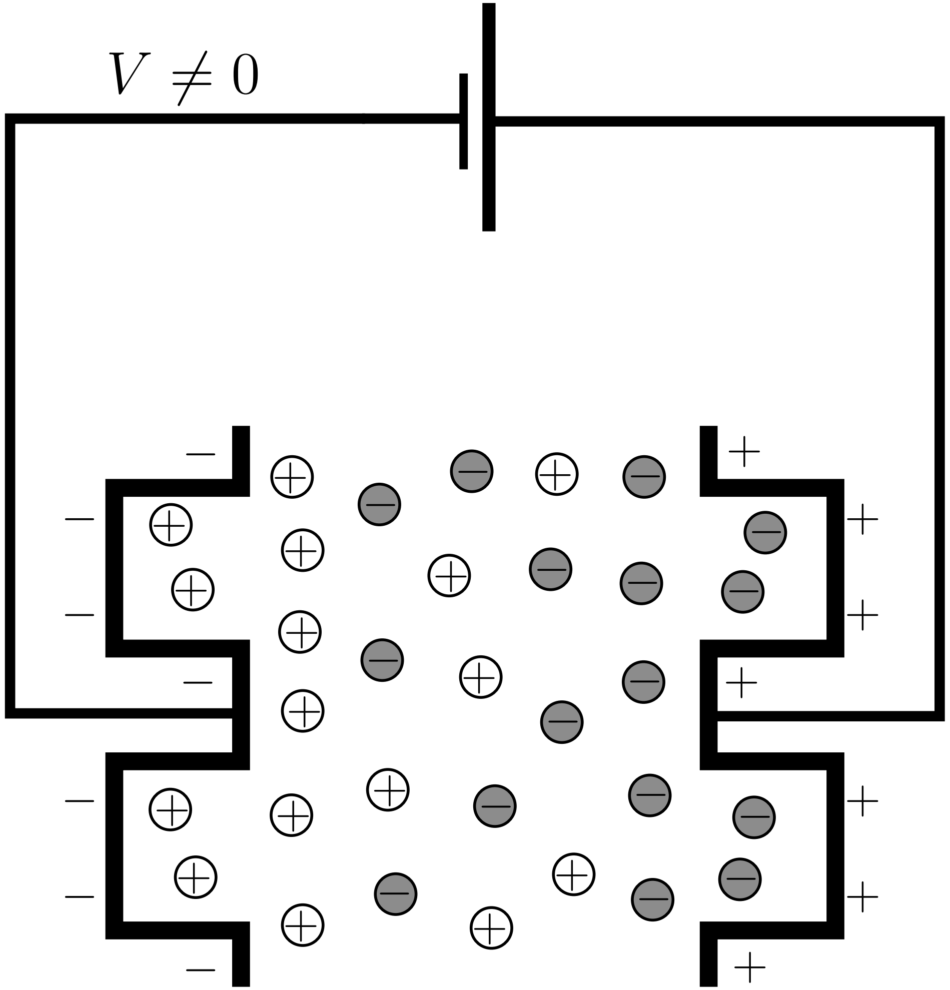


Supercaps

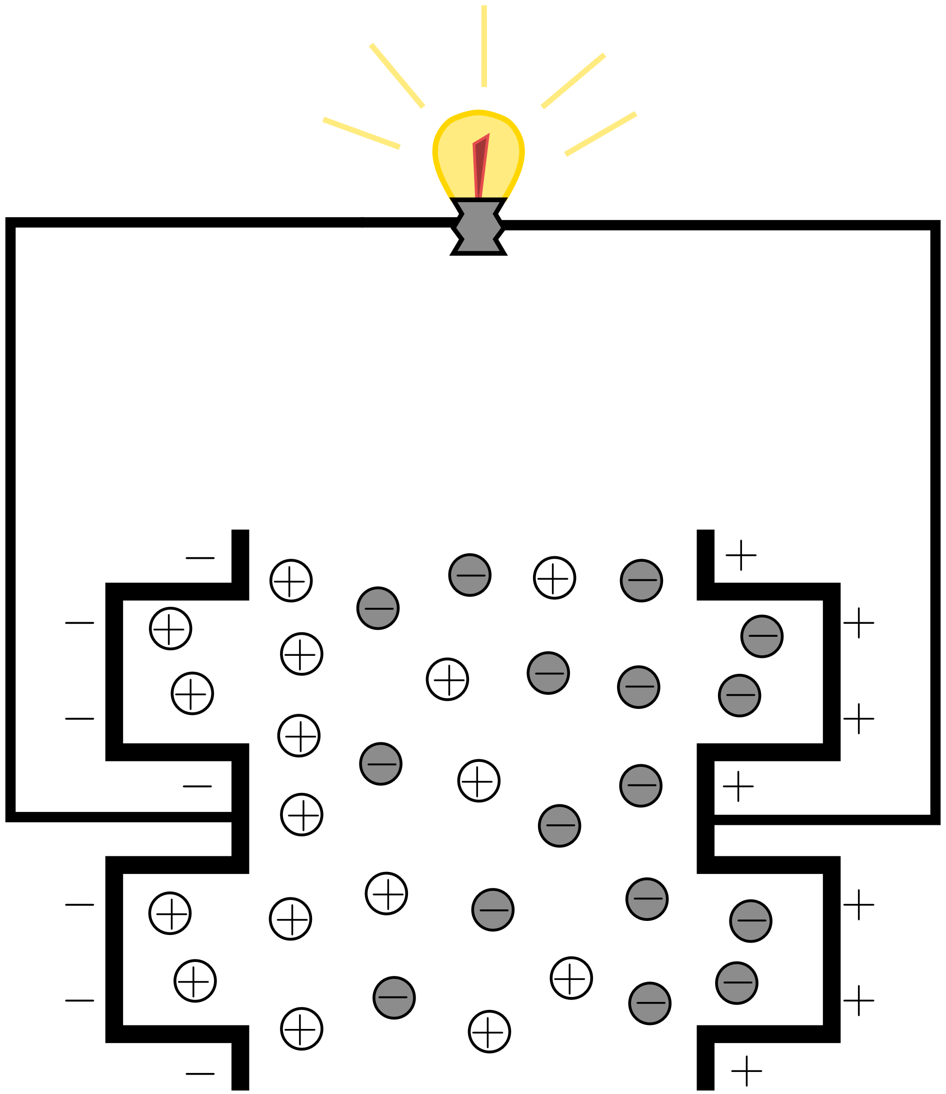
What is a Supercapacitor



What is a Supercapacitor



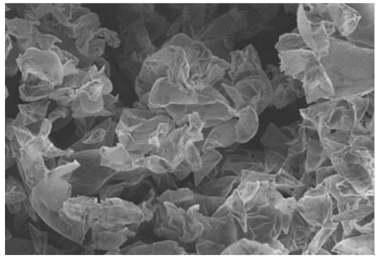
What is a Supercapacitor



Application to Supercapacitors…..

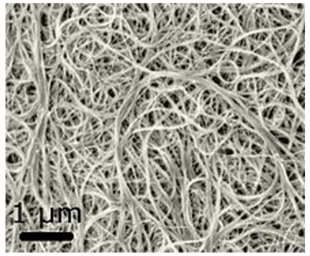
Supercapacitors are used for mobile energy storage in Electric Double Layer Capacitors / "Supercapacitors" with high specific capacitance. "Fast and Furious??"

High surface area electrode material (>1000 m^2/g)



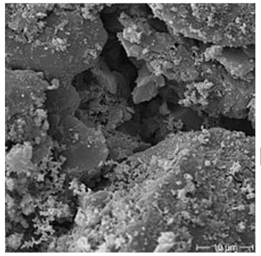
Curved graphene sheets

Liu et al., Nano Lett. (2010)



Carbon nanotubes

https://en.wikipedia.org/wiki/Carbon_nanotube



https://en.wikipedia.org/wiki/Activated_carbon

Activated carbon

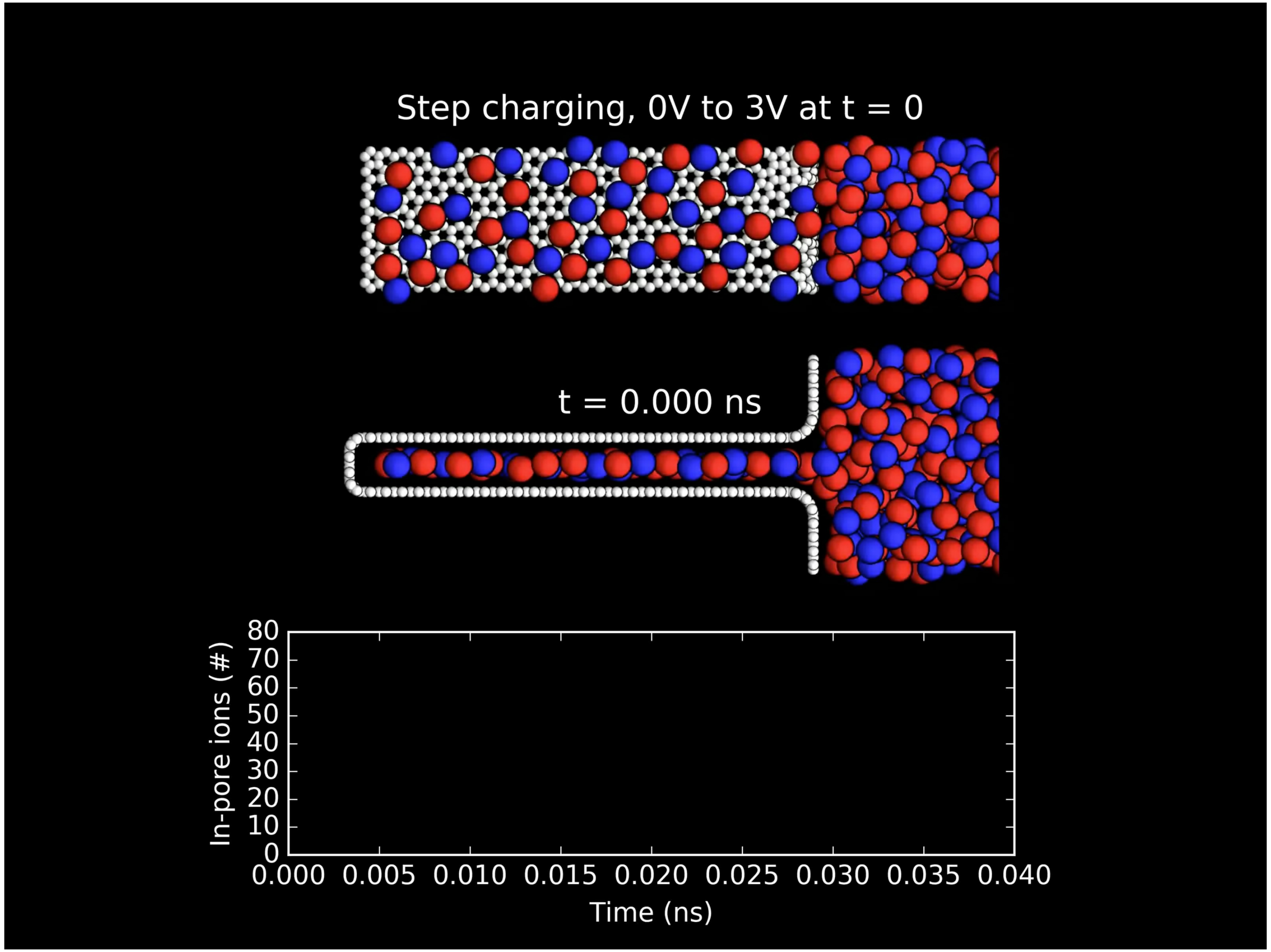
Electrolyte:

- Aqueous (e.g. Water + KOH or H_2SO_4)
- Organic solvent + Salt
- Ionic liquids

Our Goal

Understand charging mechanisms and ion dynamics in narrow charged pores for simple model systems

Voltage sweep speeds up charging of a capacitor



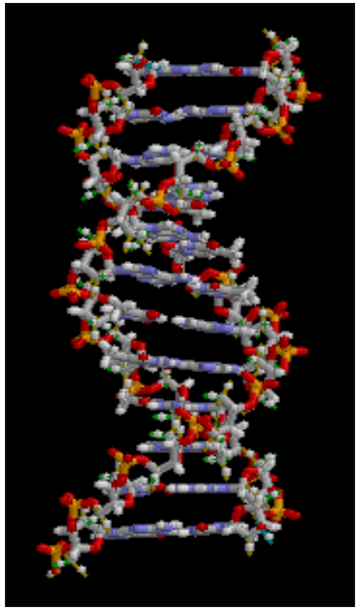
Breitsprecher, Holm, and Kondrat. "Charge me slowly, I am in a hurry: Optimizing charge–discharge cycles in nanoporous supercapacitors." ACS nano 12.10 (2018): 9733-9741.

Nanopore Sequencing

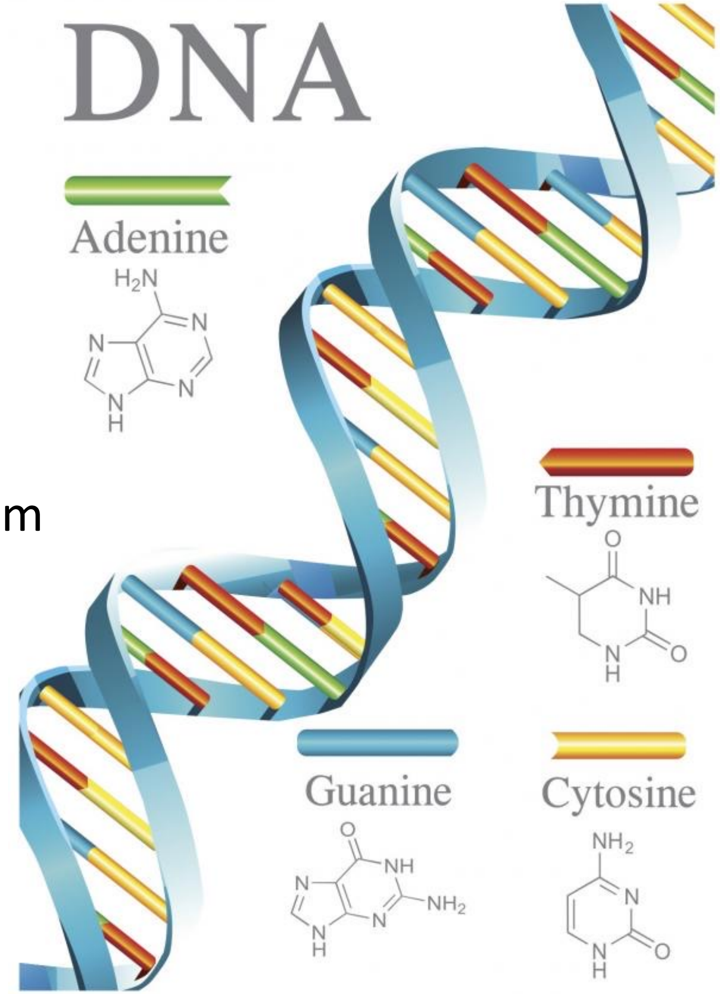
DNA Facts

dsDNA is a charged biopolymer, consisting of paired bases yielding the form of a double helix in water.

The sequence of either strand encodes our genetic information which we want to read out.

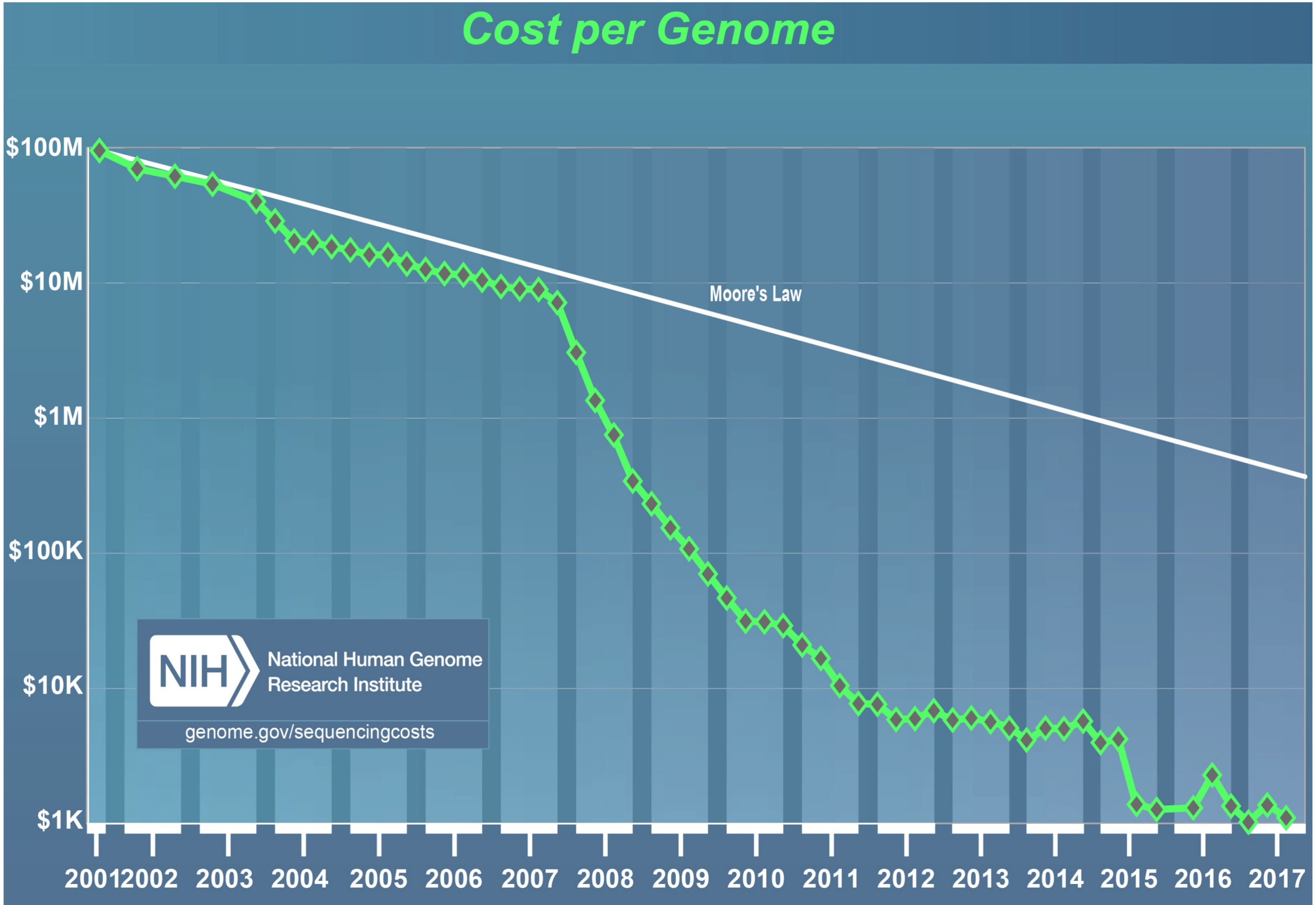


persistence length l_p=50nm



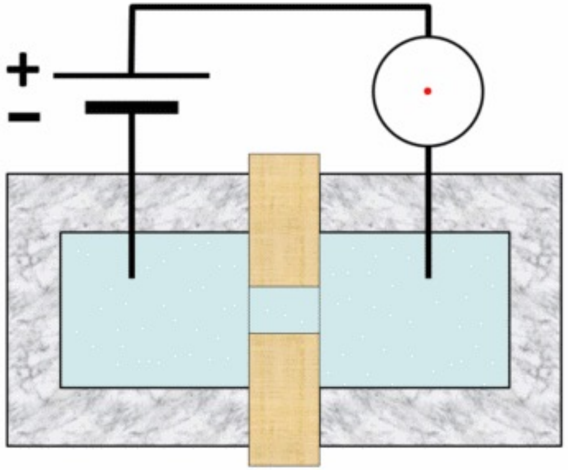
http://en.wikipedia.org/wiki/DNA

Costs of DNA Sequencing

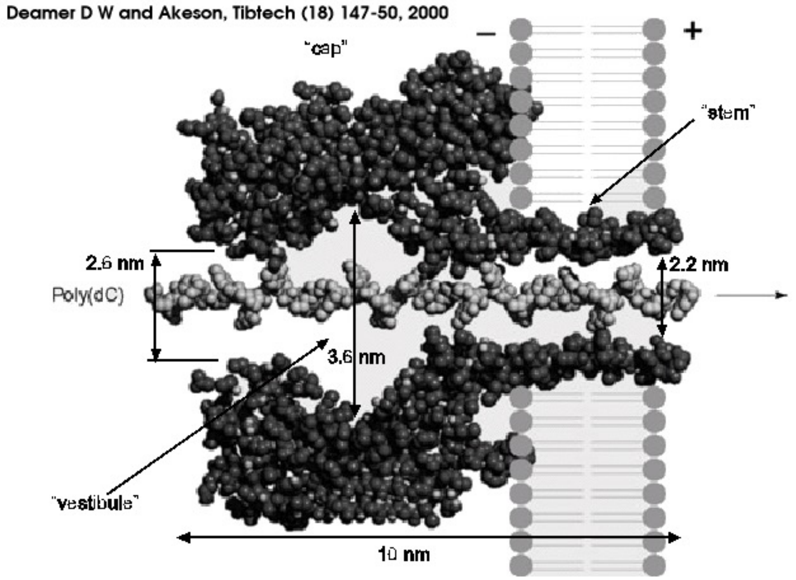


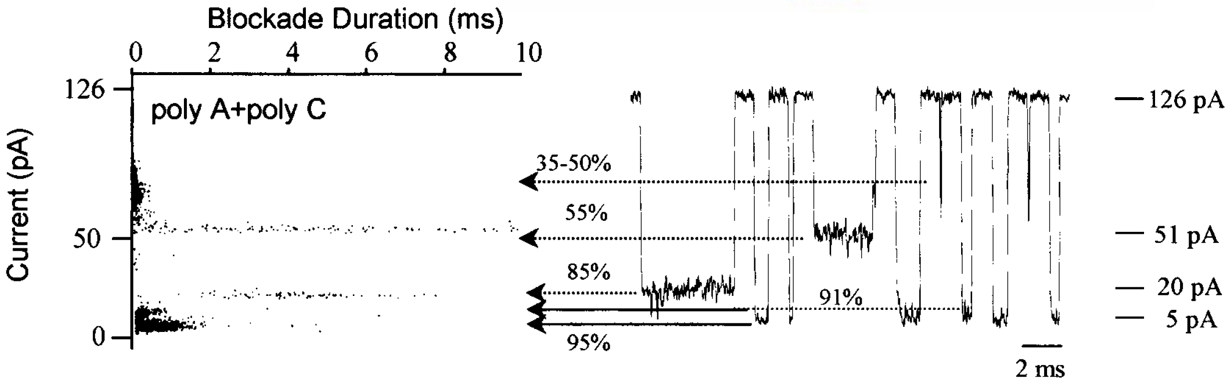
Nanopore Sequencing Approach

- acts like a more refined Coulter counter for blood cells



Electric Field



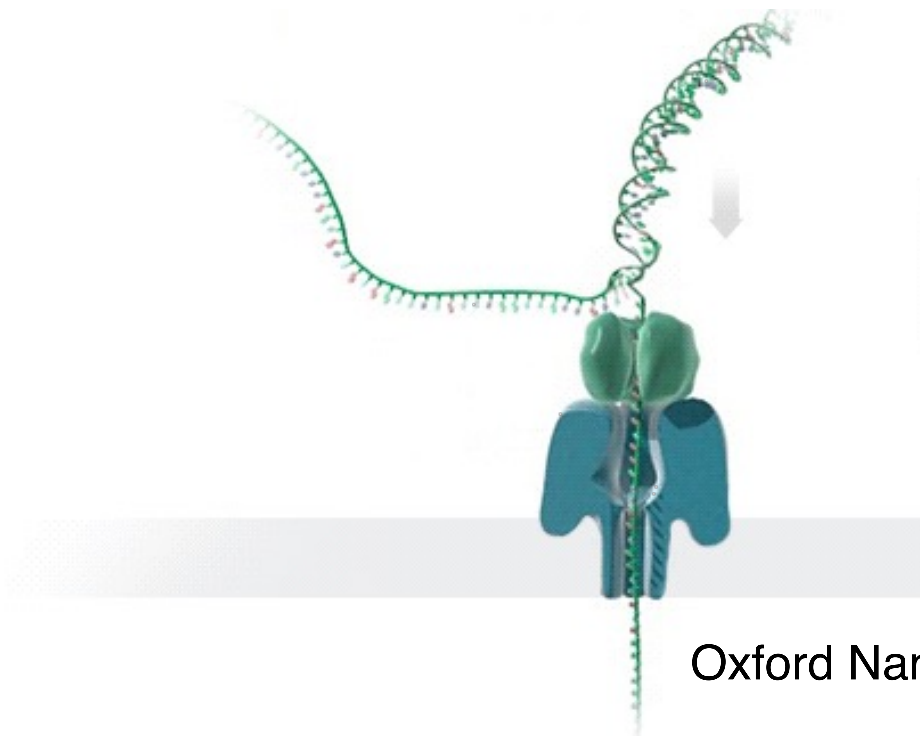


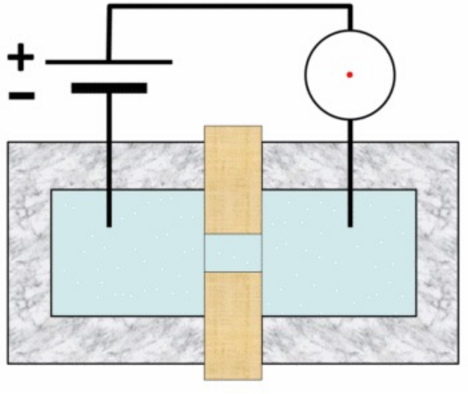
Electric Current

- conductivity measurements can reveal bp translocation of ssDNA
- Recognition of binding sites of proteins to DNA

ML Approaches for optimizing Nanopores

- acts like a more refined Coulter counter for blood cells



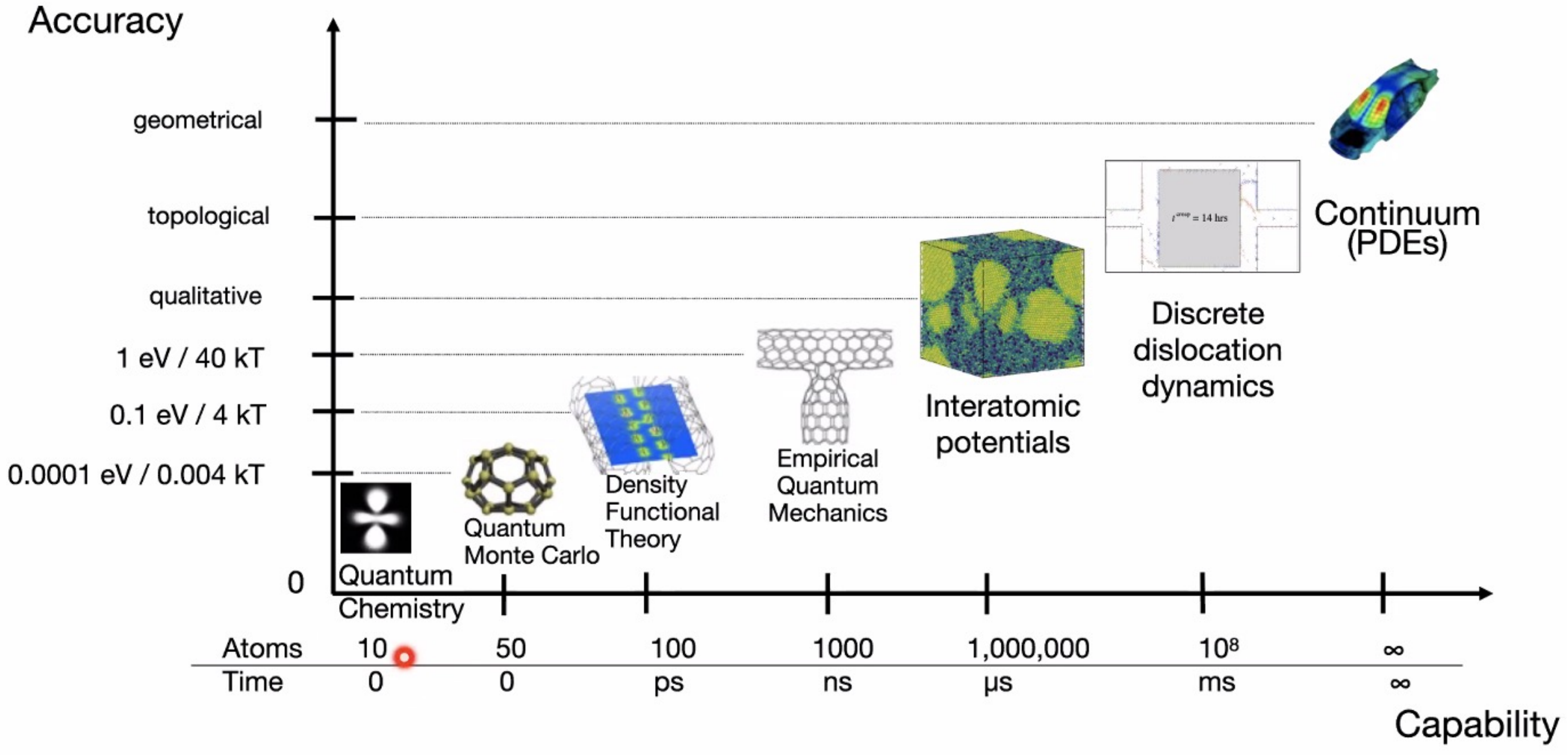


Oxford Nanopores https://nanoporetech.com

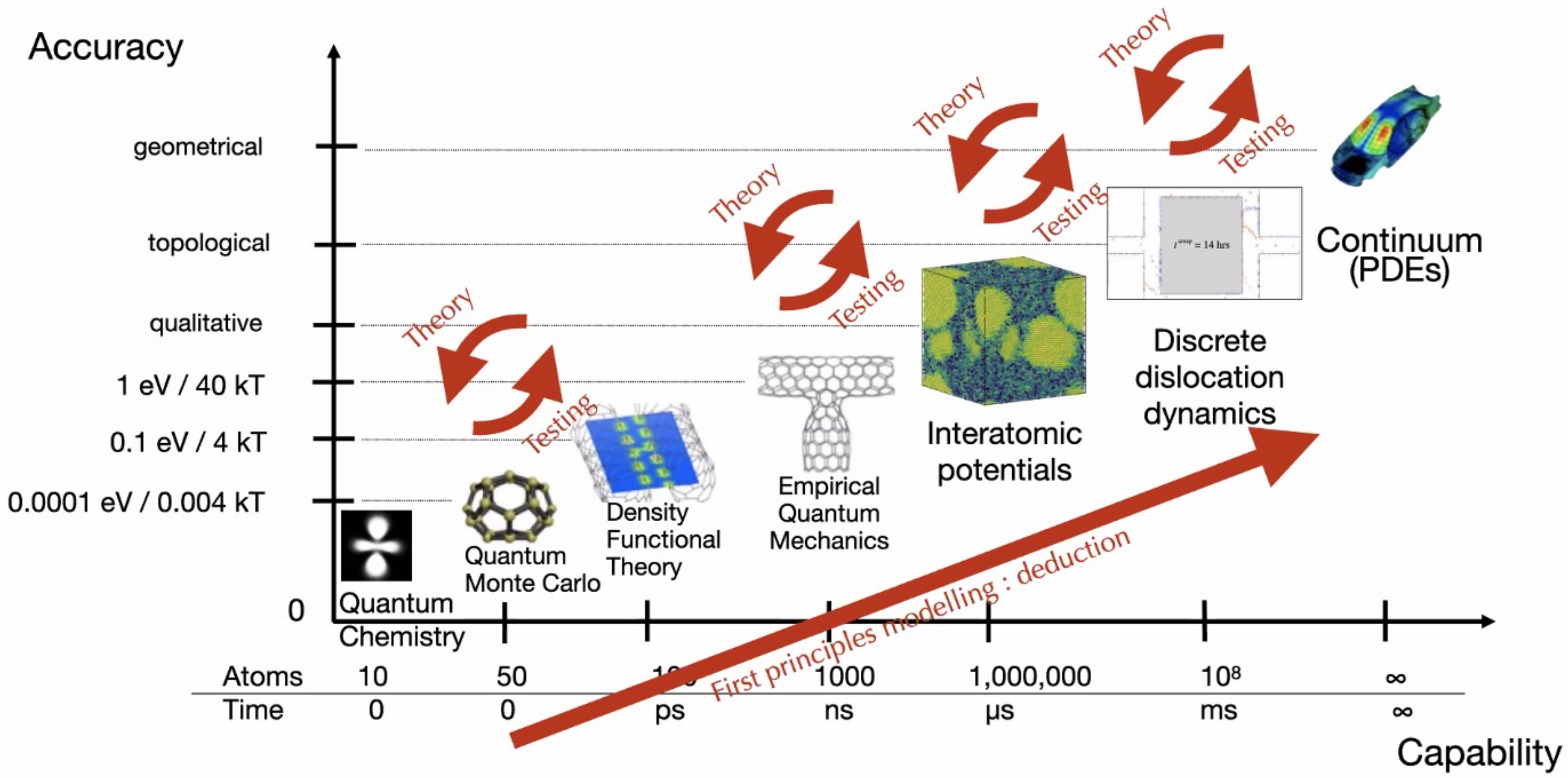
- Use ML approaches to optimize the current readout to recognize protein sequences from real experimental data provided by collaborators from Freiburg using a different biological nanopore (Aerolysine)

Oxford NANOPORE Technologies

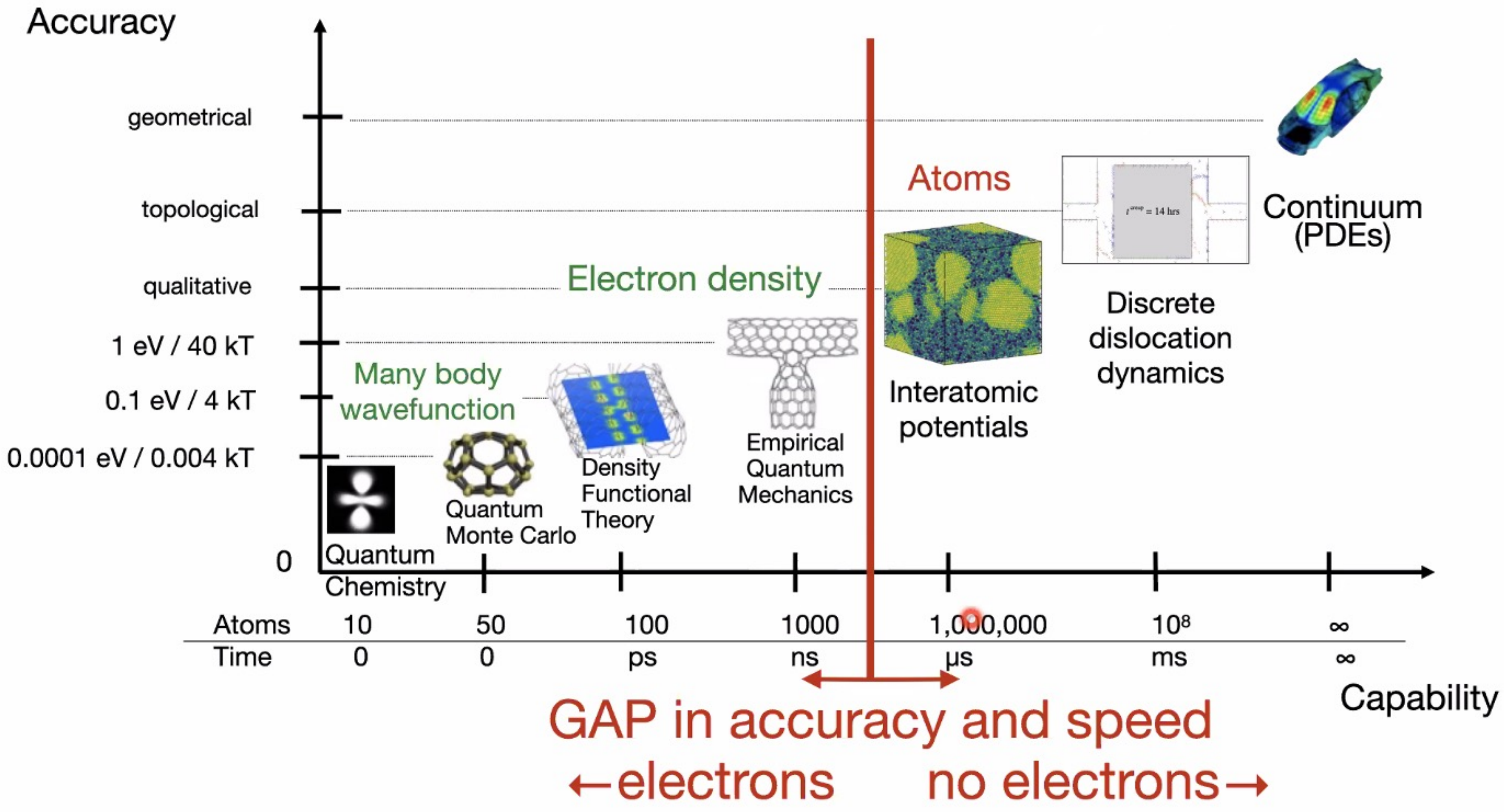
Multiple scales of materials modelling



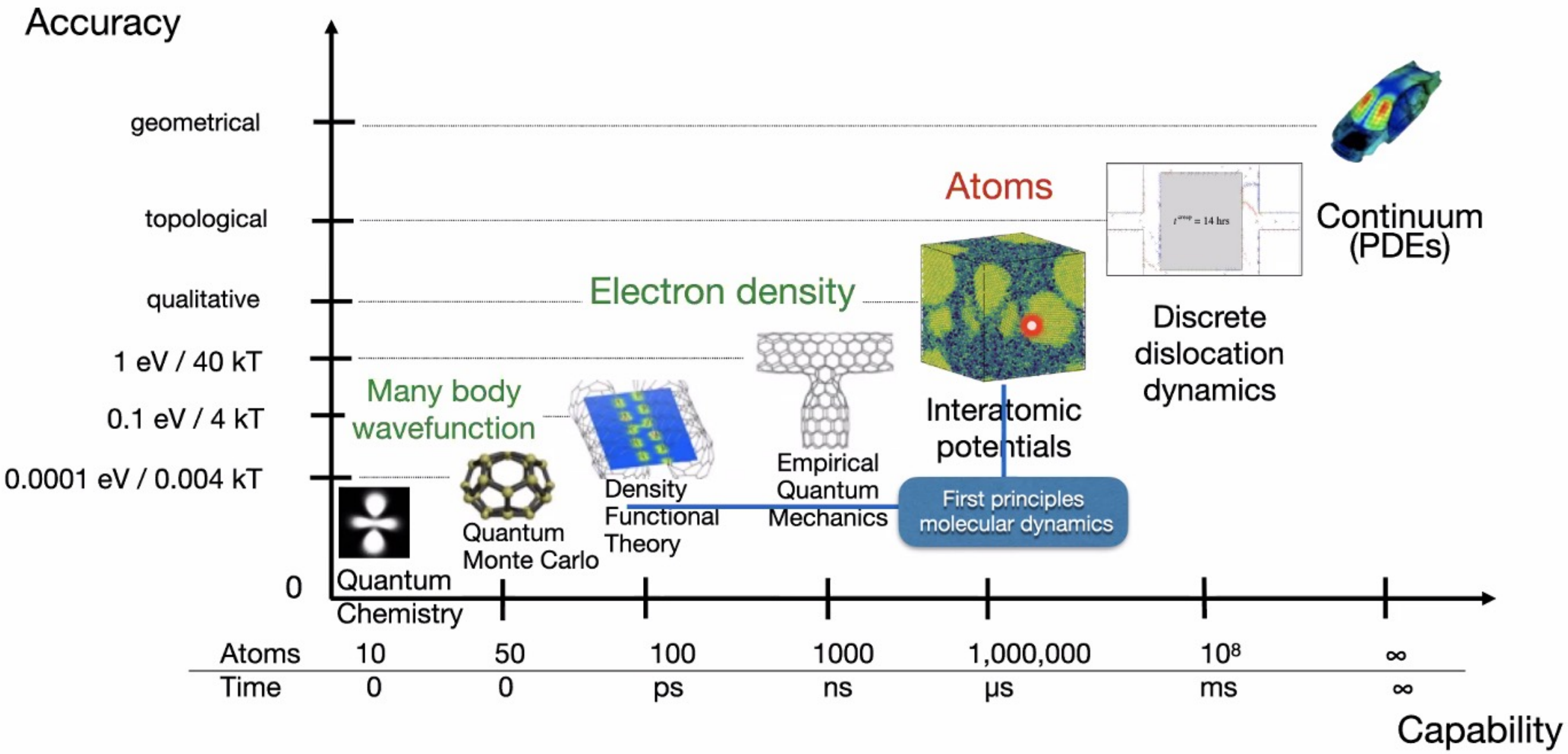
Multiple scales of materials modelling



Multiple scales of materials modelling



Multiple scales of materials modelling



Machine learned interatomic potentials from ab-initio input (often DFT)

What do we expect from you?

- Be curious for new phenomena
- Be open to use the computer as your experimental platform
- Be ready to use your imagination and physical intuition
- Some familiarity with the computer expected:
- Very helpful: Python
- Helpful C++
- We also use ready to use software suits: ESPResSo, ZnTrack, MDSuite, MLSuite, MaiCos, COMSOL, GROMACS, CP2K, PyTorch, TensorFlow…

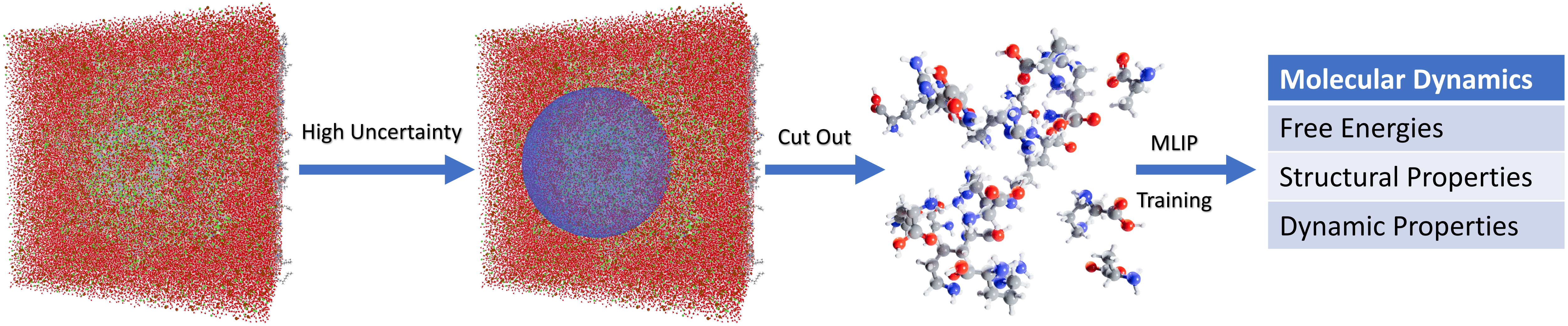
Various TOPICS Bachelor, Master, SimTech Projects

Machine-Learned Interatomic Potentials for Nanopore Protein Sequencing

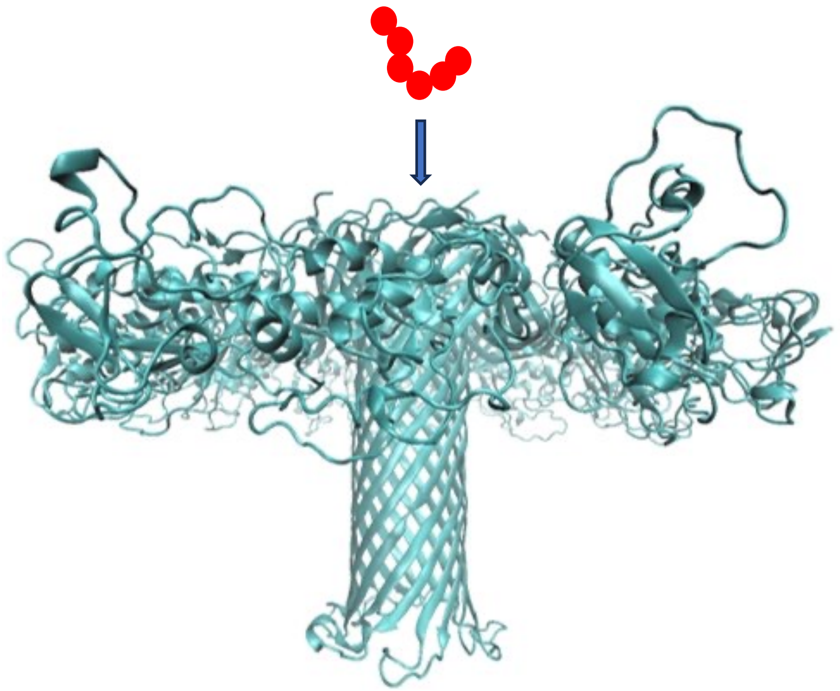
Fabian Zills *fzills@icp.uni-stuttgart.de*

- Develop Machine-Learned Interatomic Potentials (MLIPs) for biological nanopores (B.Sc. / M.Sc.)

Utilize and **develop** state-of-the-art MLIP code
https://github.com/zincware

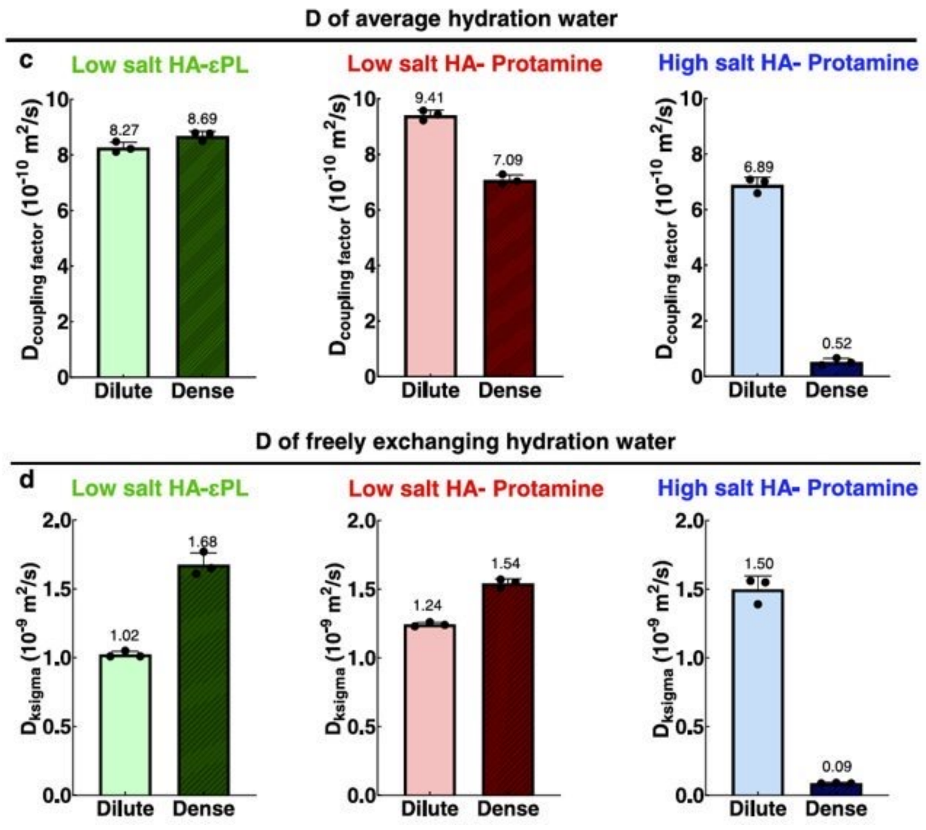


A machine-learning interatomic potential (MLIP) forcefield (FF) for charged peptides in salt solutions



Peptide enters in nanopore

Peptide dynamics in salt solution



Diffusion coefficients measured at under different exp. conditions

wenlan.liu@icp.uni-stuttgart.de

Work flow and dataset design

Initial structure/box construction

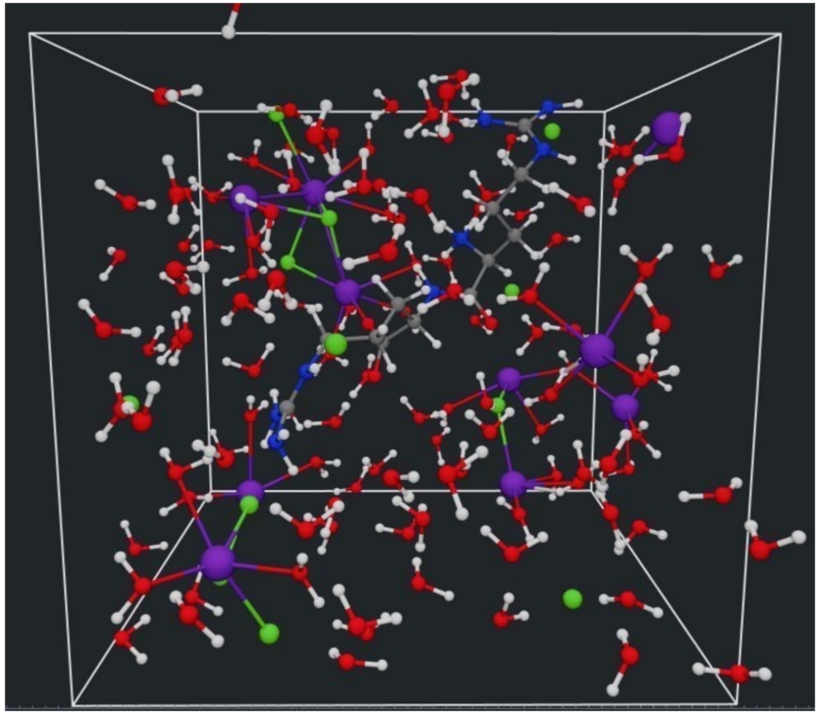
ASEGeoOpt

ASEMD

CP2K on selected snapshots

Apax check force and energy

JaxMD if runtime < 10 ns



- Low -> high salt concentration
- Different peptide chain lengths
- Peptide condensation (box size) and structure dependance

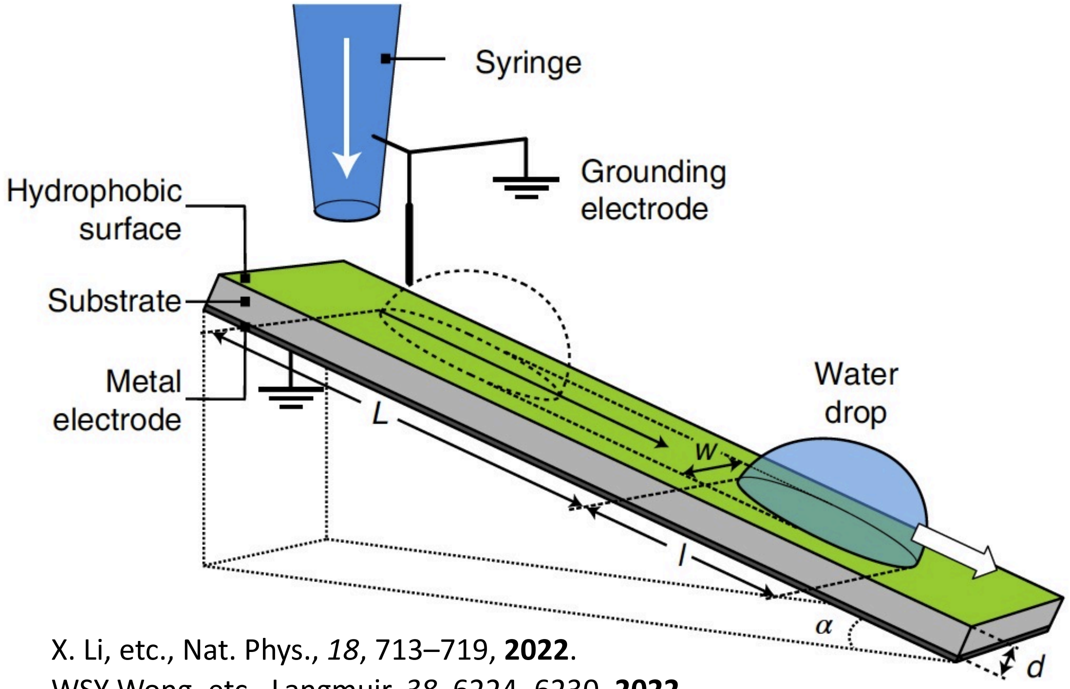
Expected goals

- Verify if MLIP-FF is reliable for peptide system in high concentration salt solution.
- Compare the peptide behavior in different salt solution, as well as in nanopore.

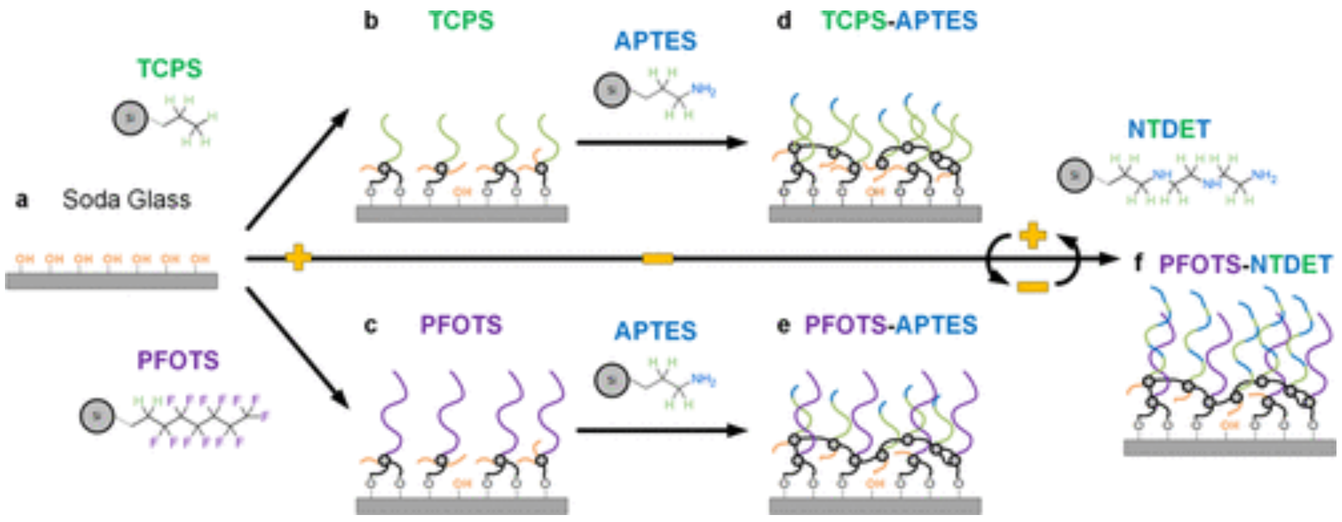
wenlan.liu@icp.uni-stuttgart.de

MLIP aided water decomposition dynamics on hydrophobic surfaces

Water drop-sliding exp.



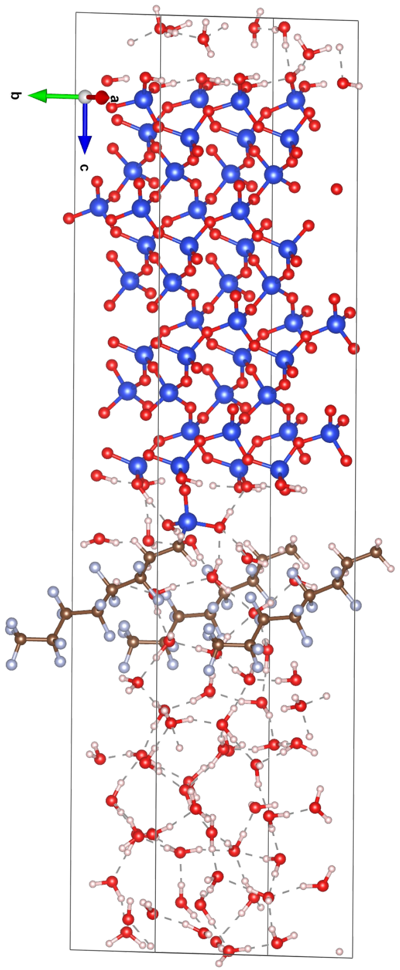
Hydrophobic surface preparation

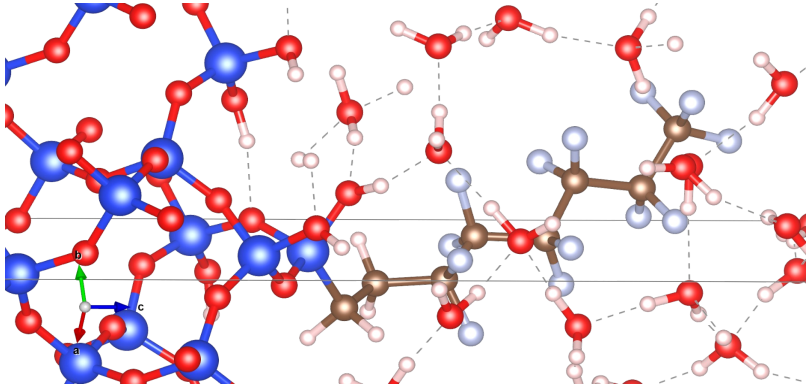


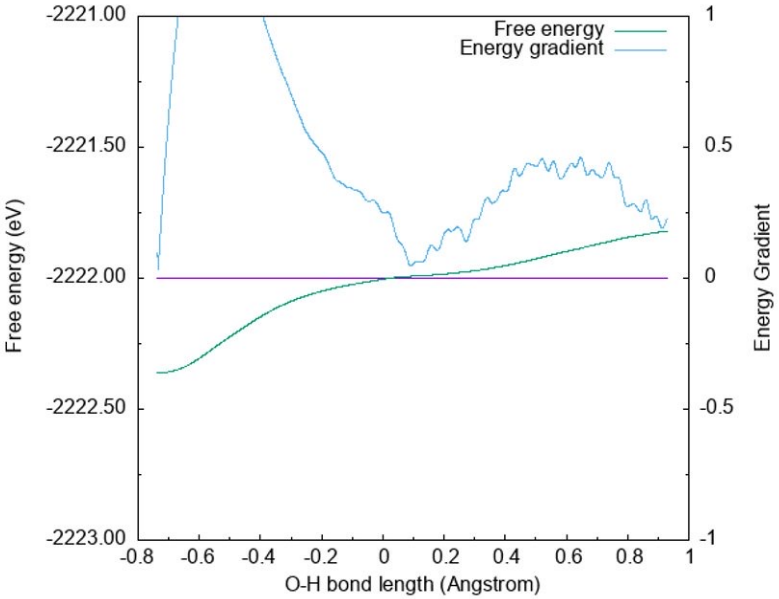
X. Li, etc., Nat. Phys., *18*, 713–719, **2022**.
WSY Wong, etc., Langmuir, *38*, 6224−6230, **2022**.

wenlan.liu@icp.uni-stuttgart.de

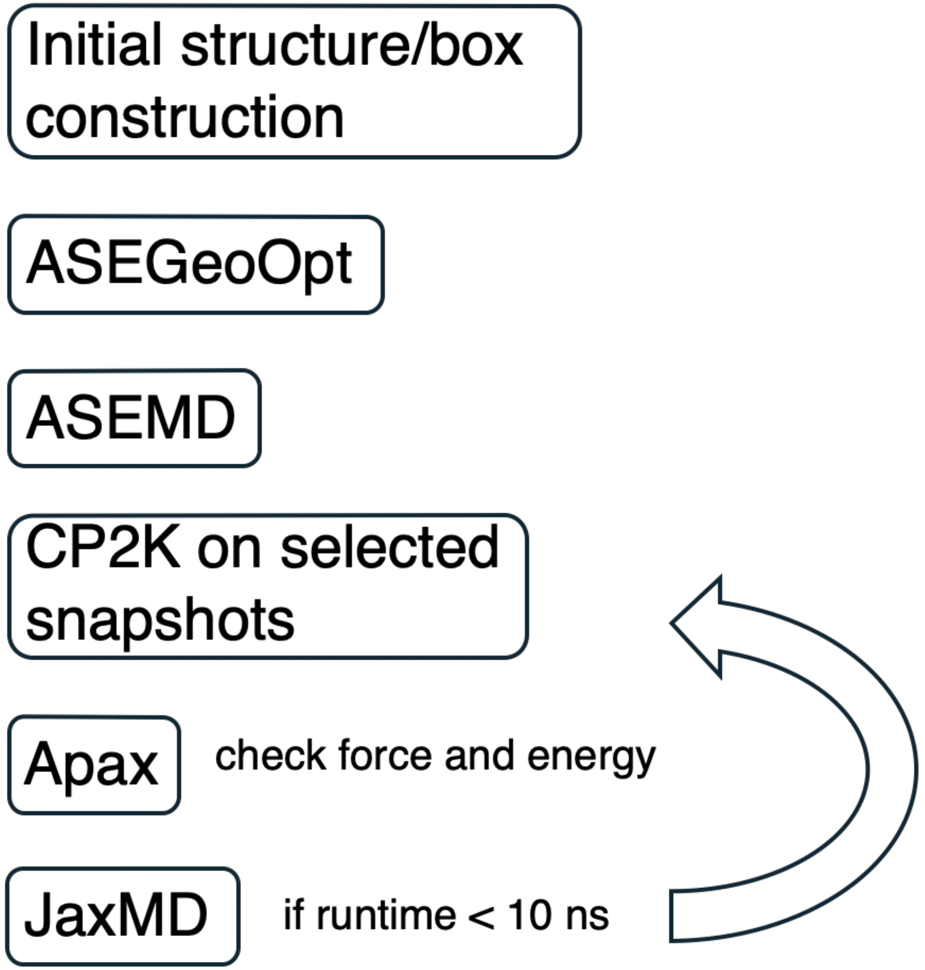
Dataset Design and Work Flow





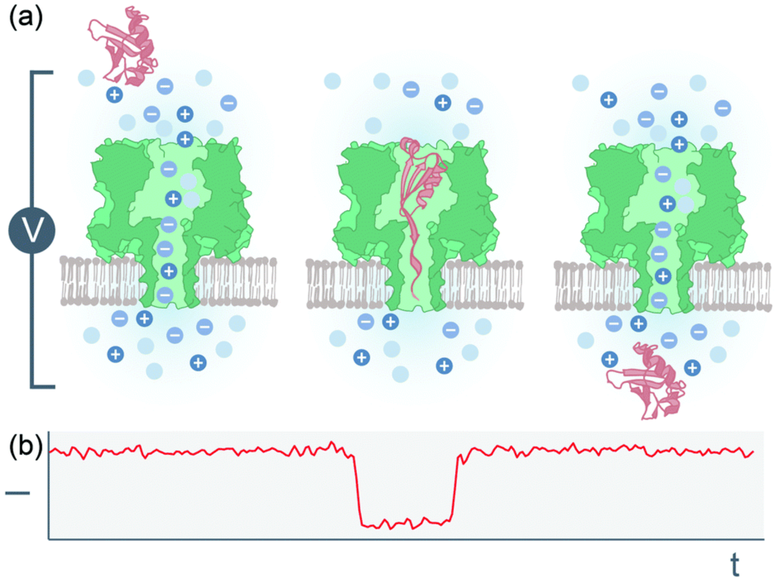


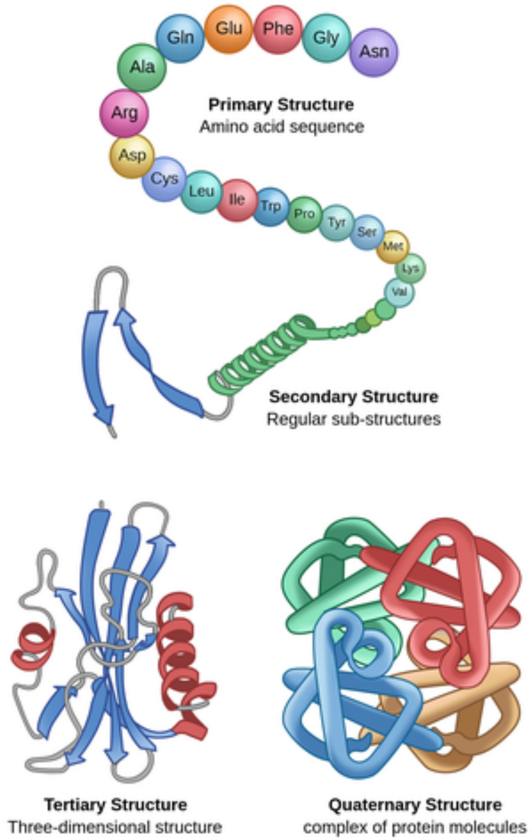
Slow-growth sampling



- Protein structure is determined by the amino acid sequence
- Mutations in the sequence can lead to malfunction and diseases

→ Fast & efficient detection of mutations can save lifes

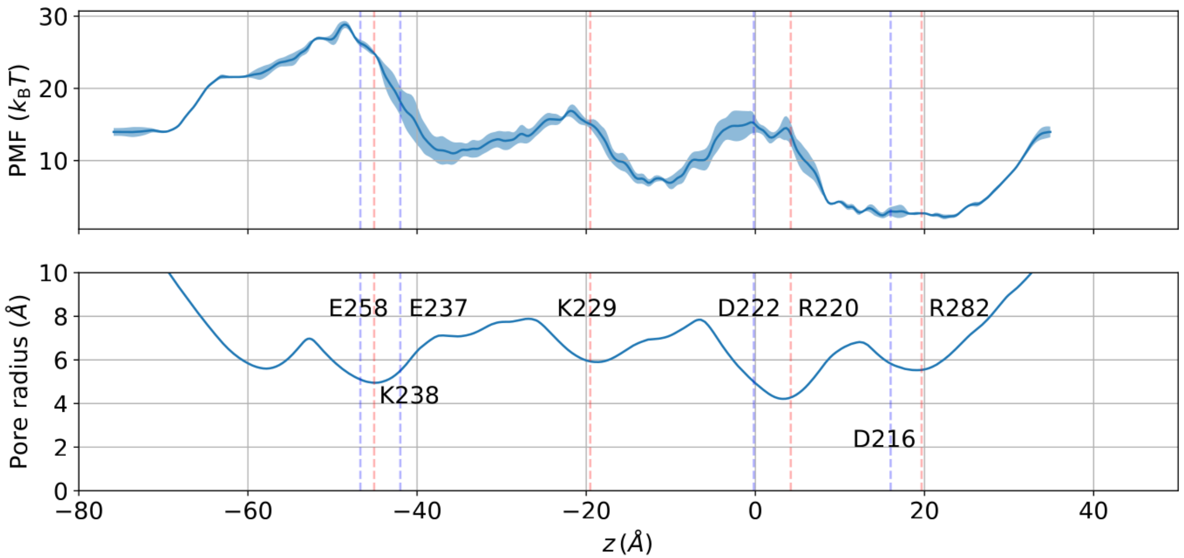


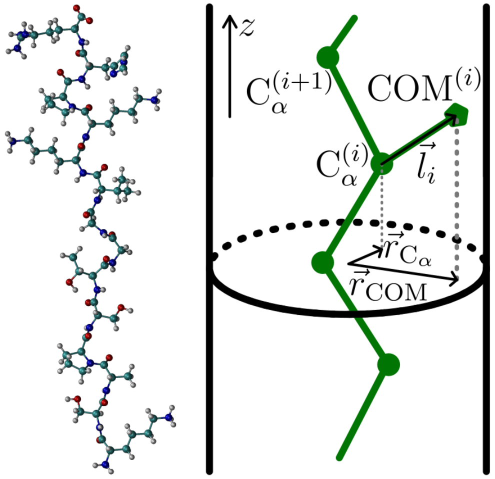


⇒ Amplitude, duration and frequency of blockade current reveal information about the protein

What did other students do?

- Computational Investigation of Methylated Histone Fragments for Nanopore Sensing Applications
- Investigation of Macromolecular Translocation Events Using Free–Energy Methods





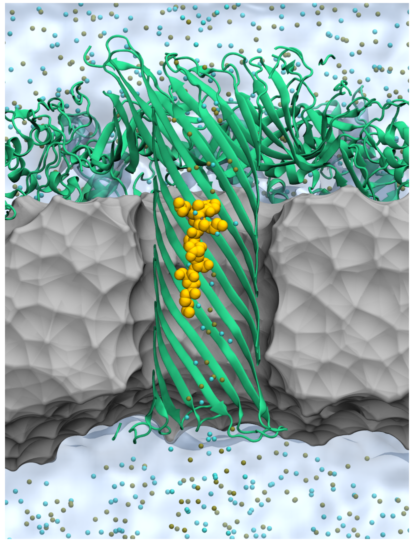
Benedikt Veit

Sylvie Eckert

What will you do?

You will learn how to ...

- Perform all–atom simulations of various nanopore systems
- Apply advanced computational techniques
- Extract physics from simulation data
- Investigate the mechanism behind nanopore sensing



For more information, please contact
michel.mom@icp.uni-stuttgart.de and visit
https://www.icp.uni-stuttgart.de/research/nanopore-sequencing/

Single-molecule protein sensing

- What features do these events have in common?
- Can we design algorithms to recognize this features?

Bachelor's Thesis: Designing artificial signals

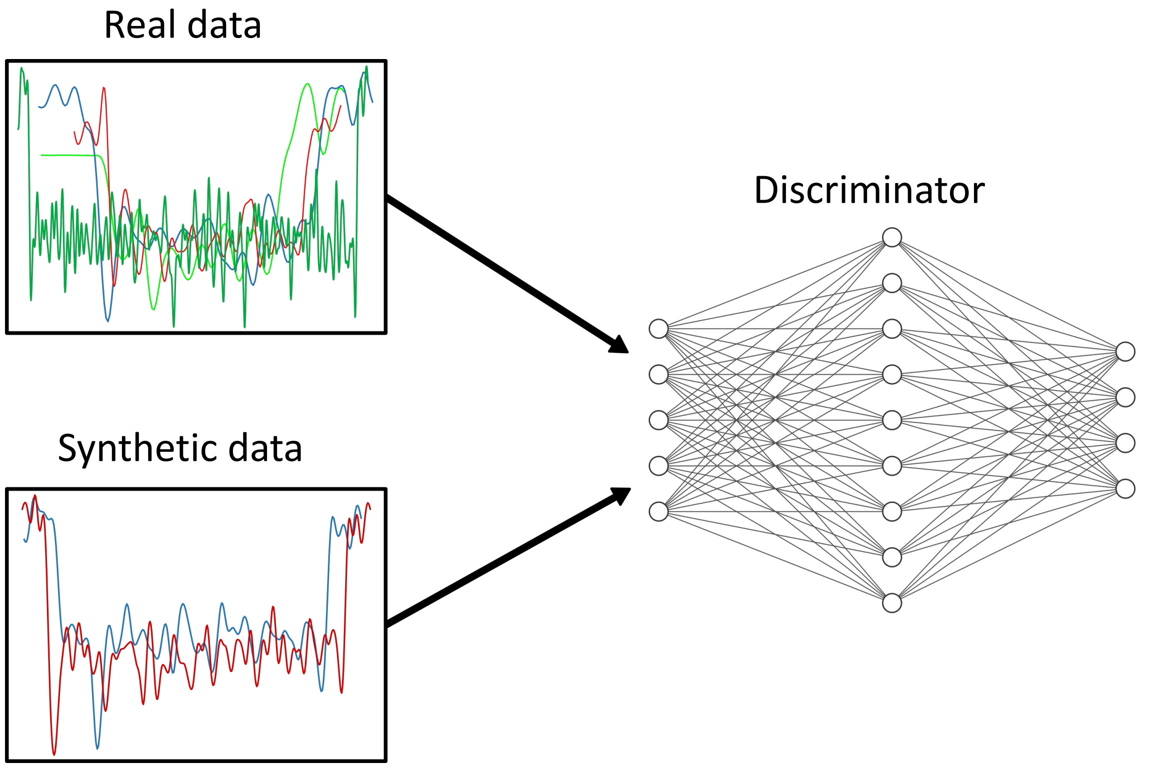
Problem:

- Experimental data requires time to acquire
- Quality of data varies between measurements

➡ Can we increase our dataset with artificial data?

Task:

- Design methods for creating artificial events
- Evaluate artificial data on classification tasks using machine learning



Contact: Julian Hoßbach
jhossbach@icp.uni-stuttgart.de

Understanding Ion Binding in Alginate via Simulations

- Alginate network formation is controlled by monomer sequence and ion-specific interactions.

- **Objective**:
  - Benchmark and compare force fields by computing ion–alginate binding free energies.

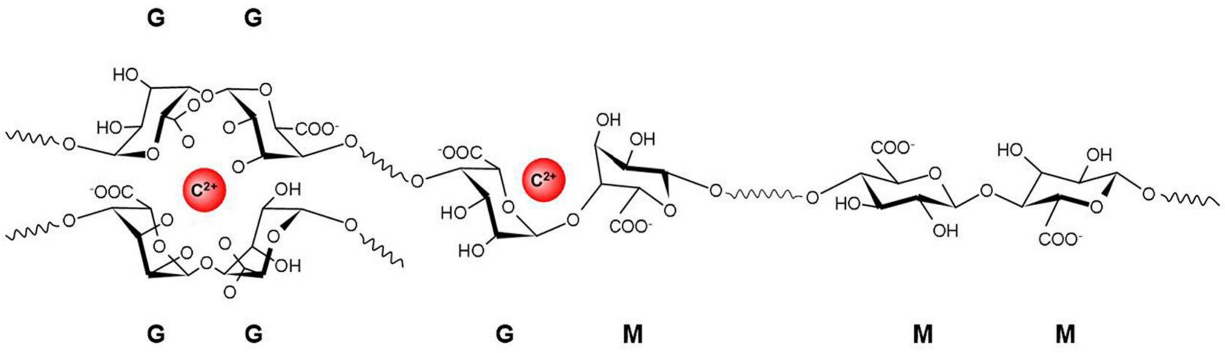


Fig. 1. Alginate molecular structure showing binding sites for divalent cations. The red circles represent cations. (C: cation; G: α-L-guluronic acid; M: β-D-mannuronic acid). DOI:10.1016/j.ijbiomac.2021.02.086

Tasks:

- Compute potential of mean force (**PMFs)** between alginate M/G monomers and multivalent ions *(CHARMM, GLYCAM, others)*
- Quantify **binding affinity differences across force fields**
- Assess consistency with **experimental ion selectivity**
- Use validated interactions to **parametrize coarse-grained potentials.**

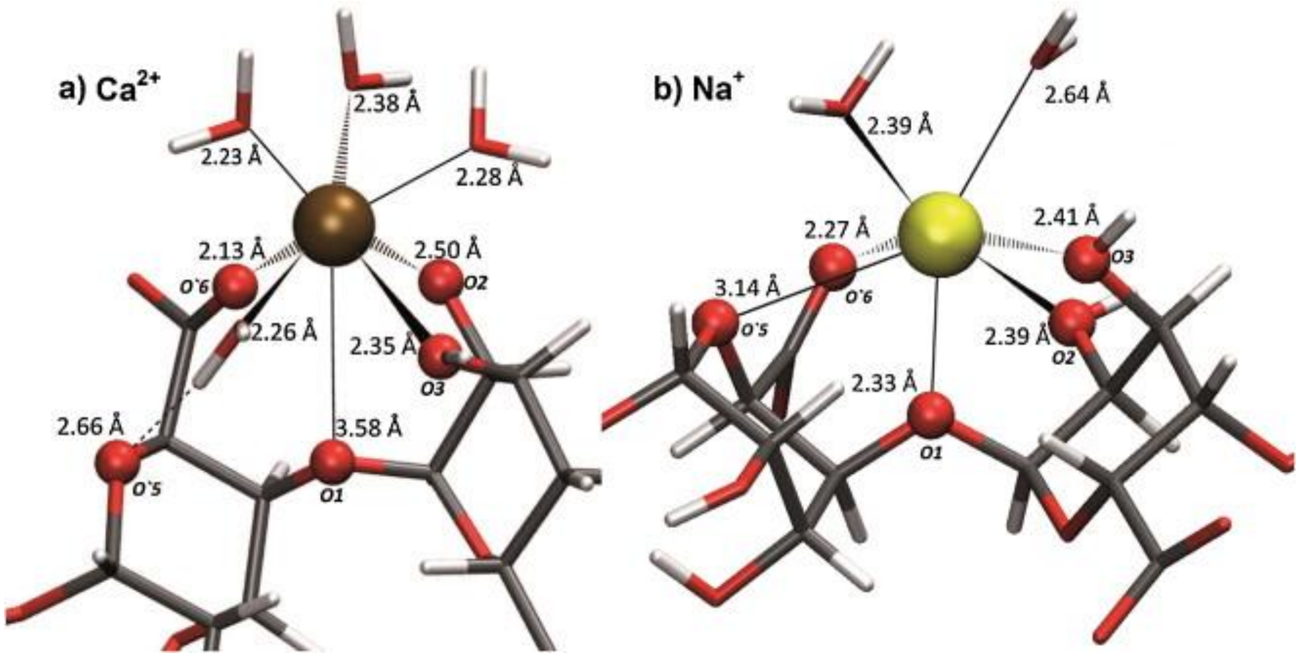


Fig. 2. Egg-box binding sites: (a) Ca^{2+} (brown) with water bridge to O’5; (b) Na^{+} (yellow). Poly-G oxygens are red; coordinated waters shown as sticks. (See web version for color references.) DOI: 10.1016/j.carbpol.2013.11.034

Outcomes:

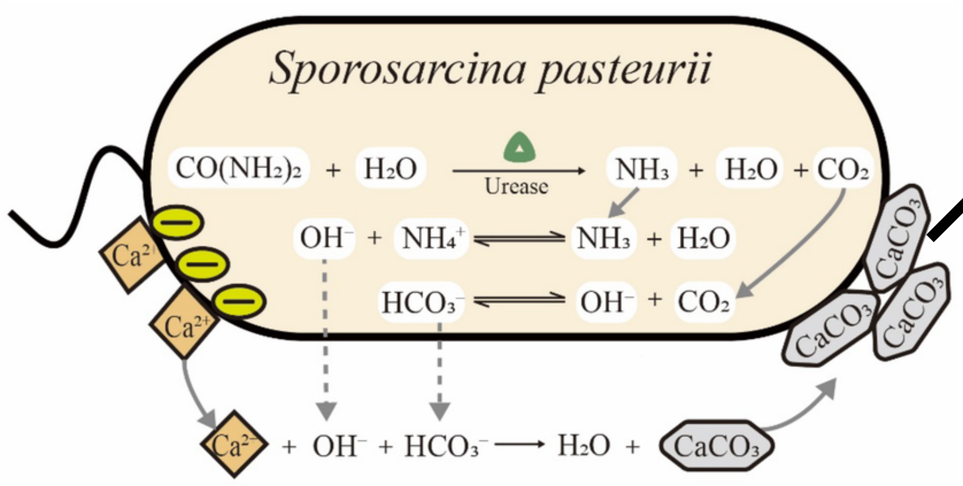
- Identify which force fields reliably reproduce ion–alginate binding trends
- Provide validated interaction parameters for coarse-grained modeling of alginate gels

Skills you will gain:

Molecular dynamics · Free-energy calculations · Force-field benchmarking ·Coarse-grained modeling

For more information, please contact hensi.gandhi@icp.uni-stuttgart.de

Microbial Induced Calcite Precipitation



Calcite precipitates
→ Clog pores

used for ↓

Self-healing concrete
CO^2 friendly bio-concrete

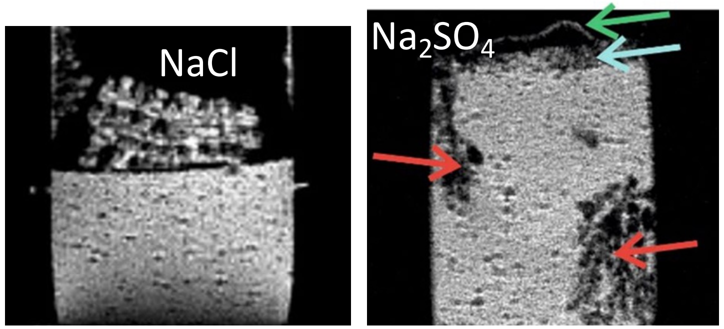
Methods

- Reactants as densities of different species localized on a grid
- Using Finite-Volume to solve the Reaction-Diffusion-Advection PDE
- Precipitation changes the system geometry and flow behavior

Ingo Tischler
itischler@icp.uni-stuttgart.de

Crystal growth dynamics in Nanopores

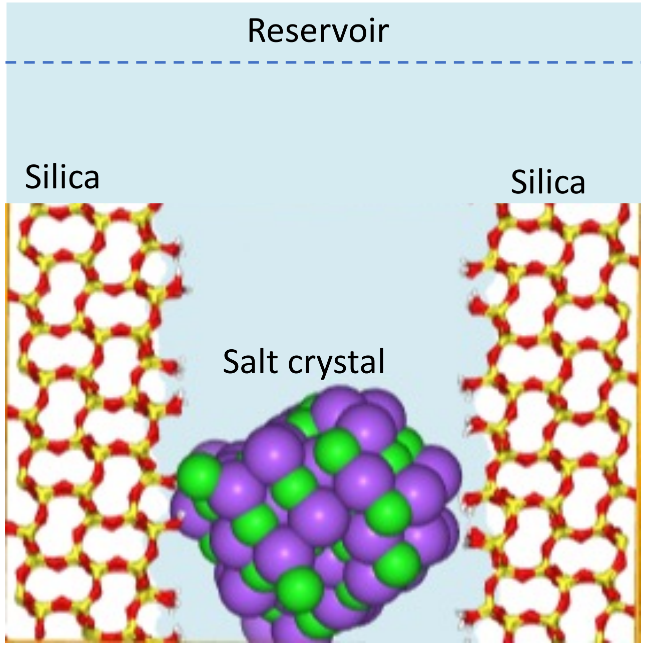
aagrawal@icp.uni-stuttgart.de



efflorescence subflorescence

The problem:
- In porous materials, salts crystallisation affects material damage, permeability, and transport
- Experiments show salt-specific behaviour -> salt can crystalise inside pores (subflorescence) or outside as crusts (efflorescence)
- But the molecular mechanism is still unclear

Goal: Identify **where crystallisation becomes irreversible** for different salts



Step 1: Model a **silica nanopore** in water with a salt solution

Step 2: **Control concentration** using a reservoir (constant supersaturation)

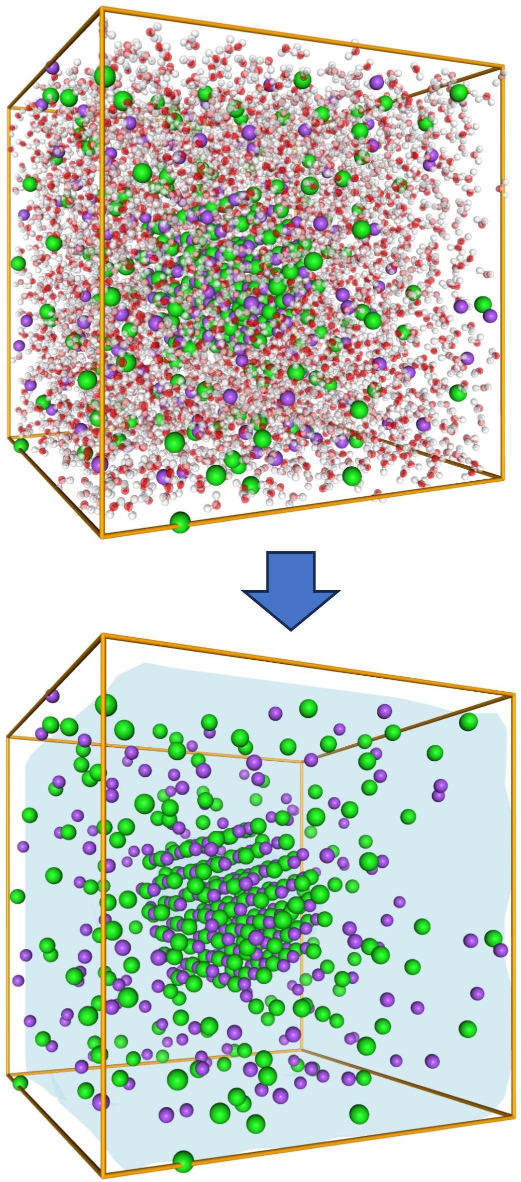
Step 3: Compare salts and **observe nucleation** and growth
– where does it start?
– how does it grow?

Machine-Learned Implicit Solvent Model for Simple Salts

The problem: Explicit-solvent MD of electrolytes is expensive

- Millions of water atoms
- Small timesteps
- Long timescales needed for nucleation/growth

Goal: Retain solvent effects on ions **without simulating water**



Step 1: Learn a **potential of mean force (PMF)** for ions from explicit-water MD

Step 2: Add **Langevin dynamics** with a friction γ

$$m\ddot{\mathbf{R}} = -\nabla U_{\mathrm{PMF}}(\mathbf{R}) - \gamma\dot{\mathbf{R}} + \sqrt{2\gamma(c)k_B T}\,\eta(t)$$

Fit γ by matching ion diffusion from explicit MD

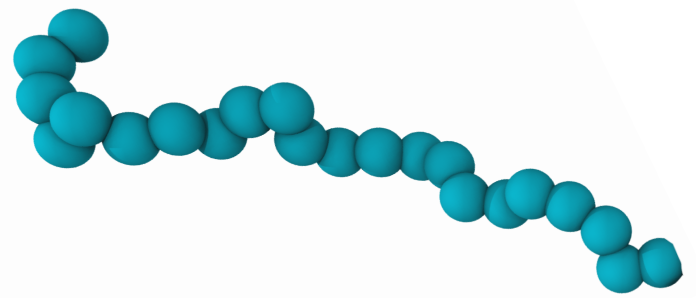
Bonus: Learn $\gamma(\xi(R))$ as smooth function of local environment

aagrawal@icp.uni-stuttgart.de

Variational Theories for Polyelectrolytes

$$\beta H_{\mathrm{t}} = \frac{3}{2l}\int_0^L \mathrm{d}s \left(\frac{\mathrm{d}\mathbf{R}(s)}{\mathrm{d}s}\right)^2 + l\int_0^L \mathrm{d}s \int_0^s \mathrm{d}s' \omega(s,s')\delta\left[\mathbf{R}(s) - \mathbf{R}(s')\right] + \frac{\lambda_{\mathrm{B}}}{l^2}\int_0^L \mathrm{d}s \int_0^s \mathrm{d}s' q(s)q(s') \frac{\exp\left(-\kappa\left|\mathbf{R}(s) - \mathbf{R}(s')\right|\right)}{\left|\mathbf{R}(s) - \mathbf{R}(s')\right|}$$

$$\longrightarrow \quad \beta H_{\mathrm{r}} = \frac{3}{2l_{\mathrm{r}}}\int_0^L \mathrm{d}s \left(\frac{\mathrm{d}\mathbf{R}(s)}{\mathrm{d}s}\right)^2$$



- Learn about the Edwards-Singh variational method
- Set up coarse-grained simulations of a polyelectrolyte for different chain lengths and salt concentrations
- Check the validity of variational calculations against your simulations

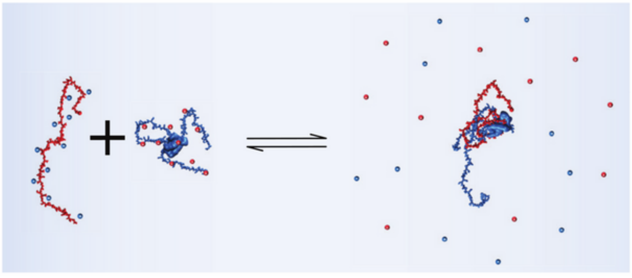
Contact:
David Beyer (dbeyer@icp.uni-stuttgart.de)
Lena Tarrach (lena.tarrach@icp.uni-stuttgart.de)

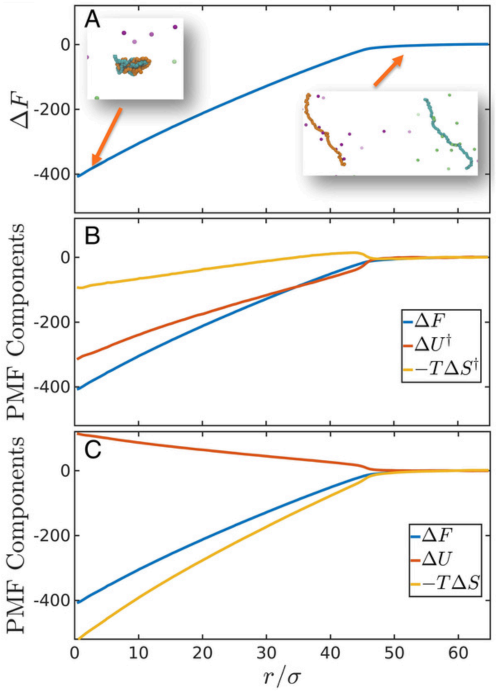
Driving Forces for Polyelectrolyte Coacervation - Enthalpy vs Entropy

- PE complex coacervate forms when oppositely charged polymers associate and phase separate.

- Disrepancy between experiments and CG simulation regarding thermodynamic driving forces on PE complex coacervation

- **Can atomistic simulation address the solvent entropy issue?**





Your Job

- Get familiar with atomistic simulation
- Calculate the PMF between ion/polyion pair
- Attribute the solvent DOF explicitly.
- Split the PMF into entropy and enthalpy contribution
- Analyze the entropy contribution further: counterion-release and electrostatic entropy

Reference: Chen et al.
https://doi.org/10.1073/pnas.2209975119

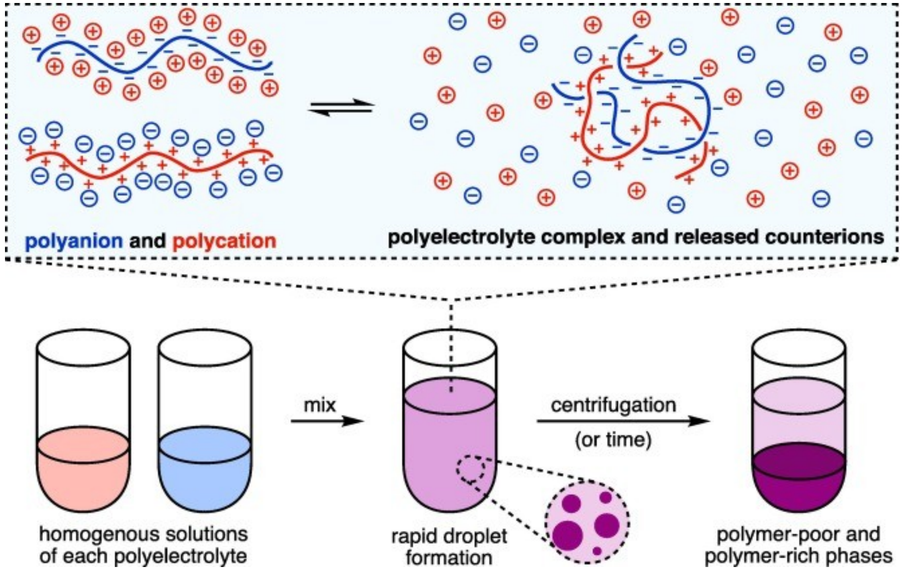
Methods and literature

- Free energy calculation
- Familiarity with electrostatic interaction
- Statistical and thermodynamic analysis of the data
- software: Lammps/Gromacs for atomistic simulation
- Python/C++ knowledge is advantageous

Somesh Kurahatti (somesh.kurahatti@icp.uni-stuttgart.de)
Lena Tarrach (lena.tarrach@icp.uni-stuttgart.de)
David Beyer (david.beyer@icp.uni-stuttgart.de)

How does the polymer architecture affect the hydrodynamic properties of polyelectrolyte complex coacervates?

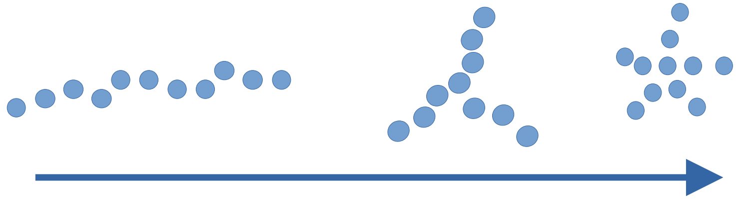
Polyelectrolyte (PE) complex coacervation



Neitzel, De Hoe & Tirrell *Current Opinion in Solid State and Materials Science* 2021 25 (2) 10089

Spruijt, Stuart & van der Gucht *Macromolecules* 2013 46 (4), 1633-1641

Polymer architecture



Why should this be interesting to you?

- Relevance in drug delivery or cell formation

What will you do?

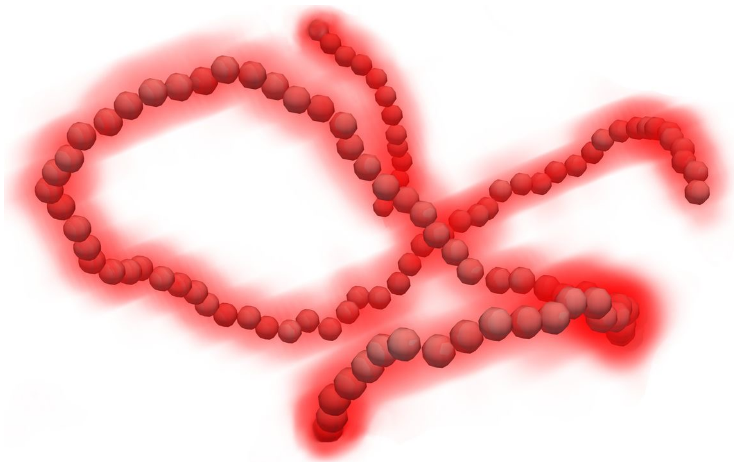
- Coarse-grained molecular dynamics simulation with ESPResSo
- Theoretical physics to compute properties
- Analysis of simulation data

What will you learn?

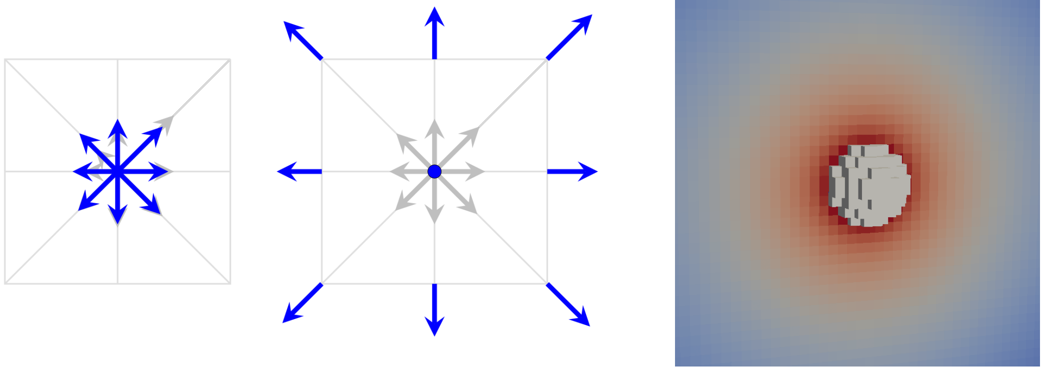
- Structure-property relations of PE complex coacervates
- Molecular dynamics simulations
- How to work on a research project

Lena Tarrach, lena.tarrach@icp.uni-stuttgart.de
David Beyer, david.beyer@icp.uni-stuttgart.de

Coupling of flexible polyelectrolytes to continuum solvent



Method: Lattice Boltzmann + Lattice Electrokinetics



How to couple particle method for charged polymers to continuum method for ions and fluid

Your Job

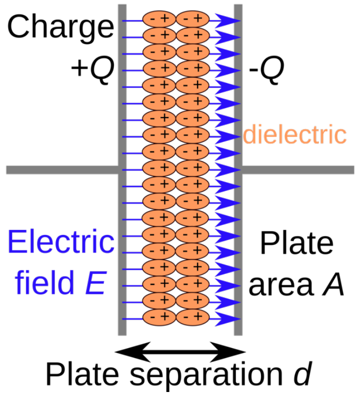
- Improve existing electrostatic coupling
- Verify against Molecular Dynamics simulations
- Implement more advanced couplings if needed

You will learn

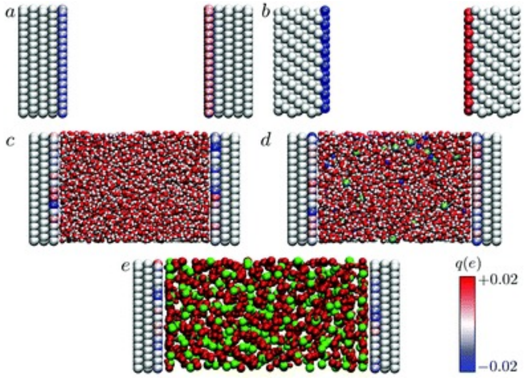
- Mesoscale lattice-based solver for hydrodynamics/Nernst-Planck equation
- Molecular Dynamics and electrostatic solvers
- Python and C++

Alexander Reinauer (alexander.reinauer@icp.uni-stuttgart.de)
Rudolf Weeber (rudolf.weeber@icp.uni-stuttgart.de)

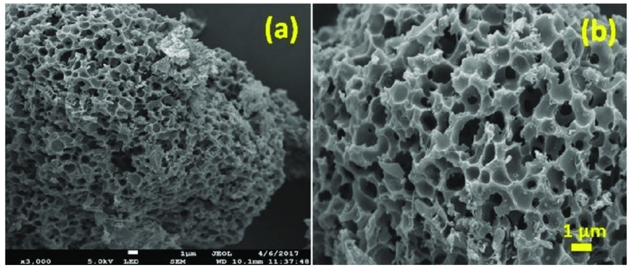
Implement high-performance constant-potential library



Wikipedia



Scalfi et al. Physical Chemistry Chemical Physics 22.19 (2020): 10480-10489.



Carbon electrode, DOI: 10.1039/C9NA00374F

What to do?

- Implementation of existing constant potential models
- High performance development
- Usable with different MD-codes

What you will learn:

- Electrostatic Solvers
- Constant Potential algorithms
- Python
- C++

Alexander Reinauer (alexander.reinauer@icp.uni-stuttgart.de)
Rudolf Weeber (rudolf.weeber@icp.uni-stuttgart.de)

Accelerate charged soft matter simulations

- The Monte Carlo (MC) method can model chemical reactions and dissociation of charged groups from polyelectrolytes
- Goal: speed up simulations by calculating electrostatic energy differences more efficiently
- Requires some C++ experience

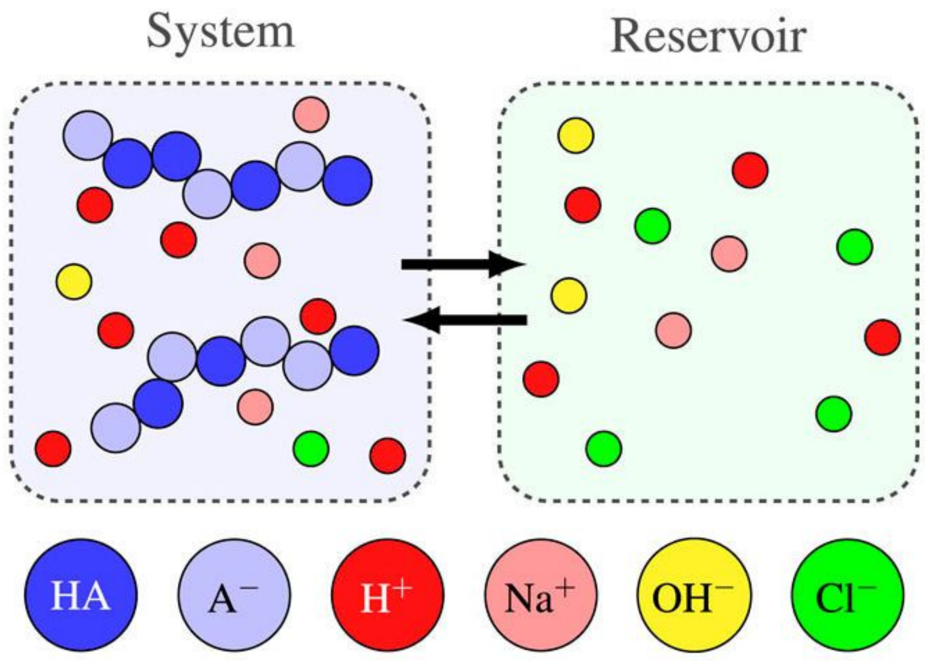


Image credit: Beyer et al. 2024, DOI:10.1063/5.0216389

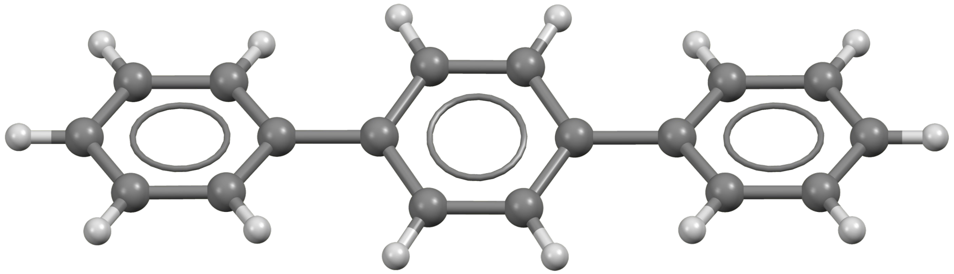
Project lead: Rudolf Weeber, Jean-Noël Grad

Rigid-Bond Molecular Dynamics in the NPT Ensemble

NPT simulations are essential to reproduce experimental conditions (constant T,P) and ensure correct system density.

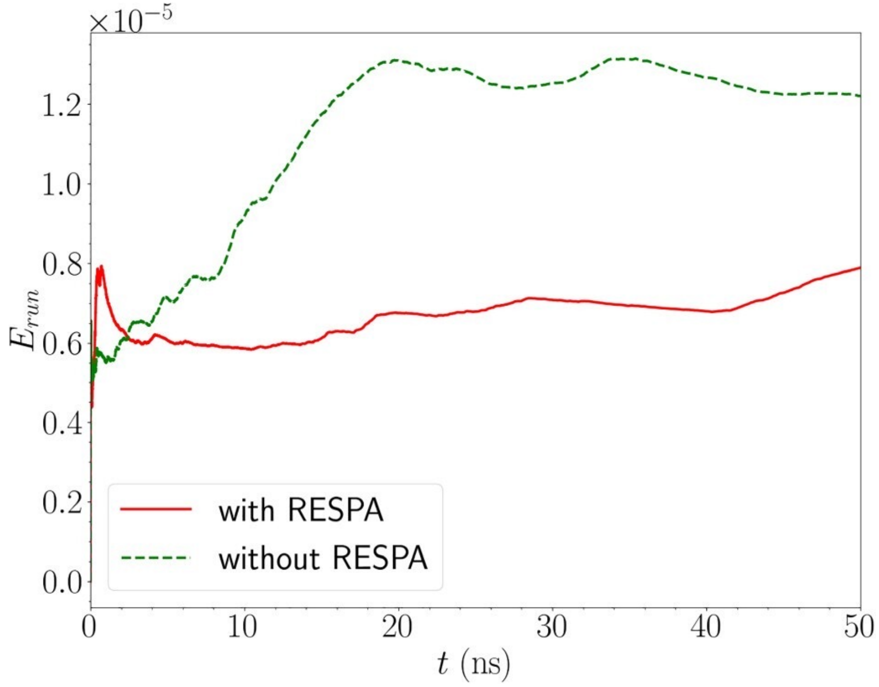
•**Challenge:** Rigid bonds allow larger timesteps, but conflict arises when the barostat scales coordinates while constraints attempt to fix bond lengths.
•**Solution:** A symplectic Trotter splitting (MTK equations + RESPA) resolves this by mathematically defining the correct order of scaling and constraining. Implement this scheme into ESPResSo!

De Michele, C., & Ciccotti, G. (2025) *Molecular Physics*, *123*(3), e2364834, (2025)



Orthotherphenyl (OTP) model
https://en.wikipedia.org/wiki/Terphenyl

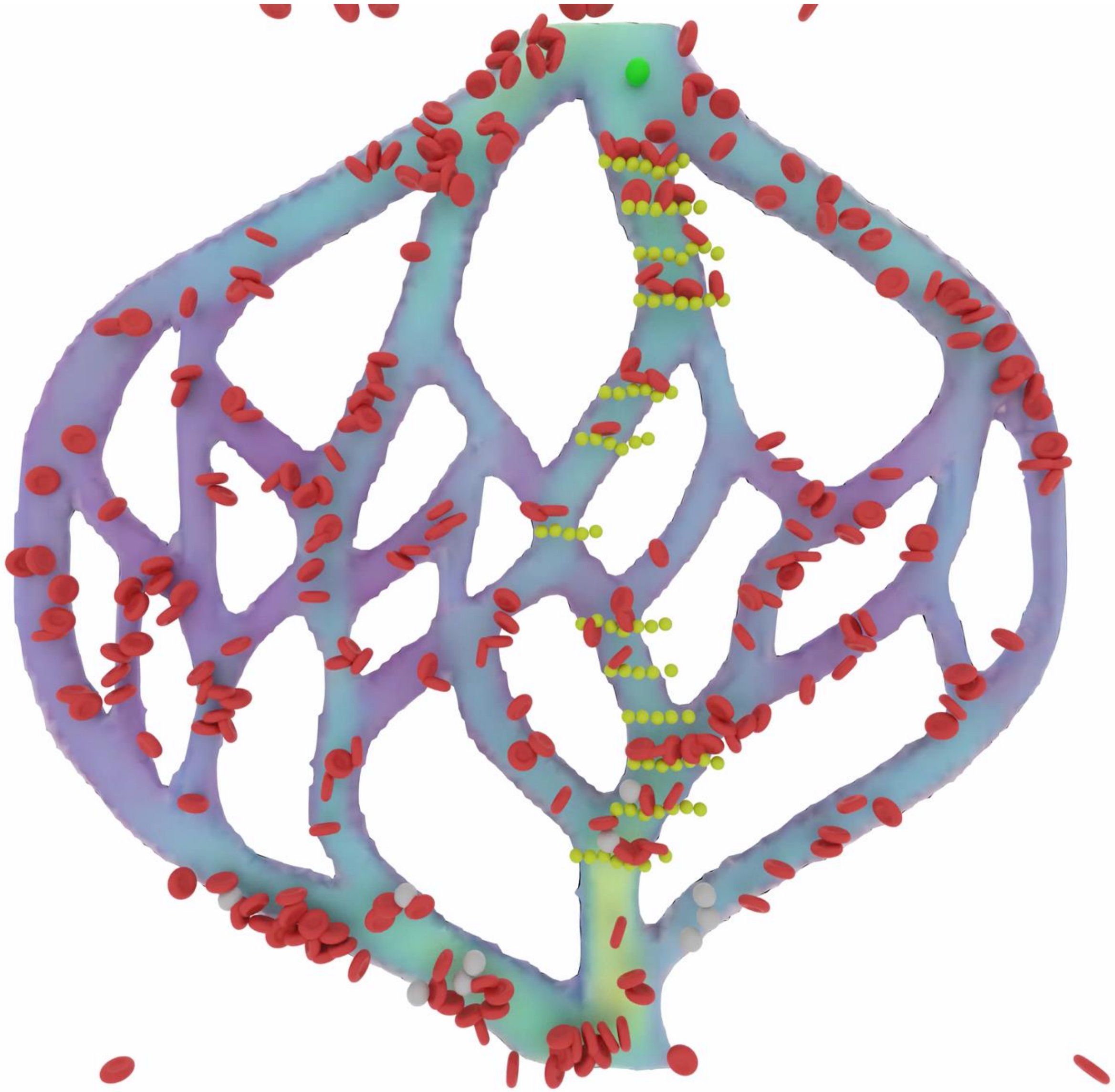
Energy conservation with OPT model in NPT



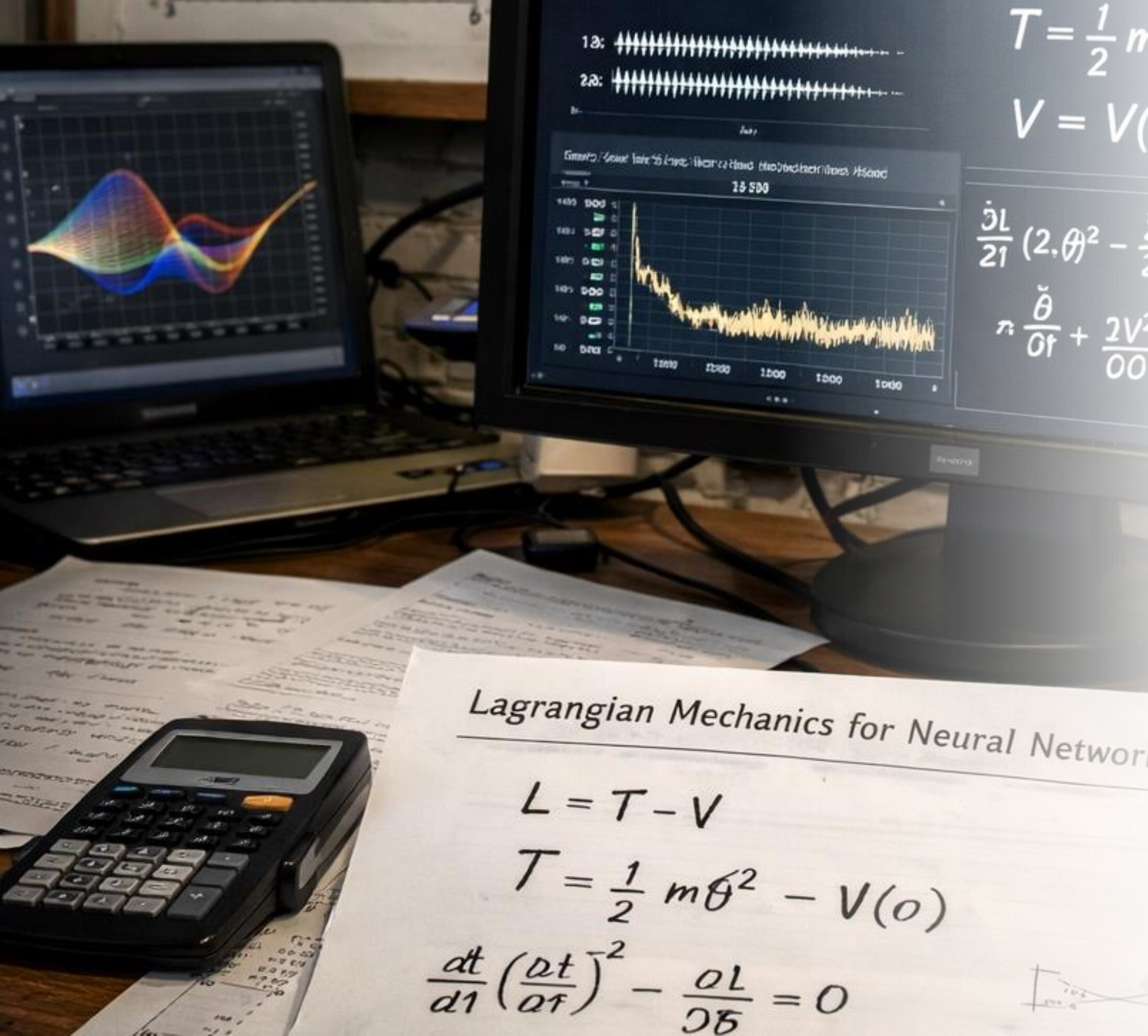
hideki.kobayashi@icp.uni-stuttgart.de

Microrobotic Control with Reinforcement Learning

- Imitation learning for microrobotic strategies
- LLM-assisted training of multi-agent simulations
- Contribute to SwarmRL software.
- Deploy models on GPU infrastructure.



Samuel Tovey, samuel-james.tovey@icp.uni-stuttgart.de



The Lagrangian of Learning

- Implement Lagrangian dynamics for a neural network.
- Explore conservation laws and Hamiltonian representations.
- Explore a vast range of neural network architectures.

Samuel Tovey, samuel-james.tovey@icp.uni-stuttgart.de

Quantum Reservoir Computing

How to teach quantum systems to predict time series?

Quantum Reservoir Computing (QRC)

Possible Topics

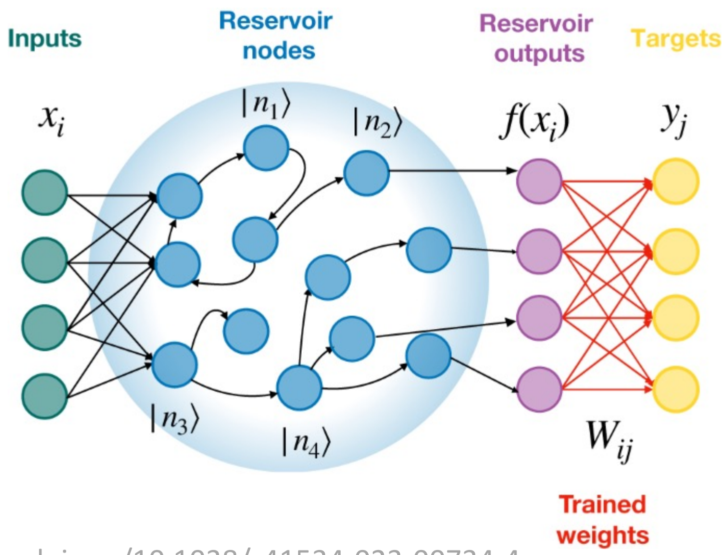
- Develop and investigate QRC with feedback
- Apply QRC to nitrogen-vacancy systems
- Study the interplay of decoherence and robustness in QRC

Requirements

- Basic understanding of quantum physics
- Good knowledge in Python

What you can learn

- Simulating quantum physical systems
- Insights into quantum computing and quantum machine learning



doi.org/10.1038/s41534-023-00734-4

tobias.fellner@icp.uni-stuttgart.de

Bachelor, Masters or PhD topics

For general contact:

Christian Holm: holm@icp.uni-stuttgart.de

Rudolf Weeber: weeber@icp.uni-stuttgart.de

Svyatoslav Kondrat: svyatoslav.kondrat@icp.uni-stuttgart.de

Samuel Tovey: stovey@icp.uni-stuttgart.de

For more informations visit the ICP website
www.icp.uni-stuttgart.de

For Teaching overview: See https://www2.icp.uni-stuttgart.de/~icp/Teaching/Overview

- Fabian Zills fzills@icp.uni-stuttgart.de — Machine learned potentials
- Konstantin Nikolaou knikolaou@icp.uni-stuttgart.de — ML for Physics
- Alexander Reinauer areinauer@icp.uni-stuttgart.de — 2-Phase LB, electrokinetic algorithms
- Michel Mom mmom@icp.uni-stuttgart.de — Nanopore and all atom simulations
- David Beyer dbeyer@icp.uni-stuttgart.de — Weak polyelectrolytes,
- Adyant Agrawal aagrawal@icp.uni-stuttgart.de — atomistic MD simulations of salt crystalization in porous media
- Tobias Fellner tfellner@icp.uni-stuttgart.de — Quantum Computing algorithms, QML
- Svyatoslav Kondrat svyatoslav.kondrat@gmail.com — Supercapcitors
- Jean-Noel Grad jgrad@icp.uni-stuttgart.de — ESPResSo, Lattice-Boltzmann
- Hideki Kobayashi hkobayashi@icp.uni-stuttgart.de — ESPResSo Software
- Rudolf Weeber weeber@icp.uni-stuttgart.de — ESPResSo, Magnetic Soft Matter, Polymer Rheology
- Julian Hossbach jhossbach@icp.uni-stuttgart.de — Machine learning for Signal processing, nanopore currents
- Yashas Ghandi yashas-tejaskumar.gandhi@icp.uni-stuttgart.de — Magnetic Gels, Viscosity simulations with LB
- Hensi Gandhi hensi.gandhi@icp.uni-stuttgart.de — Models for alginates and pectins
- Lena Tarrach lena.tarrach@icp.uni-stuttgart.de — Coacervates and weak polyelectrolytes
- Samuel Tovey stovey@icp.uni-stuttgart.de — Machine learning in Physics