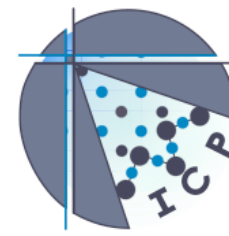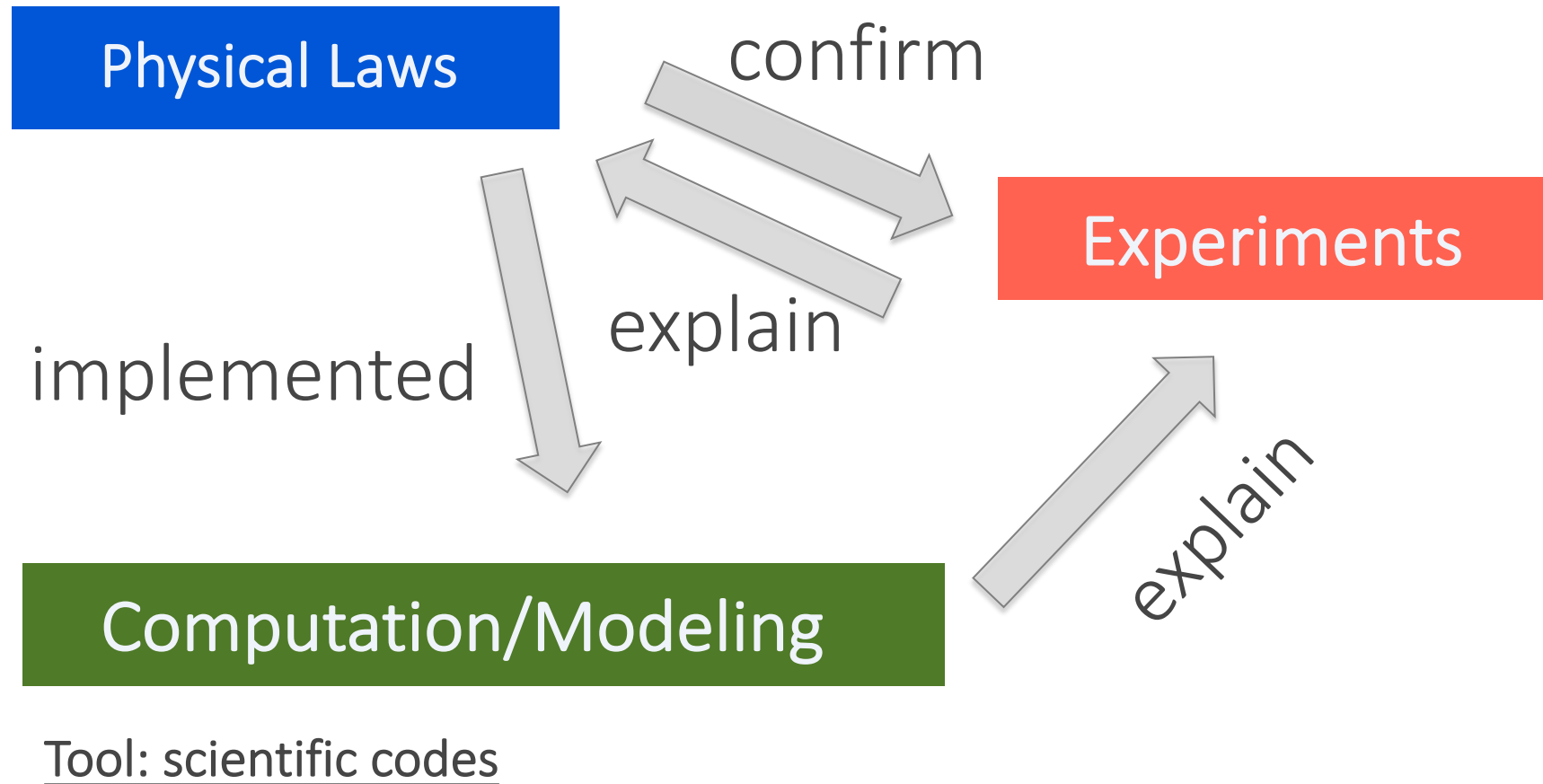**University of Stuttgart**

Germany

INSTITUTE FOR COMPUTATIONAL PHYSICS

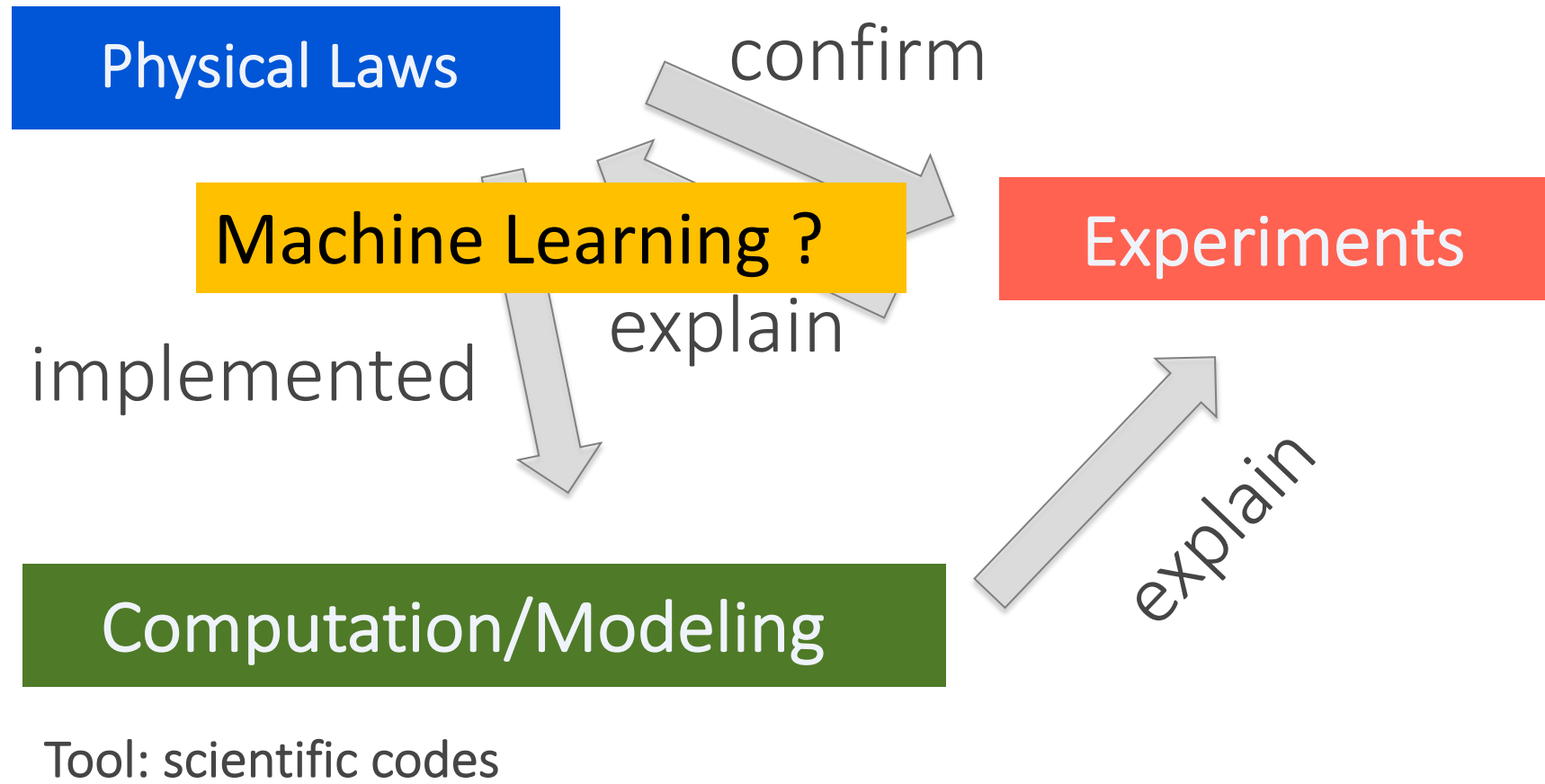# Research at the Institute for Computational Physics

Christian Holm, Rudolf Weeber, Slavko Kondrat, Alexander Schlaich (also at SimTech)

Institut für Computerphysik, Universität Stuttgart
Stuttgart, Germany

The Way Physics works today…

The Way Physics works tomorrow…??

Physical Laws

confirm

Machine Learning ?

Experiments

implemented

explain

Computation/Modeling

explain

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):
Soft Matter Theory, Supercapacitor applications

A. Schlaich (SimTech JGL):
Multiscale Materials Modelling

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

We teach on a regular basis:

- Computergrundlagen (WS) 1. FS B.Sc
- Physik auf dem Computer (SS) 4. FS B.Sc.
- Simulationsmethoden 1 + 2 elective B.Sc. und M.Sc.(WS+SS)
- Advanced Simulation Methods (SS) elective M.Sc.
- ESResSo summer school (**1. week in October before the regular start of the WS semsester** !) elective M.Sc.

Irregulary:
- Physics of Fluids 1+2 (elective Master)
- Soft and Biological Matter 1+2 (elective Master)

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

Soft Matter Physics

C. Holm

Institute for Computational Physics
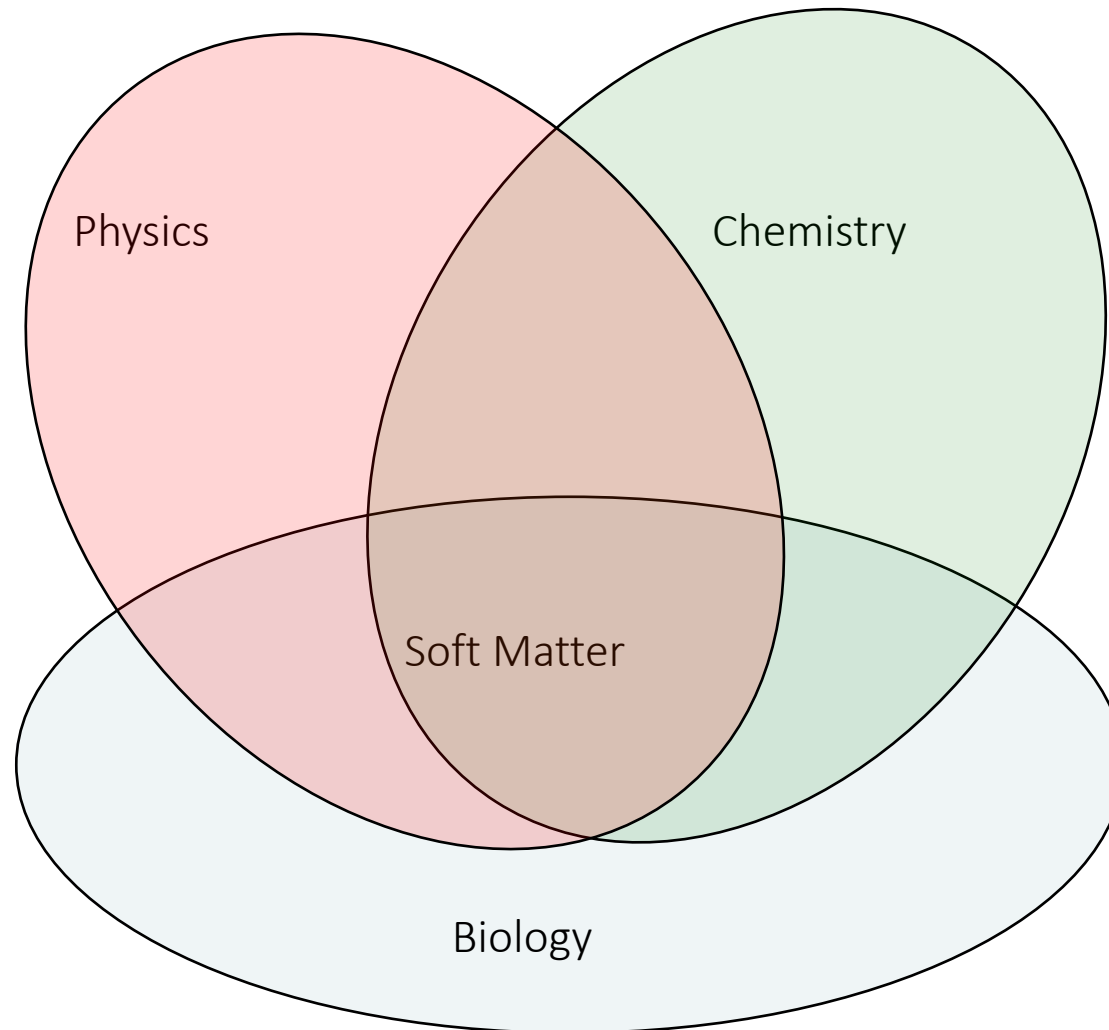Universität Stuttgart

....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), model systems for statistical physics
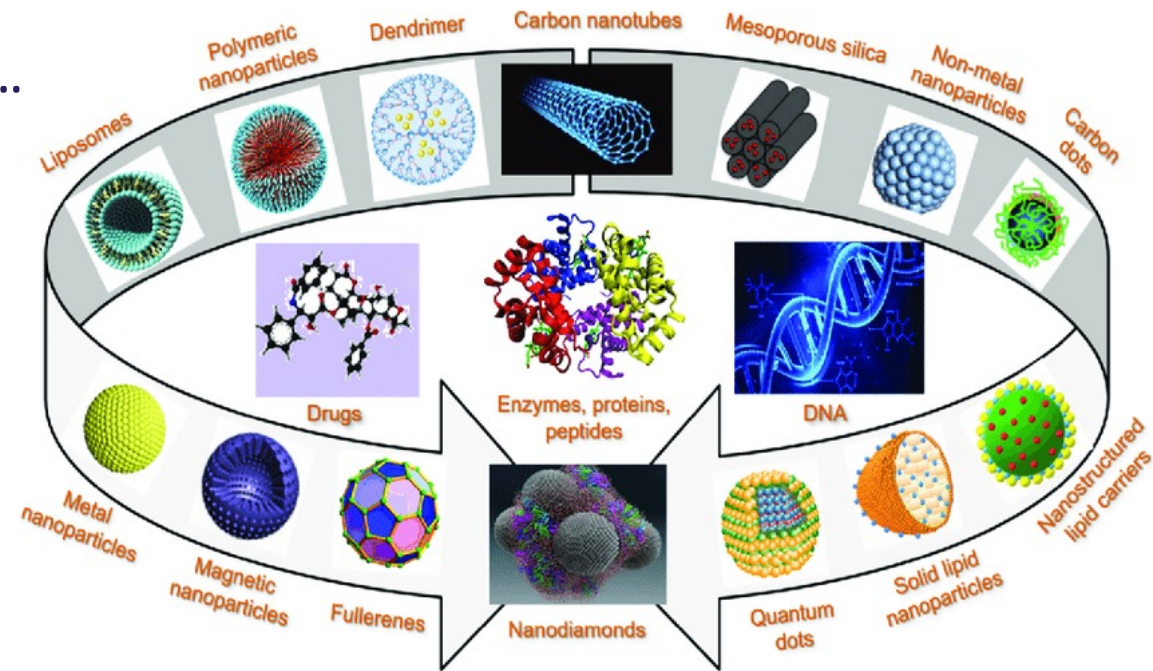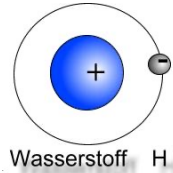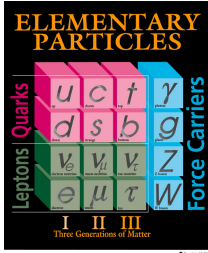

R. Kanwar et al., *Green Nanotechnology-Driven Drug Delivery Assemblies*, ACS Omega, 2019, doi:10.1021/acsomega.9b00304
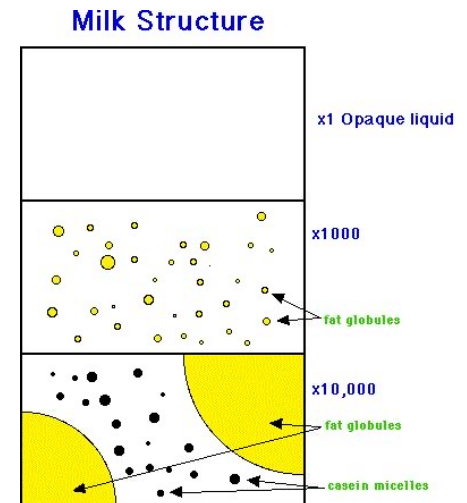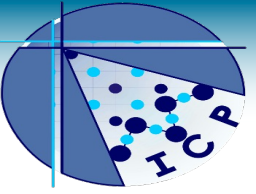
Length Scales of Soft Matter

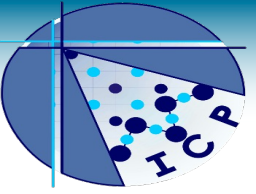1 fm   1pm   1 Å   1nm   10 μm   1mm   1m   1km 10^3km 10^6parsec
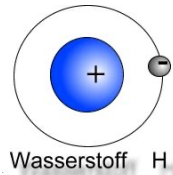
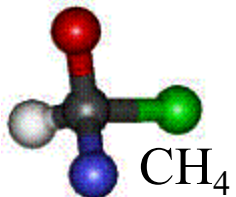**ELEMENTARY PARTICLES**

Wasserstoff   H
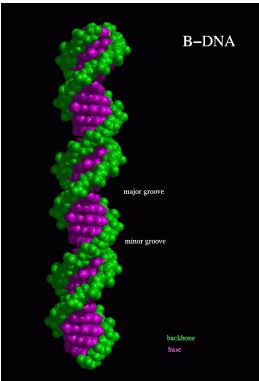
Soft
Matter

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

1 Å   1nm   10 μm 1mm

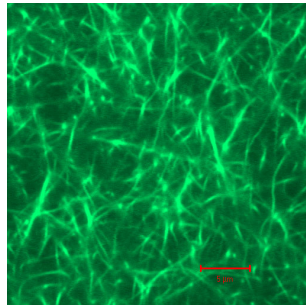Soft Matter

Wasserstoff   H

10^{-15}m 10^{-12}m 10^{-9}m 10^{-6}m 10^{-3} m 10^{0}m 10^{3}m 10^{6}m
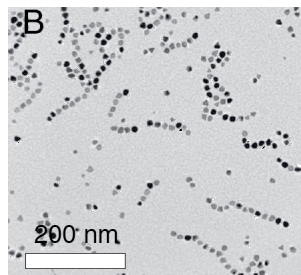
1 nm   10 nm   100 nm   1 μm   10 μm   100 μm

CH_4

B-DNA
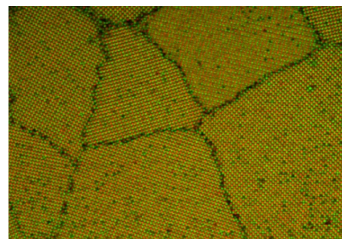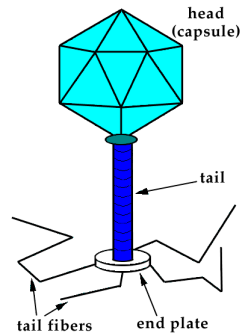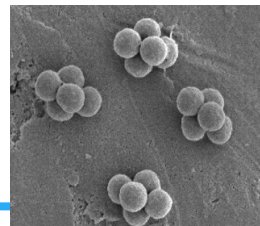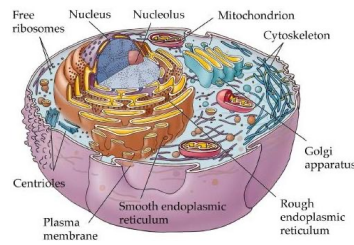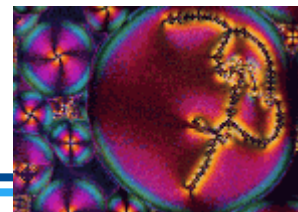
200 nm
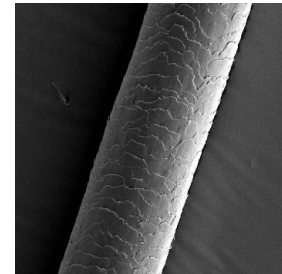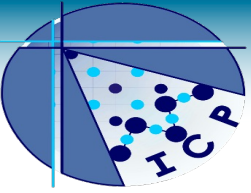
Coarse-graining

- A model consists of a number of **degrees of freedom** (e.g. atomic positions: translation) and the "**interactions**" between them.

- *Coarse-graining:*
  - 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

Quantum

All-atom

Molecular

Mesoscopic Fluid Methods

Continuum

ICP
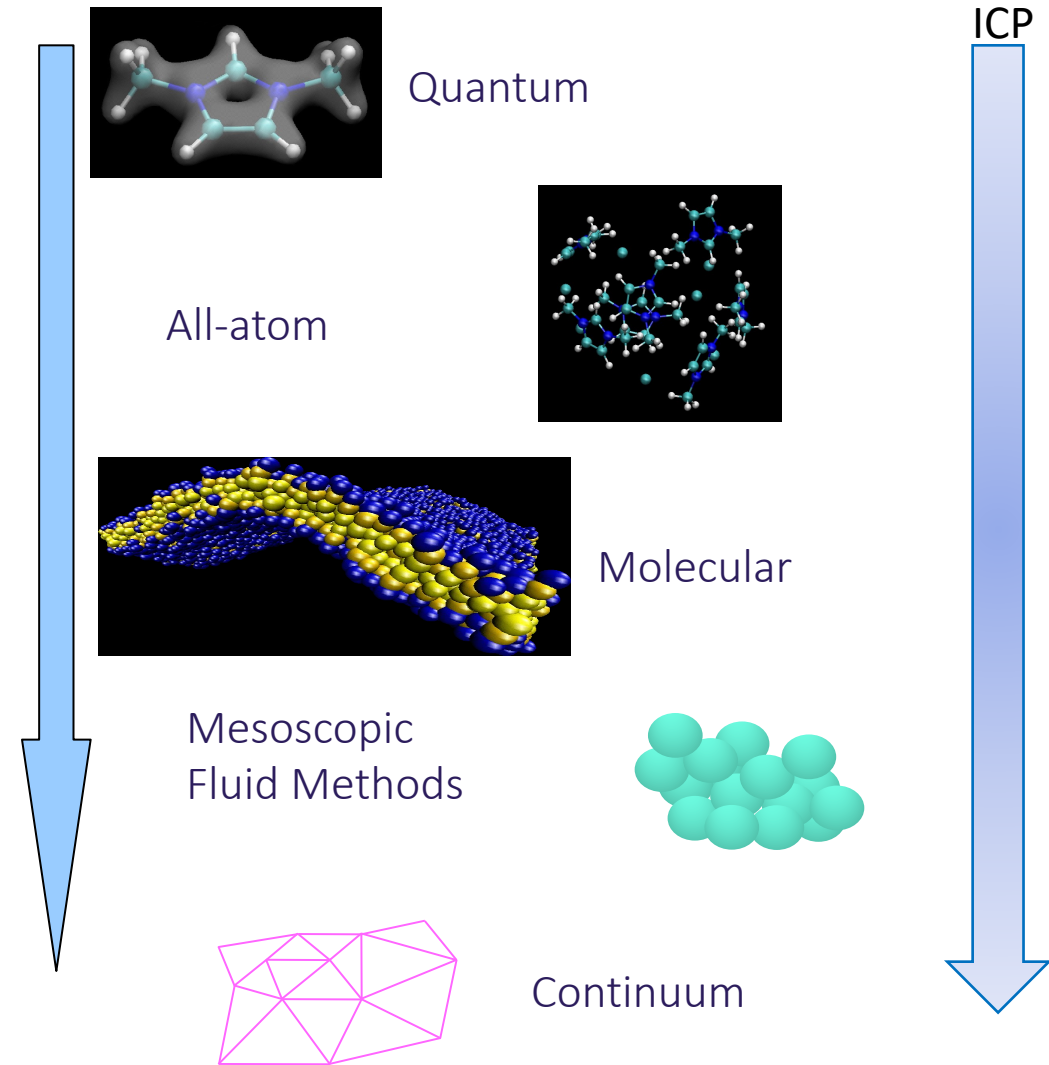
Current Research Fields (C. Holm)

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
- Fast long range solvers under various conditions

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
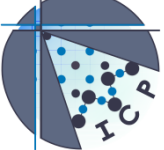
ESPResSo
The Extensible Simulation Package for Research on Soft matter

Christian Holm

Florian Weik, Georg Rempfer, Rudolf Weeber

Konrad Breitsprecher

David Sean

Michael Kuron, J. DeGraaf

Jonas Landsgesell

Kai Szuttor

Patrick Kreissl

Ingo Tischler

R. Kaufmann

Ashreya Jayaram

Miru Lee

Michael Lahnert

Milena Smiljanic

Robin Bardakcioglu

Sebastian Bindgen

Steffen Hirschmann

And many more

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

http://www.espressomd.org

Molecular Dynamics simulations

ESPResSo is capable of doing classical Molecular dynamics simulations of many types of systems in different statistical ensembles (NVE, NVT, NPT) and non-equilibrium situations, using standard potentials such as the Lennard-Jones or Morse potential. It contains many advanced simulation algorithms, which take into account hydrodynamic (lattice Boltzmann) and electrostatic interactions (P3M, ELC, MMMxD). Rigid bodies can be modelled by virtual site interactions, and it can integrate rotationally non-invariant particles.
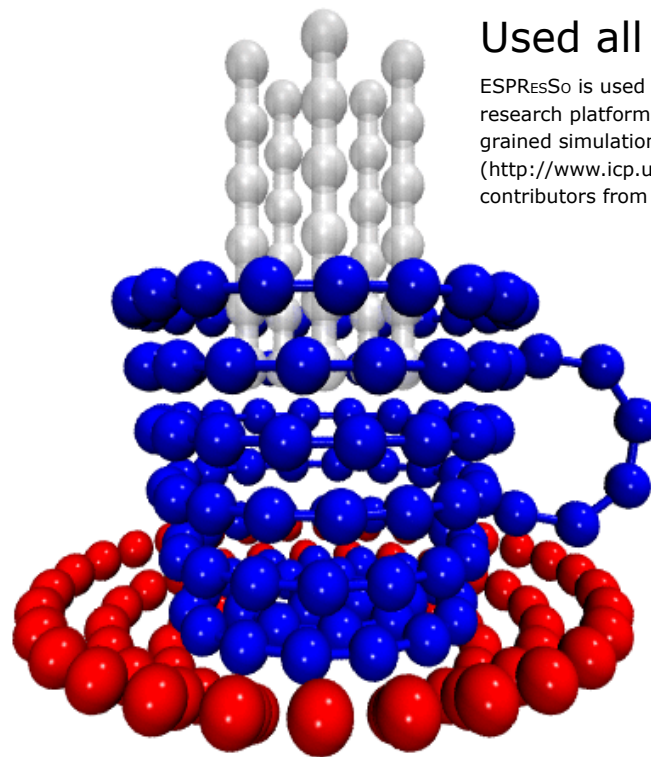
Used all over the world

ESPResSo is used in scientific working groups all over the world both as a production platform as well as a research platform for developing new algorithms and methods and designing new models for coarse-grained simulations. It is mainly developed and maintained at the Institute for Computational Physics (http://www.icp.uni-stuttgart.de)   of the University of Stuttgart (http://uni-stuttgart.de)   , but has contributors from all over the world.

Free and open-source
ESPResSo is free, open-source software published under the GNU General Public License (GPL). It is parallelized and can be employed on desktop machines, convenience clusters as well as on supercomputers with hundreds of CPUs. The parallel code is controlled via the scripting language Tcl, which gives the software its great flexibility and allows for many unconventional simulation protocols, as are often required when studying coarse-grained models.

Members of Various Research Consortia
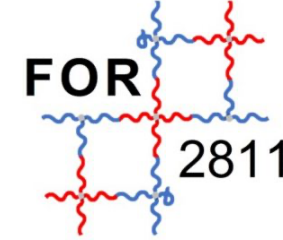
FOR 2811

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

CRC 1333

FOR 2811

3: Molecul

Multi scale

EuroHPC Centre of Excellence

nanOdiag

Nanopore technology for the molecular diagnostics of the future

cecam
Centre Européen de Calcul Atomique et Moléculaire

Cluster of Excellence EXC 2075

KEMIJSKI INŠTITUT   UNIVERSITAT DE BARCELONA

Open Positions

Universität Stuttgart   SORBONNE UNIVERSITÉ   Université de Toulouse   Consiglio Nazionale delle Ricerche

HPC Now!   university of   SURF   JÜLICH Forschungszentrum   GHENT   BSC Barcelona Supercomputing Center   LEONARDO   iit

Projects

CRC1333

Our network

CECAM Node Soft Matter and Statistical Mechanics (SMSM)
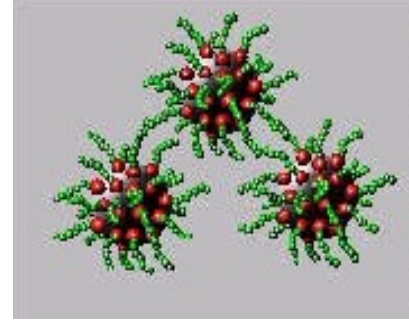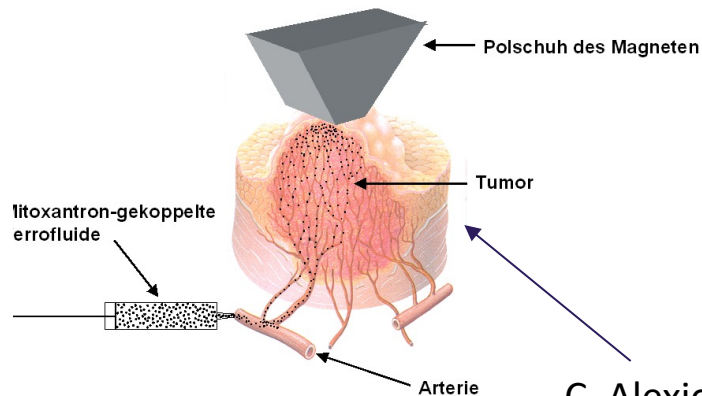
Magnetic Soft Matter

- **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)

Applications:

mechanical (*sealing of rotating shafts*);

thermal (*cooling of loud speakers*);

medical (*cancer treatment, hyper-*

*thermia, magnetic cell separation*)

Prinzip der lokalen Chemotherapie mit
Magnetischem Drug Targeting

Polschuh des Magneten

Tumor

litoxantron-gekoppelte
errofluide

Arterie

C. Alexiou (HNO- Klinikum Erlangen)
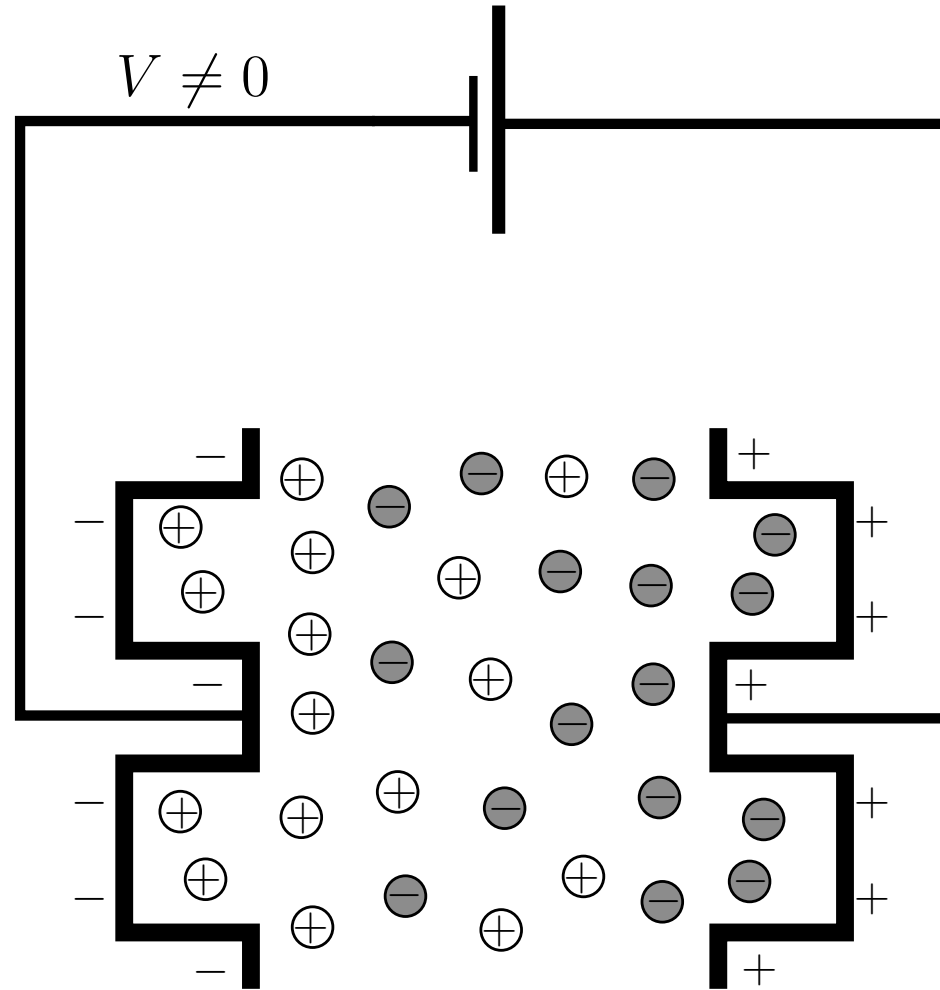
Ferrofluids can be influenced via magnetic fields

Structure Formation in Ferrofluids

Supercaps

What is a Supercapacitor

$$V = 0$$

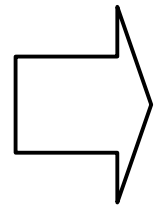# What is a Supercapacitor

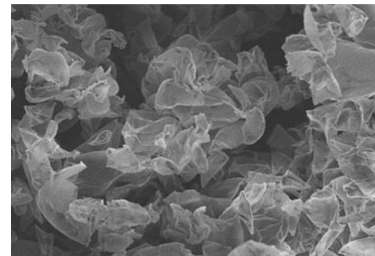$V \neq 0$
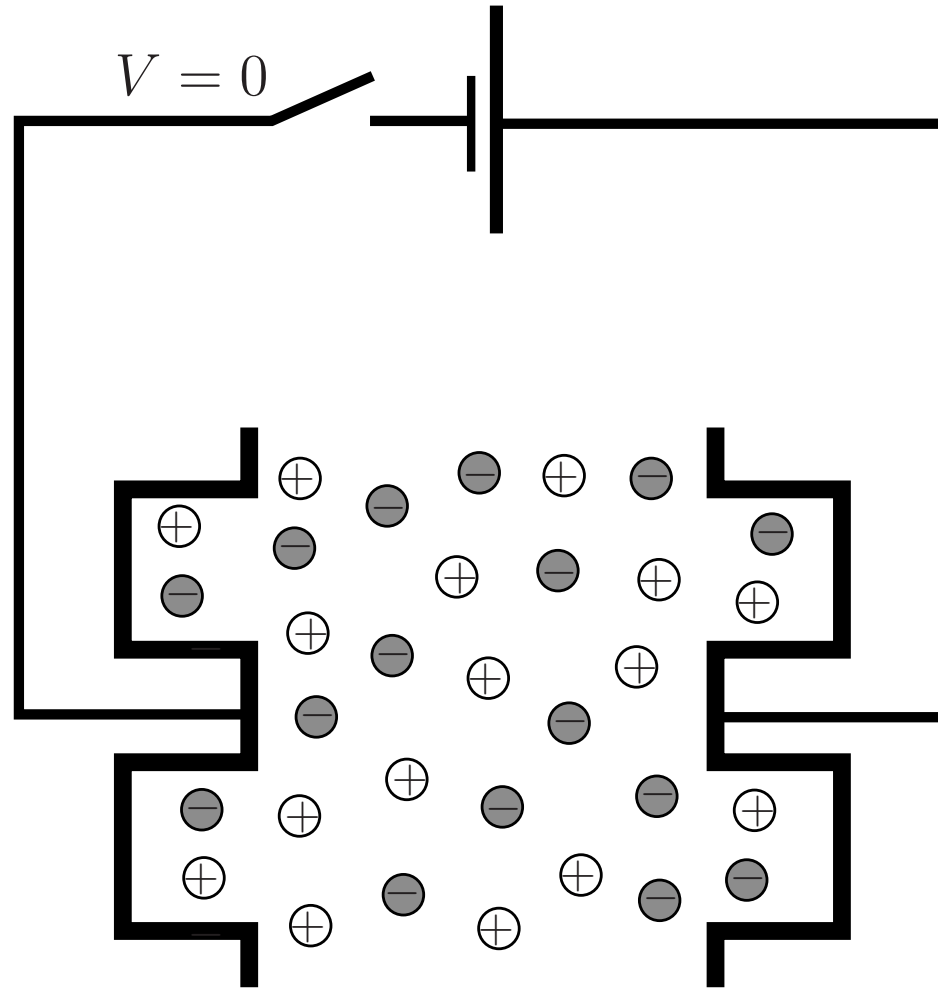
What is a Supercapacitor
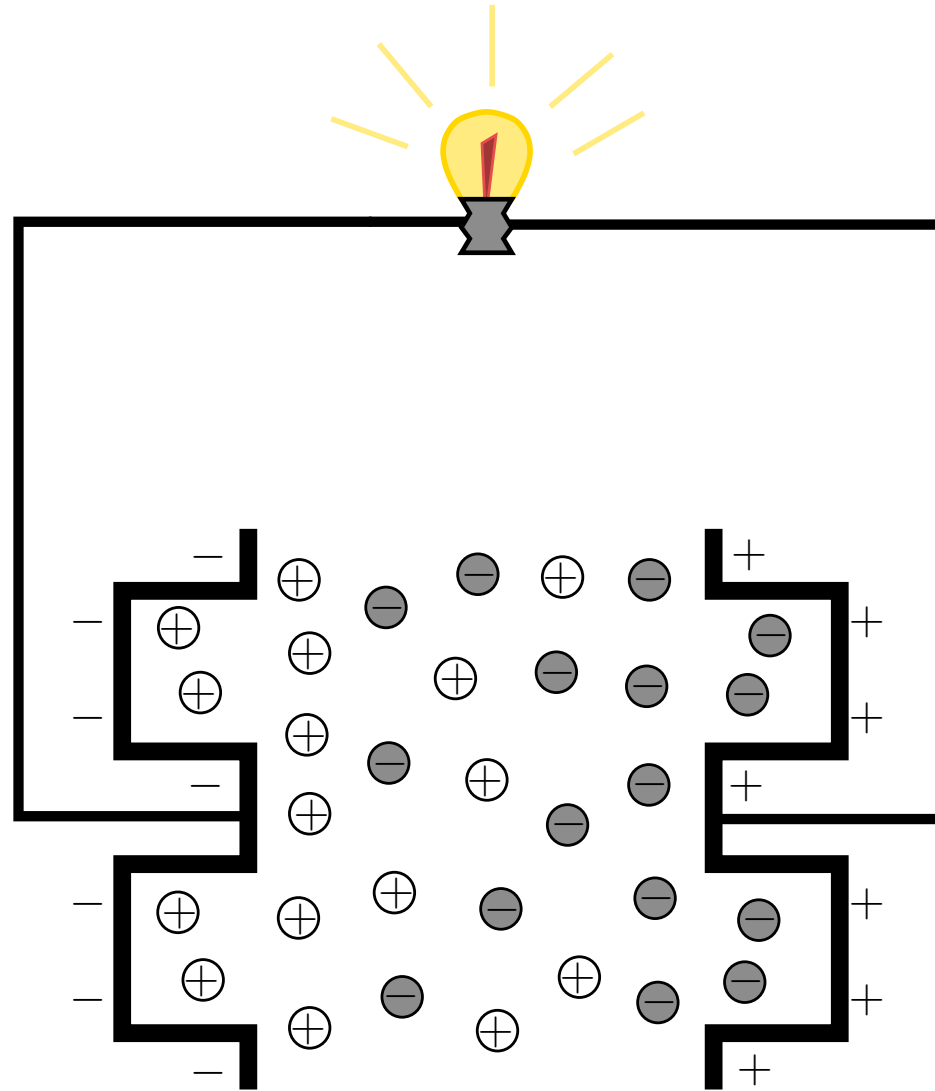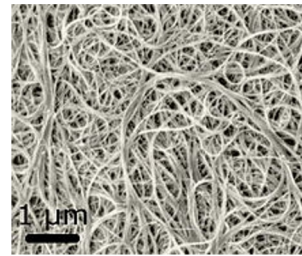
Application to Supercapacitors.....

Supercapacitors are used for mobile energy storage in Electric Double Layer Capacitors / "Supercapacitors" with high specific capacitance. "Fast and Furious??"
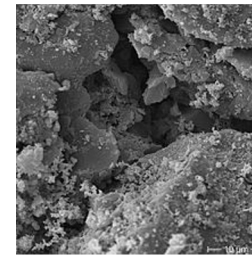
High surface area electrode material (>1000 m^2/g)

https://en.wikipedia.org/wiki/Activated_carbon
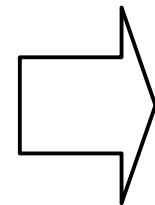
Curved graphene sheets
Liu et al., Nano Lett. (2010)

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

Activated carbon

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

Our Goal

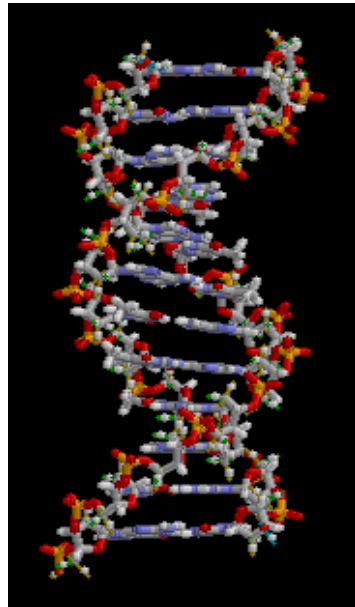Understand charging mechanisms and ion dynamics in narrow charged pores for simple model systems
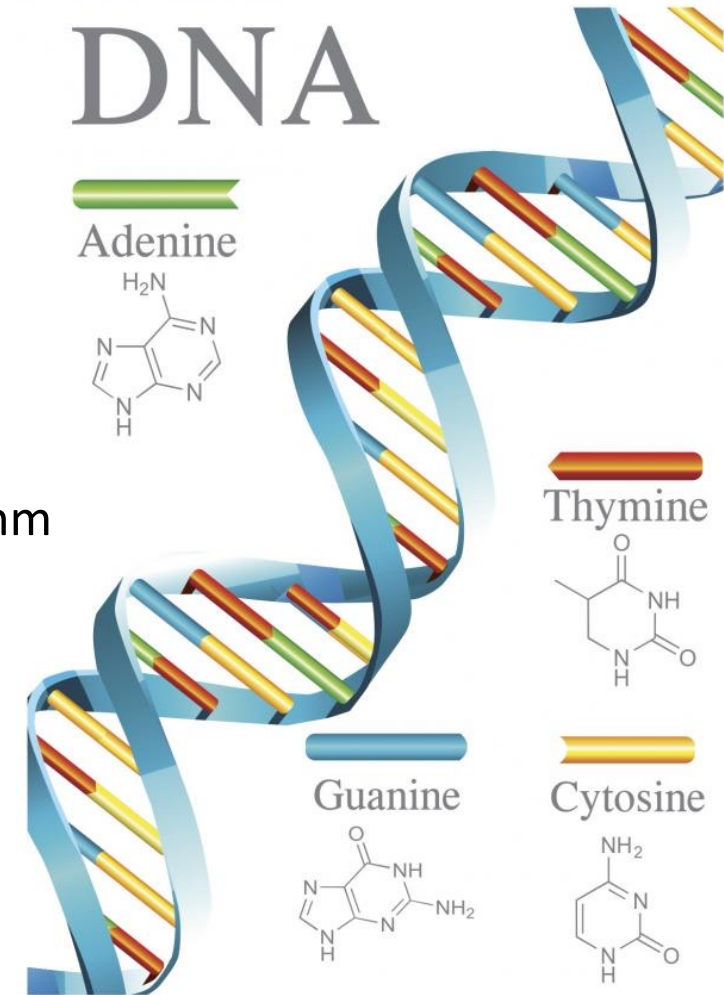
Nanopore Sequencing

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
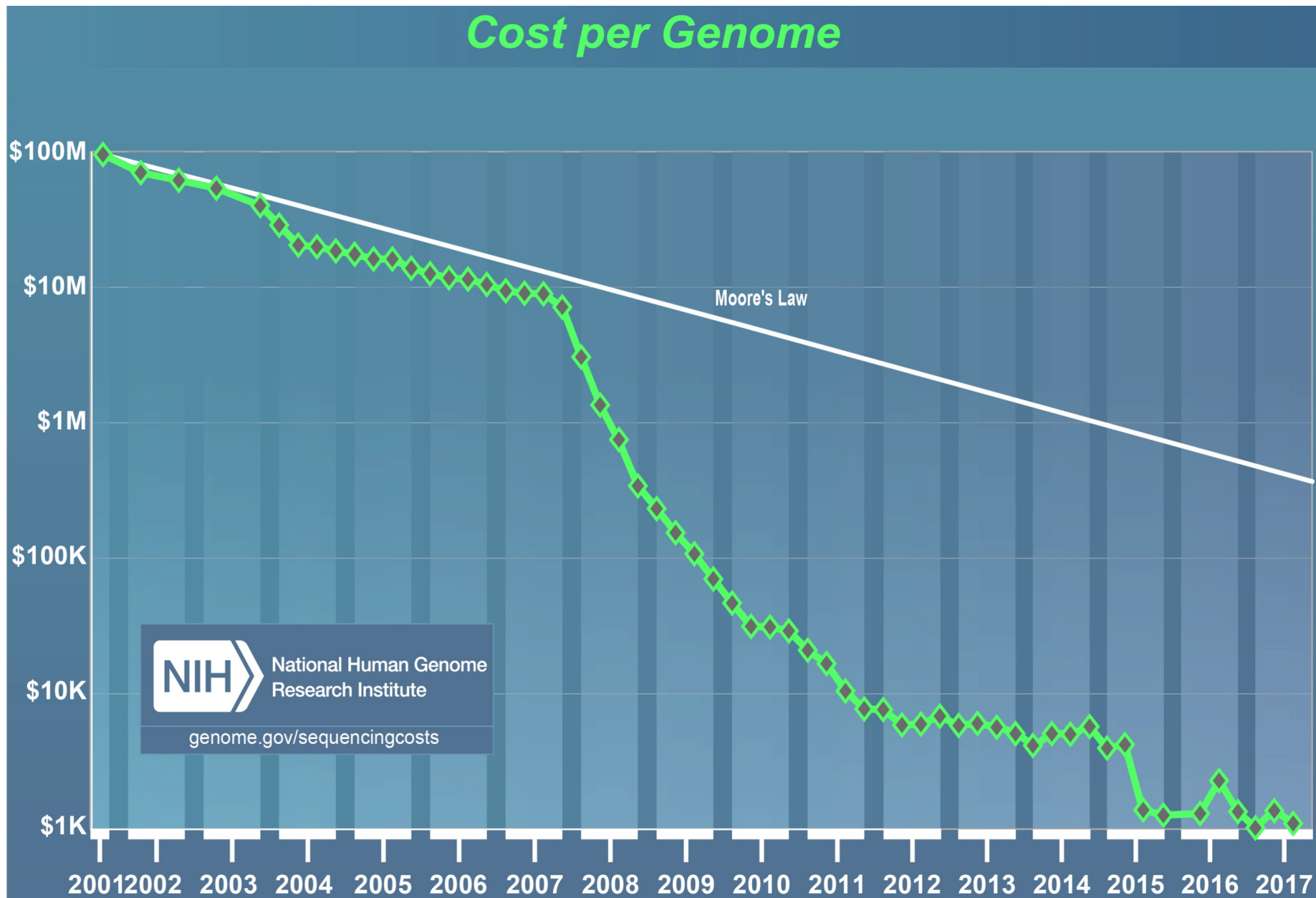
Nanopore Sequencing Approach

- acts like a more refined Coulter counter for blood cells

Deamer D W and Akeson, Tibtech (18) 147-50, 2000

Electric Field
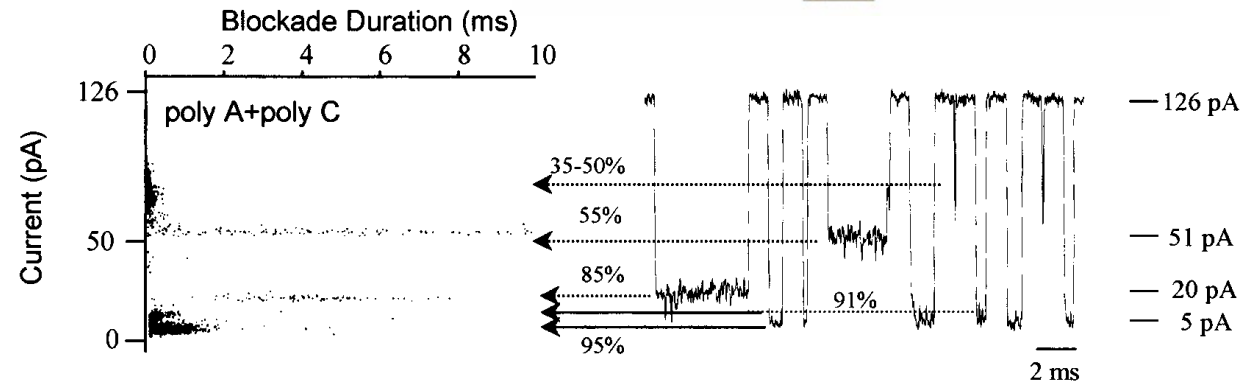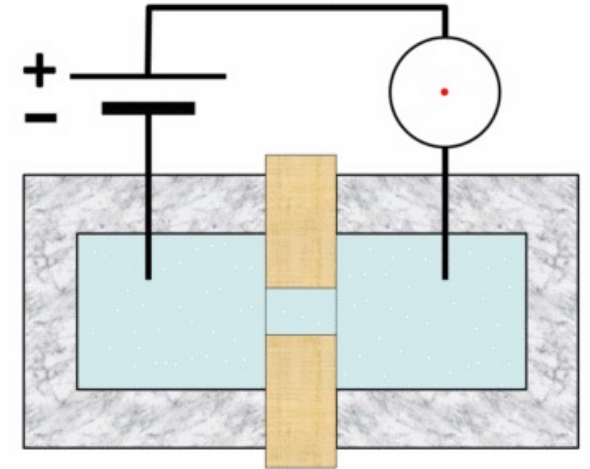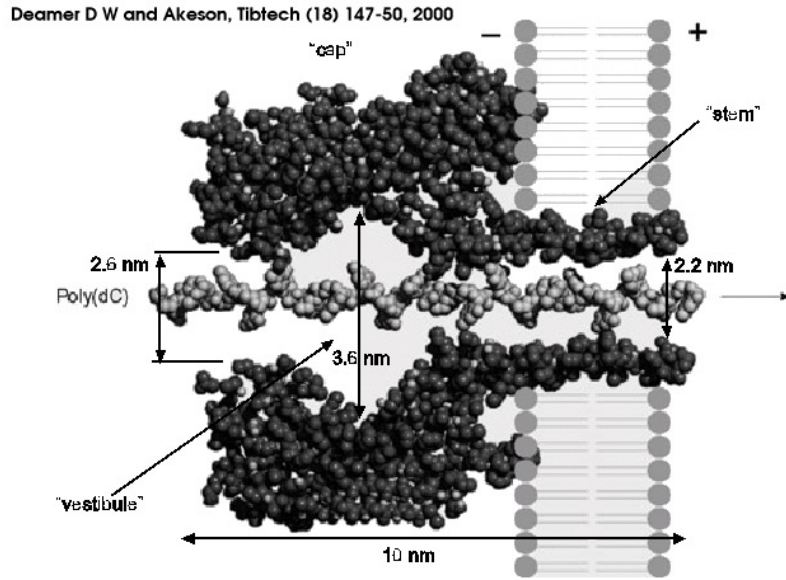
Electric Current

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

Oxford Nanopore Technologies and others
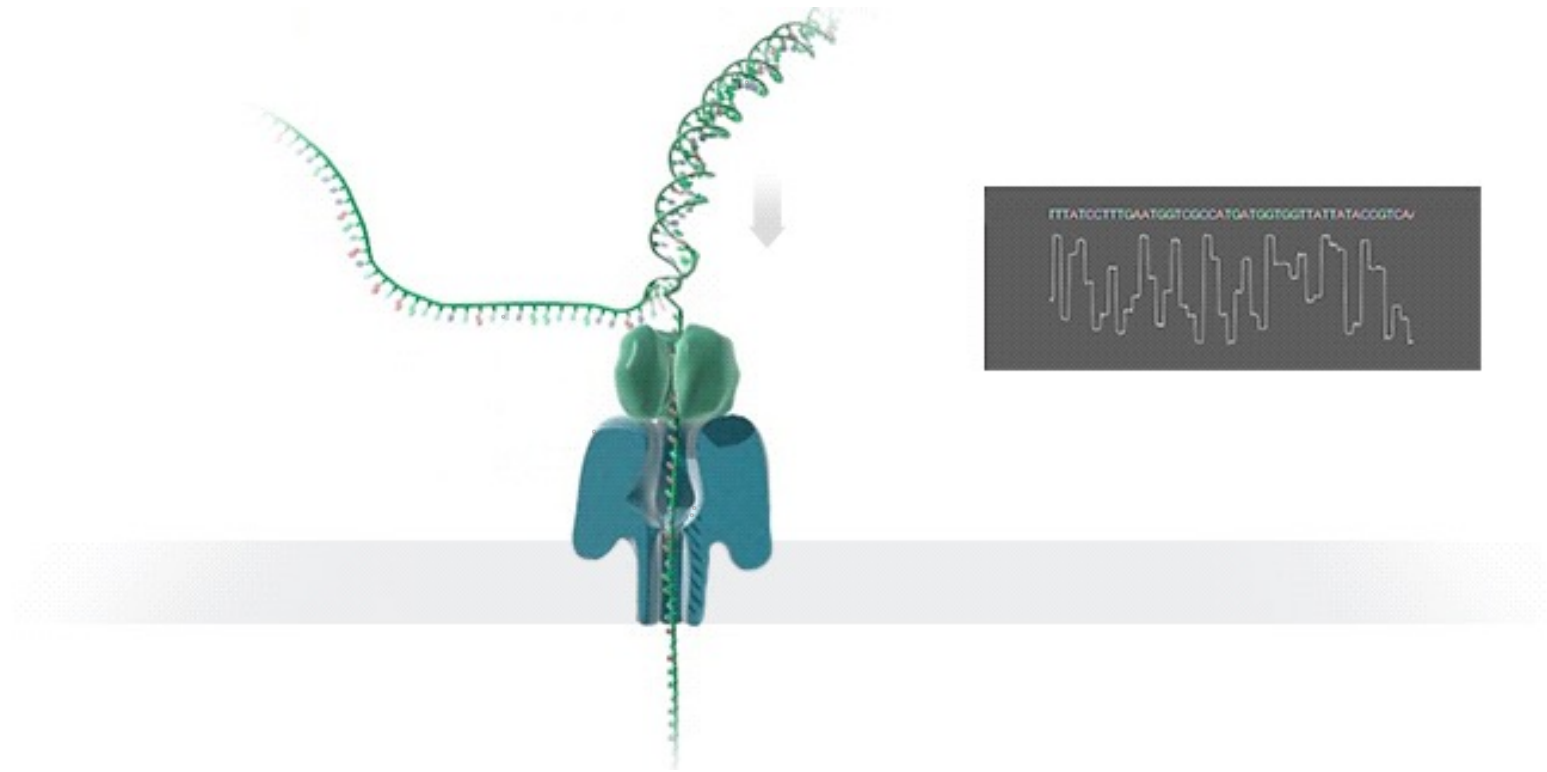
Sequencing devices on nanopore technology exists since 2016!

https://nanoporetech.com

Many efforts under way to reduce the fault rate

Multi-Scale Modelling

Time scale

Example:
DNA within a nano pore

Mesoscopical
(Finite-element)

coarse-grained

atomistic

min

s

μs

ns

ps

Å   nm μm   m   Length scale
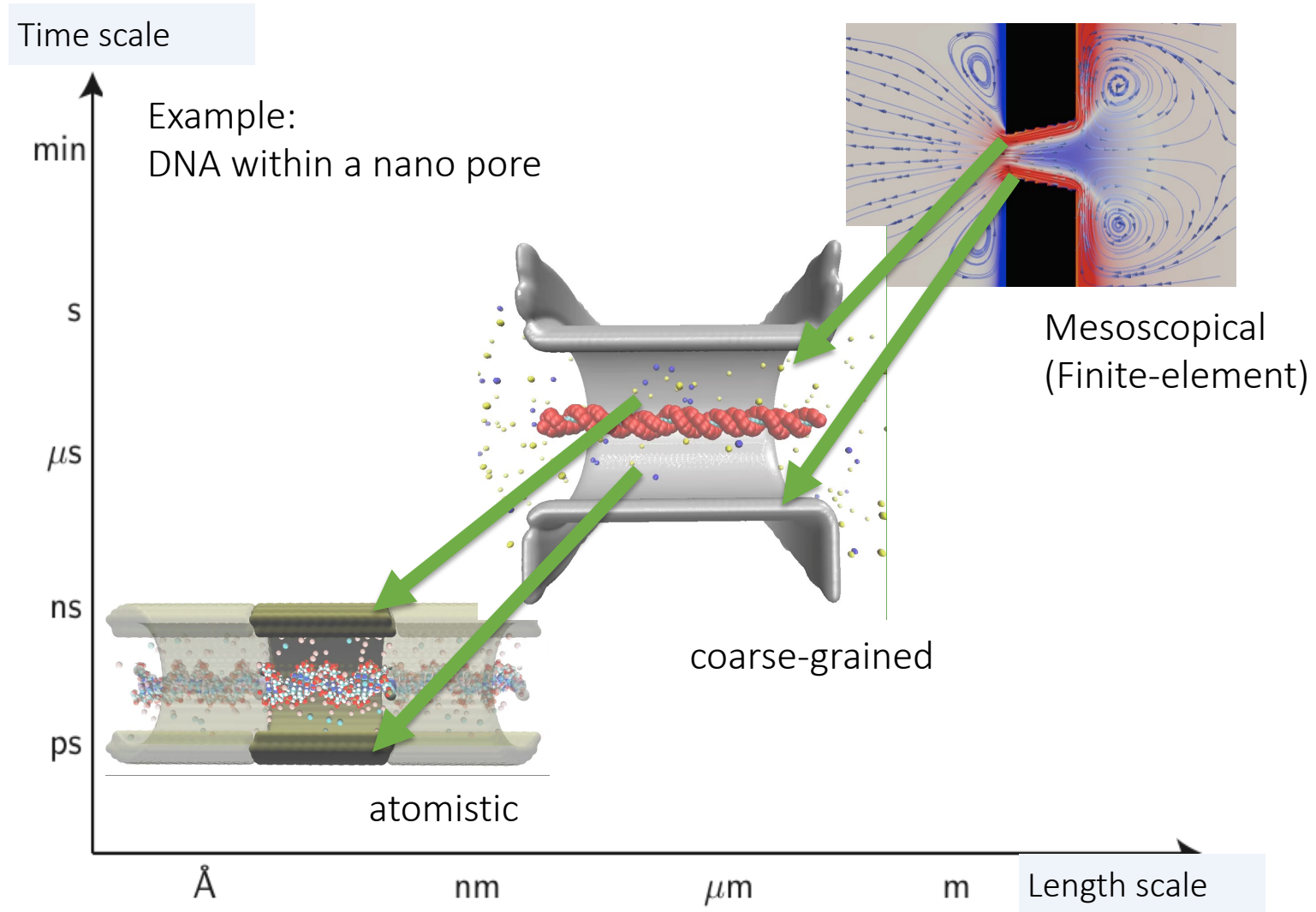
Investigations via AA Simulations
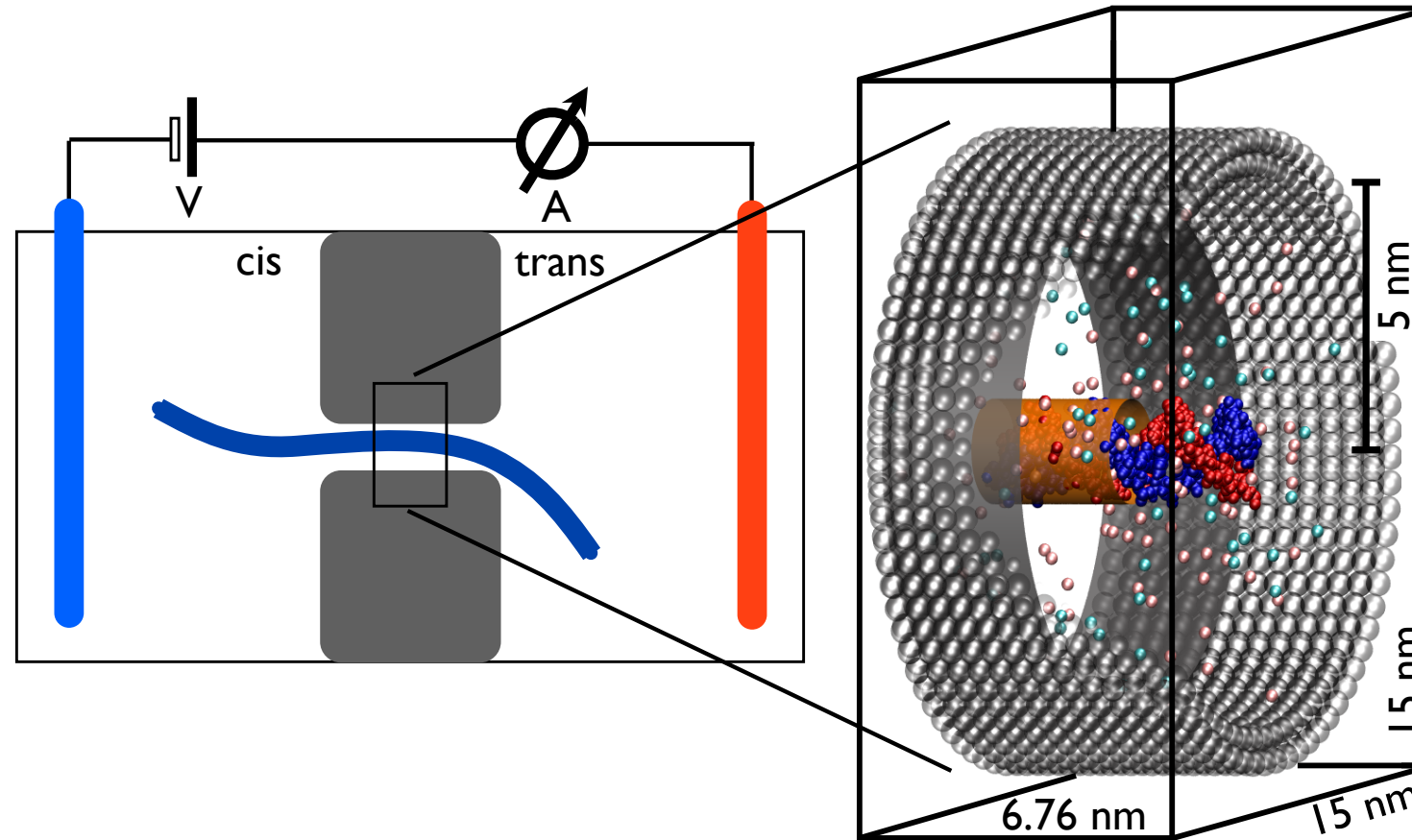
Force Field: AMBER03, Water: SPC/E
double-stranded DNA closed over PBC,consisting of 20 GC bps, P-Atoms fixed in space,
generic pore atoms
Electric field 0.2 V/nm applied along pore

Results from AA Simulations
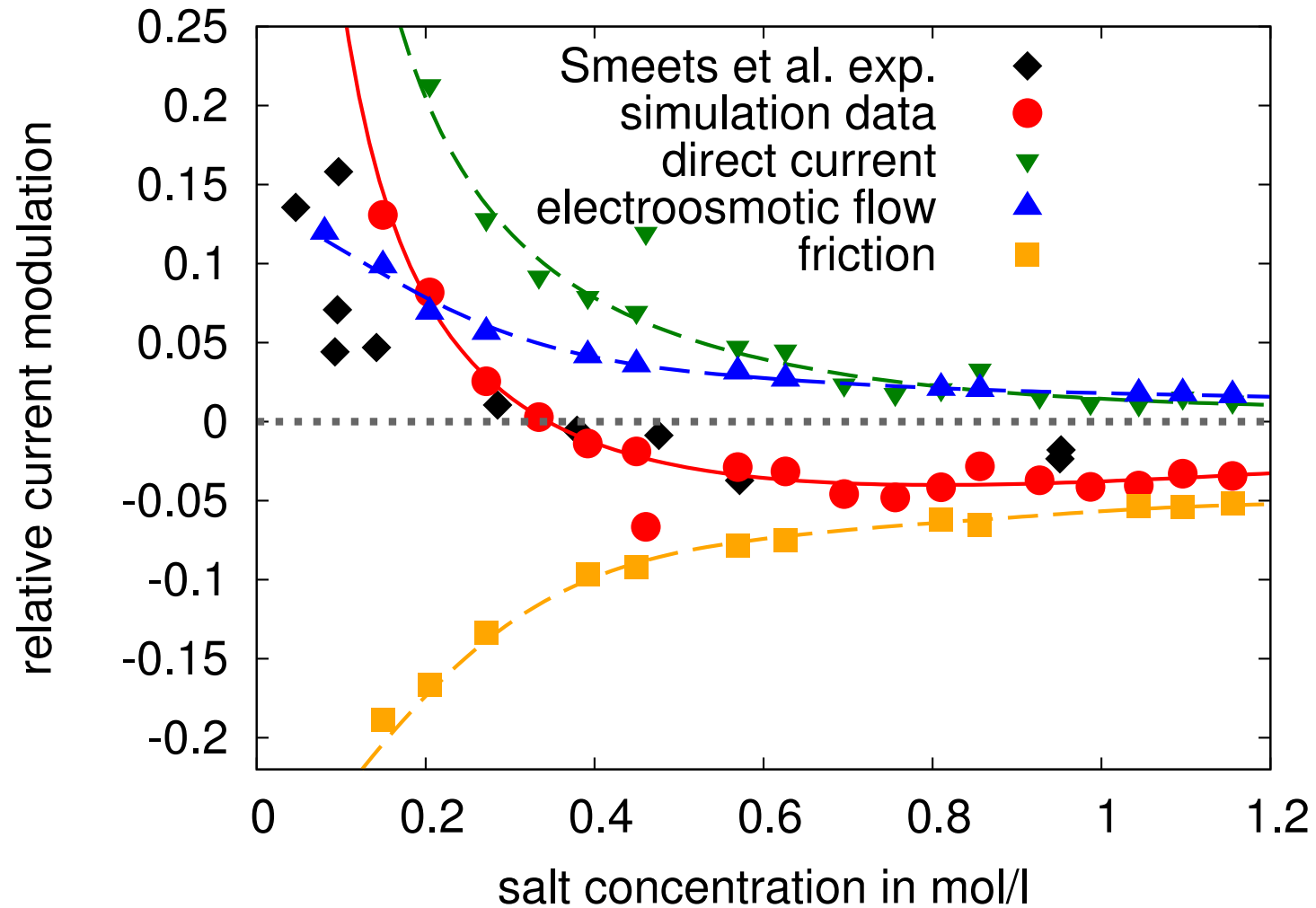
Direct current always larger with DNA inside, no blockage!

Kesselheim, Müller, Holm, *Phys. Rev. Lett.* **112,** 018101 (2014)

Ions and dsDNA in Pore- Iso-density Surfaces
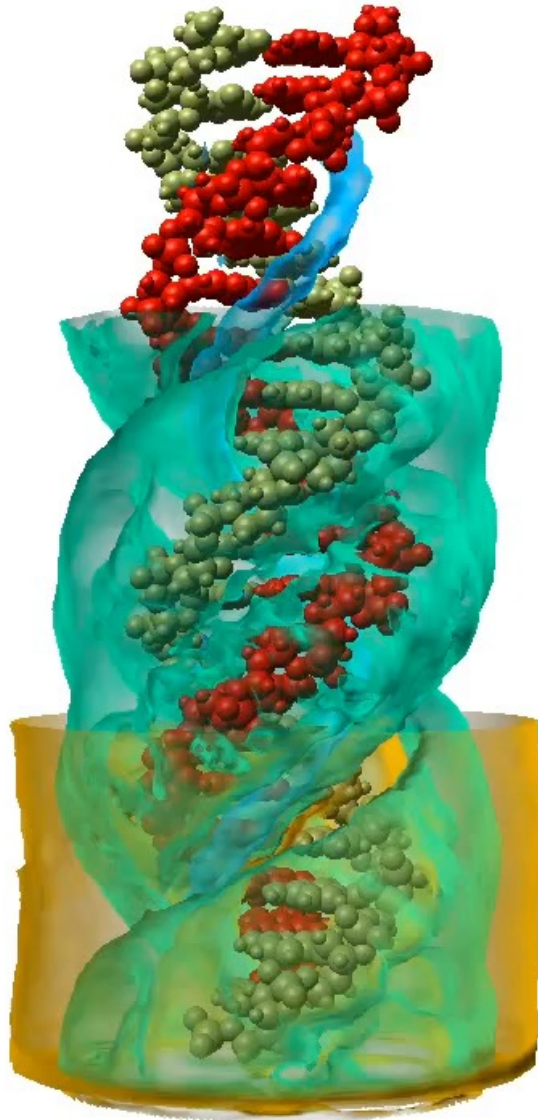
Poly-CG-DNA
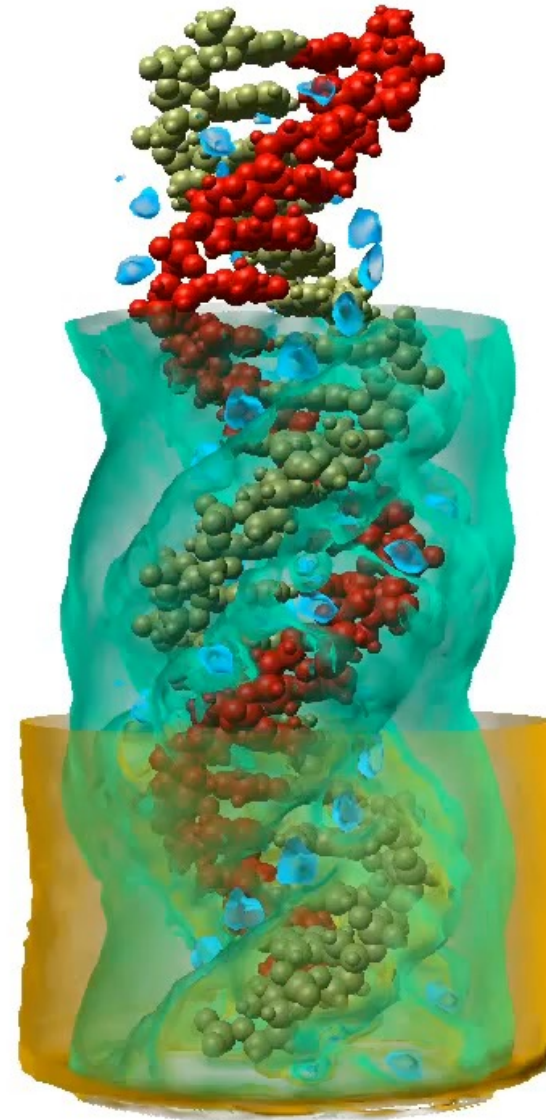
Poly-AT-DNA

ML Approaches for optimizing Nanopores

■ acts like a more refined Coulter counter for blood cells

FTTATCCTTTGAATGGTCGCCATGATGGTGGTTATTATACCGTCAI

stovey@icp.uni-stuttgart.de

holm@icp

Oxford Nanopores https://nanoporetech.com
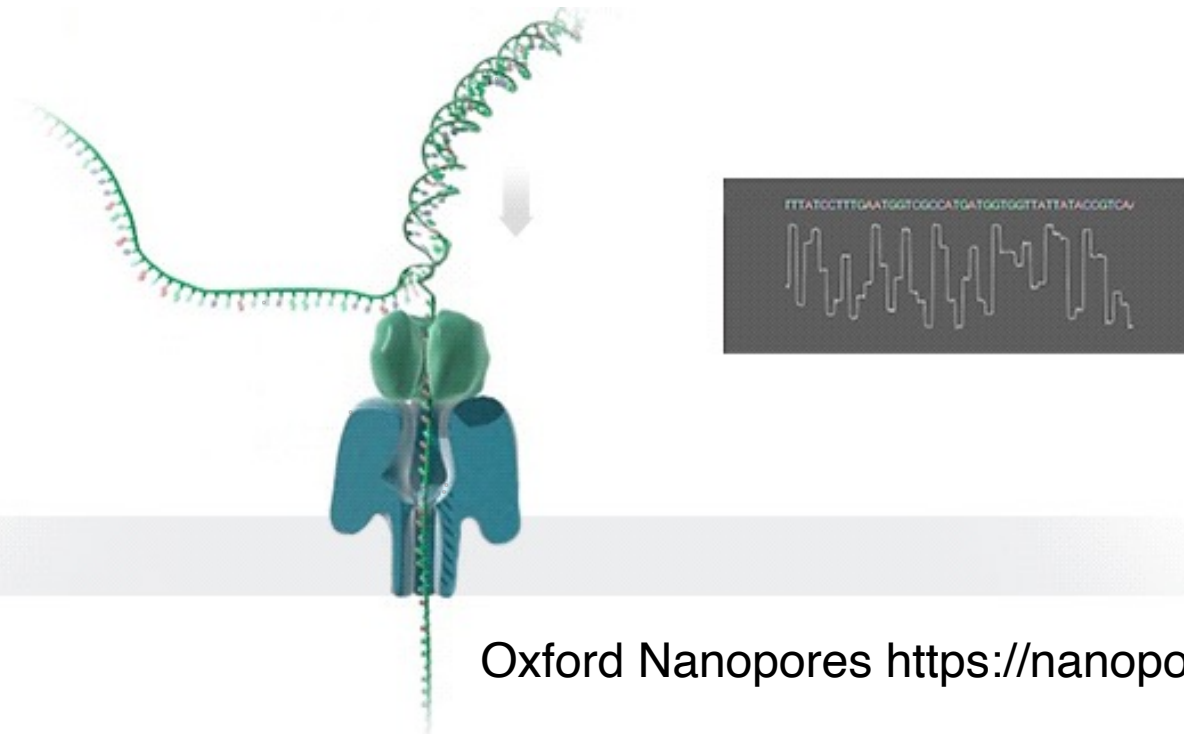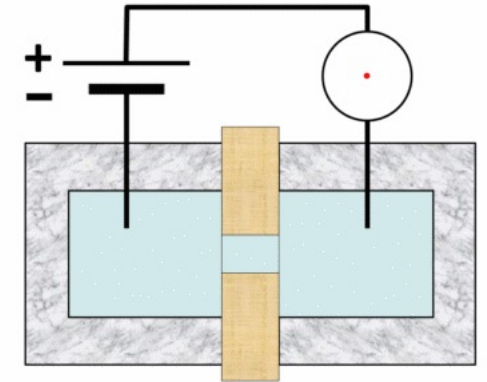
■ Use ML approaches to optimize the current readout to recognize protein sequences from real experimental data provided by collaborators from Freiburg using a different biological nanopore (Aerolysine)
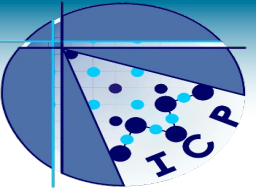
Multiple scales of materials modelling
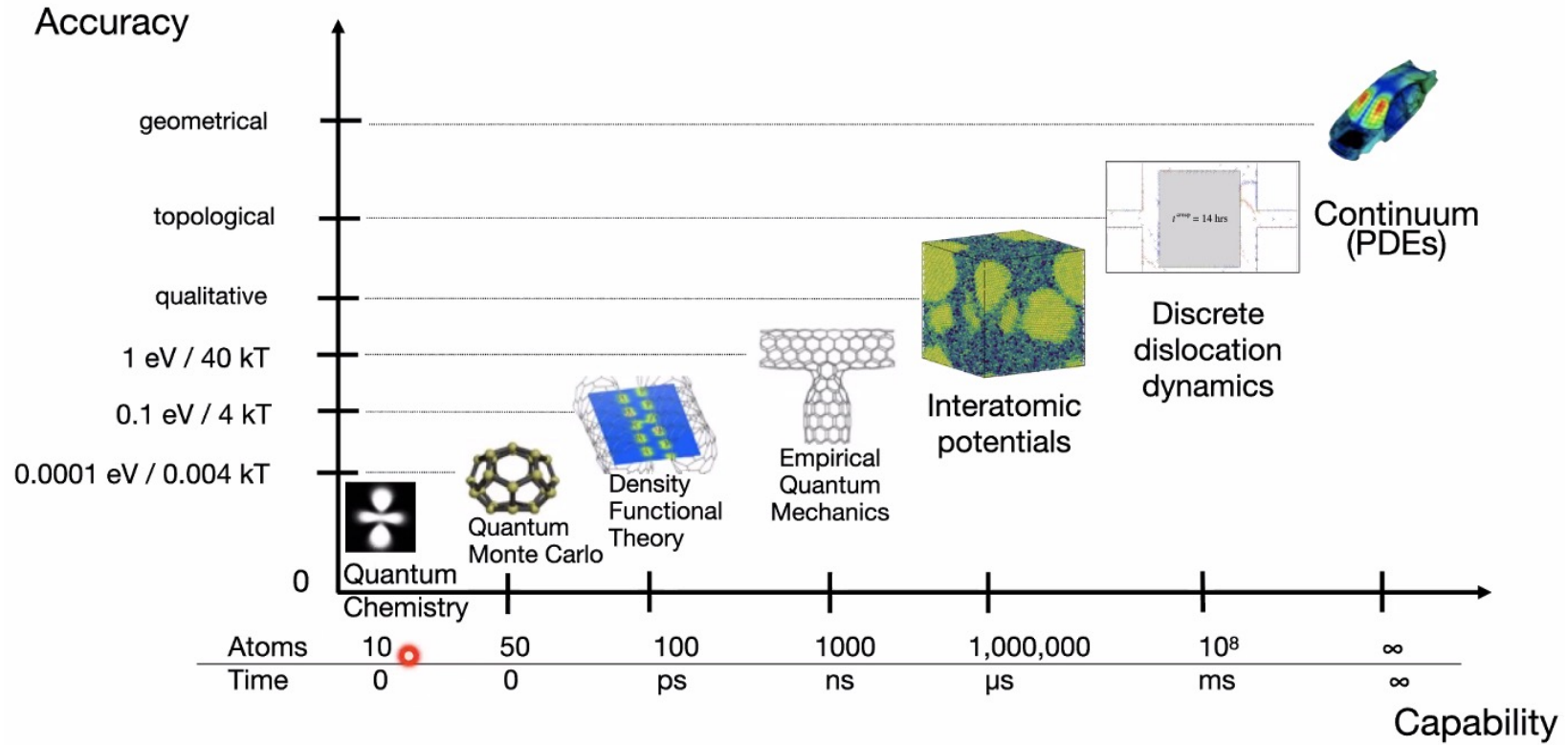
Multiple scales of materials modelling
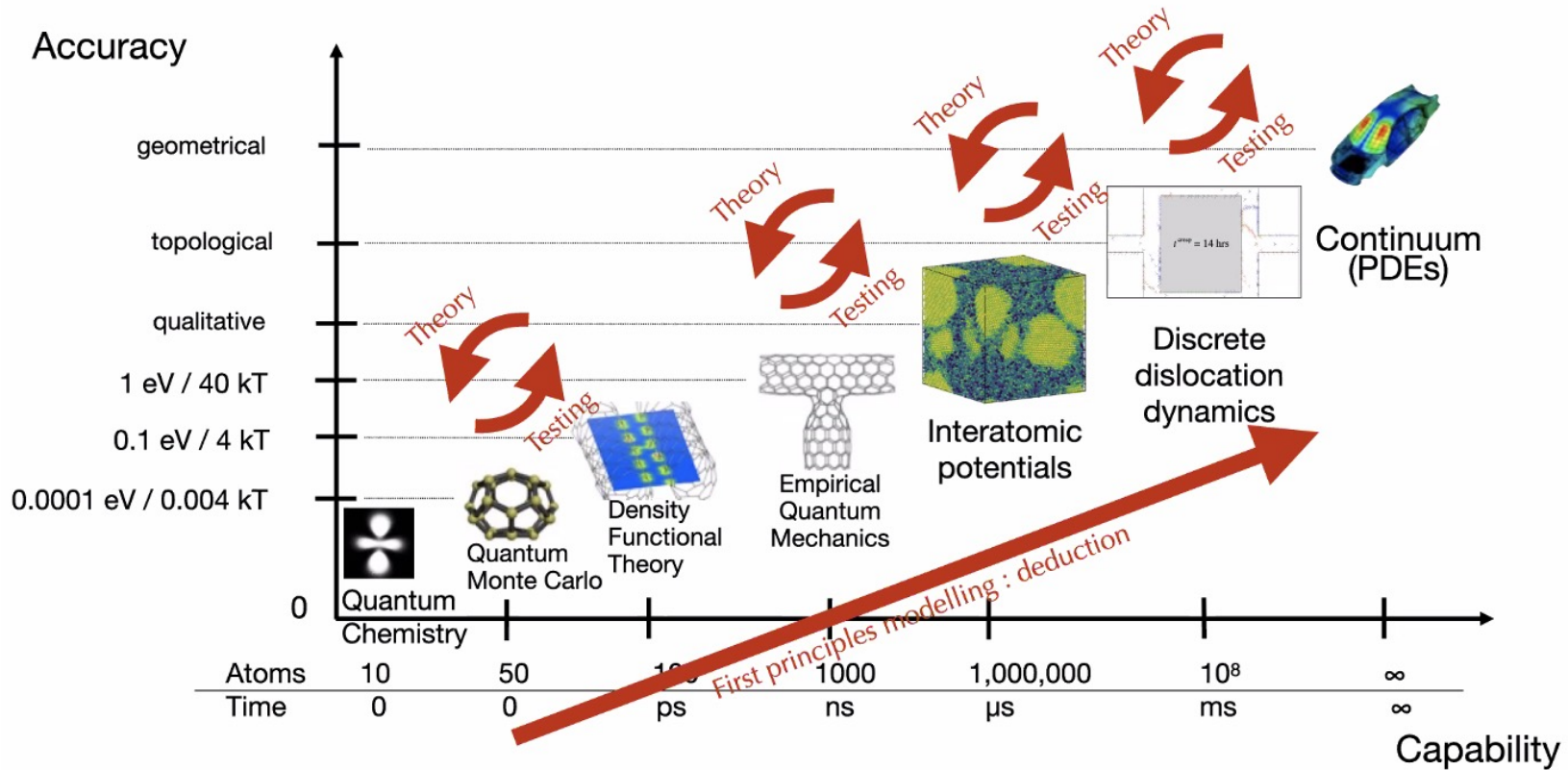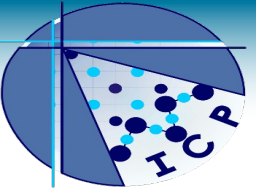
Multiple scales of materials modelling
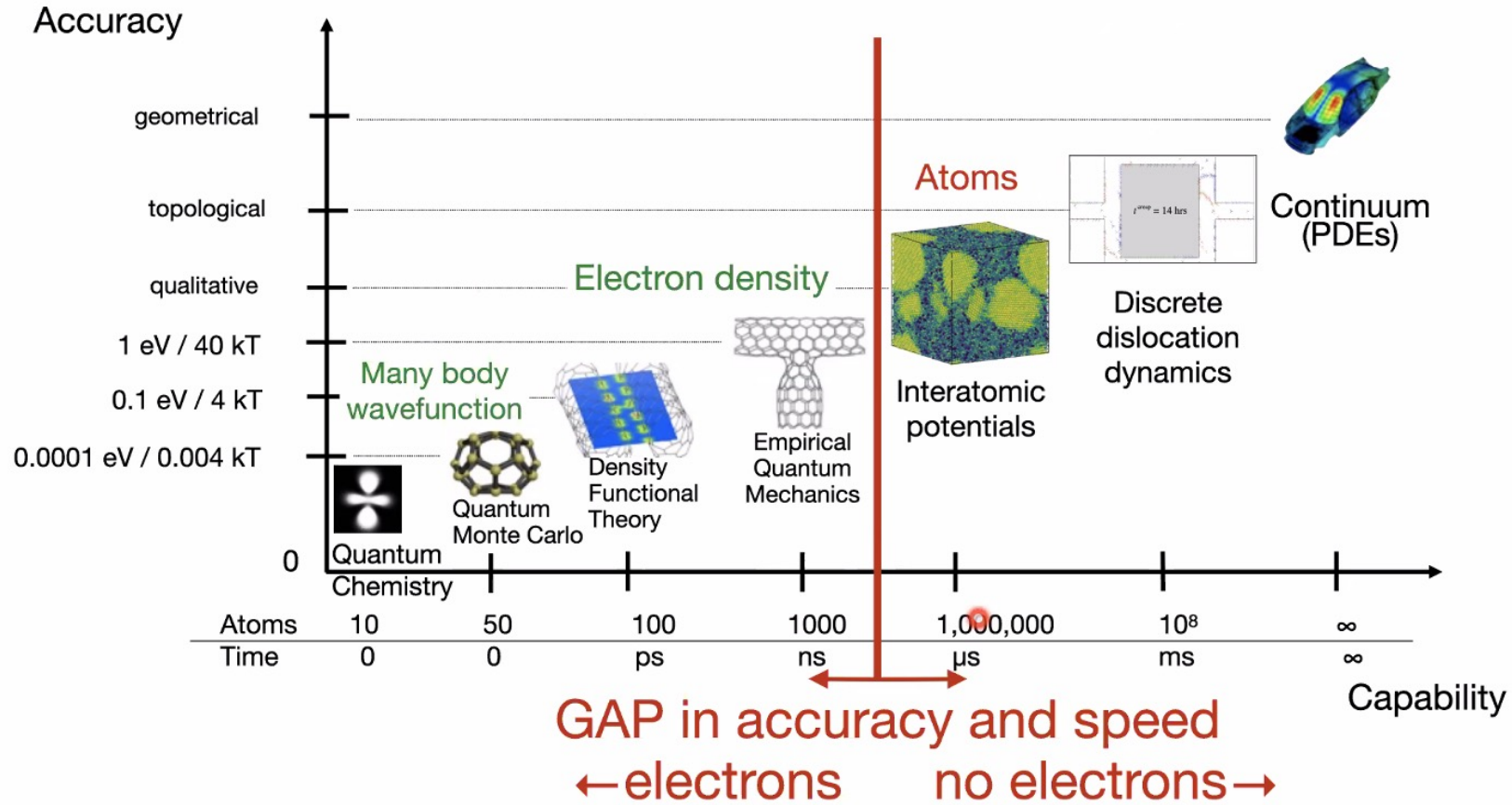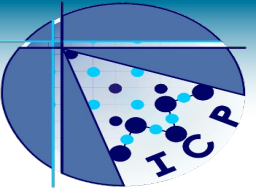
Multiple scales of materials modelling
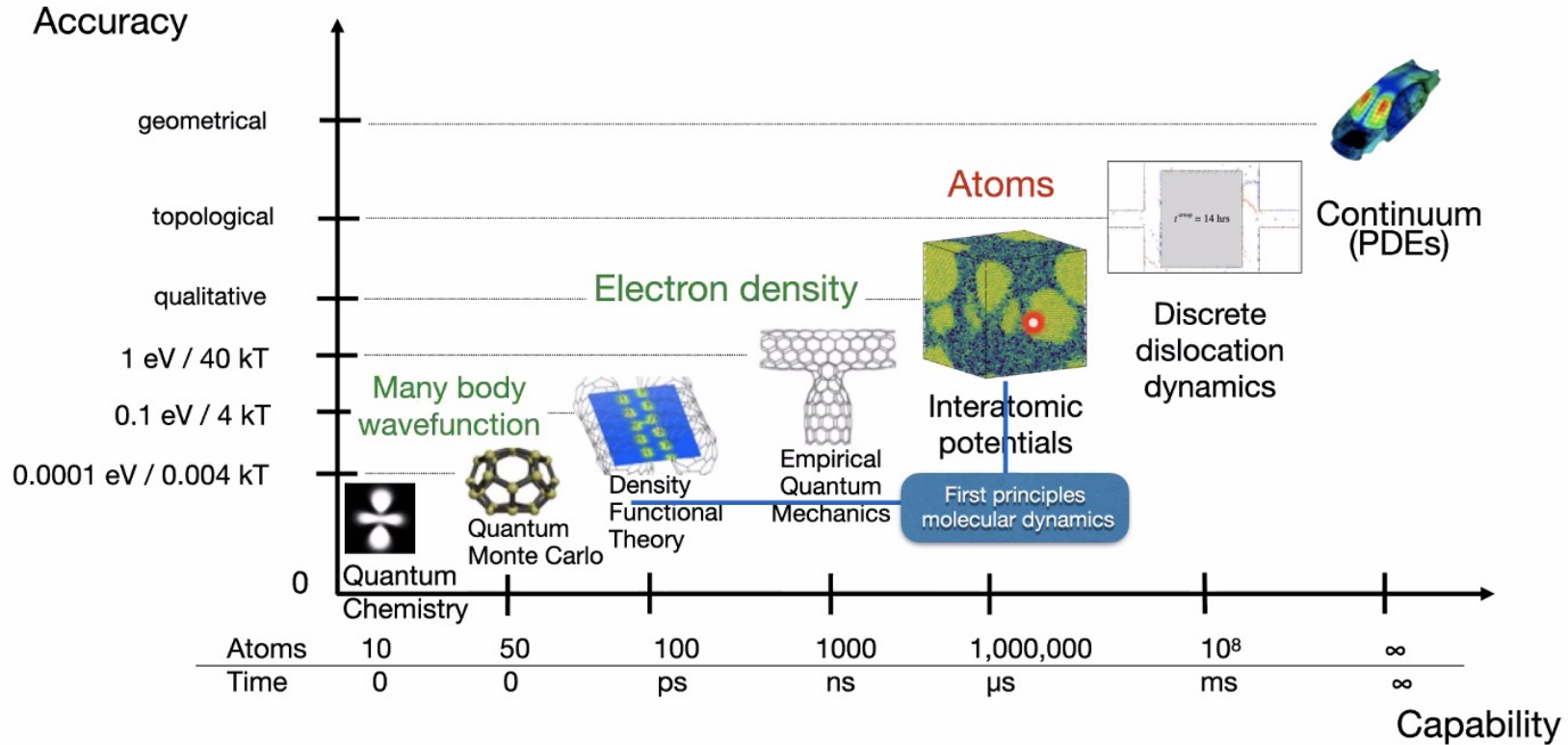
Machine learned interatomic potentials from ab-initio input (often DFT)

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…
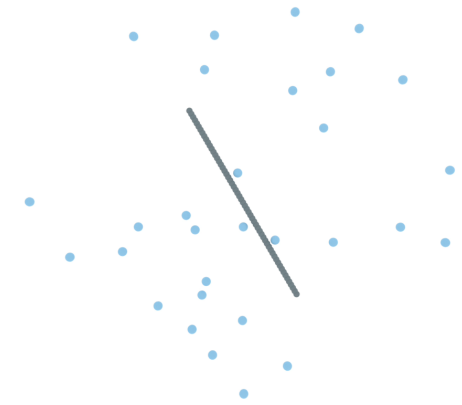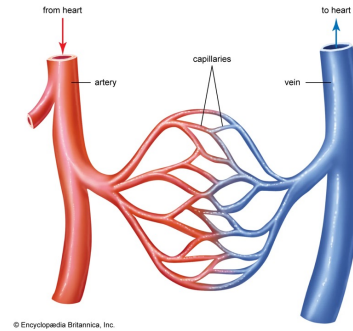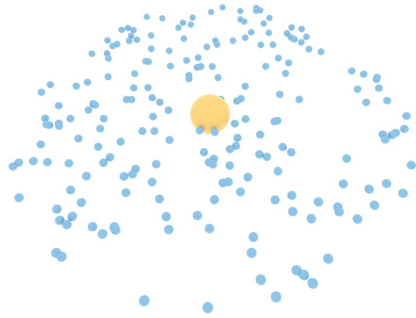
Medicinal Micro Robotics

- Implement RL training in real medical environments

- Simulation capillary blocking/clearing

- Run flow simulations using lattice-boltzmann

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

- Use Phi-2 language model to guide RL agents.

- Contribute to SwarmRL software.

- Deploy models on GPU infrastructure.

Language Models and Reinforcement Learning

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

Coarse-Graining with Hypergraphs

- Implement new ML architecture.

- Train potentials from DFT to Coarse-grained.

- Run large-scale simulations.

Samuel Tovey, samuel.tovey@icp.uni-stuttgart.de
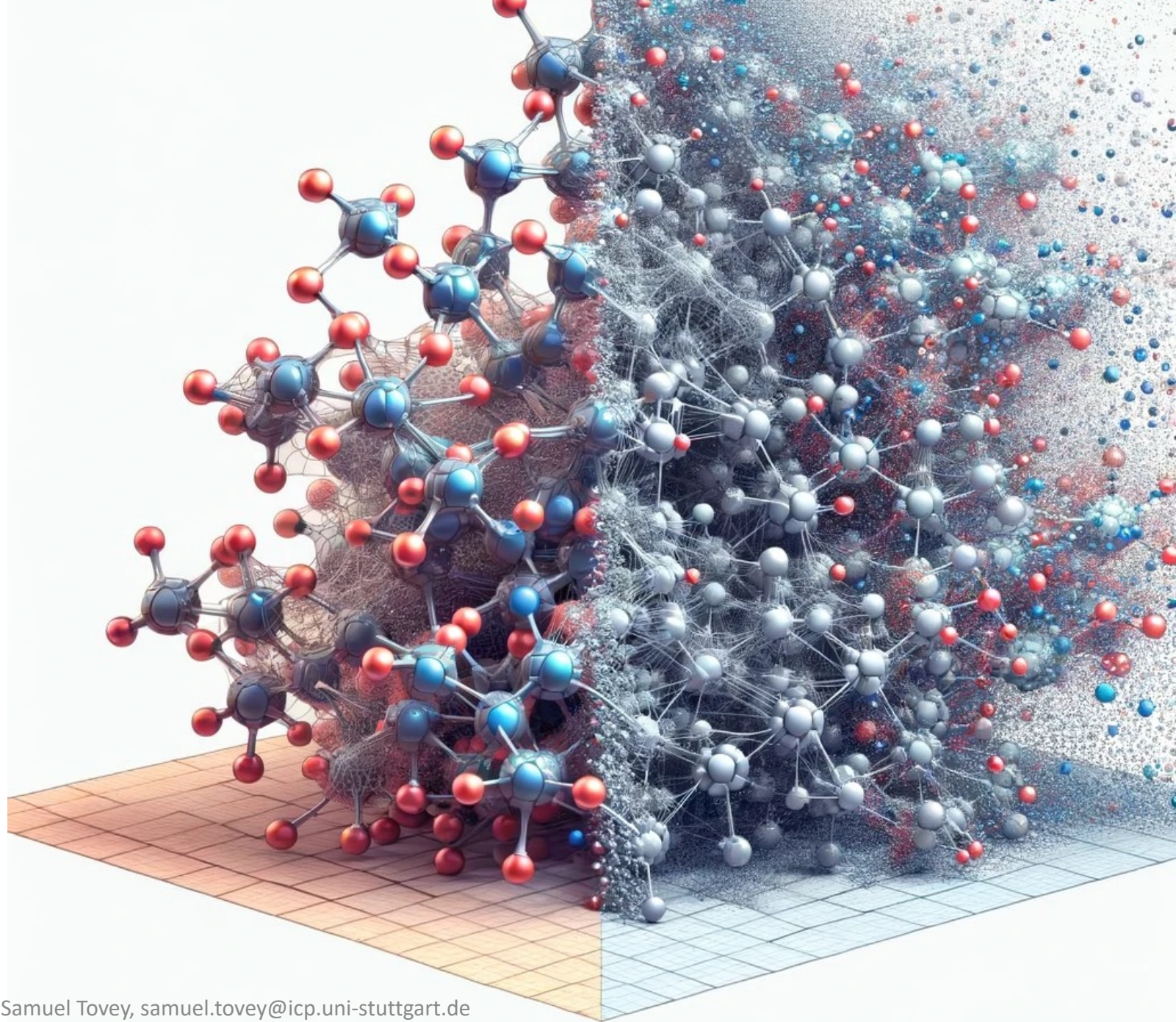
- Identify physics solutions in constrained neural networks (Occams razer).

- Investigate the role of local properties in potential fitting.

- Explore a vast range of neural network architectures.

Finding Physics in Neural Networks

Samuel Tovey, samuel.tovey@icp.uni-stuttgart.de
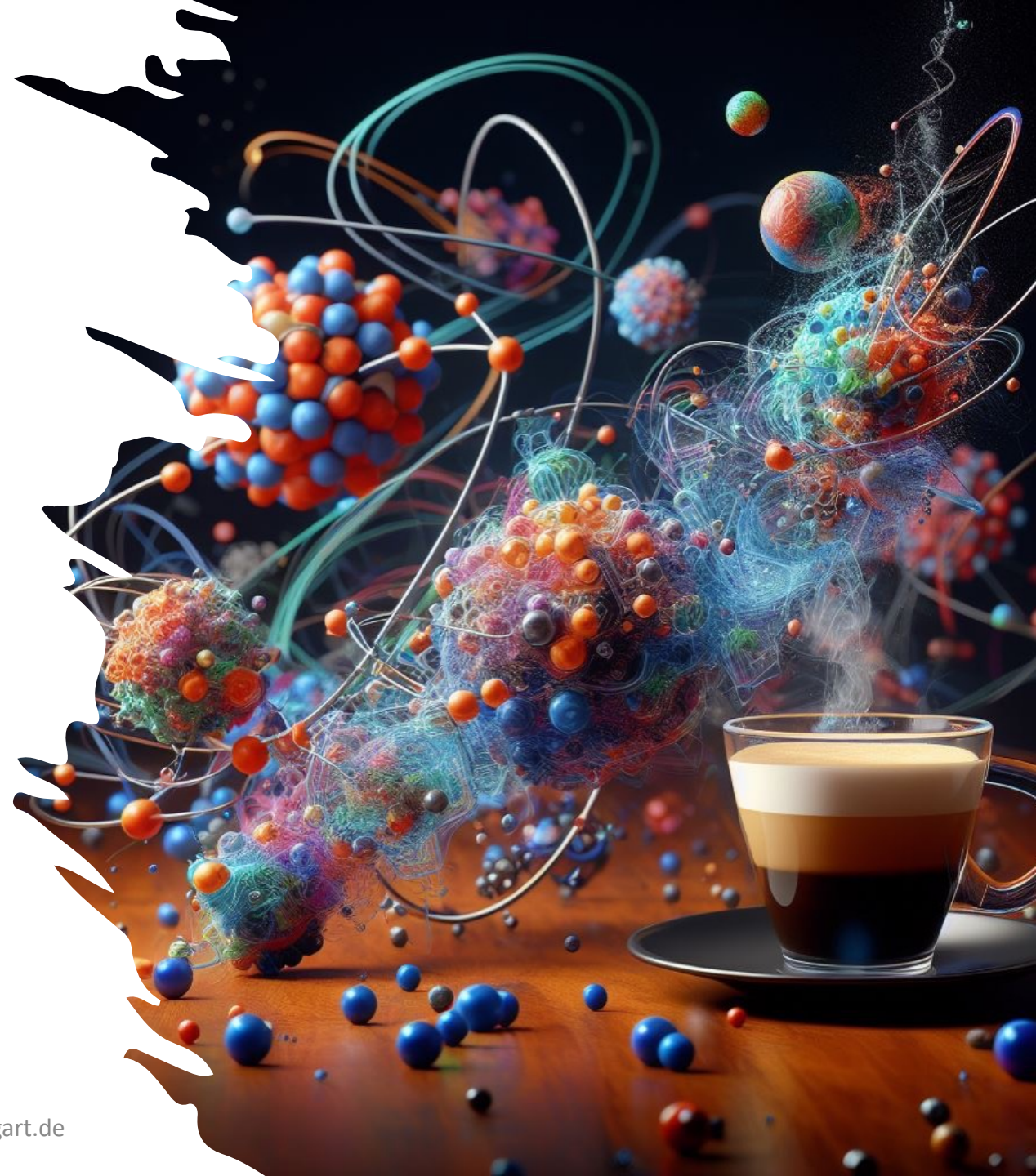
- On-line protein prediction for cancer diagnosis

- Utilize state-of-the-art time series transformers

- Deploy on data-sets in the millions

Signal Classification with Transformers

Samuel Tovey, samuel.tovey@icp.uni-stuttgart.de
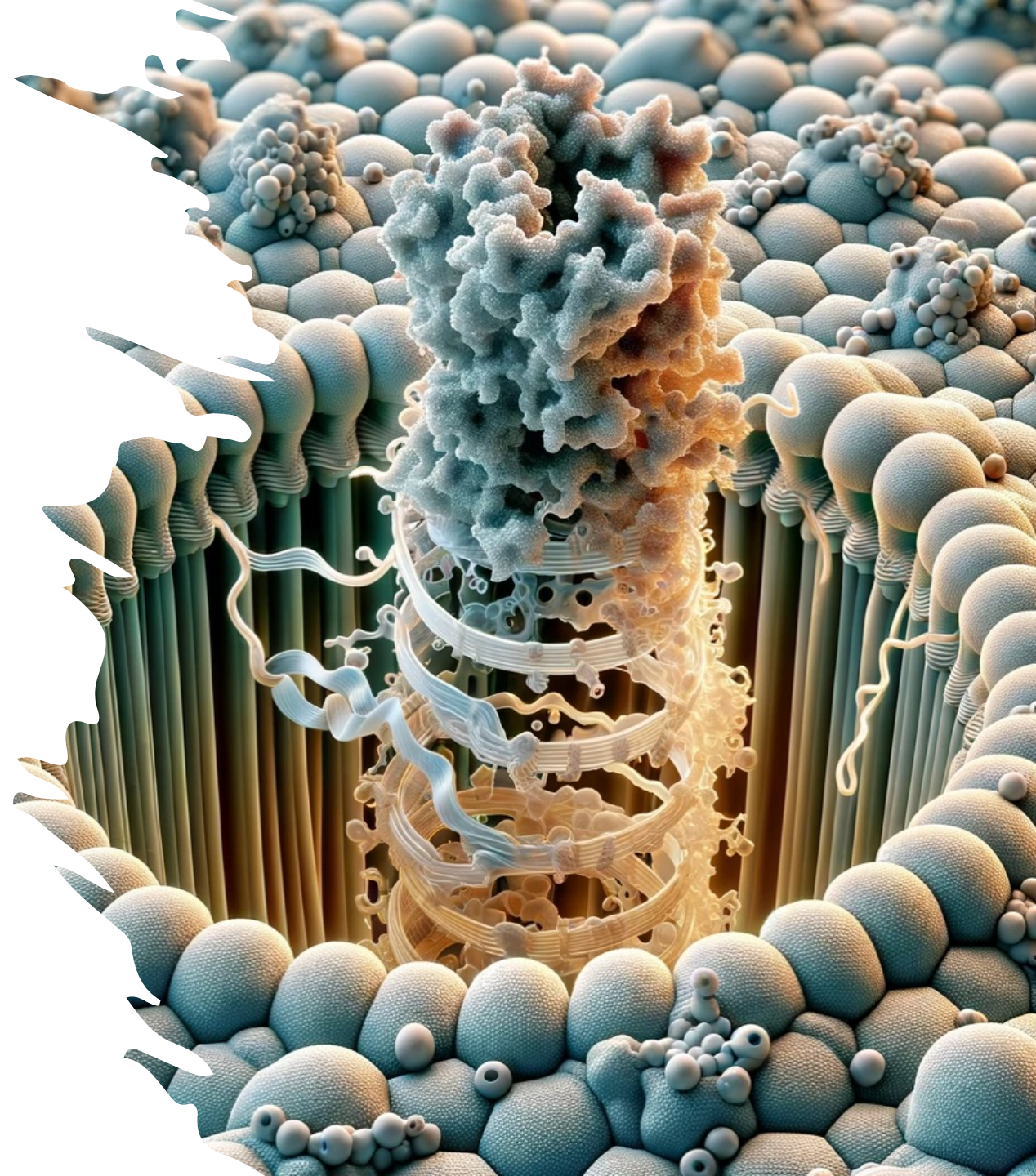
How do Neural Networks Learn ?

→ Study Learning with Collective Variables
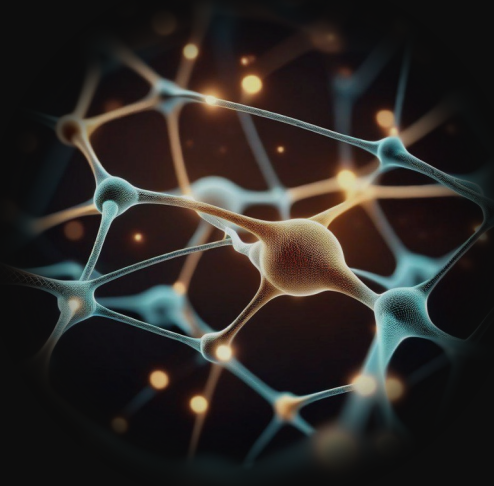
knikolaou@icp.uni-stuttgart.de

Your job is

- Analytically investigate learning behavior of linear models.
- Numerically compare linear vs. non-linear neural networks

Analytical ▬ 20

Numerical ▬▬▬ 80

Requirements: Interest

Your will learn

- Use SOTA machine learning software
- Google coding standards
- Clusters and supercomputers

Machine Learned Potentials

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

- Simulate large systems with *ab initio* accuracy.

- Investigate state-of-the-art **learning on the fly** training approaches.

- Study the benefits of transfer and Δ-learning.

- Develop packages for the Machine Learned Potential workflow.

  - Room temperature Ionic Liquids
  - Water
  - System of your choice?
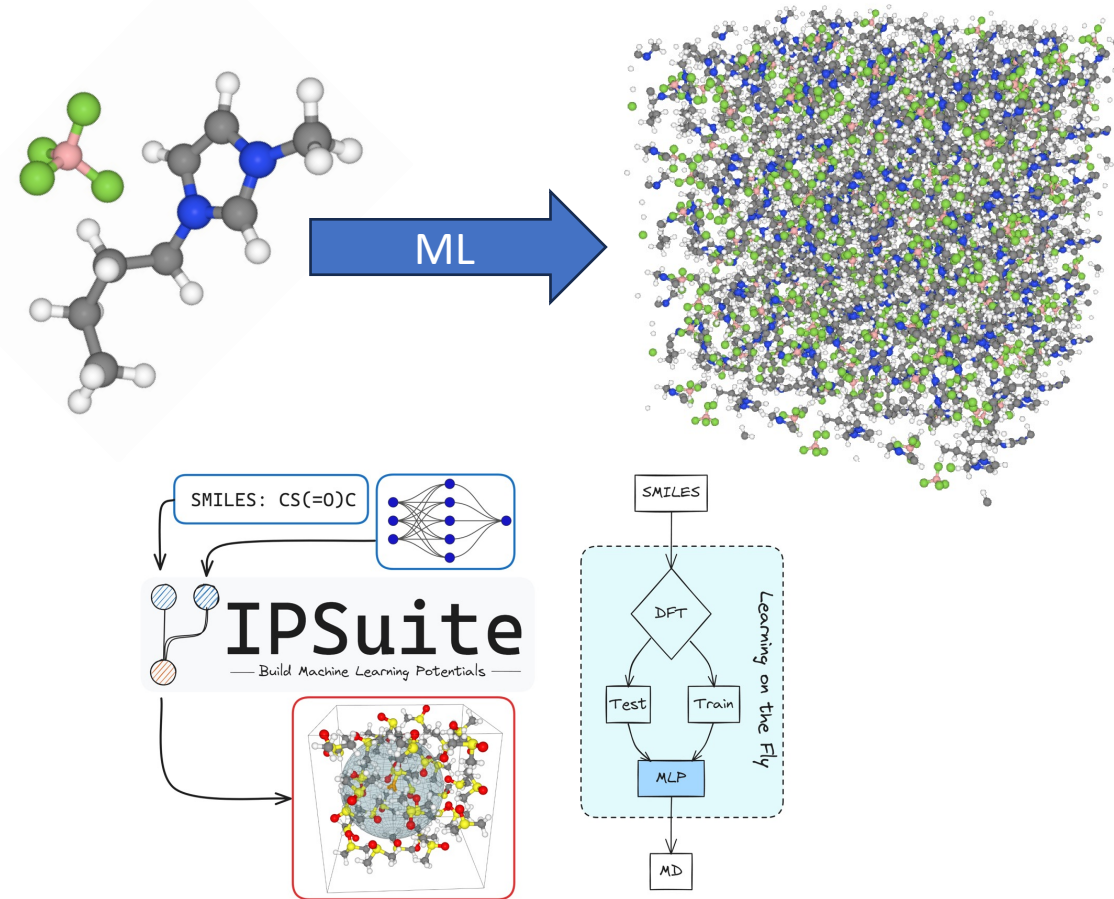
Bachelor Project: Inverse Renormalization Group using Machine Learning

- Renormalization group (RG): powerful tool to study 2nd order PT and critical phenomena

- Recent theoretical work (Bachtis et al., PRL 2022): ML can be used to invert RG flow and extract critical exponents from small-lattice simulations

- Goal of this project: investigate the asymptotic behaviour of iRG

$$L_0 \rightarrow L_1 = bL_0 \longrightarrow \cdots \longrightarrow L_j = b^{(j-i)}L_i$$
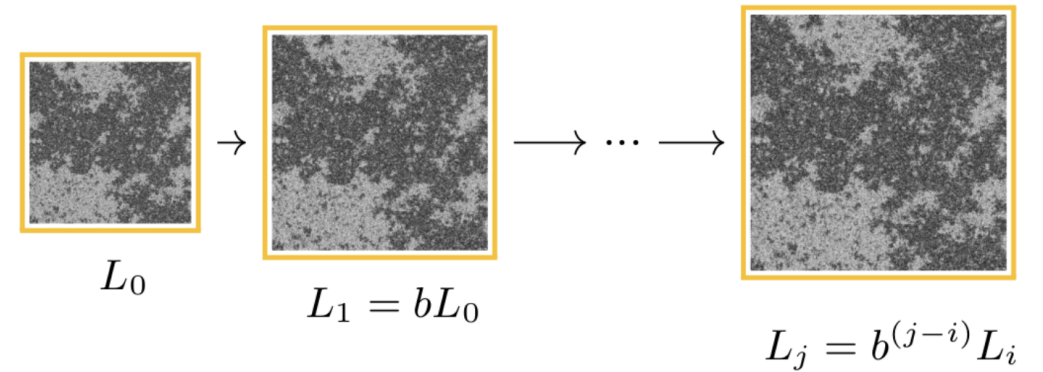
Contact:
Konstantin Nikolaou (knikolaou@icp.uni-stuttgart.de)
David Beyer (dbeyer@icp.uni-stuttgart.de)

Understanding the complexation of dendromicelles with RNA and peptides molecules

- The development of nano-carriers with programmed features is crucial when designing next-generation drug therapies.

- Dendritic micelles are promising candidates when engineering delivery carriers for RNA- and peptide-based therapeutics.

- **Bachelor/Master Project:**

  - Model complexation of linear polymeric chains with dendritic micelles via coarse-grained MD simulations.

  - Explore the effect of branching in the complexation.

Chen et al., Acc. Mater. Res. 2022, 3, 484
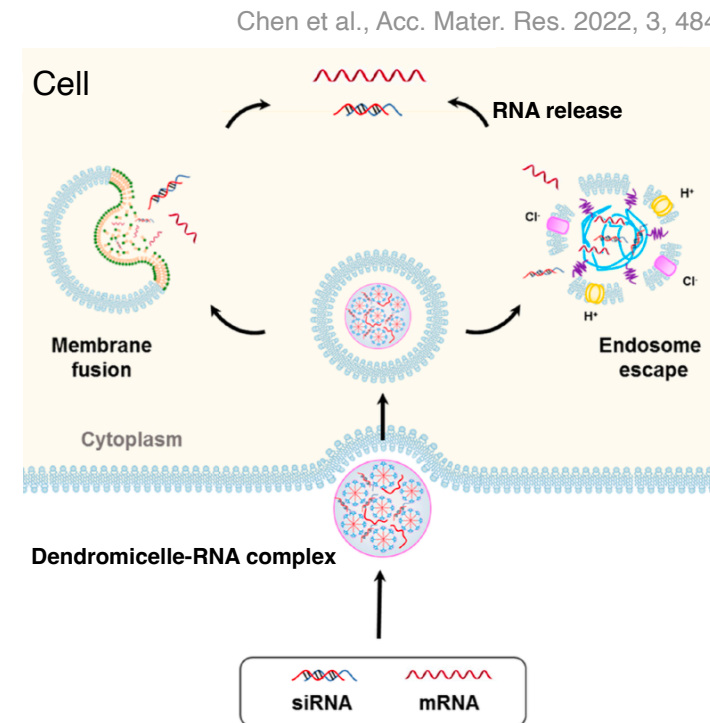
Contact: Mariano Brito (mariano.brito@icp.uni-stuttgart.de)

Develop of machine-learning-based reversed coarse-graining for gel dynamic properties

- All-atom simulations of gel systems are very expensive since they involve an enormous number of particles.

- Reverse coarse-graining provides an alternative to reconstruct gel trajectories from much cheaper coarse-grained simulations.

- **Master Project:**

  - Develop a ML-based reverse-coarse-graining method for reconstruction of gel trajectories.

  - Calculate relaxation rates of gels.

Coarse-grained gel simulation

r_{ij} r_{ij} r_{ij}

Reverse coarse graining
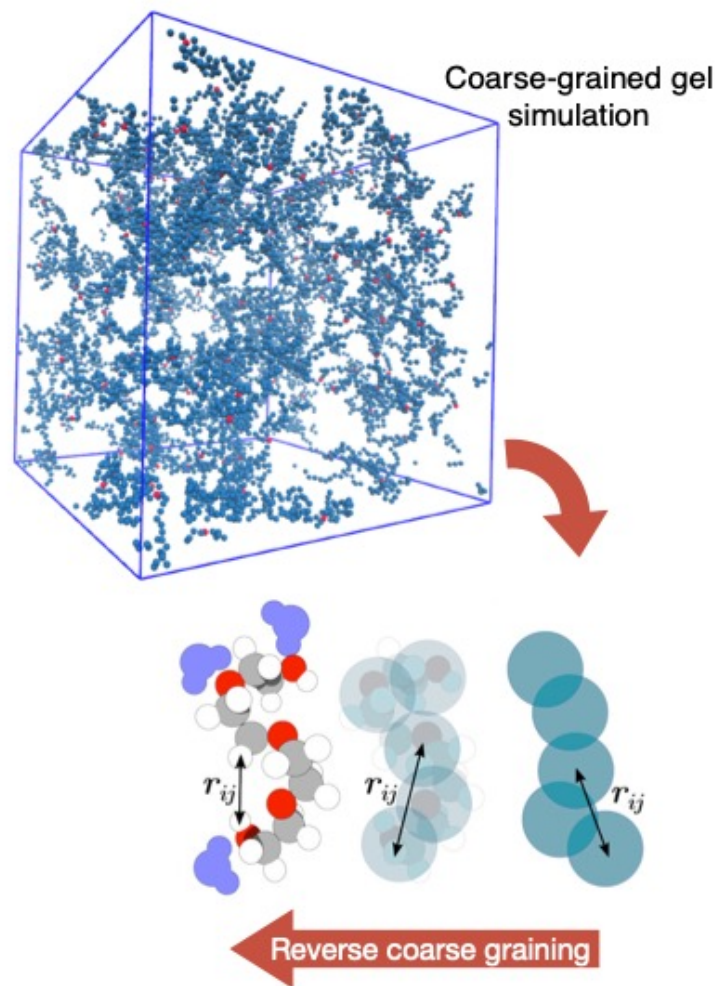
Contact: Mariano Brito (mariano.brito@icp.uni-stuttgart.de)

Electrostatic extension based on ICC* for constant-potential simulations

Energy storage: real capacitors are porous
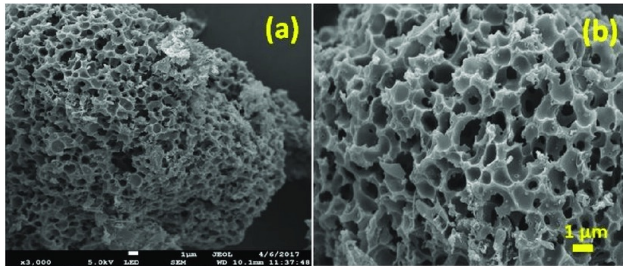
Carbon electrode, DOI: 10.1039/C9NA00374F

Develop a novel electrostatic method based on ICC* to simulate fixed-potentials on arbitrary surfaces and implement it in ESPResSo

Modeling an infinite plate capacitor with Molecular Dynamics

Your Job

- Get familiar with existing electrostatic solvers
- Adapt interfaces to compute potentials
- Implement your model
- Validation and comparison with other solvers
- Apply to complex porous electrode system

You will learn

- Molecular Dynamics and electrostatic solvers
- Python and C++
- How to write and document your own contribution to ESPResSo

Alexander Reinauer (alexander.reinauer@icp.uni-stuttgart.de)

Coupling of flexible polyelectrolytes to continuum solvent

Method: Lattice Boltzmann + Lattice Electrokinetics
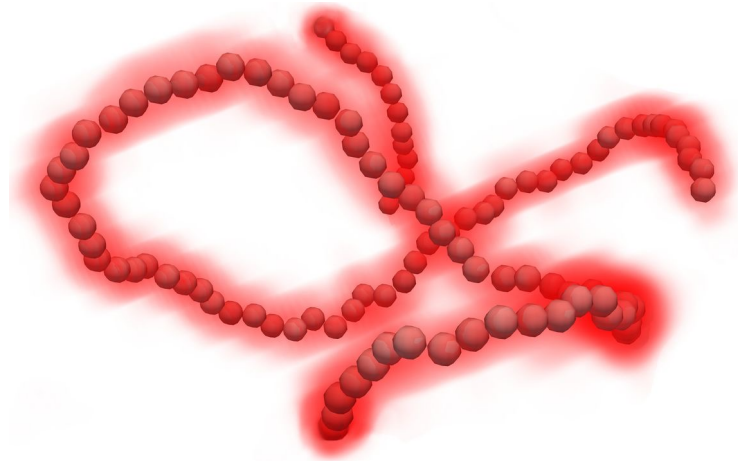
How to couple particle method for charged polymers to continuum method for ions and fluid

Your Job

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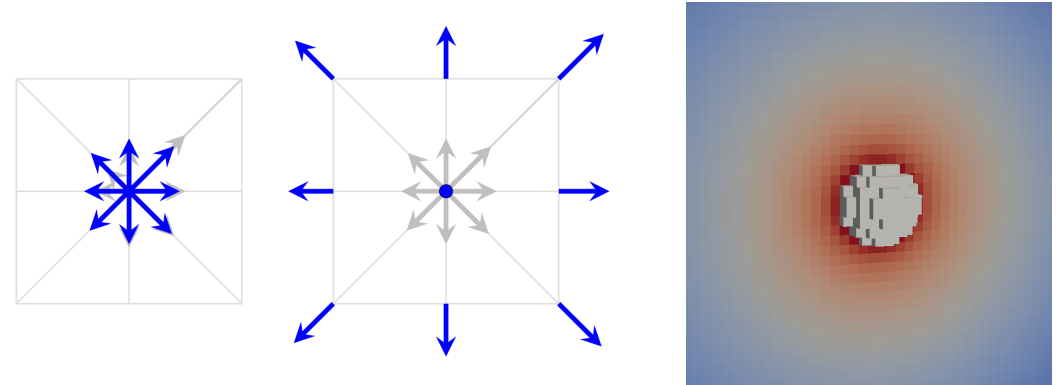
You will learn

- 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)

Simulation of imbibition experiments in model-porous media

Method: Lattice Boltzmann + Lattice Electrokinetics
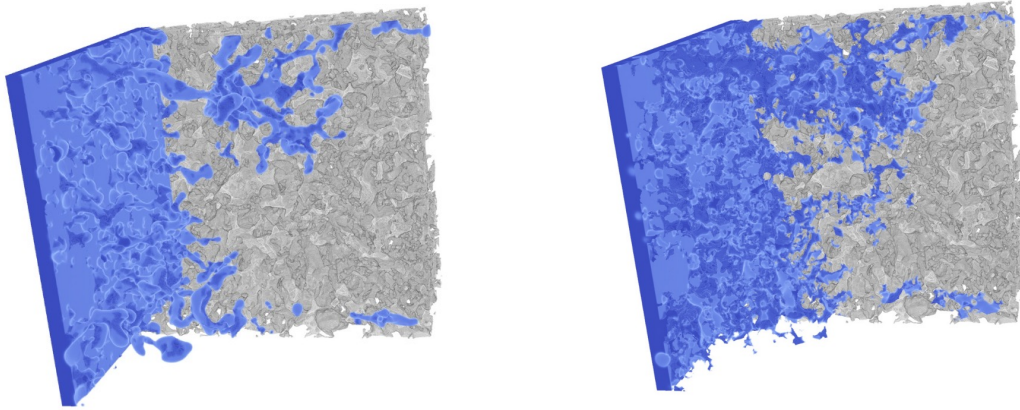
Simulate imbibition of (model) porous media using multi-phase flow model with and without implicit salt

Your Job

- Validate multi-phase flow model (Color-Gradient) for imbibition systems
- Study imbibition in sample porous media
- Comparison to experiments
- Introduce implicit salt and study surface effects
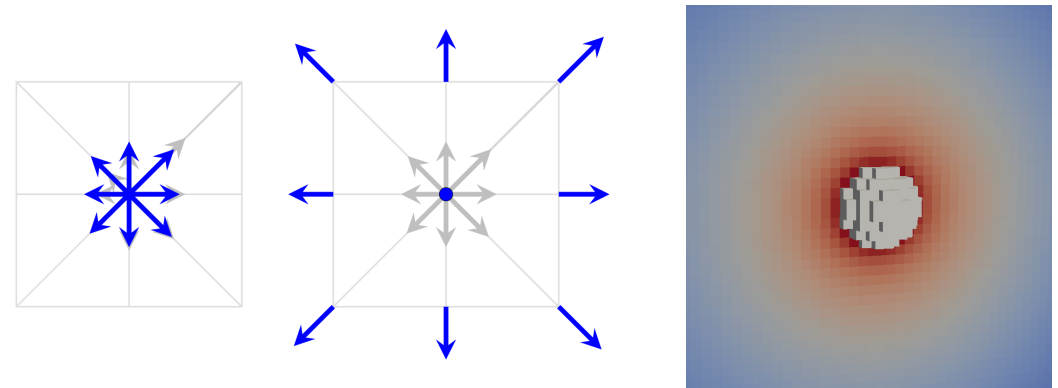
You will learn

- Mesoscale lattice-based solver for hydrodynamics and the Nernst-Planck equation
- Python and C++/CUDA
- How to use pystencils to compute on GPUs

Alexander Reinauer (alexander.reinauer@icp.uni-stuttgart.de)

Charging dynamics in charged nanopores

Method: Lattice Boltzmann + Lattice Electrokinetics
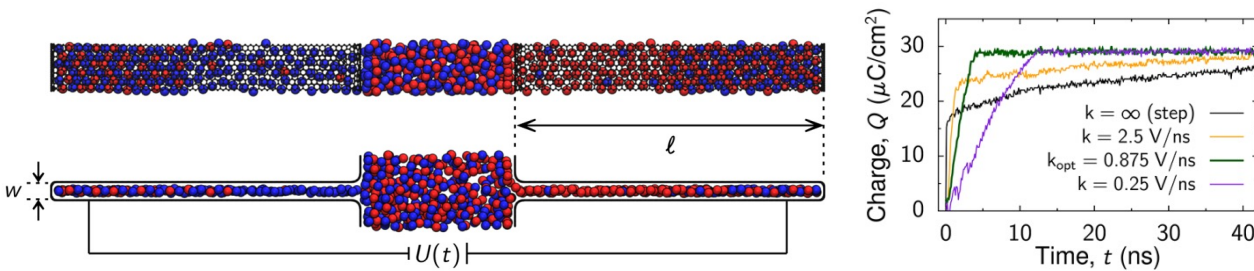
Extend existing continuum model and investigate similarity to MD simulation
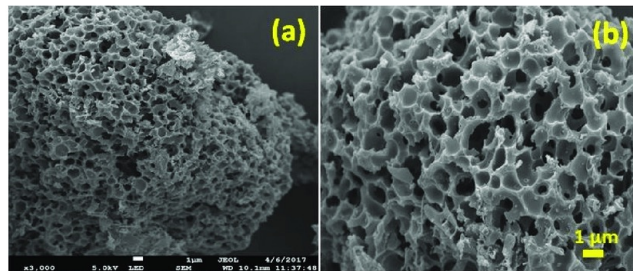
Carbon electrode, DOI: 10.1039/C9NA00374F

You will learn
- Mesoscale lattice-based solver for hydrodynamics and the Nernst-Planck equation
- Python and C++/CUDA
- How to use pystencils to compute on GPUs

Your Job
- Implement steric extensions to continuum model
- Validate system against MD data
- Apply to more complex porous electrodes
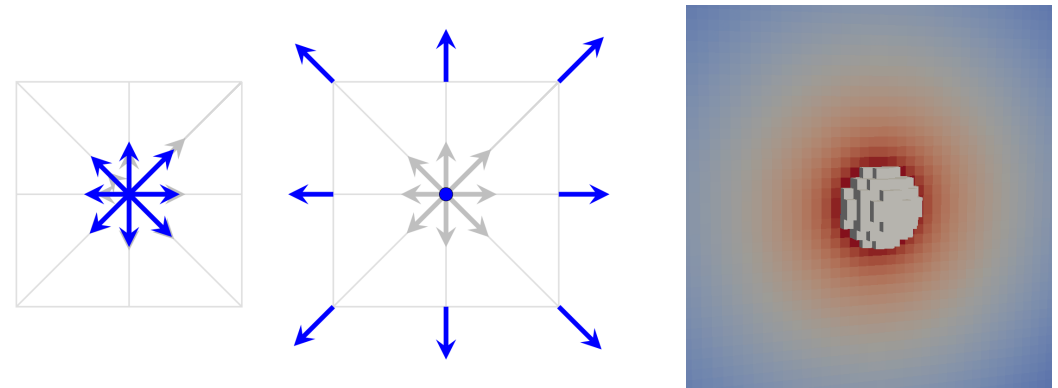
Alexander Reinauer (alexander.reinauer@icp.uni-stuttgart.de)

Implementation of dielectric ELC in ESPResSo
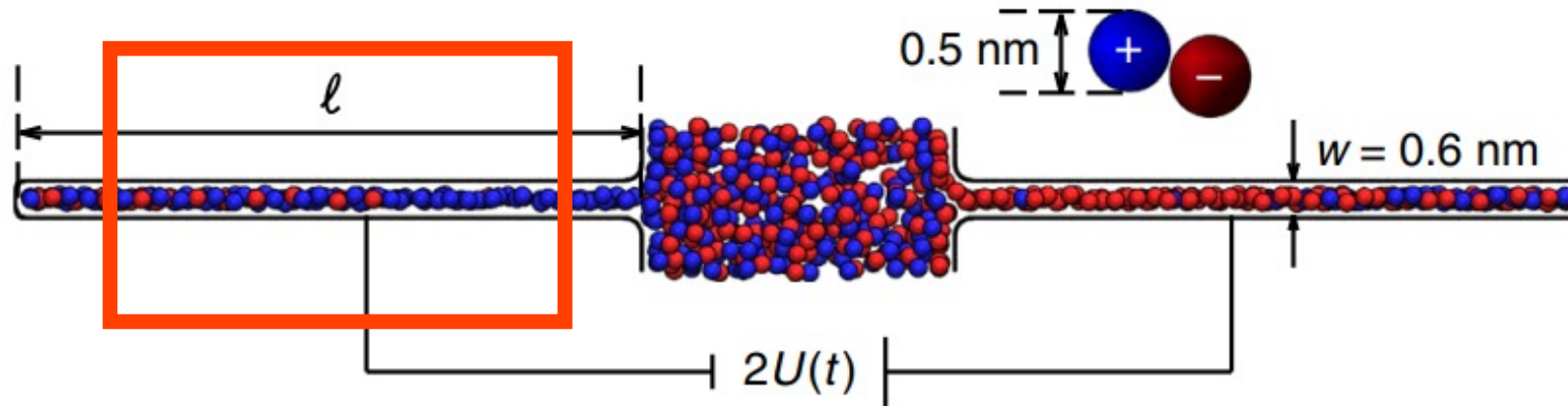
ESPResSo

Your Job

- Implement dielectric ELC into ESPResSo
- Validate code for 2D slab systems
- Apply for constant potential and constant charge simulations
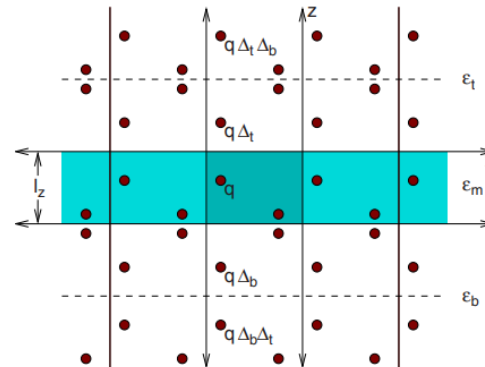
You will learn

- Molecular Dynamics
- How to use ESPResSo
- Python and C++
- How to structure code and how to document it

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

Simulating inhomogeneous systems using load-balancing

▶ In polymer networks, and many other systems like salt precipitation, soot aggregation and systems in confinement, the material is not homogeneously distributed in space

▶ The goal of this thesis is to simulate such systems efficiently on parallel computers

▶ Load-balancing: technique to distribute the work evenly among the CPU cores

▶ This thesis requires some experience in C++

Contact: J-N. Grad, R. Weeber
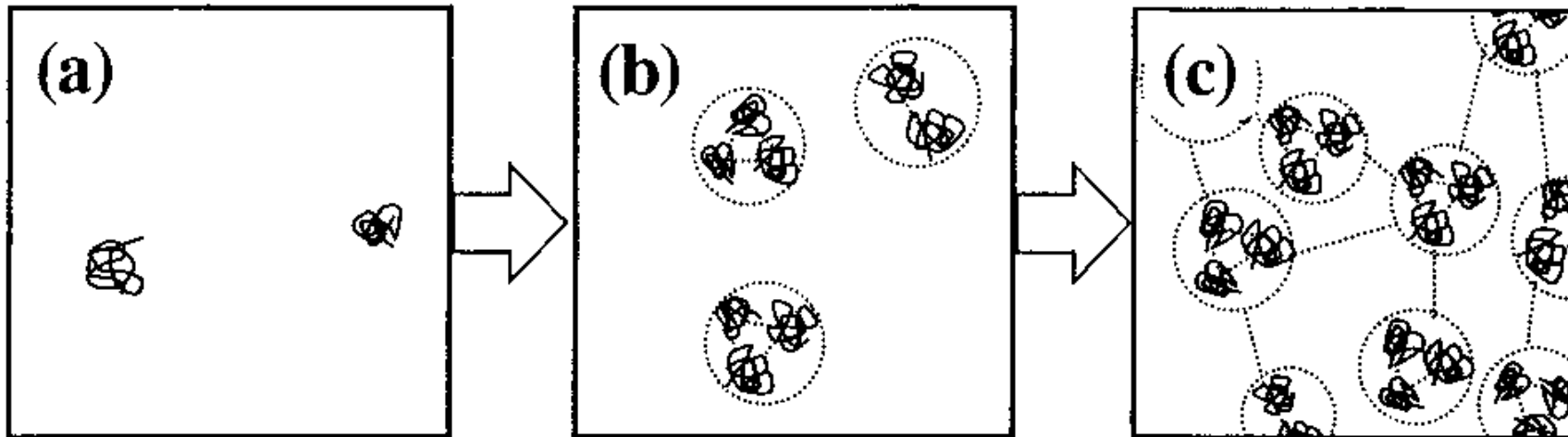
(Ide et Fukuda 1999: microgel formation during polymerization)
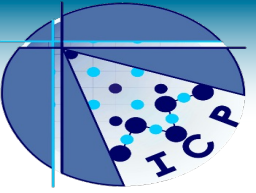
Substrate channeling in enzyme-catalysed reactions

Svyatoslav Kondrat <svyatoslav.kondrat@gmail.com>
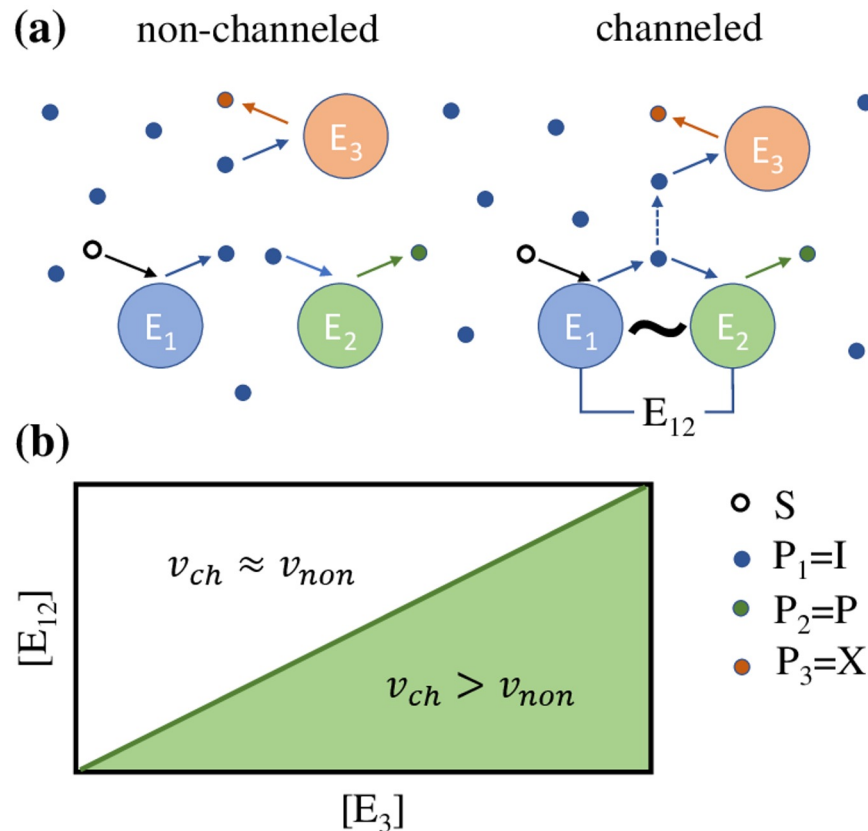
- Channeling intermediates (I) between two sequential enzymes (E_1 and E_2) can enhance the overall reaction rate
- We will use Brownian dynamics simulations to investigate such channeling effects
- In particular, how does intracellular crowding affects substrate channeling?

Kuzmak et al, *Scientific Reports* **9,** 455 (2019);
Kondrat, Kraus, von Lieres, *Current Research in Chemical Biology* **2**, 100031 (2022)

Confined Ionic liquids for energy-related applications
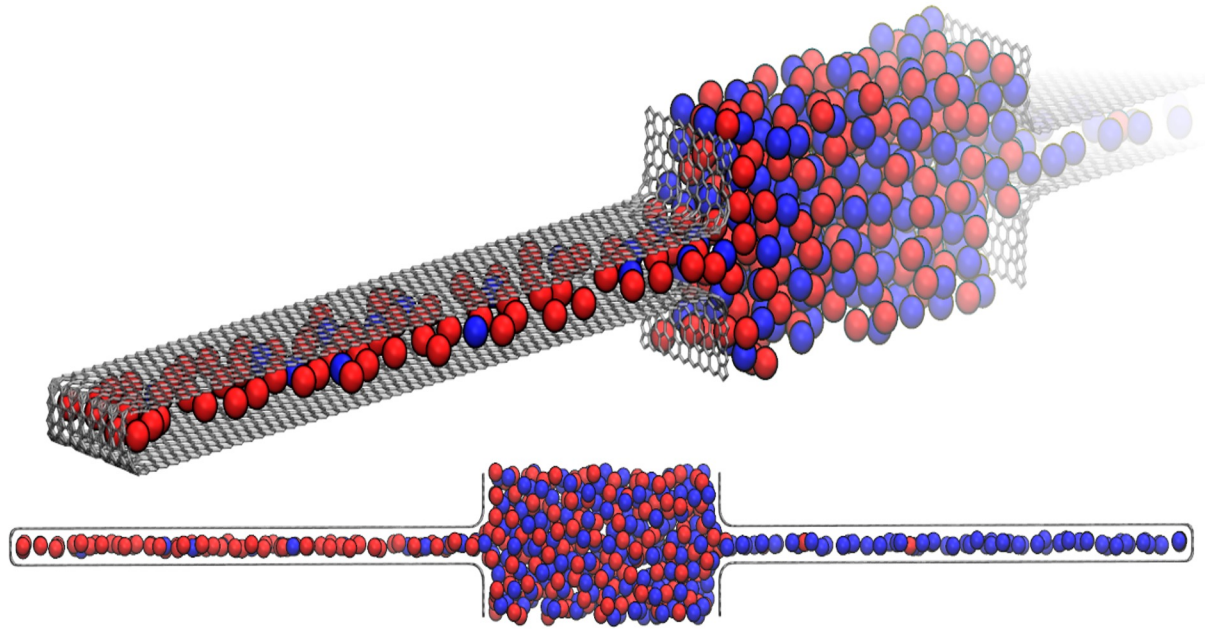
- Confined ionic liquids play the key role in many energy-related applications
- We will use molecular simulations and theory to study nanopore charging
- **Topic 1**: Confined ionic liquid mixtures for supercapacitor applications
- **Topic 2**: Charging mechanisms and performance optimisation of nanoporous supercapacitors

Breitsprecher, Holm, Kondrat, *ACS Nano* **12**, 9733 (2018)
Breitsprecher, et al, *Nature communications* **11**, 6085 (2020)

Svyatoslav Kondrat <svyatoslav.kondrat@gmail.com>

Coarse-graining and machine-learned potentials
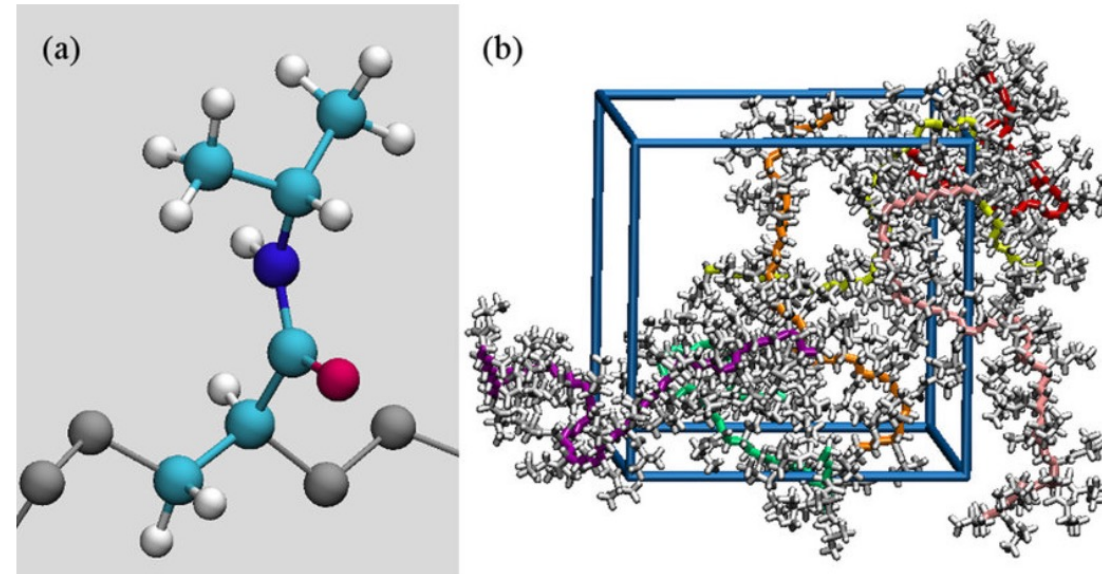
Polynipam, a polymer commonly used for hydrogels and polymer suspensions

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

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

Active particles in viscoelastic fluids
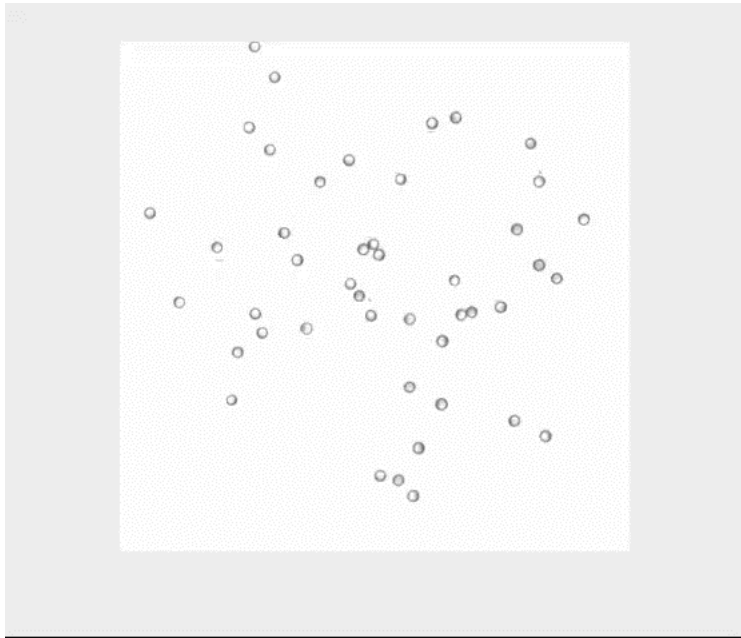
2. The Weissenberg Effect

* Active particles are particles which have a propulsion mechanisms,
e.g., by coating part of the particle surface with a catalyst
* Experiments have shown that these particles show quite unusual
behaviour in viscoelastic fluids
* Goal of the thesis is to model this using a combination of molecular
dynamics and the lattice-Boltzmann method

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

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

* hydrogels are polymer networks swollen by a carrier fluid
* magnetic gels additionally contain magnetic nanoparticles
* using an external magnetic field, the shape and elasticity can be controlled

Application: Drug release

-80°C
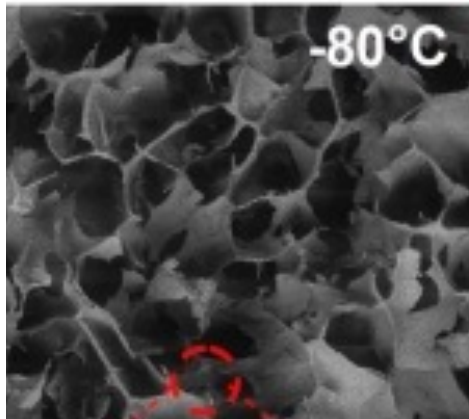
500 µm
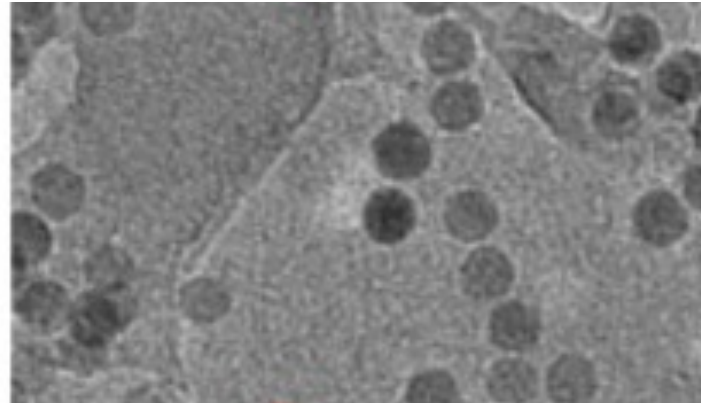
500 nm

One can store drug molecules in the porous matrix

2 min of magnetic stimulation every 30 min

No magnetic stimulation

Release can be triggered with a magnetic field

Possible thesis topics

* Model the loading and release of drugs form magnetic gels

* Understanding the influence of inhomogeneities in the network on experimentally observable properties

Contact:

Rudolf Weeber

weeber@icp.uni-stuttgart.de

Measuring chemical potentials from static structure factors – Enabling rapid sampling of the grand canonical ensemble

Background: Simulating in the Grand potential is challenging for typical systems due to sampling issues

Goal: Employ new methods that are emerging which open new ways to use statistical physics to investigate molecular systems.

Static structure factors can be used to calculate the chemical potential in a molecular dynamics simulation.
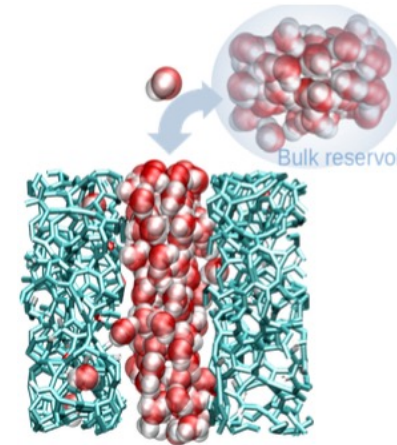
Less finite size effects and better sampling

$$N_A, N_B, P, T$$
$$\mu_A, \mu_B, V, T$$
$$(n_A, n_B)$$
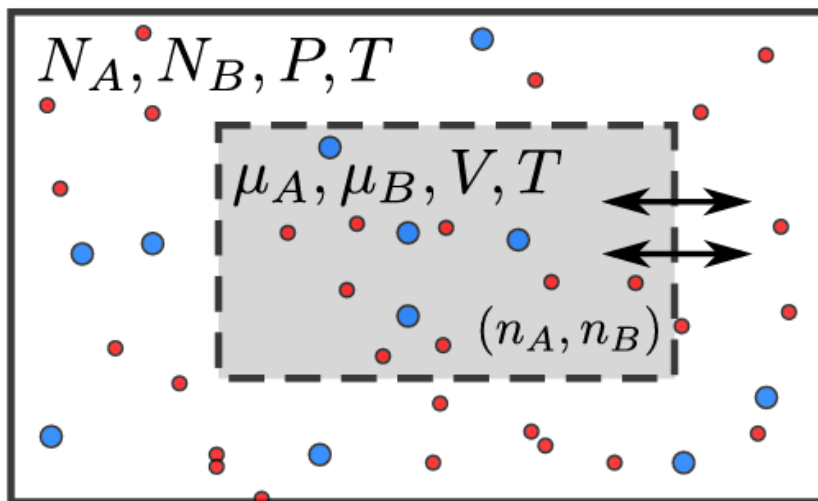
What will you do?
- Implement the S0 Method in Python
- Perform Molecular Dynamics simulations
- Adapt the methods for other ensembles/geometries

You will learn
- Thermodynamics
- Molecular Dynamics
- Python and software development

Contact
Henrik Stoß (henrik.stooss@simtech.uni-stuttgart.de
Alexander Schlaich (alexander.schlaich@simtech.uni-stuttgart.de)

Density matrix extrapolation on the Grassmann manifold for BOMD using charge dependent descriptors

Master Thesis

New scheme based on Grassmann extrapolation of density matrices for an accurate calculation of initial guesses in Born-Oppenheimer Molecular Dynamics simulations.
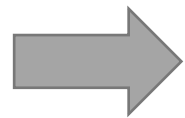The Coulomb matrix is used as a molecular descriptor for the atomic positions.

Can this scheme be applied to fluctuating charges in BOMD?

Backtransformation for use as initial guess

correction

C_n geodesic C_{n+1}

Constraint manifold for $C^\top S C = \mathbb{1}$

Grassmann manifold allows for linear superposition of density matrix states
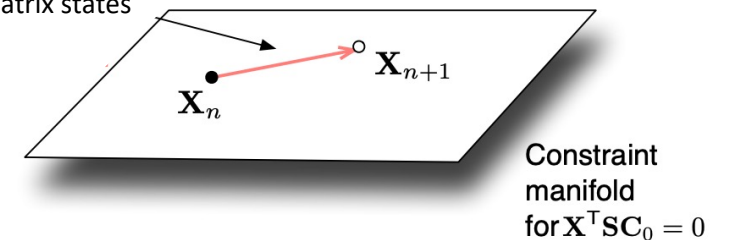
X_n X_{n+1}

Constraint manifold for $X^\top S C_0 = 0$

What you will do?
- Perform Ab-Initio Molecular Dynamics simulations
- Use Python for software development
- Simulate Solid-Liquid interfaces at constant potential

Contact
Henrik Stoß (henrik.stooss@simtech.uni-stuttgart.de
Alexander Schlaich (alexander.schlaich@simtech.uni-stuttgart.de)

Multicanonical molecular dynamics simulations using the Wang-Landau algorithm

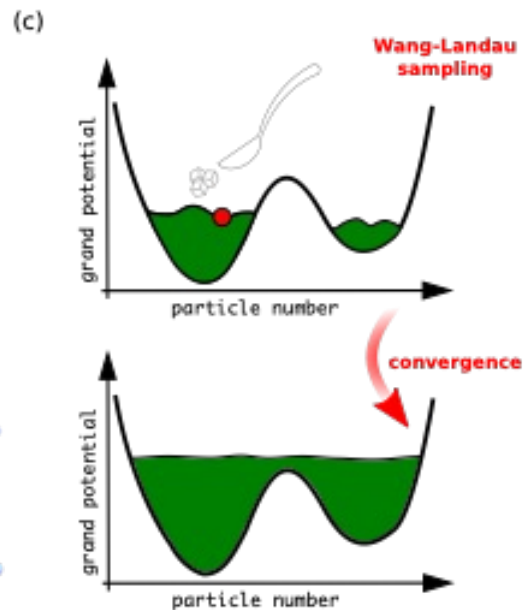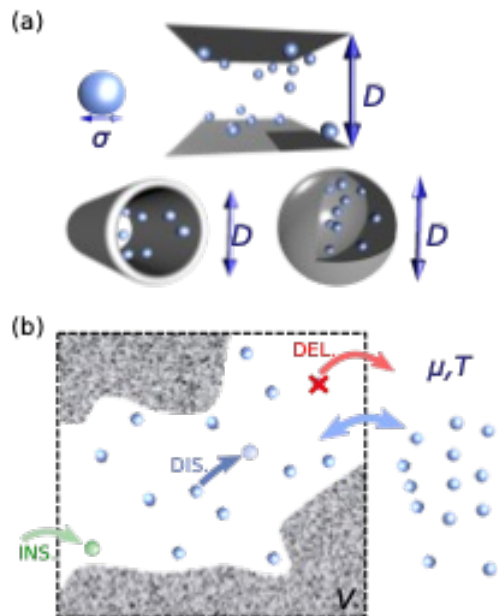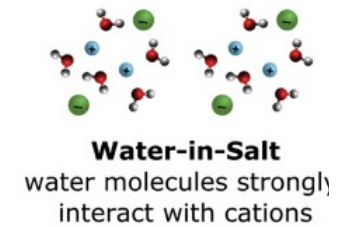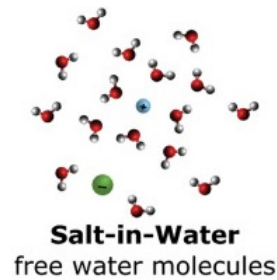**Background:** Nano-porous systems are nowadays commonly applied for energy storage. Water-in-salt solutions are a promising candidate for environmentally friendly high-efficiency charge carriers. However, compositional changes upon charge/discharge are so far poorly understood.

Goal: Implement and apply a Wang-Landau scheme for binary, ternary, … solutions.

Salt-in-Water
free water molecules

Water-in-Salt
water molecules strongly interact with cations

What will you do?
- Implement the Wang-Landau approach
- Benchmarks and tests
- Study the composition of complex solutions in confinement
- Apply machine-learning approaches to predict the composition

You will learn
- Cutting-edge energy storage problems, high performance computing, extending simulation packages

Contact
Philipp Stärk (philipp.staerk@simtech.uni-stuttgart.de)
Alexander Schlaich (alexander.schlaich@simtech.uni-stuttgart.de)

- Christoph Lohrman clohrmann@icp.uni-stuttgart.de.   Bacteria in Porous Media, Active Matter

- Mariano Brito mariano.brito@icp.uni-stuttgart.de   Hydrogels and Mean-field Theory

- Samuel Tovey stovey@icp.uni-stuttgart.de   ML for Physics, Signal analysis,, swarm computing

- 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

- Keerthi Radhakrishnan keerthirk@icp.uni-stuttgart.de   weack Polyelectrolyes

- Michel Mom mmom@icp.uni-stuttgart.de   Nanopore aa atom simulations

- David Beyer dbeyer@icp.uni-stuttgart.de   Weak polyeletrolytes, Path integral MD,

- Adyant Agrawal aagrawal@icp.uni-stuttgart.de   AA salt crystalization in porous media

- dfink dfink@icp.uni-stuttgart.de   Quantum Computing algorithms, QML

- Svyatoslav Kondrat svyatoslav.kondrat@gmail.com   Supercapcitors

- jgrad jgrad@icp.uni-stuttgart.de   ESPResSo, Lattice-Boltzmann

- Rudolf Weeber weeber@icp.uni-stuttgart.de   ESPResSo, Magnetic Soft Matter, Polymer Rheology

- Alexander Schlaich alexander.schlaich@simtech.uni-stuttgart.de JGL SimTech, Multiscale Materials Modelling

Bachelor, Masters or PhD topics

For general contact:

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

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

Alexander Schlaich: schlaich@icp.uni-stuttgart.de

Svyatoslav Kondrat: svyatoslav.kondrat@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
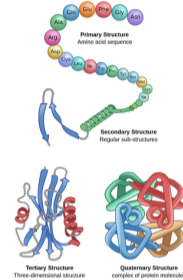
Research topic - Nanopore Sequencing

- Protein functionality is encoded in the amino acid sequence
- Mutations in the sequence can lead to malfunction and diseases (e.g. cancer)

$\Rightarrow$ Early detection of such mutations can save lifes
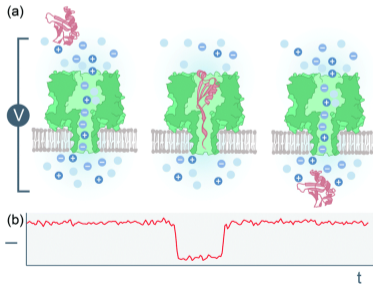
Chem. Soc. Rev. 47, 8512-8524 (2018)

https://theory.labster.com/protein-structure/

- Nanopore sequencing: Protein translocates through a biological nanopore

$\Rightarrow$ Amplitude, duration and frequency of blockade current reveal information about the protein structure

You will learn how to ...

- perform all-atom simulations using NAMD
- extract physics from simulation data
- investigate the mechanism behind protein sequencing
- collaborate with the experimentalist group from Freiburg

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