University of Stuttgart
Institute for Computational Physics

CECAM Flagship School
Simulating soft matter across scales
Book of Abstracts

Stuttgart, Germany
October 7–11, 2024

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2024 ESPResSo Summer School

CECAM Flagship School “Simulating soft matter across scales”

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Organizing committee
Jean-Noël Grad, Christian Holm,
Alexander Schlaich, Rudolf Weeber

Edited by
Jean-Noël Grad

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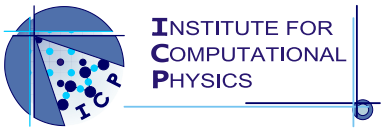

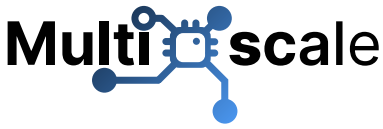

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Conference Program

Course description

Scientific content

This school teaches coarse-grained and lattice-based simulations methods suitable for modeling soft matter systems at mesoscopic length and time scales. We explore topics such as simulating coarse-grained ionic liquids in electrolytic capacitors to measure differential capacitance, simulating coarse-grained liquids with machine-learned effective potentials to match the properties of models with atomistic resolution, polymer diffusion in an implicit solvent, particle coupling to continuum hydrodynamic fields, and diffusion-advection-reaction solvers for electrokinetics and catalysis.

Lectures provide an introduction to the physics and model building of these systems as well as an overview of the necessary simulation algorithms. During the afternoon, students practice running their own simulations in hands-on sessions using ESPResSo[1] and waLBerla[2].

Many of the lectures and hands-on sessions are taught by developers of the software. Hence, the school also provides a platform for discussion between developers and users about the future of the software used in the hands-on sessions. Moreover, users can get advice on their specific simulation projects. Time is also dedicated to research talks, which illustrate how the simulation models and software are applied, and which provide further background on soft matter at different length and time scales.

Participants have the opportunity to bring a poster to introduce their work to their peers. We welcome submissions on both planned and ongoing research projects, as long as they fit to the general themes of this event. The poster session opens with 1-minute lightning talks from all presenters. The poster boards remain up for the entire duration of the school.

Teaching material

The teaching material used during the school is available online. The ESPResSo software and Jupyter notebooks are free and open-source, available on GitHub (github.com/espressomd/espresso). The lecture slides can be found on the CECAM page for the event (www.cecam.org/workshop-details/1324). The recorded lectures of past iterations of the school have been published on the YouTube channel ESPResSo Simulation Package.

Hands-on sessions

We use interactive Jupyter notebooks to teach concrete applications of the simulation methods introduced in the lectures. These notebooks outline physical systems relevant to soft matter physics and sketch simulation scripts written for the ESPResSo package using the Python language. A few parts of these scripts are hidden and need to be completed by participants, with the help of the ESPResSo user guide and tutors. These exercises can also be carried out in self-study using the web browser via Binder or Gitpod, and all exercises have hidden solutions that can be revealed at any time.

Software

In this school, participants learn to conduct coarse-grained and lattice-based simulations suitable for modeling soft matter systems using the software ESPResSo (espressomd.org) and waLBerla (walberla.net). ESPResSo is an open-source particle-based simulation package with a focus on coarse-grained molecular dynamics models. In addition, it offers a wide range of schemes for solving electrostatics, magnetostatics, hydrodynamics and electrokinetics, as well as algorithms for active matter and chemical reactions[3]. These methods can be combined to simulate different scales and recover emergent material properties at macroscopic scales.

ESPResSo consists of an MPI-parallelized simulation core written in C++ and a scripting interface in Python which integrates well with scientific packages, such as NumPy[4], pyMBE[5], PyOIF[6], VOTCA[7], ZnDraw[8], and SwarmRL[9]. ESPResSo relies on waLBerla[2], a high performance lattice-Boltzmann library for hydrodynamics and other lattice-based schemes for electrokinetics and related fields. Custom waLBerla kernels can be rapidly prototyped in symbolic form in Python and automatically converted to highly optimized, performance-portable code for CPUs and GPUs[10].

The organizing committee
Jean-Noël Grad, Christian Holm, Alexander Schlaich, Rudolf Weeber
(Institute for Computational Physics, University of Stuttgart, Germany)

Talks

Introduction to the lattice-Boltzmann method as Navier–Stokes solver

Timm Krüger[1]

I will give a concise introduction to the lattice-Boltzmann (LB) method as Navier–Stokes solver for beginners with a basic physics background. I will touch upon kinetic theory (the basis of LB), the main LB algorithm and how it asymptotically recovers Navier–Stokes behaviour. I will also present one simple boundary condition (the bounce-back method) that highlights the elegance and conceptual convenience of the LB. Finally, I will discuss advantages and disadvantages of LB and highlight various extensions that make the method so popular.

Introduction to the immersed-boundary-lattice-Boltzmann method for moving particle problems

Timm Krüger[1]

The lattice-Boltzmann method is well suited for moving boundary problems, such as suspensions of rigid or deformable particles. I will focus on the immersed-boundary method as a popular fluid-structure interaction scheme and cover the treatment of both rigid and soft objects. Advantages and disadvantages of the method will be highlighted, and other available methods for moving particles will be be mentioned.

Introduction to multi-phase models for the lattice-Boltzmann method

Alexander Reinauer[2]

This lecture reviews modeling techniques extending the lattice-Boltzmann method[11] for multi-phase and multi-component simulations, with an emphasis on the Shan–Chen method[12], the free-energy method[13] and the color gradient method[14, 15, 16].

Code generation for stencil-based methods using pystencils and lbmpy

Frederik Hennig[3]

The development of a stencil-based numerical update rule involves several steps. These include the mathematical derivation of its equations, their simplification and formulation in a programming language, and finally the mapping onto an iteration space via loop nests or some parallelization paradigm. Using the code generation software pystencils[10], these steps can be fully automated and combined into a single Python script. Therein, mathematical equations are manipulated using a computer algebra system, automatically simplified and optimized, and finally translated into a numerical kernel written in C or CUDA. In the first part of this lecture, I present the principles of pystencils and demonstrate how stencil-based methods can be derived ab inito, implemented as kernels, and immediately executed within an interactive Python environment.

The second part of the lecture is dedicated to lbmpy[17, 18]. Lbmpy builds on top of pystencils to enable the development and rapid prototyping of lattice Boltzmann methods using symbolic algebra. I will show how LB-based numerical methods can be described and manipulated using the tools provided by lbmpy. The primary focus shall be the automated derivation and implementation of LB collision kernels, while initialization procedures and boundary conditions will also be discussed.

A short introduction to waLBerla

Frederik Hennig[3]

The waLBerla[2] framework provides a platform for a wide range of multiphysics simulations, with fluid simulation using the lattice Boltzmann method at its heart. This lecture shall give an overview of waLBerla's capabilities as employed in a variety of simulation applications. Special emphasis will be put on the interaction of waLBerla with the code generation packages presented in the previous lecture, as those now drive many of the numerical methods provided within the framework.

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Introduction to ESPResSo

Jean-Noël Grad[1]

Overview of the research conducted with ESPResSo in different areas of soft matter and at different scales: supercapacitor charging dynamics[19], swelling behavior of weak polyelectrolyte stars[20], hydrogels[21] and brushes[22], DNA translocation through nanopores[23, 24], nano-particles aggregation[25] and sedimentation[3], Kármán vortex streets[3], cell membrane plasticity[26], and bacterial growth in porous materials[27]. I will discuss how the choice of algorithm is dictated by the time-scale and length-scale at which physical phenomena need to be resolved. I will also explain how to contribute new features to ESPResSo, and how to get ESPResSo installed on clusters via EasyBuild[28, 29] and EESSI[30].

Electrostatics in confinement

Christian Holm[1]

This lecture reviews algorithms available in ESPResSo[1] and ScaFaCoS[31] to model long-range electrostatic interactions in fully periodic systems (Ewald sum method[32], P^3M method[33, 34]) and in partially periodic systems (Yeh–Berkowitz[35] and ELC[36, 37] methods). In addition, methods specific to systems with planar and curved dielectric interfaces (ICC* algorithm and ELC-IC method[38, 39, 40, 41]) will be presented.

Electrostatic interactions in confinement

Alexander Schlaich[1,2,3]

This lecture presents mathematical models to solve inhomogeneous electrostatic interactions at interfaces: the Gouy–Chapman model[42, 43], the Poisson–Boltzmann equation[44], the Grahame equation[45], Derjaguin–Landau–Verwey–Overbeek (DLVO) theory[46, 47], and their applications in studying polarizable media and differential capacitance.

How to model DNA translocation through nanopores – A multiscale simulational exploration

Christian Holm[1]

In this talk I will describe our efforts to understand the current modulations a double-stranded DNA will produce when it translocates in an electrolyte bath of varying concentration via an externally applied electric field through a nanopore device. The complete understanding of this electrokinetic process is important to develop novel DNA sequencing tools, or to use the nanopore as a sensor device for various macromolecular analytes. There are by now already commercial applications of such nanosequencers available.

Understanding can be gained on various length scales, and to this end we will start with atomistic simulations of dsDNA in explicit water. The comparison with experimental results helped us in constructing an accurate electrokinetic coarse-grained model for dsDNA. Going to even larger length scales requires the usage of continuum theories which can help us to understand the electrokinetic transport of charged macromolecules through millimeter-long glass nanocapillaries[48, 49, 50, 23, 24].

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Machine-learned inter-atomic potentials

Samuel Tovey[1]

Molecular dynamics has been the workhorse of computational materials modeling for nearly half a century. Harnessing the different levels of theory, from quantum mechanics to coarse-grained representations, scientists have worked in lockstep to simultaneously produce methods for simulation and deploy them to better understand our world. In 2024, a significant step was taken in the form of a set of universal machine-learned inter-atomic potentials, referred to as foundation models.

Machine-learned inter-atomic potentials are a new player in molecular dynamics, used to maintain the accuracy of quantum mechanical simulations on the size and time scale of atomistic ones. As these models can potentially revolutionize the way materials modeling is performed and even be the "death of ab initio", they are important and useful to understand.

This talk introduces the fundamentals of machine-learned inter-atomic potentials and how they can be developed and used in research. Further, current updates in the field, such as foundation models and outlooks on coarse-graining with machine learning, are explored.

Simulating biological soft matter across scales: making use of machine learning methods

Christine Peter[2]

Coarse graining and combining particle-based models across scales has long been one important ingredient in overcoming the size and time scale limitations of purely atomistic approaches. In this context, linking the simulation scales and assessing and improving the inevitable shortcomings of the lower resolution models remains an ongoing effort in which machine learning (ML) plays an increasingly important role. Generally, in bottom-up coarse-graining, coarse-grained (CG) interactions are devised such that an accurate representation of a higher-resolution (e.g. atomistic) sampling of configurational phase space is achieved.

Recently, traditional bottom-up methods have been complemented by machine learning (ML) approaches. ML methods can be used to derive or validate CG models by matching the sampling of a (relatively complex) free-energy surface as opposed to low-dimensional target functions/properties. For example, high-dimensional free energy surfaces can be extracted from atomistic simulations with the help of artificial neural networks (NN) – which can then be employed for simulations on a CG level of resolution[51, 52].

Secondly, ML methods can also be employed to obtain low-dimensional representations of the sampling of phase space or to identify suitable collective variables that describe the states and the dynamics of a system. This information can then be directly fed into the CG potentials or be employed to identify optimal CG representations and learn CG interactions. Moreover, the so-obtained low dimensional representations enable us to assess the consistency of the sampling in models at different levels of resolution, to go back and forth between the scales and ultimately to enhance and improve the sampling of the systems. In particular, they can be used as a basis for backmapping based enhanced sampling protocols[52, 53].

Generative machine learning in multiscale molecular simulations

Tristan Bereau[3]

Generative machine learning is offering new possibilities in various scientific fields. I will describe recent efforts in the context of multiscale molecular simulations: the basin structure of a complex free-energy landscape for dimensionality reduction; a backmapping strategy that learns the atomistic distribution of atoms conditional on the coarse-grained degrees of freedom; and finally a diffusion model to efficiently compute free energies.

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Monte Carlo methods to simulate acid/base equilibria in ESPResSo

Pablo M. Blanco[1]

When chemical reactions are present in macromolecular systems, they can significantly impact the physical properties of these systems. For example, weak polyelectrolyte and biomacromolecules can modulate their charge in response to their microenvironment through the acid/base equilibrium, a phenomenon known as charge regulation. To simulate this kind of systems, the configuration space and the reaction degrees of freedom need to be simultaneously sampled because they are highly coupled.

Nowadays, Monte Carlo (MC) simulations and coarse-grained models have become a popular approach to study these systems because they permit efficient sampling of their equilibrium properties. In this lecture, we will showcase the reactive Monte Carlo methods available in ESPResSo and we will discuss their applicability for different case scenarios. Furthermore, we will present the Python-based Molecule Builder for ESPResSo (pyMBE)[5], an open source software with tools to aid the setup of these MC simulations for custom coarse-grained models and pre-defined models of peptides and globular proteins in ESPResSo.

Sub-THz acoustic excitation of protein motion

Matej Praprotnik[2]

Ultrasound is widely used as a noninvasive method in biomedical applications. Usually, continuum numerical methods are used to simulate ultrasound propagating through different tissue types. In contrast, ultrasound simulations using particle description are less common, as the implementation is challenging. In this talk, I will present a dissipative particle dynamics model for performing ultrasound simulations in liquid water. The results of our ultrasound simulations show that our particle-based approach is capable of reproducing the fluctuating hydrodynamics description of ultrasound in the continuum limit. Using the developed approach, we have studied the susceptibility of the protein's internal dynamics to mechanical stress induced by acoustic pressure waves. By analyzing the dynamic fluctuations of the protein subunits, we have demonstrated that the protein is highly susceptible to acoustic waves with frequencies corresponding to those of the internal protein vibrations. The present studies pave the way for development and optimization of a virtual ultrasound machine for large-scale biomolecular simulations.

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Poster session

Material interfaces inspired by catch bond adhesins

Kerim Dansuk[1], Sinan Keten[2]

In recent years, there has been a shift from traditional engineering materials to advanced materials with complex architectures and enhanced mechanical properties. Much of the inspiration for these new materials comes from nature, where organisms have developed a vast array of macro and nanoscale shapes and structures with ingenious mechanisms. Adhesion proteins are particularly noteworthy for novel materials because their conformational dynamics enable them to form unique non-covalent interactions known as 'catch bonds' with their ligands, wherein the dissociation lifetime of ligand-protein complexes is increased by mechanical force. Normally, one would expect that applying tensile force on a chemical bond would shorten its lifetime, making it more prone to breaking, but catch bonds contradict this expectation. When incorporated into material systems, catch bonds are anticipated to resolve the trade-offs between strength and reconfiguration, two opposing material properties mainly governed by the strength of intermolecular interactions. This study employs a multifaceted approach that combines molecular simulations and adhesion theory to develop strategies for designing material interfaces with catch bond characteristics. Drawing on adhesin properties, we proposed design guidelines to replicate the catch bond phenomenon in synthetic systems and created mechanical designs that reliably and predictably exhibited catch bond behavior under thermal excitations. Our findings show that catch bond functionality can be achieved through simple molecular mechanisms and provide design principles for creating catch bond nanoparticles and linkages, paving the way for developing synthetic materials with emergent force-tunable interfacial kinetics.

CO_2-induced drastic decharging of dielectric surfaces in aqueous suspensions

David Beyer[3], Peter Vogel[4], Thomas Palberg[4], Christian Holm[3]

We study the influence of airborne CO_2 on the charge state of carboxylate stabilized polymer latex particles suspended in aqueous electrolytes. We combine conductometric experiments interpreted in terms of Hessinger's conductivity model with Poisson–Boltzmann cell (PBC) model calculations with charge regulation boundary conditions. Without CO_2, a minority of the weakly acidic surface groups are dissociated and only a fraction of the total number of counter-ions actually contribute to conductivity. The remaining counter-ions exchange freely with added other ions like Na^+, K^+ or Cs^+. From the PBC-calculations we infer a corresponding pK_a of 4.26 as well as a renormalized charge in reasonably good agreement with the number of freely mobile counter-ions. Equilibration of salt- and CO_2-free suspensions against ambient air leads to a drastic de-charging, which exceeds by far the expected effects of to dissolved CO_2 and its dissociation products. Further, no counter-ion-exchange is observed. To reproduce the experimental findings, we have to assume an effective pK_a of 6.48. This direct influence of CO_2 on the state of surface group dissociation explains our recent finding of a CO_2-induced decrease of the ζ-potential and supports the suggestion of an additional charge regulation caused by molecular CO_2. Given the importance of charged surfaces in contact with aqueous electrolytes, we anticipate that our observations bear substantial theoretical challenges and important implications for applications ranging from desalination to bio-membranes.

Theory meets simulations: probing the thermodynamics of DNA melting via Nupack and oxDNA

Alejandro Soto[5], Iliya Stoev[5]

We compare two methods to mimic the thermodynamic properties of DNA networks using the coarse-grained model oxDNA. Using dual validation, we explore changes in the effective simulation space and its influence on finite-size effects, identifying a safe range for the simulation box from 7.5 to 9.5 µM. We also determine the model's detection limit to be four nucleotides. Our findings are relevant to the DNA nanotechnology community and oxDNA developers and can be applied to define constraints in various simulation setups and other coarse-grained molecular dynamics models.

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Successful training of a triangular swimmer: a genetic algorithm approach

Ruma Maity[1], Maximilian Hübl[2], Benedikt Hartl[1], Gerhard Kahl[1]

Natural microswimmers use various swimming gaits to propel under low Reynolds number conditions in their fluid surrounding for various reasons: search for nutrition, escape from predators or search for prey. A very common strategy for propulsion is the non-reciprocal deformation of the shape of the swimmer in an effort to realize its motion through the medium. In recent times efforts have been made to design artificial swimmers that can successfully mimic their natural counterparts and are thus able to perform specific tasks, such as targeted drug delivery in the case of nanomedical applications. In this work, we train a two-dimensional, triangular swimmer to move in a desired direction and to detect in an efficient manner nutrition sources. This is achieved – similar as in previous work on a one-dimensional linear swimmer – with adaptive neural networks (which connect the degrees of freedom and the forces acting on the swimmer), involving thereby the NEAT algorithm which optimizes the internal architecture of these networks[54]. In preceding work the one-dimensional, linear three-bead swimmer was successfully trained to swim in a chemical landscape[55]. Here we proceed to the considerably more challenging case of the triangular swimmer: now rotation, translation and the coupling of these two kinds of motion have to be taken into account. We demonstrate that also in this setup the swimmer can be trained to propagate in a desired direction and to develop swimming gaits that allows to find nutrient in a chemical landscape. Again we are able to extract valuable information about the swimmer's strategies by analyzing the internal structure of the emerging networks.

A general purpose framework for developing kinetic Monte Carlo models

Bat-Amgalan Bat-Erdene[3], Roya Ebrahimi Viand[3], Sebastian Matera[3], Karsten Reuter[3]

Many problems in condensed matter physics are characterized by the interplay of rare transitions between metastable states. Prominent examples are diffusion in solids, crystal growth, or chemical kinetics. The dynamics of such problems are typically coarse-grained Markov jump process and simulated using the kinetic Monte Carlo (kMC) methodology. A challenge here is that most models lead to only sparse changes per kMC timestep on the system's state vector. Combined with the typical stiffness, which leads to an excessive number of required timesteps, it is of utmost importance to minimize the computational footprint per step.

To address this issue, we are currently developing a software framework, that allows for the implementation of efficient kMC simulation software for almost any arbitrary Markov jump models. On an abstract level, the user specifies structural information on the specific model using a Python interface. A code generator then analyzes this information and writes an optimized software skeleton in C++ which only needs to be complemented by user-provided subroutines for the update of the propensities/process rates. When sparsity is present, e.g. for local interactions in spatially extended systems, this can be exploited leading to a code with close to constant computational complexity per step.

We demonstrate the usage and efficiency of our framework on established models such as a dynamical Ising and a CO oxidation model. Benchmarking against specialized state-of-the-art kMC software, we find that we can achieve similar efficiency. The general purpose nature of the library also allows for the implementation of long-range interactions.

LB simulation of sedimented photo-catalytic Pacman colloids

Jérémie Bertrand[4], Ignacio Pagonabarraga[4], Sara Bonella[4]

Inspired by experiments, we modeled and performed numerical simulations of photo-chemically active Pacman-shaped colloid using hybrid lattice-Boltzmann/free-energy framework (implemented in open-source code Ludwig[56]). We show that the built-in asymmetry of Pacman colloids influences the activity profile (due to geometry and shadow effects) which fosters asymmetric gradients of the photo-chemical in the vicinity of the colloid. The resulting fluid flows create torque which, via momentum balance, turn the colloid to the stable mouth up configuration. With an added interaction, we find a transient "flip" behavior and finally a stable mouth down configuration.

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Particle margination and interaction with solids in biomedical flows

Raquel Dapena García[1], Vicente Pérez Muñuzuri[1]

Cardiovascular diseases are a leading cause of death globally. Among them, some are linked to stenosis, which is an abnormal narrowing of blood vessels, as well as with other factors. Smart drug delivery systems based on micro and nanoparticles are a promising method for providing non/minimally invasive therapeutic mechanisms and are currently under active research. This proposal aims to further scientific knowledge of new strategies based on blood flow-guided drug carriers. We will study from a numerical point of view the lateral migration of particles in blood vessel flows using a lattice-Boltzmann model (LBM). The presence in the vessel of stenosis and stents will also be considered with the goal of improving the efficiency of stent localization.

In our lattice-Boltzmann Model we hope to incorporate new parametrizations, such as elastic walls and collision models for a myriad of different particles, including RBCs. The role of other blood cells, like platelets and white blood cells, and other blood particles such as fatty nanoparticles and exosomes, will also be analyzed.

Red blood cell transport in ex-vivo mouse retinal capillaries

Eren Çolak[2,3], Özgur Ekici[3], Timm Krüger[4], Şefik Evren Erdener[5]

The energy requirements of the central nervous system require a highly efficient micro-circulatory system, continuously providing oxygen and nutrients to the parenchyma. Since acute and chronic neurodegenerative conditions may be related to micro-circulatory dysfunction, it is necessary to understand the physical mechanisms governing cell transport in capillaries. Unlike blood flow in large vessels which can be described by non-Newtonian continuum models[57], the transport of red blood cells (RBCs, 8 µm diameter) in capillaries (often smaller than 5 µm in diameter) requires particulate models that can capture effects such as RBC partitioning and lingering at bifurcation[58, 59]. In this study, mouse capillaries obtained *ex vivo* are used to numerically investigate the haemodynamics within realistic capillary geometries, where the diameter of the capillary is changing in every 0.5 µm to observe the capillary transit time heterogeneity[60] (CTTH) and its effects on the neurodegenerative disorders. We employ a numerical solver based on the lattice-Boltzmann method for fluid flow, the finite-element method for the RBC dynamics and the immersed-boundary method for the fluid-cell interaction[61]. We investigate the effect of tube haematocrit (volume fraction of RBCs in blood), cell confinement and red cell distribution width (RDW) on the flow rate and discharge haematocrit (ratio of RBC flow rate to blood flow rate), and CTTH.

Implicit solvent model for ion-electrode Interactions in dilute solutions

Paul Desmarchelier[6], Benjamin Rotenberg[6,7]

The study of confined ionic solutions has gained renewed attention in the last decade, with for instance the flow through a nanopore[62] or application such as ions detection/characterization thanks to nanogap capacitors[63]. In this context, molecular dynamics has been particularly useful, in particular in the case of ions confined between metallic plates[64]. However, the case of large inter-electrode distances and dilute solutions presents a computational challenge due to the large number of particles involved. This can be addressed with an implicit solvent model drastically reducing the particle count. This has been tackled before, for instance by modeling the image charges at the liquid solid interface[40]. Our approach focuses on developing an electrostatic interaction model for ions between two metallic plates embedded in an implicit solvent under constant potential conditions. Drawing inspiration from the work of dos Santos *et al.*[65], we model the solvent as a uniform dielectric medium and employ 2D periodic boundary conditions. The metallic electrodes are represented by explicit atoms embedded in a Thomas–Fermi medium. Our solution if the electrostatic problem leverages existing Green's function solutions for these equations. We implement this implicit solvent model in the MetalWalls[66] code.

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Charge regulation in polypeptides

Ipsita Padhee[1], Vojtěch Keprta[1], Sebastian Pineda[1], Miroslav Štěpánek[1], Peter Košovan[1]

Understanding the behavior of weak polyelectrolytes, like polypeptides, as a function of pH is crucial for biological and material applications, as the charge regulation affects structure, stability and function. Therefore, we investigated the charge regulation of a polypeptide sequence of Glutamate and Tyrosine (EEEEY), focusing on its degree of ionization as a function of pH. Computationally, coarse-grain modeling was used while experimentally, potentiometric titration and fluorimetry were used to calculate the degree of ionization and p$K_a$values and compared with the Henderson–Hasselbalch equation.

The comparison between the experimental and simulation results shows that the simple models can predict the real ionization behavior of peptides by following a similar overall trend. Whereas some deviations from the simple model arise due to the complex electrostatic interactions. Qualitatively, these computational approaches are reliable in support of peptide charge regulation and ionization dynamics, but improvements in modeling are needed for quantitative accuracy.

Improved gas selectivity in SAPO-34 with ionic liquid impregnation: A Monte Carlo study

Hafsa M. Ashraf[2,3], Amro M. O. Mohamed[2], Ioannis G. Economou[2]

Small-pore zeolites like SAPO-34 are highly valued in adsorption due to their unique structural properties. In this study, Grand Canonical Monte Carlo (GCMC) simulations were employed to model the adsorption isotherms of CO_2, CH_4, C_2H_6, C_2H_4, C_3H_8, and C_3H_6 on pristine SAPO-34. The simulated isotherms for CO_2, C_2H_6, C_3H_8, and C_3H_6 showed good agreement with experimental data, while CH_4 and C_2H_4 deviated due to weaker and quadrupolar interactions. Pristine SAPO-34 demonstrated CO_2/CH_4 and CO_2/N_2 selectivities of 4.43 and 24.18, respectively, at 298 K and the simulated CO_2/CH_4 was agreeing with the experimental value. The encapsulation of 1-butyl-3-methylimidazolium acetate [Bmim][Ac] ionic liquid into SAPO-34 further enhanced gas separation performance. CO_2/N_2 selectivity was enhanced by 60 % upon the addition of 5.4 wt% ionic liquid (IL) at 10 kPa.

This improvement is attributed to the ionic liquid's ability to modify pore size and increase the number of adsorption sites, facilitating better CO_2 capture. The regenerability factor (R factor) of pristine SAPO-34 and the impregnated SAPO-34 with IL was calculated based on vacuum regenerability. R factor for pristine SAPO-34 was 86.5 % and it decreased by the addition of IL and it was 69.72 % at 5.4 wt% IL. The structural properties were calculated for pristine SAPO-34 and IL@SAPO-34. Both the pore diameter and pore-limiting diameter remain constant up to 10 wt% IL, indicating that gas diffusion is unaffected until this point upon the addition of the IL. These findings, supported by Monte Carlo simulations and experimental validation, underscore the potential of IL@SAPO-34 hybrids for efficient CO_2 separation in industrial applications, offering substantial enhancements over pristine SAPO-34.

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Bibliography

[1] Florian Weik, Rudolf Weeber, Kai Szuttor, Konrad Breitsprecher, Joost de Graaf, Michael Kuron, Jonas Landsgesell, Henri Menke, David Sean, and Christian Holm. ESPResSo 4.0 – an extensible software package for simulating soft matter systems. *European Physical Journal Special Topics*, 227(14):1789–1816, 2019. doi:10.1140/epjst/e2019-800186-9.

[2] Martin Bauer, Sebastian Eibl, Christian Godenschwager, Nils Kohl, Michael Kuron, Christoph Rettinger, Florian Schornbaum, Christoph Schwarzmeier, Dominik Thönnes, Harald Köstler, and Ulrich Rüde. WALBERLA: A block-structured high-performance framework for multiphysics simulations. *Computers & Mathematics with Applications*, 81:478–501, 2021. doi:10.1016/j.camwa.2020.01.007.

[3] Rudolf Weeber, Jean-Noël Grad, David Beyer, Pablo M. Blanco, Patrick Kreissl, Alexander Reinauer, Ingo Tischler, Peter Košovan, and Christian Holm. ESPResSo, a versatile open-source software package for simulating soft matter systems. In Manuel Yáñez and Russell J. Boyd, editors, *Comprehensive Computational Chemistry*, pages 578–601. Elsevier, Oxford, 1st edition, 2024. ISBN 978-0-12-823256-9. doi:10.1016/B978-0-12-821978-2.00103-3.

[4] Charles R. Harris, K. Jarrod Millman, Stéfan J. van der Walt, Ralf Gommers, Pauli Virtanen, David Cournapeau, Eric Wieser, Julian Taylor, Sebastian Berg, Nathaniel J. Smith, Robert Kern, Matti Picus, Stephan Hoyer, Marten H. van Kerkwijk, Matthew Brett, Allan Haldane, Jaime Fernández del Río, Mark Wiebe, Pearu Peterson, Pierre Gérard-Marchant, Kevin Sheppard, Tyler Reddy, Warren Weckesser, Hameer Abbasi, Christoph Gohlke, and Travis E. Oliphant. Array programming with NumPy. *Nature*, 585(7825):357–362, September 2020. doi:10.1038/s41586-020-2649-2.

[5] David Beyer, Paola B. Torres, Sebastian P. Pineda, Claudio F. Narambuena, Jean-Noël Grad, Peter Košovan, and Pablo M. Blanco. pyMBE: The Python-based molecule builder for ESPResSo. *The Journal of Chemical Physics*, 161(2):022502, July 2024. doi:10.1063/5.0216389.

[6] Iveta Jančigová, Kristína Kovalčíková, Rudolf Weeber, and Ivan Cimrák. PyOIF: Computational tool for modelling of multi-cell flows in complex geometries. *PLoS Computational Biology*, 16(10):e1008249, 2020. doi:10.1371/journal.pcbi.1008249.

[7] S. Y. Mashayak, Mara N. Jochum, Konstantin Koschke, N. R. Aluru, Victor Rühle, and Christoph Junghans. Relative entropy and optimization-driven coarse-graining methods in VOTCA. *PLOS ONE*, 10(7):1–20, July 2015. doi:10.1371/journal.pone.0131754.

[8] Rokas Elijošius, Fabian Zills, Ilyes Batatia, Sam Walton Norwood, Dávid Péter Kovács, Christian Holm, and Gábor Csányi. Zero shot molecular generation via similarity kernels. arXiv:2402.08708 [physics.chem-ph], 2024. doi:10.48550/arXiv.2402.08708.

[9] Samuel Tovey, Christoph Lohrmann, Tobias Merkt, David Zimmer, Konstantin Nikolaou, Simon Koppenhöfer, Anna Bushmakina, Jonas Scheunemann, and Christian Holm. SwarmRL: Building the future of smart active systems. arXiv:2404.16388 [cs.RO], 2024. doi:10.48550/arXiv.2404.16388.

[10] Martin Bauer, Johannes Hötzer, Dominik Ernst, Julian Hammer, Marco Seiz, Henrik Hierl, Jan Hönig, Harald Köstler, Gerhard Wellein, Britta Nestler, and Ulrich Rüde. Code generation for massively parallel phase-field simulations. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, New York, New York, USA, 2019. Association for Computing Machinery. ISBN 978-1-4503-6229-0. doi:10.1145/3295500.3356186.

[11] Timm Krüger, Halim Kusumaatmaja, Alexandr Kuzmin, Orest Shardt, Goncalo Silva, and Erlend Magnus Viggen. *The lattice Boltzmann method: Principles and practice*. Graduate Texts in Physics. Springer International Publishing, Switzerland, 2017. ISBN 978-3-319-44647-9. doi:10.1007/978-3-319-44649-3.

[12] Xiaowen Shan and Hudong Chen. Lattice Boltzmann model for simulating flows with multiple phases and components. *Physical Review E*, 47(3):1815–1819, March 1993. doi:10.1103/physreve.47.1815.

[13] Michael R. Swift, W. R. Osborn, and J. M. Yeomans. Lattice Boltzmann simulation of nonideal fluids. *Physical Review Letters*, 75(5):830–833, July 1995. doi:10.1103/physrevlett.75.830.

[14] Andrew K. Gunstensen, Daniel H. Rothman, Stéphane Zaleski, and Gianluigi Zanetti. Lattice Boltzmann model of immiscible fluids. *Physical Review A*, 43(8):4320–4327, April 1991. doi:10.1103/physreva.43.4320.

[15] T. Reis and T. N. Phillips. Lattice Boltzmann model for simulating immiscible two-phase flows. *Journal of Physics A: Mathematical and Theoretical*, 40(14):4033–4053, 2007. doi:10.1088/1751-8113/40/14/018.

[16] M. Latva-Kokko and Daniel H. Rothman. Static contact angle in lattice Boltzmann models of immiscible fluids. *Physical Review E*, 72(4), October 2005. doi:10.1103/physreve.72.046701.

[17] Martin Bauer, Harald Köstler, and Ulrich Rüde. lbmpy: Automatic code generation for efficient parallel lattice Boltzmann methods. *Journal of Computational Science*, 49:101269, 2021. doi:10.1016/j.jocs.2020.101269.

[18] Frederik Hennig, Markus Holzer, and Ulrich Rüde. Advanced automatic code generation for multiple relaxation-time lattice Boltzmann methods. *SIAM Journal on Scientific Computing*, 45(4):C233–C254, 2023. doi:10.1137/22M1531348.

[19] Konrad Breitsprecher, Christian Holm, and Svyatoslav Kondrat. Charge me slowly, I am in a hurry: optimizing charge–discharge cycles in nanoporous supercapacitors. *ACS Nano*, 12(10):9733–9741, August 2018. doi:10.1021/acsnano.8b04785.

[20] Peter Košovan, Jitka Kuldová, Zuzana Limpouchová, Karel Procházka, Ekaterina B. Zhulina, and Oleg V. Borisov. Molecular dynamics simulations of a polyelectrolyte star in poor solvent. *Soft Matter*, 6(9):1872–1874, 2010. doi:10.1039/B925067K.

[21] Jonas Landsgesell, David Beyer, Pascal Hebbeker, Peter Košovan, and Christian Holm. The pH-dependent swelling of weak polyelectrolyte hydrogels modeled at different levels of resolution. *Macromolecules*, 55(8):3176–3188, February 2022. doi:10.1021/acs.macromol.1c02489.

[22] David Beyer and Christian Holm. Unexpected two-stage swelling of weak polyelectrolyte brushes with divalent counterions. *ACS Macro Letters*, 13(9):1185–1191, 2024. doi:10.1021/acsmacrolett.4c00421.

[23] Kai Szuttor, Florian Weik, Jean-Noël Grad, and Christian Holm. Modeling the current modulation of bundled DNA structures in nanopores. *The Journal of Chemical Physics*, 154(5):054901, 2021. doi:10.1063/5.0038530.

[24] Kai Szuttor, Patrick Kreissl, and Christian Holm. A numerical investigation of analyte size effects in nanopore sensing systems. *The Journal of Chemical Physics*, 155(13):134902, 2021. doi:10.1063/5.0065085.

[25] G. Inci, A. Kronenburg, R. Weeber, and D. Pflüger. Langevin dynamics simulation of transport and aggregation of soot nano-particles in turbulent flows. *Flow, Turbulence and Combustion*, 98(4):1065–1085, January 2017. doi:10.1007/s10494-016-9797-3.

[26] Benedict J. Reynwar, Gregoria Illya, Vagelis A. Harmandaris, Martin M. Müller, Kurt Kremer, and Markus Deserno. Aggregation and vesiculation of membrane proteins by curvature-mediated interactions. *Nature*, 447(7143):461–464, May 2007. doi:10.1038/nature05840.

[27] Miru Lee, Christoph Lohrmann, Kai Szuttor, Harold Auradou, and Christian Holm. The influence of motility on bacterial accumulation in a microporous channel. *Soft Matter*, 17(4):893–902, 2021. doi:10.1039/d0sm01595d.

[28] Kenneth Hoste, Jens Timmerman, Andy Georges, and Stijn De Weirdt. EasyBuild: Building software with ease. In *Proceedings of the 2012 SC Companion: High Performance Computing, Networking Storage and Analysis*, Los Alamitos, California, USA, November 2012. IEEE. ISBN 978-0-7695-4956-9. doi:10.1109/SC.Companion.2012.81.

[29] Markus Geimer, Kenneth Hoste, and Robert McLay. Modern scientific software management using EasyBuild and Lmod. In *2014 First International Workshop on HPC User Support Tools*, pages 41–51, 2014. ISBN 978-1-4673-6755-4. doi:10.1109/HUST.2014.8.

[30] Bob Dröge, Victor Holanda Rusu, Kenneth Hoste, Caspar van Leeuwen, Alan O'Cais, and Thomas Röblitz. EESSI: A cross-platform ready-to-use optimised scientific software stack. *Software: Practice and Experience*, 53(1):176–210, January 2023. doi:10.1002/spe.3075.

[31] Axel Arnold, Florian Fahrenberger, Christian Holm, Olaf Lenz, Matthias Bolten, Holger Dachsel, Rene Halver, Ivo Kabadshow, Franz Gähler, Frederik Heber, Julian Iseringhausen, Michael Hofmann, Michael Pippig, Daniel Potts, and Godehard Sutmann. Comparison of scalable fast methods for long-range interactions. *Physical Review E*, 88(6):063308, December 2013. doi:10.1103/PhysRevE.88.063308.

[32] P. P. Ewald. Die Berechnung optischer und elektrostatischer Gitterpotentiale. *Annalen der Physik*, 369(3): 253–287, 1921. doi:10.1002/andp.19213690304.

[33] Markus Deserno and Christian Holm. How to mesh up Ewald sums. I. A theoretical and numerical comparison of various particle mesh routines. *The Journal of Chemical Physics*, 109:7678, November 1998. doi:10.1063/1.477414.

[34] Markus Deserno and Christian Holm. How to mesh up Ewald sums. II. An accurate error estimate for the Particle–Particle–Particle-Mesh algorithm. *The Journal of Chemical Physics*, 109:7694, November 1998. doi:10.1063/1.477415.

[35] In-Chul Yeh and Max L. Berkowitz. Ewald summation for systems with slab geometry. *The Journal of Chemical Physics*, 111(7):3155–3162, August 1999. doi:10.1063/1.479595.

[36] Axel Arnold, Jason de Joannis, and Christian Holm. Electrostatics in periodic slab geometries. I. *The Journal of Chemical Physics*, 117(6):2496–2502, August 2002. doi:10.1063/1.1491955.

[37] Jason de Joannis, Axel Arnold, and Christian Holm. Electrostatics in periodic slab geometries. II. *The Journal of Chemical Physics*, 117(6):2503–2512, August 2002. doi:10.1063/1.1491954.

[38] Sandeep Tyagi, Axel Arnold, and Christian Holm. ICMMM2D: An accurate method to include planar dielectric interfaces via image charge summation. *The Journal of Chemical Physics*, 127(15):154723, October 2007. doi:10.1063/1.2790428.

[39] Sandeep Tyagi, Axel Arnold, and Christian Holm. Electrostatic layer correction with image charges: A linear scaling method to treat slab 2D + h systems with dielectric interfaces. *The Journal of Chemical Physics*, 129 (20):204102, 2008. doi:10.1063/1.3021064.

[40] Sandeep Tyagi, Mehmet Süzen, Marcello Sega, Marcia C. Barbosa, Sofia S. Kantorovich, and Christian Holm. An iterative, fast, linear-scaling method for computing induced charges on arbitrary dielectric boundaries. *The Journal of Chemical Physics*, 132(15):154112, 2010. doi:10.1063/1.3376011.

[41] Axel Arnold, Konrad Breitsprecher, Florian Fahrenberger, Stefan Kesselheim, Olaf Lenz, and Christian Holm. Efficient algorithms for electrostatic interactions including dielectric contrasts. *Entropy*, 15(11):4569–4588, 2013. doi:10.3390/e15114569.

[42] M. Gouy. Sur la constitution de la charge électrique à la surface d'un électrolyte. *Journal de Physique Théorique et Appliquée*, 9(1):457–468, 1910. doi:10.1051/jphystap:019100090045700.

[43] David Leonard Chapman. A contribution to the theory of electrocapillarity. *Philosophical Magazine*, 25(148): 475–481, April 1913. doi:10.1080/14786440408634187.

[44] Hans-Jürgen Butt, Karlheinz Graf, and Michael Kappl. *Physics and Chemistry of Interfaces*, chapter 4: *The electric double layer*, pages 42–56. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2003. ISBN 9783527602315. doi:10.1002/3527602313.ch4.

[45] David C. Grahame. The electrical double layer and the theory of electrocapillarity. *Chemical Reviews*, 41(3): 441–501, 1947. doi:10.1021/cr60130a002.

[46] B. V. Derjaguin and L. D. Landau. Theory of the stability of strongly charged lyophobic sols and of the adhesion of strongly charged particles in solutions of electrolytes. *Acta Physicochimica (USSR)*, 14:633–650, 1941.

[47] E. J. Verwey and J. Th. G. Overbeek. *Theory of the stability of lyophobic colloids: The interaction of sol particles having an electric double layer*. Elsevier, Leiden, 1948.

[48] Tobias Rau, Florian Weik, and Christian Holm. A dsDNA model optimized for electrokinetic applications. *Soft Matter*, 13(21):3918–3926, 2017. doi:10.1039/C7SM00270J.

[49] Florian Weik, Stefan Kesselheim, and Christian Holm. A coarse-grained DNA model for the prediction of current signals in DNA translocation experiments. *The Journal of Chemical Physics*, 145(19):194106, 2016. doi:10.1063/1.4967458.

[50] Florian Weik, Kai Szuttor, Jonas Landsgesell, and Christian Holm. Modeling the current modulation of dsDNA in nanopores – from mean-field to atomistic and back. *European Physical Journal Special Topics*, 227(14): 1639–1655, 2019. doi:10.1140/epjst/e2019-800189-3.

[51] Tobias Lemke and Christine Peter. Neural network based prediction of conformational free energies - A new route toward coarse-grained simulation models. *Journal of Chemical Theory and Computation*, 13(12): 6213–6221, 2017. doi:10.1021/acs.jctc.7b00864.

[52] Simon Hunkler, Tobias Lemke, Christine Peter, and Oleksandra Kukharenko. Back-mapping based sampling: Coarse grained free energy landscapes as a guideline for atomistic exploration. *The Journal of Chemical Physics*, 151(15):154102, October 2019. doi:10.1063/1.5115398.

[53] Simon Hunkler, Teresa Buhl, Oleksandra Kukharenko, and Christine Peter. Generating a conformational landscape of ubiquitin chains at atomistic resolution by back-mapping based sampling. *Frontiers in Chemistry*, 10:1087963, January 2023. doi:10.3389/fchem.2022.1087963.

[54] Kenneth O. Stanley and Risto Miikkulainen. Evolving neural networks through augmenting topologies. *Evolutionary Computation*, 10(2):99–127, June 2002. doi:10.1162/106365602320169811.

[55] Benedikt Hartl, Maximilian Hübl, Gerhard Kahl, and Andreas Zöttl. Microswimmers learning chemotaxis with genetic algorithms. *Proceedings of the National Academy of Sciences*, 118(19):e2019683118, 2021. doi:10.1073/pnas.2019683118.

[56] Jean-Christophe Desplat, Ignacio Pagonabarraga, and Peter Bladon. LUDWIG: A parallel lattice-Boltzmann code for complex fluids. *Computer Physics Communications*, 134(3):273–290, 2001. doi:10.1016/S0010-4655(00)00205-8.

[57] Edward W. Merrill, Giles C. Cokelet, Anthony Britten, and Roe E. Wells, Jr. Non-Newtonian rheology of human blood - effect of fibrinogen deduced by "subtraction". *Circulation Research*, 13(1):48–55, July 1963. doi:10.1161/01.RES.13.1.48.

[58] Peter Balogh and Prosenjit Bagchi. Analysis of red blood cell partitioning at bifurcations in simulated microvascular networks. *Physics of Fluids*, 30(5):051902, May 2018. doi:10.1063/1.5024783.

[59] Yazdan Rashidi, Greta Simionato, Qi Zhou, Thomas John, Alexander Kihm, Mohammed Bendaoud, Timm Krüger, Miguel O. Bernabeu, Lars Kaestner, Matthias W. Laschke, Michael D. Menger, Christian Wagner, and Alexis Darras. Red blood cell lingering modulates hematocrit distribution in the microcirculation. *Biophysical Journal*, 122(8):1526–1537, 2023. doi:10.1016/j.bpj.2023.03.020.

[60] Mark B. Vestergaard, Helle K. Iversen, Sofie Amalie Simonsen, Ulrich Lindberg, Stig P. Cramer, Ulrik B. Andersen, and Henrik B. W. Larsson. Capillary transit time heterogeneity inhibits cerebral oxygen metabolism in patients with reduced cerebrovascular reserve capacity from steno-occlusive disease. *Journal of Cerebral Blood Flow & Metabolism*, 43(3):460–475, 2023. doi:10.1177/0271678X221139084.

[61] Gábor Závodszky, Britt van Rooij, Victor Azizi, and Alfons Hoekstra. Cellular level *in-silico* modeling of blood rheology with an improved material model for red blood cells. *Frontiers in Physiology*, 8:563, 2017. doi:10.3389/fphys.2017.00563.

[62] Samuel Faucher, Narayana Aluru, Martin Z. Bazant, Daniel Blankschtein, Alexandra H. Brozena, John Cumings, J. Pedro de Souza, Menachem Elimelech, Razi Epsztein, John T. Fourkas, Ananth Govind Rajan, Heather J. Kulik, Amir Levy, Arun Majumdar, Charles Martin, Michael McEldrew, Rahul Prasanna Misra, Aleksandr Noy, Tuan Anh Pham, Mark Reed, Eric Schwegler, Zuzanna Siwy, YuHuang Wang, and Michael Strano. Critical knowledge gaps in mass transport through single-digit nanopores: A review and perspective. *The Journal of Physical Chemistry C*, 123(35):21309–21326, 2019. doi:10.1021/acs.jpcc.9b02178.

[63] Serge G. Lemay, Shuo Kang, Klaus Mathwig, and Pradyumna S. Singh. Single-molecule electrochemistry: Present status and outlook. *Accounts of Chemical Research*, 46(2):369–377, 2013. doi:10.1021/ar300169d.

[64] Laura Scalfi, Mathieu Salanne, and Benjamin Rotenberg. Molecular simulation of electrode-solution interfaces. *Annual Review of Physical Chemistry*, 72:189–212, 2021. doi:10.1146/annurev-physchem-090519-024042.

[65] Alexandre P. dos Santos, Matheus Girotto, and Yan Levin. Simulations of Coulomb systems confined by polarizable surfaces using periodic Green functions. *The Journal of Chemical Physics*, 147(18):184105, 2017. doi:10.1063/1.4997420.

[66] Abel Marin-Laflèche, Matthieu Haefele, Laura Scalfi, Alessandro Coretti, Thomas Dufils, Guillaume Jeanmairet, Stewart K. Reed, Alessandra Serva, Roxanne Berthin, Camille Bacon, Sara Bonella, Benjamin Rotenberg, Paul A. Madden, and Mathieu Salanne. MetalWalls: A classical molecular dynamics software dedicated to the simulation of electrochemical systems. *Journal of Open Source Software*, 5(53):2373, 2020. doi:10.21105/joss.02373.

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