CECAM workshop

Modeling & simulation of fluid-structure interactions across scales

Book of abstracts

National Institute of Chemistry, Ljubljana, Slovenia
April 8, 2025 – April 11, 2025

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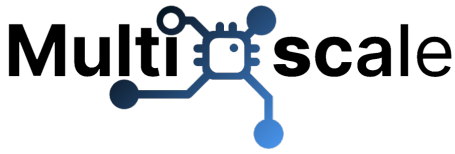

Workshop
Modeling & simulation of fluid-structure interactions across scales

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Laboratory for Molecular Modeling, National Institute of Chemistry, Ljubljana

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Contents

General Information

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Godehard Sutmann, Forschungszentrum Jülich, Jülich, Germany
Rudolf Weeber, Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

Venue

National Institute of Chemistry
Hajdrihova ulica 19, 1000 Ljubljana, Slovenia
web page: `https://www.ki.si/en`

Accommodation

Hotel Exe Lev
Vošnjakova ulica 1, 1000 Ljubljana, Slovenia
web page: `https://www.exelev.com`

How to get from Ljubljana Airport to Hotel Exe Lev?
There are several options to get from Ljubljana Airport to Hotel Exe Lev. Some of them are listed below.

Transfer by hotel shuttle
Web page: `https://www.exelev.com`
E-mail: `reservations@exelev.com`

To reserve a hotel shuttle service to the accommodation, send an email directly to the hotel with the details of the hotel reservation and the flight.

Transfer by Taxi Metro
Web page: `https://www.taximetro.si/en/company-hub-homepage/`
Phone: +386 41 240 200
E-mail: `info@taximetro.si`

The transfer costs approximately 35 EUR (one way). Airport transportation services are available 24/7 and can be booked in advance. To send an inquiry visit `https://www.taximetro.si/en/order`.

Transfer by GoOpti shuttle
Web page: `https://www.goopti.com/en`

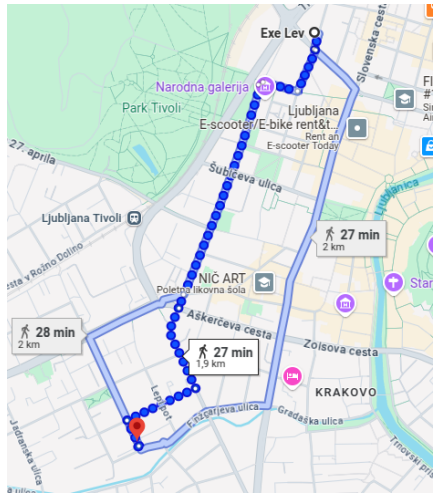
The transfer must be booked in advance at `https://www.goopti.com/en` and customers can be taken directly from the airport to their accommodation. The transfer costs approximately 11-15 EUR (one way).

Transfer by bus
Web page: `https://www.ap-ljubljana.si/en`

The departure timetables from the airport are available at `https://www.ap-ljubljana.si/en`, where passengers should select the route from Brnik/airport Ljubljana to Ljubljana AP (i.e., the main station). The main station is about a 10 minutes' walk from the accommodation (Hotel Exe Lev). Tickets can be purchased directly from the driver, but passengers are encouraged to buy them in advance at sales points.

How to get from the Hotel Exe Lev to the venue?
The accommodation is located 2 km from the venue. Below, there are several options for transportation from the accommodation to the venue.

Walk
It takes approximately a 27 minutes' walk from the hotel to the National Institute of Chemistry.



Transfer by Taxi Metro
Web page: `https://www.taximetro.si/en/company-hub-homepage/`
Phone: +386 41 240 200
E-mail: `info@taximetro.si`

The transportation services are available 24/7 and can be booked in advance. To send an inquiry visit `https://www.taximetro.si/en/order`.

Transfer by public transport
Web page: `https://www.lpp.si/en`

At Gosposvetska bus station, passengers can take bus number 1 in the direction DOLGI MOST P+R and exit at Tobačna bus station. The journey takes about 10 minutes. From Tobačna bus station to the venue is about an 8 minutes' walk (600 m). The bus ticket costs 1.30 EUR and can be paid with the Urbana card, Visa, or Mastercard. For more information on payment methods visit `https://www.lpp.si/en`. The timetables can be accessed using the LPP schedules app on Google Play or the Ljubljana Bus app on iOS App Store.

Cafes and Restaurants

The cafes and restaurants listed below are located close to the venue (up to a 15 minutes' walk).

Bar Kolezija
Gunduličeva 7, 1000 Ljubljana
(Located in front of the venue.)

Langus Kavarna
Langusova ulica 4, 1000 Ljubljana
(Approximately a 5 minutes' walk from the venue.)

Corner pub
Tržaška cesta 19, 1000 Ljubljana
(Approximately a 6 minutes' walk from the venue.)

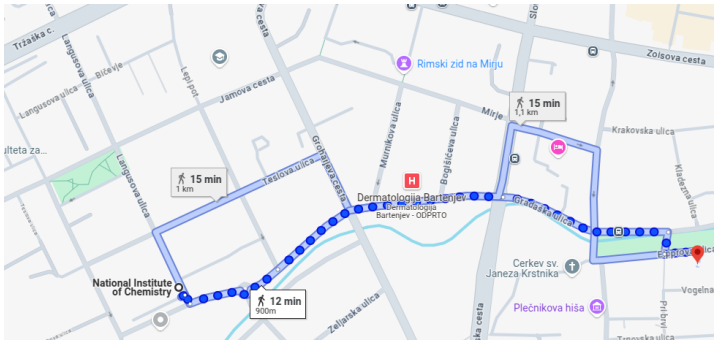
Italian restaurant Mirje
Tržaška cesta 5, 1000 Ljubljana
(Approximately a 9 minutes' walk from the venue.)

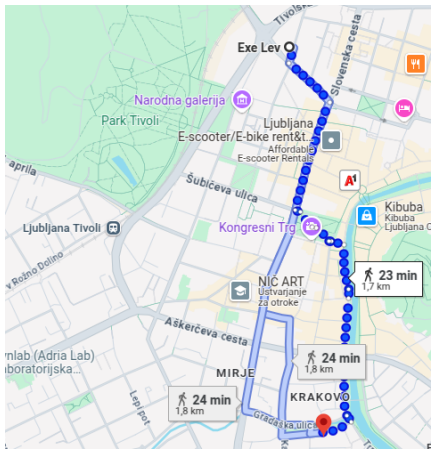
Gostilnica in pivnica Vič
Trg mladinskih delovnih brigad 8, 1000 Ljubljana
(Approximately a 15 minutes' walk from the venue.)

Gostilnica 5-6 kg
Eipprova ulica 17, 1000 Ljubljana
(Approximately a 15 minutes' walk from the venue.)

Social dinner
The workshop dinner will take place on Wednesday, April 9, at the restaurant Dežela okusov, which is located in the vicinity of the venue. More information about the restaurant is available at `https://dezela-okusov.si`.

The restaurant is about a 12 minutes' walk (see the upper map) from the venue and about a 23 minutes' walk from the Hotel Exe Lev (see the bottom map).





Description

In today's world, the modeling and simulation of complex systems span a wide range of disciplines, from biology and chemistry to engineering and beyond. Understanding these systems requires a multiscale approach that integrates knowledge from various levels of organization, from molecular interactions to macroscopic behavior. This approach is crucial for tackling challenges in diverse fields such as bioliquids, energy storage devices, and helicopter dynamics. In the realm of bioliquids, such as biomolecules and cellular components, multiscale modeling plays a pivotal role in unraveling the complexities of biological processes. From protein folding to membrane dynamics, researchers employ techniques ranging from atomistic simulations to coarse-grained models to capture the intricate interplay of molecules within cellular environments. These models not only enhance our fundamental understanding of biological systems but also have practical applications in drug design and personalized medicine. Similarly, the design and optimization of batteries demand a multiscale perspective to address issues ranging from electrode materials to system-level performance. Atomistic simulations provide insights into the behavior of ions and electrons within electrode materials, guiding the development of novel chemistries with enhanced energy storage capabilities. Meanwhile, continuum models facilitate the prediction of battery performance under various operating conditions, aiding in the design of safer and more efficient energy storage devices. In the field of helicopter dynamics, multiscale modeling enables engineers to simulate the interaction between aerodynamics, structural mechanics, and control systems. By integrating these disparate disciplines, engineers can optimize helicopter design for improved performance, maneuverability, and safety. Despite significant advancements, multiscale modeling of complex systems still faces challenges. Bridging the gap between different scales, accurately representing system dynamics, and incorporating uncertainty remain areas of active research. Furthermore, the increasing complexity of modern systems demands innovative computational techniques and interdisciplinary collaboration. In conclusion, the state of the art in multiscale modeling and simulation of complex systems encompasses a diverse range of applications, from

bioliquids and batteries to helicopters. By integrating knowledge across multiple scales, researchers strive to unravel the mysteries of nature, optimize technological innovations, and address pressing societal challenges.

Program

All listed times are in Europe/Ljubljana - GMT+02:00 (CEST).

Tuesday April 8th 2025 - Day 1

14:00 to 14:45	Registration
14:45 to 15:00	Welcome & Introduction
15:00 to 15:45	**Matevž Dular** *Interaction of a cavitation bubble and a nearby structure*
15:45 to 16:30	**Sergey Karabasov** *Fluid dynamics modelling from micro to macro scales*
16:30 to 16:45	Coffee break
16:45 to 17:30	**Jens Harting** *Capillary interactions between soft capsules, hard particles and droplets at thin fluid films*
17:30 to 18:15	**Marco Ellero** *Lagrangian Heterogeneous Multiscale Method for the simulation of polymeric fluids*
18:15 to 20:00	Poster session & Aperitif

Wednesday April 9th 2025 - Day 2

09:00 to 09:45	**Alan O'Cais** *Scientific Software made EESSI*

09:45 to 10:30	**Laura Grigori** *Randomization techniques for solving high dimensional problems*
10:30 to 11:00	Coffee break
11:00 to 11:45	**Paul Desmarchelier** *From explicit to implicit models of electric double-layer nanocapacitors with tunable metallicity*
11:45 to 12:30	**Rocio Semino** *Multiscale Modeling of Metal-Organic Frameworks and their Composites*
12:30 to 14:00	Lunch
14:00 to 15:00	Discussion
15:00 to 15:45	**Céline Merlet** *Simulations of carbon-electrolyte interfaces in supercapacitors across scales*
15:45 to 16:30	**Matija Gatalo** *Black powder at the 'heart' of the hydrogen technologies*
16:30 to 16:45	Coffee break
16:45 to 17:30	**Robert Dominko** *How a computational approach can accelerate the development of batteries*
17:30 to 18:15	**Marta Klanjšek Gunde** *Influence of microencapsulation on the phase change of the core material*
19:30 to 00:00	Social dinner

Thursday April 10th 2025 - Day 3

09:00 to 09:45	**Horacio V Guzman** *Fine Tuning the Adsorption of Biomacromolecules at the Solid Liquid Interfaces*
09:45 to 10:30	**Jean-Philip Piquemal** *Large-scale simulations for biophysics: from polarizable force fields to neural networks*
10:30 to 11:00	Coffee break

11:00 to 11:45	**Carlo de Falco** *Performance portability in a compressible fluid simulator based on the material point method*
11:45 to 12:30	**Marco Aldinucci** *Streaming Workflows: From Scientific Applications to AI and Back*
12:30 to 14:00	Lunch
14:00 to 15:00	Discussion
15:00 to 15:45	**Sergio Decherchi** *NanoShaper: A Tool for Molecular Surface Computation and Pocket Detection*
15:45 to 16:30	**Miha Ravnik** *Passive and active topological soft matter*
16:30 to 16:45	Coffee break
16:45 to 17:30	**Tilen Potisk** *Learning macroscopic equations of motion from dissipative particle dynamics simulations of fluids*
17:30 to 18:15	**Jean-Noël Grad** *Simulating solid/liquid interfaces across scales with ESPResSo*
18:15 to 20:00	Poster session & Aperitif

Friday April 11th 2025 - Day 4

09:00 to 09:45	**Mojca Benčina** *Ultrasound-Controlled Gene Regulation in Mammalian Cells*
09:45 to 10:30	**Daniel Svenšek** *Modeling ultrasonic metafluids: The significance of discrete oscillators*
10:30 to 11:15	**Hari Haran Sudhakar** *Development and implementation of hybrid atomistic / coarse-grained modelling applied to complex interfaces*
11:15 to 11:45	Coffee break
11:45 to 12:00	Discussion
12:00 to 12:15	Closing word

Abstracts – talks

Interaction of a cavitation bubble and a nearby structure

Matevž Dular
University of Ljubljana, Ljubljana, Slovenia

Cavitation, a formation of small vapor bubbles inside an initially homogeneous liquid medium, can occur on different complexity scales - the simplest one being a single cavitation bubble. Yet, even here a plethora of phenomena are present.

In the 60', the first recordings of the bubble collapse by a high-speed camera, revealed a formation of high-velocity jets (>100 m/s) directed toward the nearby solid surface. These was associated with one of the most ubiquitous issues of cavitation – cavitation erosion, which causes failure of pumps, turbines, marine propellers and even rocket engine turbopumps.

In the talk we will discuss recent developments understanding the interaction of a single cavitation bubble with i) a rigid surface, ii) a compliant structure and iii) the bubble collapse in broken symmetry conditions. The results show a promise of controlling the bubble shape and the collapse direction, which may lead to developments in engineering, chemistry and medicine.

Fluid dynamics modelling from micro to macro scales

Sergey Karabasov
Queen Mary University of London, London, United Kingdom

High-resolution fluid dynamics simulations across the scales play an important role in many areas of science and engineering. In particular, flow interaction with solid surfaces is important in aeronautics, where bio-inspired surfaces are used for efficient noise mitigation as well as high-speed atomic force microscopy, where hydrodynamic interactions must be considered for correct characterisation of materials. In this talk, we will review recent activities in our group on both fronts, which rely on application of GPU-accelerated Large Eddy Simulations as well as hybrid continuum-molecular dynamics modelling.

Capillary interactions between soft capsules, hard particles and droplets at thin fluid films

Jens Harting
Forschungszentrum Jülich, Jülich, Germany

The ordering of particles in the drying process of a colloidal suspension is crucial in determining the properties of the resulting film. For example, microscopic inhomogeneities can, lead to the formation of cracks and defects that can deteriorate the quality of the film considerably. We study this multiscale problem using our recently developed lattice Boltzmann method, which allows for the simulation of soft deformable particles, hard colloids or even droplets (liquid lenses) attached to liquid interfaces. Although capillary interactions between rigid particles are well studied, much is still to be understood about the behavior of soft particles or liquid lenses and the role of their softness during the final stages of film drying. This includes the effect of menisci deformations and lateral capillary forces on the final film, the impact of the particle softness on the film formation or the interplay of fluid viscosity and surface tension on the coalescence of droplets.

Lagrangian Heterogeneous Multiscale Method for the simulation of polymeric fluids

Marco Ellero
Basque Center for Applied Mathematics, Bilbao, Spain

This study investigates the rheological behavior of polymer melts under complex shear flow conditions using a Lagrangian Heterogeneous Multiscale Method (LHMM). The approach combines Dissipative Particle Dynamics (DPD) and Smoothed Particle Hydrodynamics (SPH) to model the non-Newtonian behavior of polymer melts. The LHMM addresses the limitations of traditional Eulerian-based HMM methods, which often struggle to accurately simulate history-flow dependent fluids such as polymer melts. This integration effectively captures both microscopic stress contributions and macroscopic flow dynamics. Polymer chains, composed of 4 to 32 beads connected by FENE bonds, exhibit distinct relaxation dynamics under varying shear rates. As a preliminary step, DPD simulations using arbitrary flow conditions act as a virtual rheometer to determine fundamental rheological properties, including shear-dependent viscosity, mean relaxation time, and zero-shear-rate viscosity. These properties provide essential microscopic calibration for the LHMM framework, enabling accurate characterization of the Weissenberg number (Wi) and viscosity scales. The LHMM combines macroscopic shear rates and velocity gradients from SPH with microscopic stress contributions computed directly in DPD along Lagrangian trajectories using the Irving-Kirkwood (IK) method. This coupling effectively integrates polymer chain dynamics and macroscopic flow behaviors, capturing contributions from both scales under complex flow conditions. The framework is validated using Poiseuille Flow and the Flow Around a Cylinder. These tests demonstrate the LHMM's ability to model polymer melts transient and steady-state behavior. By bridging micro- and macroscales, this methodology provides valuable insights into polymer melts rheological properties and dynamics under complex flow conditions, as well as it paves the way for a general multiscale coupling in molecular fluids with memory.

Scientific Software made EESSI

Alan O'Cais
University of Barcelona, Barcelona, Spain

The **European Environment for Scientific Software Installations** (**EESSI**) is revolutionizing how researchers and HPC users create and deploy scientific software. By providing a centrally managed, collaboratively maintained software stack that is portable, performant, and reproducible across different computing environments, EESSI eliminates many of the traditional pain points in software development and deployment.

In this talk, we will explore how EESSI leverages technologies such as **EasyBuild**, **Lmod**, and **CernVM-FS** to deliver optimized software environments that work seamlessly across clusters, cloud platforms, and even personal workstations. We'll discuss the benefits of a community-driven approach to scientific software, share real-world use cases, and provide insights into how you can integrate EESSI into your own workflows.

Randomization techniques for solving high dimensional problems

Laura Grigori
EPFL, Lausanne, Switzerland
PSI, Villigen, Switzerland

In this talk we will review recent advances in using randomization for solving high dimensional problems as arising in molecular simulations. Randomization is a powerful technique that allows to leverage optimized kernels, reduce communication on large scale computers. It can be used to solve linear systems of equations, eigenvalue problems, regression problems, computing low rank approximations to deal with large volumes of data, while exploiting mixed precision arithmetic.

From explicit to implicit models of electric double-layer nanocapacitors with tunable metallicity

Paul Desmarchelier

PHENIX, Paris, France

Understanding the behaviour of electrolytes confined between metallic surfaces separated by distances between a few nm to ∼100 nm is crucial for the development of nanocapacitors and other nanoelectrochemical devices used in applications from sensing to desalination. At the nanoscale, particle-based modeling, particularly molecular dynamics in the constant-potential ensemble, has been instrumental in simulating these systems, as it allows for a realistic description of ions in a molecular solvent next to electrodes, whose metallic character can be tuned via the Thomas-Fermi model [1,2,3]. The statistical mechanics of this constant-potential ensemble further provides a direct link between the dynamics of the equilibrium fluctuations of the electrode charge and the electrical impedance of the system, which can in turn be analyzed in terms of microscopic mechanisms [4,5,6,7].

Molecular dynamics simulations are however limited to length scales smaller than ∼10 nm and time scales shorter than a few 100 ns, restricting them to sufficiently large concentrations, as well as frequencies larger than typical electrochemical impedance experiments. To overcome these constraints while capturing the dynamics of the ions on sufficiently long time scales, it is essential to reduce the number of explicitly modeled particles by implicitly representing the solvent and/or electrodes. For dilute systems, modeling the solvent's screening effect with a homogeneous dielectric constant is a reasonable approach. Several models exist for electrodes, and we demonstrate that the effects of planar electrodes with tunable metallicity can be incorporated by adding a correction to the existing Ewald summation for systems with 2D periodic boundary conditions. By not explicitly accounting for electrode atom/ion interactions, significant computational speed-ups can be achieved while retaining the effects on Coulombic interactions. We have implemented this new implicit solvation/implicit electrode scheme within the MetalWalls simulation code [8,9] and we will provide some first illustrations of this approach.

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Multiscale Modeling of Metal-Organic Frameworks and their Composites

Rocio Semino
PHENIX, Sorbonne Université, Paris, France

The unique structural diversity of metal-organic frameworks (MOFs) makes them very promising for applications in many environmental and industrial fields, such as carbon capture, drug delivery and generation of renewable energies. Despite the intense activity at electronic and atomistic resolutions, coarse grained (CG) modeling of MOFs has only very recently began being explored. The main reason for this was the lack of adequate CG force fields. In this seminar, I will first discuss the development of CG force fields for MOFs by applying CG strategies that are well known in the polymers and biomolecules communities but were never before tested for porous solids. Specifically, I will present MARTINI, Iterative Boltzmann inversion and force matching force fields for modeling ZIF-8 at three different coarse-grained resolutions [1,2], and critically compare their abilities to reproduce structure, elastic tensor, thermal expansion and the swing effect, a subtle phase transition ZIF-8 undergoes when loaded with guest molecules. Overall, all our force fields reproduce structure reasonably well. Elastic constants and volume expansion are more challenging, while force matching has proven promising for capturing the swing effect.

In the second part of the seminar, I will discuss how these force fields can be applied to model MOF/polymer composites. These composite materials are widely popular, as they ally good mechanical properties of polymers with MOF's high separation selectivities. I will summarize our most recent findings concerning the influence of MOF nanoparticle size and morphology on compatibility and gas separation performances of MOF/polymer composites via simulations at the CG level [3]. Finally, I will discuss current efforts for combining atomistic and CG resolutions within the same simulation box to study these composites. This will enable us to keep atomistic resolution at the interface between both solids, while the bulk phases can be modeled at a lower resolution to increase computational efficiency.

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[3] C. Alvares, R. Semino, under review

Simulations of carbon-electrolyte interfaces in supercapacitors across scales

Céline Merlet
CIRIMAT - CNRS - Université de Toulouse, Toulouse, France

Electrochemical double layer capacitors, often called supercapacitors, are energy storage systems which accumulate and release energy through reversible ion adsorption at electrode/electrolyte interfaces. Porous carbons are commonly used as electrode materials due to their relatively low cost and good electronic conductivity. Over the past decade, most of the simulations of supercapacitors were performed at the microscopic scale, using Molecular Dynamics (MD) simulations. This allowed to understand the adsorption of ions and the effect of surface porosity on some electrochemical properties. However it is well known from experiments that commercial materials are highly inhomogeneous, while molecular simulations, where electrode sizes are a few nanometers, only allow for the inclusion of a few pores. It is therefore necessary to simulate electrodes and supercapacitors at larger scales.

To this end, we develop a software, Lattice Porous Carbon 3D (LPC3D), designed for mesoscopic simulations of capacitive properties of carbon-carbon capacitors, based on a lattice-gas model. The code calculates properties such as quantities of adsorbed ions, diffusion coefficients and Nuclear Magnetic Resonance (NMR) spectra for ions adsorbed in porous carbons. I will show how the mesoscopic model allows to bridge the gap between the time and length scales of atomistic simulations, accurate but computationally expensive, and experimental results such as electrochemical measurements and nuclear magnetic resonance spectroscopy. I will then describe how the latest code improvements, realised in the context of the MultiXscale project, allowed us to simulate systems with length scales up to hundreds to thousands of microns and how we are moving towards coupling LPC3D with molecular simulations codes (molecular DFT and MD simulations) to increase the accuracy of the model.

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E. Lahrar, C. Merlet, Faraday Discuss. **255**, 355-369 (2025)

Black powder at the 'heart' of the hydrogen technologies

Matija Gatalo
ReCatalyst D.o.o., Ljubljana, Slovenia

In the realm of hydrogen technologies, fuel cells and water electrolysis stand out as pivotal innovations for a sustainable future in the energy and transport sectors. At the 'heart' of these technologies lies a critical component: the catalyst, often referred to as 'black powder.' This composite material, composed of high surface area carbon and platinum-based nanoparticles, plays an essential role in determining the efficiency and durability of hydrogen production and utilization processes in fuel cells and water electrolysers.

In this presentation, we will delve into the significance of this 'black powder' catalyst and its impact on hydrogen technologies. We will also introduce ReCatalyst d.o.o., a seed-stage start-up from Slovenia and a spin-out from the National Institute of Chemistry. Our journey, from inception to our current endeavours as well as future inspirations to advance the 'hearts' of hydrogen technologies. Furthermore, we will also briefly touch upon our technological relationship with various forms of modelling and how this reflects in our scale-up and product development efforts.

ReCatalyst is REvolutionising the way we make CATALYSTs for hydrogen technologies. In 2023, we have become the Slovenian Start-up-of-the-year, started with the coordination of the prestigious EIC Transition project ENABLER and also closed an oversubscribed Seed funding round co-led by reputable early-stage financial investors such as High-Tech Gründerfonds, xista science ventures and OCCIDENT.

How a computational approach can accelerate the development of batteries

Robert Dominko, Ervin Rems, Aiping Wang, Anja Kopač Lautar
National Institute of Chemistry, Ljubljana, Slovenia

Battery research is shifting from lab-scale component design to more controlled development, where innovative approaches are investigated in realistic prototype cells with well-defined electrode technology and the controlled ratio between active materials and electrolyte. This requires equipment that enables the controlled production of battery slurry and electrodes, as well as stacking machines that can be used to produce cell prototypes. The National Institute of Chemistry in Ljubljana is building a new infrastructural center where single or multi-layer battery cells (pouch or prismatic design) will be prepared and studied. With such an approach, we can expect a better understanding of how different parameters in battery design influence the quality, reliability, durability, and safety (QRLS) of the cells.

In addition to well-designed cells, we also need an understanding of the stability of the interfaces and interphases between the various components in the battery for a detailed investigation of QRLS. In the transition from liquid electrolytes to solid-state electrolytes, we are confronted with various instabilities at the interfaces. Some of them are inherently present, while others can be mitigated by appropriate pre-treatment of the cell components. Another technology that is still at an early stage of development are multivalent batteries, where the interfacial stability is completely different from lithium-ion battery technology. A few selected cases are used to explain how the expertise gained through calculations can accelerate the development of batteries.

Influence of microencapsulation on the phase change of the core material

Marta Klanjšek Gunde, Barbara Šumiga, Eva Pogorelc, Ondrej Panák
MyCol D.o.o., Ljubljana, Slovenia

Microencapsulation is used in many applications, from pharmaceuticals and cosmetics to construction and energy conservation. The phase change of the core material is of central importance in some of them, e.g. in heat storage and in reversible thermochromics. Microcapsules are almost perfectly round particles, the size of which can range from a few mm to a few 10 mm or even a few 100 mm in some cases. The polymer shell is usually thin, typically around 100 nm.

It has been shown that microencapsulated organic material crystallises at a much lower temperature than in bulk form (shifting as large as 15–20 °C towards lower values in the studied case) [1]. A similar effect has been demonstrated for miniemulsion droplets of some alkanes. Here, the liquid droplets have no polymer shell and are at least one order of magnitude smaller than the microcapsules in our example [2-5]. Thus, super-cooling effects reported in the literature did not show such large effects and were studied only for nanostructured materials.

It is likely that the effects observed in a large scale of material are due to the spatial confinement of the organic phase change material that occurs in microcapsules or in a porous medium (e.g. in chromatography paper). However, the typical sizes are far from nanodimensions, thus the phase changes have to be analysed across scales, from nano- to bulk behaviour. This includes modelling and simulation of complex systems, using multiscale approaches of a bulk material confined in different types and sizes. Therefore, various levels of organization, from molecular interactions to macroscopic behaviour is to be considered.

The expected results are important for the development of various applications using an organic material in microencapsulated form. MyCol has a great deal of experimental evidence, where a shift in crystallization temperature of up to 50 °C, which can be used to model the material properties across scales, i.e. to use multiscale calculations.

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Fine Tuning the Adsorption of Biomacromolecules at the Solid Liquid Interfaces

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General understanding of the interactions between biomacromolecules and materials remains limited, particularly in environments involving polarizable surfaces. In this study, we employ molecular simulations to examine the role of spike proteins, including its glycan, across open, closed and transitory configurations and their response during adsorption onto hydrophobic and hydrophilic surfaces. Our findings reveal stable adsorption to hydrophobic surfaces of both open and closed configurations. However, both exhibit tractable differences in the dynamics of adsorption, as for example, the contact region of the closed-conformation shows no significant structural changes, while flexibility is the driving force of adsorption for the open-conformation [1]. The residues involved in the contact with surfaces differ significantly from those interacting with its native biological interface, the ACE2 receptor [1]. Hydrophilic surfaces are clearly less prone to adsorption, especially in the closed-spikes. The influence of glycans on adsorption of open-configurations is negligible, however, in the closed-configurations they finely tune the adsorption process.

These findings show the complex interplay between a semi-flexible polymer (protein part) and flexible polymers (the glycans), which require the development of novel 2D analysis methods, as well as, combining multiple spatial resolution models based on their flexibility characteristics. Here, we developed a 2D analysis approach for the adsorption processes of biomacromolecules onto flat surfaces, which quantifies the molecular flexibility [2,3], electrostatics forces (based on Poisson-Boltzmann solvers) [4] and formation of hydrophilic interactions. Finally, I will discuss the potential role of combining protein and glycans for the design of viral trapping inanimate surfaces.

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Large-scale simulations for biophysics: from polarizable force fields to neural networks

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I will discuss our strategy for high-resolution molecular dynamics towards biophysical applications. As I detail the various protein targets that are currently under study, I will show how the newly developed multi-GPUs version of the Tinker-HP software can accelerate high-resolution molecular dynamics simulations. Indeed, thanks to adaptive sampling and new generation many-body polarizable force fields such as AMOEBA, long (μs) molecular dynamics simulations at enhanced accuracy become possible. As I detail the currently available other enhanced sampling capabilities of the software, I will present results related to the use of new physically-driven machine learning approaches for efficient and accurate condensed phase biomolecular simulations.

Performance portability in a compressible fluid simulator based on the material point method

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Politecnico di Milano, Milan, Italy

Ongoing rapid and continuous development of hardware acceleration technologies has recently increased the importance of implementation strategies that strike a reasonable balance between strong performance acceleration and future-proofing.

We present here an example of applying such approach to the development of a simulator for compressible gas dynamics problems base on the Material Point Method (MPM). The choice of the MPM, which is a special class of Particle In Cell (PIC) methods, was motivated by the fact that it can be cast in a form suitable for the requirements of data locality and fine-grained parallelism of modern hardware accelerators such as Graphics Processing Units (GPUs). The code developed is a proof of concept aimed at assessing the viability for this method to serve as the core for the development of a monolithic MPM solver for Fluid-Structure Interaction (FSI) problems at all Mach numbers up to the supersonic regime.

Streaming Workflows: From Scientific Applications to AI and Back

Marco Aldinucci
University of Turin, Turin, Italy

Within the Italian National Center in HPC and Quantum Computing (ISCS), the University of Turin and Pisa have co-developed two cloud-HPC development tools. The first is StreamFlow, an implementation of the open standard CWL (Common Workflow Language) that makes it possible to design scientific workflows that can be seamlessly ported on different platforms. StreamFlow fosters declarative workflows that can be executed on HPC platforms (e.g., based on SLURM), cloud platforms (e.g., based on K8S, AWS), and hybrid platforms without code modification. The second tool is CAPIO (Cross-Application Programmable I/O), which transforms files exchanged between parallel applications into streams, introducing further parallelism and helping to avoid the I/O bottleneck. StreamFlow+CAPIO has many applications, from genomics pipelines to astrophysics and materials science workflows to AI for science pipelines.

NanoShaper: A Tool for Molecular Surface Computation and Pocket Detection

Sergio Decherchi
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NanoShaper is a robust computational tool designed for the efficient and accurate generation of molecular surfaces and the detection of pockets, playing a crucial role in applications ranging from computational biophysics to molecular visualization. By leveraging advanced geometric and numerical techniques, NanoShaper constructs solvent-excluded and "skin" surfaces with high precision, enabling downstream analyses such as electrostatics calculations and molecular interactions.

In this talk, I will provide an overview of NanoShaper's core methodology, highlighting its unique capabilities in molecular modeling. Additionally, I will present our recent optimizations, which further enhance its computational efficiency and improve numerical accuracy, making NanoShaper even more suitable for large-scale molecular computations. These advancements significantly expand its applicability in molecular simulations, drug discovery, and structural biology.

Passive and active topological soft matter

Miha Ravnik
University of Ljubljana, Ljubljana, Slovenia

Topological soft matter presents distinct class of materials capable of diverse material mechanisms and characteristics, ranging from internal order, self-assembly, topology, defects and notably, activity. Here, I will give a selected overview of recent and emergent directions in passive and active topological soft matter, with particular emphasis on structures in passive and active nematics and their capability to perform as photonic or micro-electronic elements. Singular and nonsingular topological defects are shown to perform as objects that can affect or even control the material performance and response, both in passive and active systems.

Learning macroscopic equations of motion from dissipative particle dynamics simulations of fluids

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Macroscopic dynamic models of complex materials often rely on a set of phenomenological parameters, which must be determined either through costly and time-consuming experiments or extensive numerical simulations. For novel materials or biological systems, these macroscopic descriptions may be unavailable or even unknown. Coarse-grained particle-based methods can help address these challenges, but extracting phenomenological parameters from simulations requires full knowledge of the governing macroscopic laws and carefully designed simulations tailored to measure specific parameters.

In this work, we apply a data-driven approach, Sparse Identification of Nonlinear Dynamics (SINDy), to directly infer macroscopic dynamic laws from mesoscopic simulation data. To generate this data, we utilize dissipative particle dynamics (DPD), a method with a strong theoretical foundation, and investigate transient flows in a simple fluid system. We derive dynamic equations for mass density and linear momentum density, capturing both non-phenomenological (convective) and phenomenological (viscous) terms. Furthermore, we observe excellent agreement between the extracted pressure-density relation and its well-established semi-empirical relation for single-component DPD fluids. Since our method requires only a single simulation, it presents a computationally efficient alternative for measuring the equation of state.

Simulating solid/liquid interfaces across scales with ESPResSo

Jean-Noël Grad
University of Stuttgart, Stuttgart, Germany

The solid/liquid interface is host to a wealth of molecular mechanisms such as adsorption, reactions, charge regulation and molecular recognition. With ongoing development in the fields of nanoporous materials and nanofluidics, specific surface phenomena are now routinely investigated *in silico* for applications in energy storage, catalysis, and dialysis.

Particle-based and lattice-based simulations lend themselves particularly well to the study of soft matter, as they abstract away chemical detail and focus on the overall dynamics of the macromolecular system. Coarse-graining in particular allows for complex arrangements such as groups of atoms to be represented efficiently by a smaller number of particles, e.g. a two-bead model for each monomer of a polymer chain. Chemical detail can be re-introduced in a region of interest via machine-learned interatomic potentials, at a fraction of the cost of traditional ab initio calculations.

Particles can be further coupled to continuum fields to recover hydrodynamic and electrokinetic effects in solution, making simulations computationally tractable at the micrometer scale. Practical applications include the swelling behavior of weak polyelectrolyte gels, ultrasound-driven nanoparticle transport in human tissue, and bacterial growth in porous media.

Within MultiXscale, ESPResSo [1] provides a scalable multiphysics and multiscale simulation platform for soft matter research, with an emphasis on energy storage and hydrogels. The software leverages the lattice-Boltzmann method for continuum hydrodynamics and diffusion-advection-reaction equations for electrokinetics and catalysis. Its flexible Python interface [2] and lattice-based code-generation toolbox [3] allows for the rapid prototyping of new simulation setups and facilitates its integration in third-party scientific codes, such as VOTCA [4] for systematic coarse-graining, pyMBE [5] for hydrogel and protein modelling, pyOIF [6] for red blood cell simulations, and SwarmRL [7] for bacterial motion modelling.

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Ultrasound-Controlled Gene Regulation in Mammalian Cells

Mojca Benčina, Filip Ivanovski, Nina Varda, Vid Jazbec, Duško Lainšček, Roman Jerala

National Institute of Chemistry, Ljubljana, Slovenia

Remote control of cell activity in deep tissue with precise spatial and temporal control remains a major challenge. Ultrasound is a promising tool for non-invasive therapeutic applications in vivo, as it can precisely stimulate cells in deep tissues. In this study, we have developed a genetic circuit that enables mammalian cells to respond to ultrasound stimulation in vivo. Instead of increasing cellular mechanosensitivity, we have developed a calcium-responsive NFAT-based transcription factor with a customisable DNA-binding domain. This approach enables selective gene regulation while preventing broad activation of endogenous NFAT-responsive genes. We have identified ultrasound parameters that promote calcium entry into mammalian cells without triggering the native NFAT signalling pathway. The functionality of the system was validated in vivo by inducing anti-inflammatory interleukin-10 expression in transplanted artificial cells in a mouse model. This sonogenetic platform offers a non-invasive method for precise, ultrasound-guided stimulation of artificial cells in deep tissue.

Modeling ultrasonic metafluids: The significance of discrete oscillators

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National Institute of Chemistry, Ljubljana, Slovenia
University of Ljubljana, Ljubljana, Slovenia

Suspending tiny, subwavelength-size discrete micro-oscillators in a fluid can significantly alter its acoustic response. We explore how the topological properties of these oscillators, such as mass distribution and connectivity of their components, influence the effective dynamic density and compressibility of the embedding fluid. We demonstrate a metamaterial-like behaviour of suspension of micro-oscillators with a high density of low-frequency modes, occurring in loosely connected microstructures. This low-frequency resonant response, combined with the absence of a need for intricate structural design, brings experimental realization within closer reach.

Development and implementation of hybrid atomistic / coarse-grained modelling applied to complex interfaces

Hari Haran Sudhakar, Alessandra Serva, Rocio Semino
Sorbonne Université, Paris, France

Multiscale simulations combine different levels of detail to understand the behaviour of a system at different time and length scales at the same time. The term "system" includes, but is not limited to, soft matter, polymers, electrolytes, colloids, and biomolecules. To study the physical, kinetic, and thermodynamic properties of these systems thoroughly, several scales need to be sampled, and this requires a compromise between resolution and computational cost. Along with the advent of modern computers and high-performance facilities, different strategies were developed to improve the model in terms of both accuracy and computational efficiency.

We are working on the development and implementation of a hybrid coupling scheme that combines atomistic and particle-based coarse-grained resolution in the same simulation box, allowing the particles in the system to change their resolution "on the fly" during the course of the simulation. This method has already been developed for bulk liquids but never for solid/solid or solid/liquid interfaces. However, implementing a dual resolution in the same simulation box, while ensuring the chemical and thermodynamic equilibrium across the resolution, presents its own challenges. This requires special treatments on the non-bonded interactions, long-range electrostatics, neighbour lists, thermostats, additional forces introduced in the coupling regions, among others. This method will be implemented in the latest stable version of LAMMPS. In this talk, I will discuss the theoretical framework, implementation, and some of the benchmark studies performed on different systems along with the scope of this method to study complex heterogeneous interfaces such as those encountered in mixed matrix membranes and electrochemical systems.

Abstracts – posters

Hierarchical bayesian inference for parameter estimation in a water model

Brieuc Benvegnen[1], Nikolaos Ntarakas[2], Tilen Potisk[2], Ignacio Pagonabarraga[1], Matej Praprotnik[2]

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Coarse-grained water models are widely employed across physics, chemistry, and biology, providing simplified yet efficient representations of water's behavior. Here we calibrate a dissipative particle dynamics (DPD) fluid to accurately reproduce water's viscosity and speed of sound. Using a Hierarchical Bayesian framework, we infer the conservative and dissipative forces governing the DPD fluid. We show that the calibrated model matches the expected thermodynamic properties of water and we rigorously quantify the uncertainty in the predictions.

Open-boundary molecular dynamics of ultrasound using supramolecular water models

Maša Lah, Nikolaos Ntarakas, Tilen Potisk, Petra Papež, Matej Praprotnik
National Institute of Chemistry, Ljubljana, Slovenia

We introduce a first step toward a general particle-based approach for modeling ultrasound at the mesoscale, where particle interactions and boundary conditions pose significant implementation challenges. Using open-boundary molecular dynamics (OBMD), we simulate ultrasound waves in liquid water under ambient conditions, focusing on wave attenuation and velocity dispersion in the sub-THz range. We use three different supramolecular water models: dissipative particle dynamics (DPD), many-body DPD, and Martini 3 [1].

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Protein rotational and vibrational dynamics unveiled using OBMD method

Petra Papež, Franci Merzel, Matej Praprotnik
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Proteins are natural polymers that play an essential role both in living organisms and in biotechnological applications. They are dynamic entities, and their 3D structure encodes motions that determine their activity. The protein function and activity can be impaired by mechanical stress (e.g., shear flow or mechanical pressure waves), and the open-boundary molecular dynamics (OBMD) method represents a promising computational tool to investigate such effects.

Here, we use the OBMD method as a virtual rheometer to study rotational dynamics of a protein and as a virtual ultrasound machine [1] to inspect susceptibility of the protein internal dynamics to induced sub-terahertz acoustic waves. Our results show that extraordinarily high shear rates must be applied to observe protein unfolding [2] and that acoustic waves enhance its internal dynamics [3].

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Toward transferable force fields for biological membrane simulations

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Biological membranes are a crucial component of all cellular organisms and mediate many essential cellular functions. Detailed atomistic insight into their structural and dynamical properties are of significant interest to many fields of research, such as biology, medicine, biotechnology and drug development.

Studying biological membranes with atomistic molecular dynamics (MD) simulations is a commonly employed strategy to provide such insight, which are difficult to obtain via experimental means. Simulations have also been used to aid the interpretation of experimentally obtained raw data (incl. those from neutron scattering) in order to provide more detailed understanding of the structure of model membranes.

The utility of MD simulations, however, depends on the accuracy and transferability of the underlying force field description (e.g., parameters, functional forms etc.). Specifically, the fidelity with which the potential energy landscape can be represented, the consistency with which interaction parameters can be assigned, and the extent to which parameters can be transferred between chemical entities. Currently available lipid force fields, while able to model simple membranes with adequate accuracy, lack sufficient transferability, rendering them unreliable for modelling more realistic and complex membrane systems and their interaction with other biologically relevant molecules.

In this study, I take a robust bottom-up approach to re-examine and re-parameterize force field terms used in small molecule analogues of common components in different lipid species by comparing to their experimentally derived properties (e.g., pure liquid and solvation properties). Refinements for the force field descriptions of small molecules, including hydrocarbons and esters, are proposed. The effect of the refined parameters in lipid bilayer systems is also assessed. A key element of this work is minimizing confounding variables that can mislead parameterization efforts. This was done by ensuring that the calculation of observables is performed in a regime that reduce their sensitivities to the precise choice of simulation settings, and explicitly considering the correlations between different force field parameters.

Transport of acetylene adsorbed in CuBTC metal organic framework

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[2] BARC, Mumbai, India

Metal organic frameworks (MOFs) are an important class of material which has a potential to be used for variety of applications such as in storage materials, pollution control, etc. Here we report a molecular dynamics simulation study investigating dynamical behaviour of the smallest and linear hydrocarbon, acetylene, adsorbed in CuBTC MOF. CuBTC has complex network structure consisting of large pores and tetrahedral pockets connected by windows. Calculated mean squared displacements of the acetylene molecules adsorbed in CuBTC showed anomalous behaviour with change in concentration. This has been understood by studying the evolution of the trajectories and free energy map. There are two pathways for an acetylene molecule to diffuse inside CuBTC. One is through tetrahedral pockets and other is through large pores. It is found that tetrahedral pockets are potential minima sites and most of the molecules reside there at low concentration. Free energy map also showed that there exists a higher energy barrier if diffusion occurs through tetrahedral pockets rather than large pores. Relative population of acetylene molecules in large pores is found to increase with the concentration and since energy barrier is less while diffusing through large pores, it leads to increase in the average diffusivity at higher concentration. It is found that relative population of acetylene molecules diffusing through different pathways and collision between the molecules decide the average diffusivity of the molecules inside CuBTC. Analysis of intermediate scattering function indicated that there exist three time scales associated with the centre of mass diffusion of the acetylene molecules in CuBTC framework.

Transport-structure relationship in diglyme-based electrolytes for lithium-sulfur batteries

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Lithium-sulfur batteries represent a promising alternative to state-of-the-art Li-ion batteries due to their energy density and low cost. However, the grand challenge of Li-S batteries is their poor cycle life [1]. An electrolyte formulation based on high concentrations of lithium nitrate ($LiNO_3$) and low concentrations of lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) in diglyme has been shown to improve the cycle life of Li-S battery by order of magnitude, though at the cost of poor ionic conductivity [2]. In this work, we investigate transport in LiTFSI $-$ $LiNO_3$-diglyme electrolytes through classical molecular dynamics simulations. Specifically, we show that the LiTFSI $-$ $LiNO_3$ ratio strongly affects the ionic conductivity of the electrolyte due to the peculiar correlations in ion-ion transport. Correlated movements are directly linked to the ion-ion structural ordering, which strongly depends on the LiTFSI $-$ $LiNO_3$ ratio.

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Viscoelastic channel flows during solidification: modelling viscoelastic phenomena with variable-order fractional calculus

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Theoretical modelling of viscoelastic flows during phase transformations is difficult due to rheological models of viscoelasticity requiring a large number of experimentally-determined material constants and a lack of a clear way of coupling the phase transformation to the mechanical response. One solution is the use of variable-order fractional models, which require less experimental data and enable clear coupling to the phase transformation, and are also fundamentally more accurate at modelling viscoelastic phenomena. In this contribution, we consider the flow of a viscoelastic fluid in a rectangular channel driven by a pressure gradient, with photopolymerization occuring in the channel in the transversal direction due to irradiation by an external light source. We assume a simple photopolymerization reaction which is decoupled from the mechanical response, with light transmissivity governed by the Beer-Lambert law and constant luminous flux along the domain boundaries. We further assume a fully developed time-dependent flow, and employ a model of viscoelastic response based on the formalism of variable-order fractional calculus, which is analogous to the Bagley-Torvik model for polymer solutions. The variable order of the Caputo-like differential operator appearing in the model depends on the spatially- and temporaly-dependent extent of polymerization. In solving the problem, we obtain physically sound solutions, as the velocity field corresponds to viscous flows in parts of the domain where the extent of the phase transformation is low and diminishes in magnitude where its extent is high.

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