Perspectives and challenges of future HPC installations for atomistic and molecular simulations

CECAM Flagship Workshop, Zuse Institute Berlin (19–21 February, 2024)

Organisers: F. Höfling, P. Imhof, and T. D. Kühne

Mon 13:30 – 15:20 Hybrid QM/MM methods and their applications

- Opening (10')
- **Giulia Palermo** (UC Riverside) – *online*
  Dynamics and mechanisms of CRISPR-Cas9 through the lens of computational methods
- **Dmitry Morozov** (Univ. Jyväskylä)
  Scalable simulations of biological processes with GROMACS–CP2K interface and enhanced sampling methods
- **Flash talks on posters** (2' each)

Coffee and discussion break

Mon 16:00 – 17:40 Highlights in classical molecular simulations

- **James C. Phillips** (Univ. Illinois) – *online*
  Sustainable Software Lessons from Scaling and Accelerating NAMD
- **Hector Martinez-Seara** (IOCB CAS Prague)
  Challenges and Prospects in Molecular Dynamics: Scaling Computational Resources for Complex Biological Systems
- Dmitry Nerukh (Aston Univ.)
  Approaching exascale: MD and hybrid MD/hydrodynamics modelling of large biomolecular systems in solution

Mon 18:30 – 20:30 Posters and Reception (from 19:00)

Tue 09:00 – 10:00 Advances in quantum mechanical modelling

- **Christian Carbogno** (FHI Berlin)
  Efficient All-electron Hybrid Density Functionals for Atomistic Simulations Beyond 10,000 Atoms
- Ji Liu (Tyndall Nat. Inst.)
  Ab initio molecular dynamics simulations on the N-plasma cycle of plasma-enhanced atomic layer deposition of Co thin film

Tue 10:00 – 10:40 Parallel processors and programming frameworks I

- **Michael Klemm** (AMD, OpenMP ARB)
  AMD EPYC processors and Instinct accelerators – the journey to exascale and beyond

Coffee and discussion break

Tue 11:20 – 12:40 Parallel processors and programming frameworks II

- **Tom Deakin** (Bristol Univ.)
  Performance Portability for Next-Generation Heterogeneous Systems
- **Michèle Weiland** (EPCC Edinburgh)
  Performance portable optimisation of sparse matrix operations

Lunch break and discussions

Tue 14:00 – 15:40 Technology trends

- **Michael Hennecke** (Intel Germany)
  More than a faster filesystem – exploring DAOS storage APIs to accelerate domain specific I/O workloads
- **Hans-Christian Hoppe** (FZ Jülich)
  The DEEP Series of Projects – Application-Driven Co-Design Towards Exascale
- **Panel discussion**

Coffee and discussion break

Tue 16:10 – 17:30 Algorithms and software for simulations at multiple scales

- **Rommie Amaro** (UC San Diego) – *online*
  SEEKR package for simulations at multiple scales
- **Andrej Antalík** (EPFL Lausanne) – ASC Lecture
  MiMiC, a flexible and scalable framework for multiscale modeling

Tue 19:30 – 22:00 Social Dinner

Wed 09:00 – 11:00 Molecular simulations with advanced force fields

- **Sereina Riniker** (ETH Zürich)
  Learning physical interactions for molecular dynamics simulations
- **Julien Steffen** (Univ. Erlangen) – ASC Lecture
  Computational Challenges in Machine-Learning Force Field Simulations of Liquid Interface Catalyst Systems
- Kosuke Nakago and Rudy Coquet (Preferred Networks, Inc.)
  Matlantis – Million years of research acceleration with universal neural network potential-based SaaS
- Samuel J. Newcome, M. Mühlhäusser, F. A. Gratl, M. Mishra, P. Neumann, H.-J. Bungartz (TU Munich)
  Simulation-Tuned Time and Energy Optimisation for Multi-Site and 3-body Molecular Dynamics Simulations with AutoPas

Coffee and discussion break

Wed 11:40 – 13:05 Innovative hardware and emerging computing paradigms

- **Martin Herbordt** (Boston Univ.)
  Scalable Molecular Dynamics with Ultra-Low Latency Communication: Implementation and Utilization
- Xin Wu, T. Kenter, R. Schade, T. D. Kühne, C. Plessl (Paderborn Univ.)
  Energy efficient FPGA-accelerated computation of electron repulsion integrals
- Mario Hernandez Vera (LRZ Munich)
  Exploring opportunities and challenges of hybrid quantum-classical algorithms for electronic structure calculations: the case of the Variational Quantum Eigensolver (VQE)
- Closing remarks (5')

Posters

(1) Killian Babilotte, Alizée Dubois, Thierry Carrard, Jean-François Molinari, Laurent Soulard (CEA)
Multi-billion atoms simulations: an in-situ analysis framework to unveil new physical phenomena

(2) Ryan Brook, (University of Leeds)
Dissociation of PPVE plasma after electron excitation

(3) Nicholas Charron, Félix Musil, Andrea Guljas, Yoayi Chen, Klara Bonneau, Aldo Pasos-Trejo, Jacopo Venturin, Daria Gusew, Iryna Zaporozhets, Andrea Krämer, Clark Templeton, Atharva Kelkar, Aleksander Durumeric, Simon Olsson, Adrìa Pérez, Maciej Majewski, Brooke Husic, Ankit Patel, Gianni De Fabritiis, Frank Noé, Cecilia Clementi (Zuse Institute Berlin)
Navigating protein landscapes with a machine-learned transferable coarse-grained model

(4) Steffen Christgau, Viktor Skoblin, Tilmann Ehrlich (Zuse Institute Berlin)
Experiences with Cross Platform GPU support for HAL's MD package using SYCL

(5) Rudy Coquet, Hiroki Iriguchi, Akihiro Nagoya, Yusuke Asano, Taku Watanabe (Preferred Computational Chemistry, Inc.)
Applicability of universal neural network potential to organic polymer materials

(6) Alireza Ghasemi, (Friedrich-Alexander-Universität Erlangen-Nürnberg)
Title: Machine Learning Interatomic Potentials: Workflow for Generating Training Dataset on Massively Parallel Computers

(7) Eirini Gkolfi, Petra Bačová, Vagelis Harmandaris (Foundation for Research and Technology - Hellas (FORTH))
Advancing structural analysis in complex polymeric systems through high-performance computing

(8) Munavvar Husain, Tatiana Korona (University of Warsaw)
Quantum Topology Study for Unveiling the Charge Transfer Excitation in the Complex of Ethylene and Tetrafluoroethylene

(9) Sophia Johnson, Murat Kılıç, Polydefkis Diamantis, Oliver Toth, Ursula Rothlisberger (EPFL)
Redox-Based Defect Detection in Packed DNA: Hybrid Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation & Feature Selection Studies

(10) Anna Kahler, Thomas Zeiser, Gerhard Wellein (Friedrich-Alexander-Universität Erlangen-Nürnberg)
Improving MD performance on HPC clusters through in-depth hardware knowledge and advanced program usage

(11) Sadra Kashef Ol Gheta, Tobias Morawietz (Bayer AG)
!AIQU: Bridging Artificial Intelligence and Quantum Chemistry for Faster Conformation Search and Enhanced Property Prediction

(12) Rasmus Kronberg, (CSC – IT Center for Science Ltd.)
Atomic-scale simulations on the LUMI supercomputer: Performance and best practices

(13) Andrea Levy, Andrej Antalík, Ursula Rothlisberger (EPFL)
Interfacing OpenMM to MiMiC for Efficient Multiscale Simulations

(14) Diego Liberati, (National Research Council of Italy)
Inference and simulation in understanding and designing bioproteins

(15) Conor Price, Piotr Kowalski, Tobias Binninger, Yin-Ying Ting (Forschungszentrum Jülich)
Atomistic Modeling of Energy Materials on Emerging Computational Infrastructures

(16) Dusan Racko, Renáta Rusková (Slovak Academy of Sciences)
Using HPC in modeling compression of DNA inside finite versus infinite nanochannels

(17) Ruben Raffelsieper, Fabian Tipp, Mohammad Eslamibidgoli, Kourosh Malek, Michael Eikerling (Forschungszentrum Jülich)
Computational assesment of snythesizability and solubility descriptors for imidazolium-based ionic compounds

(18) Anita Ragyanszki, Hongchen Ji, Rene Fournier (Zuse Institute Berlin)
Understanding the Origins of Life - A Machine learning approach to estimate reaction mechanisms of biotic precursors

(19) Christopher Secker, Konstantin Fackeldey (Zuse Institute Berlin)
A multi-objective affinity approach to identify pH-specific μ-opioid receptor agonists

(20) Fabian Tipp, Mohammad Eslamibidgoli, Kourosh Malek, Michael Eikerling (Forschungszentrum Jülich)
High throughput simulation-based approach to predict the alkaline stability and guide the design of imidazolium-based anion exchange membranes

(21) Mahesh Yadav, Roberto Covino, Dorothee Dormann, Lukas Stelzl, Friederike Schmid (Johannes Gutenberg-University of Mainz)
Phase behavior of RNA-binding proteins using coarse-grained simulations and machine learning

(22) Xin Zhong, Felix Höfling, Timm John (Freie Universität Berlin)
Molecular dynamics simulation of hydrogen diffusion in garnet