

CECAM Tutorial: Atomistic Monte Carlo Simulations of Bio-Molecular Systems

The CECAM tutorial "Atomistic Monte Carlo Simulations of Bio-molecular Systems" took place at Forschungszentrum Jülich from September 15 to 19, 2014 and was attended by scientists from seven countries. The five days of the tutorial featured a range of lessons and hands-on practical sessions to provide scientists with everything necessary to apply this technique to their own research topics.

After the initial presentation by Prof. Anders Irbäck (Lund University) on the first afternoon that summarized the theory of Monte Carlo (MC) simulation and its application to biological macromolecules, the participants were introduced to the open source Monte Carlo simulation package ProFASi that served as the basis for the hands-on parts of the tutorial. ProFaSi is under active development by the organizers from the Simulation Laboratory Biology at JSC. It is a powerful alternative to molecular dynamics (MD), in particular for cases where the underlying process is too slow to be simulated by classical MD, such as in protein folding and peptide aggregation.

Two introductory sessions enabled the participants to set up, monitor, and analyze MC simulations of protein folding, peptide aggregation with ProFASi on the HPC resources of JSC. The following sessions addressed several advanced features including advanced error analysis and visualization. Wouter Boomsma (Univ. Copenhagen) demon-

strated the use of different constraints obtained from predictions and experiments in connection with MC simulations. Finally, the programming interface of ProFASi was introduced that allows for rapid development of new algorithms and simulation strategies using atomistic Monte Carlo.

The CECAM tutorial concluded with some recent research highlights using atomistic MC simulations, and a lively discussion of best practices and future developments with the participants.

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UNICORE Summit 2014

The UNICORE Summit is a unique opportunity for users, developers, administrators, researchers, service providers, and managers to meet. Its objective is to exchange and share experiences, new ideas, and latest research results on all aspects of UNICORE [1]. Since the first Summit in 2005, the organisers have received and reviewed a significant amount of distinguished contributions. Those selected and presented, complemented by invited talks, guarantee exciting Summits and lively discussions about the state-of-the art and the future of UNICORE, Grids, and distributed computing in general. The tenth edition, the UNICORE Summit 2014 [2] has been held on 24 June 2014 in Leipzig, Germany.

The invited talk "HPC Applications in Biophysics, Material Science and Biomedicine - enabled by UNICORE" by Borries Demeler, PhD, Associate Professor from University of Texas

Health Science Center at San Antonio, focused on applications of the UltraScan XSEDE Science gateway [3] for high-resolution modelling of hydrodynamic experiments. The UltraScan software is used by scientists across the globe for research in biophysics, biochemistry, biomedicine, and material science to study the structure and function of biological macromolecules, investigate nanomaterials, and develop cures for diseases [4]. The keynote provided an overview of the integration of UNICORE into the gateway architecture in order to facilitate job submission and workflow management and discussed examples of science and discovery enabled by this implementation.

A second interesting use case was presented in the talk "A Workflow for Polarized Light Imaging Using UNICORE Workflow Services". The Polarized Light Imaging of brain slices is used to understand the anatomical structure of the human brain on the level of single nerve



Figure 1: Participants of UNICORE Summit 2014.

fibres and is nowadays one of the most challenging tasks in neuroscience. The application of the UNICORE workflow system for this particular use case resulted in minimizing user interaction and time to completion of the scientific workflow. The next presentations highlighted current state, new ideas and concepts for the future development of the UNICORE portal [5], experiences with certificate-free user-friendly HPC access based on LDAP with UNICORE and UNITY [6], perspectives for REST services in the UNICORE environment, integration of UNICORE services in a private cloud computing platform and resource scheduling algorithms in distributed problem-oriented environments. Finally, the UNICORE roadmap and future developments were discussed by the attendees from Germany, Poland, Russia, and the United States.

The slides to the presentations can be found on the web at <http://www.unicore.eu/summit/2014/schedule.php>

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References

- [1] UNICORE Web Page: <http://www.unicore.eu>
- [2] UNICORE Summit 2014 web page: <http://www.unicore.eu/summit/2014/>
- [3] XSEDE Science Gateway: <https://portal.xsede.org/science-gateways>
- [4] UltraScan-III: <http://www.ultrascan.uth-scsa.edu>
- [5] UNICORE Portal: <http://sourceforge.net/projects/unicore/files/Servers/Portal>
- [6] UNITY Web Page: <http://www.unity-idm.eu>

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"Bernstein Network - Simulation Lab Neuroscience" HPC Workshop

Neuroscience today is attacking problems of increasing complexity and scale as exemplified by projects like the Human Brain Project, which require computationally intensive simulations and the analysis of large data sets. However, many projects currently using local clusters for these purposes have not yet adapted their software and theoretical approaches to take advantage of HPC systems such as those available at the Jülich Supercomputing Centre (JSC).

The "Bernstein Network - Simulation Lab Neuroscience" HPC Workshop on June 4th and 5th at the JSC brought together Jülich computational neuroscientists and HPC experts with neuroscience domain experts from across Germany who are interested in developing petascale simulations and analyses. An important goal of this meeting was to find ways for the neuroscience community to fully exploit available JSC resources by catalyzing collaborations and adapting tools to supercomputer scales.

A total of 32 participants shared their perspectives on HPC in neuroscience. Members of the SimLab Neuroscience [1] and the JSC's HPC in Neuroscience Division delivered presentations covering a range of issues regarding the use of computing facilities at the JSC, in addition to describing work being currently done by the SimLab which leverages these resources such as structural plasticity modeling in the visual cortex using the NEST simulator [2].



Figure 1: Participants of the "Bernstein Network - Simulation Lab Neuroscience" HPC Workshop.