JÜLICH
FORSCHUNGSZENTRUM

JSCNews
Jülich
Supercomputing
Centre

No. 226 • Nov. 2014

Jülich School on Computational Science 2015

From 23 to 27 March 2015, the IAS School on "Computational Trends in Solvation and Transport in Liquids" will take place at JSC. This event is part of a series of Schools in Computational Science, which have been regularly organized at Jülich since 2000. More than 20 renowned scientists from seven countries will present lectures on modern methods and algorithms for treating solvents most efficiently on different time and length scales. The school is part of the activities of the Jülich CECAM node and is co-supported by the Cluster of Excellence RESOLV at Ruhr University Bochum.

"Solvation Science" is increasingly recognized as an important research area addressing a variety of different computational and simulation methods which were designed for scale-bridging investigations of complex systems. Solvation and transport problems arise in many fields of application, ranging from fundamental problems in chemistry or soft matter physics to industrial processes. The IAS School 2015 will focus on computational trends, multi-method approaches, and modelling in this interdisciplinary area. The full range from large-scale modelling on a coarse grain level down to fully quantum-mechanical simulations of liquids at the level of electrons and nuclei will be addressed. Not only will bulk liquids and homogeneous solutions be discussed, but also heterogeneous systems such as liquid/solid interfaces and solvated (bio)molecules.

The IAS School is intended for PhD students and postdocs. Applications for participation can be sent until the end of January 2015. Based on the required application documents, about 50 participants will be selected by the organizers. Details can be found at *http://www.fz-juelich.de/stl-2015*.
(Contact: Dr. Godehard Sutmann,
g.sutmann@fz-juelich.de)

JSC @ SC14

SC14, the premier international exhibition and conference on high-performance computing, networking, storage, and analysis, will take place in New Orleans, Louisiana, USA, from 16 to 21 November 2014, where JSC will present its supercomputing activities at booth #639. JSC staff will demonstrate scientific simulations on supercomputers and the software solutions LLview, Scalasca, SIONlib, and UNICORE, all developed in-house. JSC's activities in current European supercomputing initiatives will also be showcased, particularly its involvement in the Human Brain Project. The HPC section of the Jülich Aachen Research Alliance (JARA-HPC) is a guest at JSC's booth and will present its projects on visualizing complex data, in particular of neural networks and brain regions.

JSC staff will also be on hand continuously at the joint booth of the European Exascale Projects (#1039), and at the PRACE booth (#2215). As part of the conference programme, JSC staff will give tutorials on "Hands-On Practical Hybrid Parallel Application Performance Engineering" and "Debugging and Performance Tools for MPI and OpenMP 4.0 Applications for CPU and

Forschungszentrum Jülich GmbH
in der Helmholtz-Gemeinschaft
Jülich Supercomputing Centre
52425 Jülich I Germany

Phone +49 2461 61-6402

jsc@fz-juelich.de
www.fz-juelich.de/jsc

Accelerators/Coprocessors", present talks, and participate in numerous special interest group sessions. For up-to-date information on JSC's activities at SC14, see *http://www.fz-juelich.de/ias/jsc/events/sc14*
(Contact: Dr. Walter Nadler, *w.nadler@fz-juelich.de*)

CECAM Tutorial "Atomistic Monte Carlo Simulations of Bio-molecular Systems"

The CECAM tutorial "Atomistic Monte Carlo Simulations of Bio-molecular Systems" took place at JSC from 15 to 19 September 2014 and was attended by 25 scientists from seven countries. 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 an intensive introduction to the theoretical foundations of Monte Carlo (MC) simulations by Prof. Anders Irbäck (Lund University), the participants consolidated their knowledge in the hands-on sessions using the open source MC simulation package ProFASi. This software is under active development at the Simulation Laboratory Biology at JSC. The participants learned to set up, monitor, and analyse MC simulations with ProFASi on the HPC resources of JSC. The exercises introduced scientifically interesting all-atom protein folding and aggregation simulations. Such processes are often too slow to be simulated by classical molecular dynamics, and the tutorial presented MC as a powerful alternative tool. Wouter Boomsma (University of Copenhagen) showed how to integrate available experimental information with the MC sampling procedure as an advanced application. Finally, the programming interface of ProFASi was introduced to encourage research and experimentation with new MC techniques. 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.

Overall, it proved to be a significant community-building event for the ProFASi software package, and provided much stimulus for future development work by the SimLab Biology.
(Contact: Dr. Sandipan Mohanty, *s.mohanty@fz-juelich.de*)

Review of the CECAM Workshop on Many-Core Computing at Daresbury

From 10 to 12 September, the workshop "Exploiting heterogeneous multi-core and many-core platforms for atomic and molecular simulations" was held at STFC Daresbury Laboratory in the UK. The workshop was organized together by the Jülich and UK Hartree CECAM nodes. The motivation for the workshop arose from Daresbury and Jülich Simulation Laboratories to account for the transition from homogeneous parallel clusters to heterogeneous architectures and to discuss experiences and recent developments in the user community. Members from JSC together with other participants from five countries presented in 16 talks their recent work and the progress of implementations and software design for heterogeneous computers. Introductory talks about new developments in processor architecture were given by experts from Intel and NVIDIA on the first day. Follow-up talks by practitioners then focused on experiences in porting, optimizing and the performance of simulation codes and scheduling tools. New developments were seen in task based hybrid programming models to facilitate exploitation of the potential of multi-core architectures. Contributions from participants were mainly focused on recent experiences with GPU accelerators and the Intel Xeon-Phi processor. Discussions were particularly fruitful between the scientific disciplines, including soft matter science, plasma physics, biophysics, engineering and material sciences, where similar methods are sometimes developed and applied in a different type of problem context. Since heterogeneous multi-core architectures are of high interest for JSC, the success of the event in terms of information exchange and networking within the user community has provided motivation to organize workshops with a similar focus in Jülich in future.
(Contact: Dr. Godehard Sutmann, *g.sutmann@fz-juelich.de*)

New GCS Large-Scale Projects

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers, currently JUQUEEN (JSC), HORNET (HLRS), and SuperMUC (LRZ). Projects are classified as large-scale if they require at least 35 million core hours. At its October meeting at JSC, the GCS Peer Review Board decided to award the status of a large-scale project to 17 projects from various fields of the simulation sciences. Three projects were granted a total of 308 million compute core hours on HORNET, nine projects were granted a total of about 541 million compute core hours on JUQUEEN, and six projects were granted a total of 180 million compute core hours on SuperMUC. For more details on these projects, see *http://www.gauss-centre.eu/large-scale*.
(Contact: Dr. Walter Nadler, *w.nadler@fz-juelich.de*)

Events

Data analysis and data mining with Python
Instructors: Dr. Jan Meinke, Dr. Olav Zimmermann, JSC
Date: 17-19 November 2014, 09:00-16:30
Venue: Jülich Supercomputing Centre, Ausbildungsraum 1
Registration: *j.meinke@fz-juelich.de*

Editor: Dr. Sabine Höfler-Thierfeldt, ext. 6765