

JSCNews

Jülich
Supercomputing
Centre

No. 198 • Oct. 2011

Jülich LOFAR Station Opened

On 5 October 2011, the LOFAR station was officially opened on the campus of Forschungszentrum Jülich. The antenna station is an integral part of the digital radio telescope and the European large-scale project LOFAR (Low Frequency Array). It will contribute to measuring long-wave radio signals from the dawn of the universe. The Jülich LOFAR station was built as part of a cooperation between Ruhr University Bochum, Jacobs University Bremen and Forschungszentrum Jülich with funds provided by the Federal Ministry of Education and Research (BMBF).

JSC is contributing to the organization and operation of the antenna station. Furthermore, JSC will function as a computing and storage centre for the German LOFAR stations in Effelsberg, Garching, Potsdam, Tautenburg, and Jülich, which are organized in the GLOW (German Long Wavelength) consortium, as well as for the international LOFAR project. The data communication traffic of these stations to the central computing system in Groningen is also managed by JSC.

Within LOFAR, key science projects will investigate the cosmological epoch of reionization, transient sources, ultra-high energy cosmic rays and cosmic magnetic fields. Furthermore, LOFAR is an instrument for solar science, space weather and deep extragalactic surveys. More information and pictures of the station can be found at <http://www.fz-juelich.de/ias/jsc/lofar>. (Contact: Dr. Thomas Fieseler, ext. 1602)

JSC Participates in Mont-Blanc

In October, the EU-funded project Mont-Blanc started as one of three exascale projects within the research theme "Information and communications technologies" of the 7th Framework Programme of the European Commission. The objectives of Mont-Blanc are the development of a fully functional energy-efficient HPC prototype based on the low-power embedded ARM technology, the design of a next-generation HPC system in order to overcome the limitations identified in the prototype system, and the development of a portfolio of exascale applications to be run on this new generation of HPC systems. The project is coordinated by the Barcelona Supercomputer Centre; the partners from industry are ARM, GNODAL, and BULL, and from research CNRS, Forschungszentrum Jülich, GENCI, LRZ, and CINECA.

JSC contributes the performance analysis tool Scalasca and exascale applications from different areas of research like the parallel Coulomb solver PEPC, the massively parallel multi-particle collision software MP2C, the software for molecular mechanics of proteins SMMP, and the protein folding and aggregation simulator ProFASi. (Contact: Dr. Thomas Fieseler, ext. 1602)

JSC at SC11 in Seattle

SC11, the premier international exhibition and conference on high-performance computing, networking, storage, and analysis, will take place in Seattle, Washington, USA,

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

Phone +49 2461 61-6402

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

from 12 to 18 November 2011. JSC will present its wide-ranging supercomputing activities at booth #535. There, JSC staff will demonstrate scientific simulations on supercomputers and on the supercomputing tools UNICORE, LLview and Scalasca developed in-house. JSC staff will present protein folding on the Knights Ferry processor at the Intel booth (#2121) and on Grid Interoperability at the EMI (#763) and XSEDE (#5415) booths. JSC staff will also be continuously on hand at the PRACE booth (#5001).

As part of the conference programme, JSC staff will give tutorials on "Supporting Code Development on Extreme-scale Computer Systems" and on "Practical Hybrid Parallel Application Performance Engineering", present posters, and will participate in numerous special interest group sessions ("Bird-of-a-Feather", BoF). In particular, JSC is organizing the BoF session on "Community-Oriented Scientific Support Structures for HPC" and co-organizing the sessions on "European Exascale Research", on "The European HPC Infrastructure PRACE", and on the HPC monitoring and performance analysis projects "HOPSA" and "Score-P".

For up-to-date information on JSC's activities at SC11 see: <http://www.fz-juelich.de/ias/jsc/events/sc11>. Do pay us a visit if you're attending the conference and don't forget to join in the PRACE treasure hunt!

(Contact: Dr. Walter Nadler, ext. 2324)

CECAM Summer School in Retrospect

From 12 to 16 September 2011, the Jülich CECAM Node organized a Summer School on Fast Methods for Long-Range Interactions in Complex Systems at JSC. Around 37 participants from 14 countries came to learn about state-of-the-art methods and algorithms for efficiently solving the Coulomb problem. Lectures and tutorials on this pervasive topic were held by experts from the universities of Bielefeld, Chemnitz, Mainz, Stuttgart and Wuppertal as well as by experts from JSC.

During the week, morning sessions were devoted to the mathematical principles, algorithmic implementations and parallelization issues of each method. The latter comprised simple cut-off methods, Fourier-based methods, mesh-based Maxwell solvers, multigrid techniques and mesh-free techniques, such as the Barnes-Hut tree method, and the fast multipole method FMM. This theoretical material was complemented by hands-on sessions, including introductions to parallel programming models like MPI, OpenMP, and P-threads and performance analysis tools, followed by practical applications of the above Coulomb solvers contained within the recently established ScaFaCoS library.

The attendees came from a broad range of disciplines (engineering, astrophysics, biophysics, plasma physics, soft matter physics) and had the opportunity to present their own

scientific work during a poster session. The diversity of the participants' scientific backgrounds combined with their strong interest in the methods covered by the school (some of which were developed at JSC) is testament to the interdisciplinarity of computational science activities at JSC. The Lecture Notes are available as a publication in the IAS Series at <http://hdl.handle.net/2128/4441>.

(Contact: Dr. Godehard Sutmann, ext. 6746)

PRACE-1IP and PRACE-2IP Meetings

From 14 to 16 September 2011, more than 200 participants from the 21 PRACE member countries met at the Barcelona Supercomputing Center for a three-day project meeting of PRACE-1IP and PRACE-2IP, the first and second implementation phase projects for the PRACE Research Infrastructure. The European Commission is providing funding worth € 20 million and € 18 million for both two-year projects, respectively. These projects, coordinated by JSC, support and accelerate the implementation of the pan-European High-End Computing Research Infrastructure created and operated by PRACE (Partnership for Advanced Computing in Europe).

At the project meeting, the current status and future work of PRACE-1IP, which started in July 2010, was discussed in an all-hands meeting, covering the first one and half days. This was followed by the kick-off of PRACE-2IP and the welcoming of Hungary as the 21st partner country in the PRACE projects. PRACE-2IP will extend the work of PRACE-1IP by providing access to national HPC resources (Tier-1), building on the successful work of the former DEISA projects. The project will offer application-enabling and scaling support in partnership with scientific communities, and it will create a coordinated European HPC training programme. Dr. Florian Berberich (JSC) was appointed project manager of PRACE-2IP.

(Contact: Tanja Weber, ext. 2959)

Prof. Rollnik Passed Away

Prof. Dr. Dr. h.c. mult. Horst Rollnik was a tireless advocate for computational science and supercomputing in Germany. He was one of the founding fathers of the John von Neumann Institute for Computing (NIC), and for a long time, he headed the NIC Scientific Council. Even in recent years, he continued to contribute his experience to this panel as a honorary member. Two years ago, NIC and JSC paid homage to his contributions to NIC and to computational science in Germany in an Honorary Colloquium (see <http://www2.fz-juelich.de/nic/events/colloquium.html>).

Horst Rollnik died on 28 September 2011 at the age of 80. JSC will always remember him with gratitude.

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