

JSCNews

Jülich Supercomputing Centre

Looking Back on SC12

Supercomputing 2012, the premier international conference and exhibition on high-performance computing and networking, took place in Salt Lake City, Utah, USA, from 10 to 16 November 2012. JSC participated in the conference and exhibition for the fourteenth time in succession.

The role of JSC as a leading European high-performance computing centre was highlighted by it receiving the award for the "Fastest Supercomputer in Europe" from the TOP500 committee, the new 5 Petaflop IBM Blue Gene/Q installation JUQUEEN having become operational and accessible for users just before the conference.

JSC also received HPCwire's 2012 Reader's Choice Award for "Best use of HPC in life sciences" for using NVIDIA Tesla GPUs to uncover causes of and treatments for autism, Alzheimer's, and other neurological diseases. The application is currently being developed at Jülich's Institute of Neuroscience and Medicine (INM-1).

JSC staff members actively contributed to the conference's programme, to tutorials and to various special interest meetings. Bernd Mohr, the only European member on the SC Steering Committee, acted as chair for the Awards Session.

At its booth, JSC presented its broad spectrum of activities together with scientific results obtained on its supercomputers in the form of displays, movies, animated presentations, and in individual consultations. Particular emphasis was placed on LLview, the

interactive monitoring software for supercomputers. LLview is currently being used at a large number of supercomputing sites and it is also part of the Eclipse PTP environment for developing supercomputing applications. JSC also showcased DEEP, the European Exascale project coordinated by JSC. Next year, at SC13, all European Exascale projects will be presented jointly at a new dedicated booth.

JSC staff gave presentations at the Intel and NVIDIA booths and demonstrated the interoperability of the UNICORE middle-ware with other international technologies in the context of XSEDE at the University of Virginia booth as well as at the Italian Grid Initiative booth. Finally, JSC staff also managed the PRACE booth.

More detailed information and pictures are available at:

http://www.fz-juelich.de/ias/jsc/events/sc12. (Contact: Dr. Walter Nadler, w.nadler@fz-juelich.de)

Workshop "Lattice Practices 2012" a great success

In October 2012, the workshop "Lattice Practices 2012" at Zeuthen was organized by the emerging SimLab "Nuclear and Particle Physics" as a joint activity between JSC, DESY, and the Cyprus Institute. The workshop provided 30 students and researchers with practical training as well as theoretical background for their own research. Speakers from different institutions all over Europe gave lectures on topics in

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jsc@fz-juelich.de www.fz-juelich.de/jsc their own field of expertise and prepared hands-on exercises with strong emphasis on this practical training. The topics covered ranged from computer architecture, optimization and simulation algorithms to hot topics in quantum chromodynamics that are presently attracting great attention within the field.

The participants' evaluations showed that the workshop was a great success and provided encouraging feedback for the next workshop, which is planned to take place at JSC. Further information can be found at http://www.desy.de/LAP2012

(Contact: Dr. Stefan Krieg, s.krieg@fz-juelich.de

New GCS Large-Scale Projects at JSC

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers JUQUEEN (JSC), HERMIT (HLRS), and Super-MUC (LRZ). Projects are classified as "large-scale", if they require more than 2% of the available CPU cycles, corresponding, e.g., to 36 million core hours on JUQUEEN. This time around, six additional projects were able to achieve the status of a large-scale project on JUQUEEN, with a total of about 380 million core hours being awarded. Four projects are from high-energy physics, submitted by Prof. Zoltan Fodor, Dr. Kalman Szabo (both Bergische Universität Wuppertal), Prof. Gerrit Schierholz (DESY), and Prof. Hartmut Wittig (Johannes Gutenberg University Mainz), all dealing with various problems in the theory of strong interactions. One project is from the field of chemistry, submitted by Prof. Dominik Marx (Ruhr-Universität Bochum), about mechanochemistry, i.e. the mechanical manipulation of covalent bonds. Finally, one project is from condensed matter physics, submitted by Dr. Jens Harting, (University of Stuttgart), dealing with the simulation of complex fluids and their flow through porous media.

For more details on these projects and also on projects at HERMIT and SuperMUC, see http://www.gauss-centre.eu/. (Contact: Dr. Walter Nadler, w.nadler@fz-juelich.de)

NIC Excellence Projects 2012

At its meeting on 18 October 2012 at Jülich, the NIC Peer Review Board decided to recognize another outstanding simulation project by awarding it the title of a NIC Excellence Project. "Non-linear single particle response of glass-forming systems to external fields", submitted by Prof. Kurt Binder (Johannes Gutenberg University Mainz), aims to investigate the active nonlinear microrheology in glass-forming systems using non-equilibrium molecular dynamics simulations. For more details, see http://www2.fz-juelich.de/nic/Projekte/exzellenz-2012.html, in German.

(Contact: Dr. Walter Nadler, w.nadler@fz-juelich.de)

Awards for Bachelor's and Master's Students

On 23 November 2012, four students from Forschungszentrum Jülich received an award – the Ehrenplakette – from Aachen University of Applied Sciences (FH Aachen). In a ceremony at Aachen's historical town hall, Prof. Baumann, rector of FH Aachen, honoured Ingo Heimbach (PGI), Florian Rhiem (PGI), and Martin Vieten (IEK-5) as the best graduates of the bachelor's course Scientific Programming, and Carsten Karbach (JSC) as the best graduate of the master's course Technomathematics. Carsten Karbach's master's thesis has been published and is available at: http://hdl.handle.net/2128/4703

(Contact: Prof. Johannes Grotendorst, *j.grotendorst@fz-juelich.de*)

End of Year Colloquium 2012

Date: Thursday, 13 December 2012, 10:00-16:00

Venue: Hörsaal, JSC

Most talks will be given in German.

10:00 Thomas Lippert: Welcome

10:15 Robert Speck: The simultaneity of the non-

simultaneous

10:45 Carsten Karbach: PTP is watching your supercom-

puter

11:15 Jedrzej Rybicki: DARIAH - a case for Big Data

14:00 Maik Boltes: Menschen von oben

14:30 Dirk Brömmel: HPC goes Win95

15:00 Jiri Kraus: Das NVIDIA Jülich Application Lab

15:30 Thomas Lippert: God save the Queen

Info: http://www.fz-juelich.de/ias/jsc/events/eyc-2012

Events

Workshop "Blue Gene Active Storage"

Date: 10-11 January 2013

Venue: Rotunda, Jülich Supercomputing Centre Info: http://www.fz-juelich.de/ias/jsc/events/bgas

Opening Event for the Simulation Lab Neuroscience

Date: 14-15 January 2013

Venue: Rotunda, Jülich Supercomputing Centre Info: http://www.fz-juelich.de/ias/jsc/events/slns2013

First JUQUEEN Porting and Tuning Workshop

Date: 4-6 February 2013

Venue: Lecture room 1, Jülich Supercomputing Centre Info: http://www.fz-juelich.de/ias/jsc/events/juqueenpt13

Application deadline: 11 January 2013

If you would like to receive regular information on our events, please send an e-mail to *jsc-events-join@fz-juelich.de*.

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