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Exascale Project DEEP Started

The EU-funded project DEEP started on 1 December 2011 with the goal of developing a Dynamical Exascale Entry Platform over the next three years.

In the DEEP project, partners from all over Europe (8 research centres, 3 universities, and 5 industrial companies) have joined forces to build the prototype of a novel supercomputing architecture for exascale: the DEEP system. Its innovative design consists of two parts, which are connected to each other but can also be operated autonomously: Cluster and Booster. DEEP aims to bridge the gap between today's highly scalable architectures and less scalable cluster machines. In the DEEP system, applications will run those parts of their code with regular communication patterns (typically highly scalable) on the Booster, leaving their less scalable complex kernels on the Cluster. While the Cluster is an off-the-shelf component, the Booster will be designed and built by the DEEP project partners using Intel MIC processors and the novel EXTOLL interconnect. To increase energy efficiency, the DEEP system will be cooled using the "hot water" concept, which significantly reduces the energy needed for cooling. However, DEEP is not only a hardware project. To run the DEEP system, a programming and run-time environment will be created, and mathematical libraries and performance analysis tools will be adapted. Furthermore, six scientific applications, selected based on their high relevance for industry and society, will be ported to the DEEP system to demonstrate the validity of the DEEP concept and its scalability towards exascale.

JSC is coordinating the DEEP project and is participating in the architectural (both hardware and software) design, the development of the lower layers of the programming environment, and the adaptation of mathematical libraries and the performance analysis tool Scalasca to the new platform. The DEEP system will be installed at JSC.
(Contact: Wolfgang Gürich, ext. 6540;
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NIC Symposium 2012

The 6th NIC Symposium will be held at Forschungszentrum Jülich from 7 to 8 February 2012. The talks will inform a broad audience of scientists and interested members of the public about the activities and results obtained in the last two years by research projects supported through the John von Neumann Institute for Computing (NIC) on the supercomputers JUROPA and JUGENE at Jülich. Invited talks and a poster session will cover topics in the fields of astrophysics, biophysics, chemistry, elementary particle physics, condensed matter, materials science, soft matter science, environmental research, hydrodynamics and turbulence, plasma physics, and computer science. To accompany the conference, a comprehensive proceedings volume will also be published and copies made available to the participants. It will cover an even wider range of projects than given by the talks.

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This symposium will also mark the 25th anniversary of the founding of the Höchstleistungsrechenzentrum (HLRZ), which in 1998 became NIC. The detailed programme and the registration form are available at:
http://www2.fz-juelich.de/nic/symposium.
(Contact: Dr. Walter Nadler, ext. 2324)

Winter School on Hierarchical Methods for Dynamics

Jülich will continue its successful series of winter schools in computational science. From 5 to 9 March 2012, the winter school on "Hierarchical Methods for Dynamics in Complex Molecular Systems" will be held at Jülich Supercomputing Centre. The school is organized by the Jülich CECAM node and Ruhr-Universität Bochum and is tailored to PhD students and young postdocs. The scientific programme offers 25 lectures including an introduction to parallel computing.

Generating and analysing the dynamics of molecular systems is a true challenge for molecular simulation. It includes processes that happen on the femtosecond scale, such as photoinduced nonadiabatic (bio)chemical reactions, and touches the range of seconds, e.g. relevant to cellular processes or crack propagation. Thus, many orders of magnitude in time need to be covered either one by one or concurrently. This winter school will focus on hierarchical methods for dynamics with a view to systems described in terms of many atoms or molecules. Examples will come from materials science, soft matter and life science and fluid dynamics, such as the simulation of blood flow on the cell scale. The programme is complemented by lectures on modern numerical methods and parallel computing techniques.

Applications for participation can be sent until 27 January 2012. Based on the required application documents, about 50 participants will be selected by the organizers. Details about the school and the application process can be found at: *http://www.fz-juelich.de/wshd*.
(Contact: Prof. Dr. Johannes Grotendorst, ext. 6585)

Looking Back on SC11

Supercomputing 2011, the premier international conference and exhibition on high-performance computing and networking, took place in Seattle, Washington, USA, from 12 to 18 November 2011. Conference attendance at this year's event set a new record with about 11,500 attendees, 15% above last year's number. JSC participated in the conference and exhibition for the thirteenth time in succession.

JSC highlighted its role as one of the leading European high-performance computing centres at the exhibition, where a record 351 exhibitors, research institutions as well as hardware and software companies, were represented. 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 individual consultations. Particular emphasis was placed this year on tools developed by JSC for the performance analysis of parallel programs, monitoring supercomputers, and Grid activities under the motto "It's More Than Hardware". LLview, the interactive monitoring software for supercomputers, was presented in live demonstrations on the JSC systems JUGENE, JUROPA, and HPC-FF and on various systems of the US university HPC environment XSEDE. It drew an extraordinarily large response from visitors. Incidentally, LLview was also showcased at the IBM booth as part of the Eclipse PTP environment. In addition, JSC presentations were given at the Intel, European Middleware Initiative (EMI), and XSEDE booths, and JSC staff were also present at the PRACE booth.

JSC staff members contributed actively 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 Poster Session and presented the Best Poster Award. Furthermore, Prof. Achim Bachem, chairman of the Board of Directors of Forschungszentrum Jülich and chairman of the PRACE AISBL council, gave a keynote speech.

More detailed information and pictures are available at:
http://www.fz-juelich.de/ias/jsc/events/sc11.
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PhD Student Seminar on Fluid Dynamics

On 29 November 2011, the first PhD student seminar entitled "Fluid dynamics on supercomputers" took place at the Jülich Supercomputing Centre. PhD students from JSC and the DLR Center for Computer Applications in AeroSpace Science and Engineering ($C^2A^2S^2E$) in Braunschweig reported on research projects in aerodynamics, propulsion technology, flow simulation and numerical methods. The goal of the joint seminar is to exchange ideas and to improve networking between young researchers from $C^2A^2S^2E$ and JSC. Since 2010, DLR and Forschungszentrum Jülich cooperate in the field of aircraft simulations on supercomputers. Numerical simulations promise to reduce the development risks and to shorten the development cycles of aircrafts. It is expected that the next generation of aircrafts will be developed and tested completely on the computer ("digital aircraft"). Further information can be found at:
http://www.fz-juelich.de/ias/jsc/events/dlr-fzj-phd.
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