

JSCNews

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High-Q Club Launched

Following the first JUQUEEN Porting and Tuning workshop in February, a number of applications have since been scaled across the entire 28-rack BlueGene/Q machine at JSC. To encourage other developers to invest in tuning and scaling their codes and to promote the idea of exascale computing, JSC has established the High-Q Club, an exclusive set of codes capable of utilizing all of the 458,752 cores – and typically more than 1 million threads – of JUQUEEN.

Members so far include: **waLBerla**, a Lattice Boltzmann solver from the University of Erlangen-Nürnberg; **Terra-Neo**, a multi-grid solver for geophysics applications, also from the Erlangen group; **Gysela**, a gyrokinetic code from CEA, France, for modelling fusion core plasmas; **dynQCD**, a Lattice QCD code developed at the University of Wuppertal and JSC; and **PEPC**, a tree algorithm developed at JSC for electrostatic and gravitational N-body problems. In the last example, PEPC was able to utilize a total of 458,752 MPI tasks and 1,668,196 parallel threads to compute long-range electrostatic forces between 65 billion particles – a new record for this class of N-body code.

To qualify for High-Q Club status, application developers should submit evidence of scalability across all available cores on JUQUEEN, preferably including multithreading capability. High-Q Club membership updates including technical details of applications' performance and qualification rules are available at

<http://www.fz-juelich.de/ias/jsc/high-q-club>.

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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 JUQUEEN (JSC), HERMIT (HLRS), and SuperMUC (LRZ). Projects are classified as large-scale, if they require more than 35 million core hours.

After the last call, seven projects achieved the status of large-scale project on JUQUEEN, with a total of about 380 million core hours being awarded. One project from the field of chemistry, submitted by Prof. Dominik Marx (Ruhr-Universität Bochum), deals with prebiotic peptide synthesis. The second project is from the field of astrophysics, submitted by Dr. Hubert Klahr (MPI for Astronomy, Heidelberg), and simulates planet formation. Another project, from condensed matter physics, submitted by Dr. Jens Harting, (University of Stuttgart), simulates complex fluids and their flow through porous media. The project headed by Prof. Jörg Schumacher (Technische Universität Ilmenau) is from the field of fluid dynamics and analyzes strong fluctuations in turbulent convection. Three projects are from the field of high-energy physics, submitted by Dr. Stephan Duerr, Prof. Zoltan Fodor, and Dr. Christian Hoelbling (all from the University of Wuppertal), and all involve investigating various aspects of hadronic properties in lattice QCD.

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

JUROPA Successor Prototype Installed

In preparation for the upcoming replacement of the JUROPA HPC cluster, a prototype system called JUROPA-3 has recently been installed and successfully accepted at JSC. JUROPA-3 is the outcome of a cooperation between JSC, ParTec Cluster Competence Center GmbH, and T-Platforms. The purpose of the cooperation is to study possible solutions for fundamental questions in large-scale cluster computing. Topics like application check-point/restart, end-to-end data integrity, network topology, failure prediction and energy efficiency will be addressed. JUROPA-3 will serve as a testbed for these investigations.

In addition, a small sub-partition of JUROPA-3 will be used as a platform for long-running application codes solving static non-linear structural mechanics problems with high memory demands. This partition, financed by ZEA-1 (Engineering and Technology) at Jülich, will be hosted by JSC.

JUROPA-3 comprises 60 compute nodes, each equipped with two Intel Xeon E5-2650 CPUs (Sandy Bridge-EP) providing a total of 960 processor cores with a peak performance of 15.3 teraflops. In addition, eight compute nodes are each enhanced with either two NVIDIA Tesla K20X GPUs or two Intel Xeon Phi 5110P co-processors. The co-processors amount to an extra performance of 18.5 teraflops peak. Further details can be found at

<http://www.fz-juelich.de/ias/jsc/juropa-3>.

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PRACE Conference in Varna

From 3 to 5 June 2013, more than 100 participants from the 25 member countries and the Brussels office of PRACE (Partnership for Advanced Computing in Europe) met in Varna, Bulgaria, for a project meeting of the three PRACE implementation phase projects.

On the first day, the highlights of PRACE-1IP, which started in July 2010, were presented. Up until the end of 2013, the evaluation of prototypes for multi-petascale technology and the porting of applications to the emerging Intel MIC technology will complete the work. Prof. Thomas Lippert, coordinator of the project, stressed that PRACE-1IP has been an indispensable step in the implementation of the PRACE Research Infrastructure. Among its many achievements, he highlighted in particular the initiation of and support for the update of the Scientific Case for HPC in Europe, which supports the efforts of PRACE AISBL to maintain HPC as a high-priority item on the political agenda in Europe.

The remaining two days were dedicated to discussions of the current status and future work of the PRACE-2IP and

PRACE-3IP projects. PRACE-2IP will end in August, and therefore an important topic was the handover to PRACE-3IP of ongoing activities. A new element of PRACE-3IP is a joint pre-commercial procurement (PCP) pilot, focusing on whole system design for energy-efficient HPC. It is planned to publish the PCP tender in July, and the meeting provided a good opportunity to finalize the preparations.

The European Commission is providing € 57 million funding in total for the three projects which support and accelerate the implementation of the pan-European high-end computing research infrastructure created and operated by PRACE. JSC is the coordinator of all three PRACE projects.

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News from the NIC Scientific Council

The Scientific Council of the John von Neumann Institute for Computing (NIC) held its annual meeting on 18 April 2013 at Jülich. New members Dr. Christian Beck (Siemens AG), Dr. Marc-Oliver Gewaltig (EPFL Lausanne), and Prof. Hartmut Wittig (Johannes Gutenberg-University Mainz) were elected and will begin their term in January 2014. Two new members were also elected to the NIC Peer Review Board: Prof. Michael Rohlfing (University of Münster) and Prof. Andreas Kempf (University of Duisburg-Essen). They will begin their term of office at the next meeting of the NIC Peer Review Board in October.

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NIC Excellence Project 2013

At its April meeting at JSC, the NIC Peer Review Board decided to award an outstanding simulation project with the title of NIC Excellence Project. "First-principles modeling of minerals, melts and fluids at high pressures and high temperatures", submitted by Dr. Sandro Jahn (German Research Centre for Geosciences GFZ, Potsdam), investigates material properties and chemical processes under extreme temperatures and pressures in order to understand geochemical and geodynamic processes in the Earth's crust and mantle. For more details, see

<http://www.fz-juelich.de/nic/Projekte/exzellenz-2013.html> (in German).

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Events

NVIDIA Application Lab at Jülich: First Annual Workshop

Date: 8-9 July 2013

Venue: Jülich Supercomputing Centre, Rotunda

Info: <http://www.fz-juelich.de/ias/jsc/events/nvidia-ws>

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