JUQUEEN – Jülich's New Green Flagship

As a result of the strong collaboration between JSC and IBM in the Exascale Innovation Centre, Forschungszentrum Jülich procured an IBM Blue Gene/Q system, known as JUQUEEN. Systems of this type are currently the most energy-efficient supercomputers according to the Green 500 List (*http://www.green500.org*). The machine is being installed for researchers at Jülich and for researchers working in the HPC branch of the Jülich-Aachen Research Alliance (JARA).

The structure of the Blue Gene/Q is similar to that of the Blue Gene/P with increased performance metrics and on-board water cooling. The system will consist of eight racks and will have a peak performance of 1.6 petaflops. One rack contains 32 node boards with 32 compute nodes each. A node consists of a processor comprising 16 IBM PowerPC A2 cores (1.6 GHz, 64 bits) for the execution of user applications; one additional core is used for the operating system. Each core can execute four processes/threads and has a quad floating point unit. The maximal performance of the processor is 204.8 Gflop/s. The main memory per node is 16 GB and an integrated 5D torus provides 50 GB/s bandwidth and 2.5 μs latency (worst case). I/O nodes supply the connection to the JUST fileserver via 10 gigabit Ethernet technology.

JUQUEEN will be installed in two batches with four racks each, one in mid-April and the second one in June. Production will start mid-May. Further information can be found at *http://www.fz-juelich.de/ias/jsc/juqueen*.

Furthermore, Jülich intends to procure a second Blue Gene/Q system, funded by GCS, for national (GCS/NIC) and European (PRACE) users. It will succeed JUGENE and should be accessible in November 2012. To prepare for the replacement, the final shutdown of JUGENE has been scheduled for 31 July 2012, i.e. before the end of the allocation periods expiring in autumn 2012. All JUGENE users with ongoing projects will receive compensation of their "dropped" JUGENE compute time. Emails to this effect have been sent to the users affected. All project data accessible on JUGENE will also be accessible on the Blue Gene/Q system.

To allow for maximum capability, JUQUEEN and the GCS-funded Blue Gene/Q system will be coupled in October 2012. No user access to these machines will be possible during this time. After the replacement has been completed in November 2012, we at JSC are looking forward to presenting an improved leadership-class supercomputer infrastructure to our users.
(Contact: Dr. Norbert Attig, n.attig@fz-juelich.de)

Guest Student Programme 2012 – Call for Application

During summer 2012, JSC will once again be offering a guest student programme. It will be supported by the Centre Européen de Calcul Atomique et Moléculaire (CECAM) and the German Research School for Simulation Sciences (GRS).

Within this programme, students with a major in natural sciences, engineering, computer science or mathematics will have an opportunity to familiarize themselves with different aspects of scientific computing. Together with local scientists, the participants will work on different current topics in research and development. Depending on their previous knowledge and on the participant's interests, the assignments can be taken out of different areas. These fields include mathematics, physics, chemistry, software development tools, visualization, distributed computing, operating systems and communication. Special emphasis is placed on the use of supercomputers.

The participants are expected to be familiar with and have experience in the computer-oriented branches of their subjects. The students should already have completed their first degree but have not yet finished their master's course. Additionally, a letter of recommendation from a university lecturer or professor is required for application.

The programme will last ten weeks and will take place from 6 August to 12 October 2012. Students are encouraged to apply for the programme in writing (English or German). The closing date for applications is 9 May 2012. Further information can be found on the web at
http://www.fz-juelich.de/ias/jsc/gsp/.
(Contact: Mathias Winkel, *jsc-gsp@fz-juelich.de*)

First EUDAT User Forum in Barcelona

The pan-European EUDAT project aims to establish a collaborative data infrastructure (CDI) to serve the needs of a wide variety of research communities, including those in the roadmap released by the European Strategy Forum on Infrastructures (ESFRI).

In Barcelona from 7-8 March, EUDAT held its first user forum together with more than 60 participants including representatives of 18 ESFRI projects and other research communities. The requirements for a set of initial cross-disciplinary data services the EUDAT CDI aims to deliver were discussed in four different user forum tracks. The user communities presented their different data model approaches and research activities from a wide range of scientific disciplines.

The deployment of cross-disciplinary EUDAT services is driven by the strong demand from research communities. Several EUDAT user communities (CLARIN, ENES, EPOS, VPH) identified a common need to replicate their scientific data from their community centres to data centres (CINECA, CSC, JSC, RZG, SARA) in a safe way, leading to a better accessibility of the data. The demands of the user communities and the capabilities of the data centres are aligned in task forces. These activities are coordinated by the 'replication task force' that is led by JSC. The initial approach for data replication was presented at the user forum in order to get feedback and discuss possible extensions for further

user communities. The task force aims to provide pilot services in autumn 2012. At the same time, the requirements from user communities attending the user forum will be assessed to pave the way for new communities.
(Contact: Morris Riedel, *m.riedel@fz-juelich.de*)

IAS Winter School 2012

From 5-9 March 2012, the Winter School and CECAM tutorial "Hierarchical Methods for Dynamics in Complex Molecular Systems" of IAS (Institute for Advanced Simulation) took place at JSC. It continued the successful series of biennial Winter Schools at JSC and was organized by the Jülich CECAM node. The focus of this year's school was on hierarchical simulation methods for dynamics in hard and soft materials, biomolecular systems, flow simulation and transport. The programme was complemented by lectures on advanced methods (fast algorithms for DFT on modern HPC systems, multigrid QM/MM approaches, accelerated molecular dynamics methods), numerical software for supercomputers and an introduction to parallel computing followed by a hands-on programming session. The scientific programme was compiled by Johannes Grotendorst, Godehard Sutmann, Gerhard Gompper (Forschungszentrum Jülich) and Dominik Marx (Ruhr-Universität Bochum). Leading scientists in computational physics, chemistry, biology and mathematics presented lectures for 50 PhD students and young postdocs from eleven different countries. The young scientists were encouraged to present their own research in short oral presentations and subsequently to discuss methods and results in poster sessions. The lecture notes from the school have been published as volume 10 in the IAS book series; see *http://hdl.handle.net/2128/4545*.
(Contact: Prof. Dr. Johannes Grotendorst, *j.grotendorst@fz-juelich.de*).

Events

IAS Seminar: FLAME - Modern Alternatives to (Sca)LAPACK
Speaker: Robert van de Geijn, University of Texas, Austin
Date: 12 April 2012, 14:00
Venue: Hörsaal, Jülich Supercomputing Centre

HPC-Technologie für die Wissenschaft – Festkolloquium
Date: 25 April 2012, 14:00
Venue: Hörsaal, Jülich Supercomputing Centre

Further events, talks, and training courses:
http://www.fz-juelich.de/ias/jsc/events

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