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NVIDIA Application Lab at JSC

During ISC 2012, Forschungszentrum Jüich and NVIDIA announced a multi-year collaboration. Together, the two organizations launched the "NVIDIA Application Lab" which is based at JSC. The primary goal of the lab is to broaden the application basis for GPGPUs (General-purpose computation on graphics processing units) and to provide support for the optimization of applications using such devices. Enabling the efficient use of parallel multi-GPU architectures will be the key focus of the lab, as will the analysis of new features of next-generation hardware (such as the upcoming Kepler GK110) and programming models. The lab will use the JUDGE cluster (Jülich Dedicated GPU Environment) at JSC, which comprises 206 nodes with 2 NVIDIA GPGPUs per node.

The lab will work on applications from different research areas including astrophysics and astronomy, biology, elementary particle physics and materials science. It will initially concentrate on a pilot application from Forschungszentrum Jülich in the field of medicine and neuroscience. The group headed by Prof. Katrin Amunts (INM-1, Structural and Functional Organization of the Human Brain) plans to extend the use of GPGPUs for their JuBrain project. Within this project, a large number of histological brain sections will be scanned and rendered to create a high-definition, structurally accurate and realistic model of the human brain. (Contact: Prof. Dr. Dirk Pleiter, *d.pleiter@fz-juelich.de*)

Farewell JUGENE

Installed in October 2007, JUGENE with its 16 racks became the most powerful supercomputer in Europe and was ranked second in the international Top500 list in November 2007. As the concept of this Blue Gene/P system proved very successful and the user demand was overwhelming, JUGENE was later expanded to 72 racks in the context of the Gauss Centre for Supercomputing (GCS). User operation of what was the first petaflop system in Europe started in June 2009.

On 31 July 2012, having been in use for nearly five years, what is still the largest Blue Gene/P in the world will be shut down. JUGENE's 72 water-cooled racks will then be removed to make room for the superseding Blue Gene/Q system.

Managing the huge number of components was a challenge when operation began, but JUGENE proved to be an extremely stable system after the start-up period. Many scientific user groups from GCS, PRACE, and Forschungszentrum Jülich ran production jobs, pushing the usage to an average of over 95% of the computing time, and quite a few successfully ran jobs in parallel on all 294,912 cores. The results of these scientific applications have been published in several articles in renowned magazines such as Nature and Science.

We bid this workhorse farewell, and welcome the new Blue Gene/Q (JUQUEEN), which will provide even more computing power to our users in the future.
(Contact: Jutta Docter, *j.docter@fz-juelich.de*)

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FIT4Green Project Successfully Completed

FIT4Green – a 30-month EU project that started in January 2010 – was successfully completed in June 2012. JSC collaborated in this project with partners from GFI Informatica Spain, HP Italy, University of Passau, University of Mannheim, Imperial College London, VTT Technical Research Centre Oulu, Create-net Italy, ENI Italy, and Almende Rotterdam. FIT4Green contributed to ICT energy reducing efforts by creating an energy-aware layer of plug-ins for data centre automation frameworks, to improve the energy efficiency of existing IT deployments. It also minimizes the overall power consumption by moving computation and services around a federation of IT data centres. The FIT4Green optimization layer does not compromise Service Level Agreements (SLA) and Quality of Service (QoS) metrics, and it operates on top of current data centre resource management software to orchestrate the allocation of ICT resources and turn off the under- or unused equipment. Energy savings varied between 5% in a fully utilized HPC environment and up to 50% in a federation of data centres and they strongly depended on the availability of energy-saving mechanisms on the resources. More information can be found at *http://www.fit4green.eu/*.
(Contact: André Giesler, *a.giesler@fz-juelich.de*).

GCS Steering Committee founded

After all partners in the Gauss Centre for Supercomputing (GCS) – JSC, HLRS and LRZ – installed petaflop supercomputers funded by the Bund-Länder project PetaGCS, a common steering committee for computational science projects was established on 2 July 2012 at a meeting at LRZ in Garching. The committee will award computer time grants on the GCS petaflop systems to excellent GCS large-scale projects which do best in a rigorous scientific and technical evaluation. Chairman of the GCS Steering Committee is Prof. Siegfried Wagner from the University of Stuttgart, and Prof. Kurt Binder from the Johannes Gutenberg University of Mainz is Vice Chairman. The complete list of committee members is available at *http://www.gauss-centre.de/sc*.
(Contact: Dr. Norbert Attig, *n.attig@fz-juelich.de*)

2nd Call for High-Level Support from JSC SimLabs

Following their successful high-level support initiative in 2011, the four JSC Simulation Labs (Computational Biology, Molecular Systems, Plasma Physics, and Climate Science) are again inviting current and potential supercomputer users to apply for expert help in adapting and optimizing their applications for state-of-the-art HPC architectures. In this second call, the emphasis will be on longer-term projects aimed at designing new computational methods or improving existing algorithms capable of exploiting highly parallel architectures – in particular the JUROPA and BlueGene/Q machines hosted at JSC. Proposed work packages may involve up to 6 person-months of SimLab staff resources and are expected to take the form of a scientific cooperation, ideally culminating in joint publications or follow-up projects with external funding.

The present call is open-ended and is expected to run until at least mid-2013. Proposals will be assessed at regular intervals depending on demand and staff availability. Further information can be found at
http://www.fz-juelich.de/ias/jsc/simlab-call2.
(Contact: Dr. Paul Gibbon, *p.gibbon@fz-juelich.de*)

International Workshop CQDC'12

The "International Workshop on Cooperative Quantum Dynamics and Its Control (CQDC'12)" will take place from 29 to 31 October 2012 at JSC. The goal of the workshop is to discuss the possibility of essentially new quantum phenomena, and observations/operations that would be required for their realization, detection, and understanding.

Quantum dynamics and novel quantum states in systems of many particles or spins, many of which had been beyond the reach of experimental realization, are now becoming more realistic due to recent advances in experimental techniques, such as the synthesis of molecular magnets, the nano-engineering of quantum dots, time-resolved measurements with ultra-short pulses, and optical lattices of cold atoms.

In addition, new numerical methods, such as the tensor-network variational approximation, are making many previously hard problems now tractable. The talks, given by invited speakers only, will highlight recent developments in quantum annealing, open quantum systems, quantum computer hardware, optical lattices, equilibration and thermalization of quantum systems, tensor network simulations, and related topics. All participants are invited to present a poster in the poster session. More information can be found at *http://www.fz-juelich.de/ias/jsc/events/cqdc12*.
(Contact: Prof. Dr. Kristel Michielsen, *k.michielsen@fz-juelich.de*)

Events

Introduction to parallel programming with MPI and OpenMP
Instructors: Dr. F. Janetzko, Dr. A. Schnurpfeil, JSC
Date: 7-10 August 2012, 09:00-16:30
Venue: Ausbildungsraum 1, Jülich Supercomputing Centre
Registration: *f.janetzko@fz-juelich.de*, ext. 1446

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