



Jülich Supercomputing Centre

Blue Gene/P Scaling Workshop 2011

Continuing our very successful series of Blue Gene Scaling Workshops, JSC has announced the next "Blue Gene/P Extreme Scaling Workshop", which will take place at JSC from 14 to 16 February 2011. The purpose of the workshop is to give application teams an opportunity to scale their code across the full Blue Gene/P system JUGENE, which consists of 72 racks with a total of 294,912 cores – still the highest number of cores worldwide. Appropriate hardware, software and support personnel will be provided to assist participants.

Workshop attendees will be selected on the basis of written proposals, which must be submitted by 30 November 2010. Participation is limited to six application teams. Selection criteria are: a high level of confidence that the code will scale across 294,912 cores or at least a large proportion of them; the JUGENE infrastructure (OS, compilers, libraries) must support user requirements; and the code should be able to produce a significant scientific impact. Priority will be given to new applicants who have not yet participated in one of the previous workshops.

To apply for the workshop send a short proposal (about two pages including a scaling plot/table) by email to sc@fz-juelich.de using "ScalingWS11" as part of the subject. The proposal should contain a description of the application to be scaled, scaling plots showing a good scaling of at least up to 64k tasks, code requirements (e.g. spe-

cial libraries, compiler versions, I/O needs, and other requirements beyond a "standard" BlueGene/IBM setup), contact data and references. If accepted, we expect that at least one team member will register and attend the workshop. More information can be found at:

http://www.fz-juelich.de/jsc/bg-ws11 (Contact: SC Support, ext. 2828)

Heraeus Summer School

From 6 - 10 September 2010 Jülich Supercomputing Centre organized a Summer School on Fast Methods for Long-Range Interactions in Complex Systems, which was financially supported by the Wilhelm and Else Heraeus Foundation. Thirty participants from five countries came to Jülich to learn about modern algorithms which efficiently solve the Coulomb problem by reducing its algorithmic complexity from $O(N^2)$ to $O(N \log N)$ or O(N). Ten lecturers from universities all over Germany and from Forschungzentrum Jülich presented state-of-the-art methods, algorithms and implementations of various approaches to tackle the long-range interactions between particles.

The motivation for organizing this Summer School arose from the BMBF-funded network project ScaFaCoS (Scalable Fast Coulomb Solver), which aims to develop a freely available scalable library for various fast methods solving the long-range interactions between particles in complex systems. No. 189 • Oct. 2010

Forschungszentrum Jülich GmbH in der Helmholtz-Gemeinschaft Jülich Supercomputing Centre 52425 Jülich I Germany

Phone +49 2461 61-6402

jsc@fz-juelich.de www.fz-juelich.de/jsc The wide spectrum of the participants' scientific fields reflects the interdisciplinary nature of computational science activities at JSC. Many of the participants expressed strong interest in incorporating the advanced methods presented at the school in their own applications. The proceedings of the Summer School will be published as a volume in the IAS Series. We intend to repeat the school with a similar focus next year.

(Contact: Dr. Godehard Sutmann, ext. 6746)

Best Paper Award at ICPP 2010 Conference

Researchers from the Jülich Supercomputing Centre received the Best Paper Award from the International Conference on Parallel Processing (ICPP) 2010 in San Diego, California, a forum for scientists and engineers in academia, industry and government to present their latest findings in parallel and distributed computing. The award was given to the authors David Böhme, who is funded through a scholarship from the RWTH graduate school AICES, Dr. Markus Geimer, Prof. Felix Wolf, and Dr. Lukas Arnold for their paper entitled "Identifying the root causes of wait states in largescale parallel applications". The article introduces a scalable technique that enables an improved understanding of how the effects of load imbalance slow down program execution - a well-known problem with many simulation programs that prevents them from exploiting the full power of large and expensive supercomputers such as JUGENE. The new approach, which is currently being integrated into Scalasca, a widely-used performance-analysis tool developed at the Jülich Supercomputing Centre and the German Research School for Simulation Sciences in Aachen, will allow more target-oriented optimizations of such phenomena. (Contact: Prof. Felix Wolf, ext. 1583)

New 100 Gigabit/s Ethernet Successfully Tested between JSC and KIT

The German Research Net Provider DFN, JSC, KIT at Karlsruhe and the industrial partners Cisco Systems and Huawei Technologies jointly tested newly developed 100 gigabit/sec Ethernet components in the beta state in a real-life scenario on a fibre link between JSC and KIT.

While the JSC designs and operates terabit networks as part of its supercomputer and storage cluster setup, it also acts as a leading project partner responsible for the planning, deployment and operation of demanding Europeanscale research networks like the DEISA network or the German part of the LOFAR network. In this role, JSC works in close cooperation with leading manufacturers as a research partner for designing and deploying new network technologies. The testbed between JSC and KIT was one of the first real-world wide-area deployments of the recently finalized IEEE802.3ba standard for 100 Gbit/s Ethernet. Based on development versions of Cisco Systems CRS-3 and Huawei DWDM equipment, the project partners evaluated the interoperability of the 100GE components in a heterogeneous environment. After several months of planning, preparation and the installation of several racks of network equipment at both sides of the testbed, the actual tests were conducted in a three-week test window. They revealed that, despite some minor interoperability issues on the optical layer, the newly built pre-production versions of 100GE network inter-faces were able to offer sustainable and reliable 100 Gbit/s bandwidth to real-world IP-based applications at a distance of 447 km.

The results of these tests are important for the future development of research network infrastructures as well as for dedicated networks in the all-demanding area of supercomputers and data centres.

(Contact: Olaf Mextorf, ext. 2519)

JSC at SC10 in New Orleans

SC10, the premier international conference on highperformance computing, networking, storage, and analysis, will take place in New Orleans, Louisiana, from 13 to 19 November 2010. There, JSC will present its wide-ranging supercomputing activities in booth #1451. One focus will be the supercomputers JUGENE, JUROPA, and QPACE, which are again expected to attain a high ranking on the next Top500 and Green500 lists. JSC will also highlight how its advanced application-enabling support structures, in particular its newly created simulation labs, drive the advance of simulation science. JSC staff will give presentations at the booth about simulation labs, supercomputing tools, and about Grid activities and Grid tools developed in-house. JSC staff will also be present at the PRACE booth (#4021).

For up-to-date information on JSC's activities at SC10 see: *http://www.fz-juelich.de/jsc/news/sc10*.

Do pay us a visit if you're attending the conference and also join in the PRACE treasure hunt! (Contact: Dr. Walter Nadler, ext. 2324)

Events

UNICORE 6 – uniform access to the supercomputer systems

Speaker: Michael Rambadt, JSC Date: Tuesday, 26 October 2010, 9:00 - 12:00 Venue: Ausbildungsraum 2, Jülich Supercomputing Centre Registration: *M.Rambadt*@*fz-juelich.de*, ext. 4340

Jülich-Chernogolovka Seminar

Topic: Protein Folding

Date: Wednesday, 3 November 2010, 14:00 Venue: Hörsaal, Jülich Supercomputing Centre