JÜLICH
FORSCHUNGSZENTRUM

JSCNews
Jülich
Supercomputing
Centre

No. 187 • July 2010

Heraeus Summer School at JSC

JSC will host a Wilhelm und Else Heraeus Summer School on "Fast Methods for Long-Range Interactions in Complex Systems" from 6 to 10 September 2010. The focus of this school is parallel computing and computer simulations of complex charged particle systems, a recurring topic in a wide range of physical sciences, such as astrophysics, statistical physics, plasma physics, material sciences and physical chemistry. Important methods and algorithms for reducing the computational complexity of evaluating long-range interactions will be covered including fast multipole and tree methods along with multigrid or FFT-based methods and their parallelization. Sessions will include both lectures from JSC and invited speakers, together with hands-on training with selected techniques.

The school is open to PhD students and postdocs working in computational science, in particular physics, computational chemistry or numerical mathematics, who wish to learn about these state-of-the-art techniques or who want to apply them to their own simulation codes.

Further information and advice on how to apply is available from
http://www.fz-juelich.de/wehss
(Contact: Dr. G. Sutmann, ext. 6746)

Application for Computing Time

Applications for computing time on the supercomputers JUGENE and JUROPA in Jülich can be made for the next granting period (1 November 2010 - 31 October 2011). Researchers working on simulation-intensive projects in the natural and engineering sciences can apply in several different ways:

Projects on JUROPA and national projects on JUGENE
Proposals are eligible from academic and research institutions. The electronic application forms will be open starting from 30 July 2010 and can be accessed through: *http://www.fz-juelich.de/jsc/computing-time*. Deadline for submissions is 31 August 2010.

GCS large-scale projects on JUGENE
Additionally, the Gauss Centre for Supercomputing (GCS) is issuing its fourth call for large-scale projects. Projects are classified as "large-scale" if they require more than 5 % of the potentially available CPU cycles on the high-end system of a member centre, for example more than 70 million processor core hours or 24 rack months on JUGENE within the granting period. Further details can be found at: *http://www.gauss-centre.eu/computing-time/call*. Deadline for submissions is 31 August 2010.

These proposals for JUROPA and JUGENE will be evaluated by the peer review board of the John von Neumann Institute for Computing (NIC).

PRACE call for projects on JUGENE
The Partnership for Advanced Computing in Europe (PRACE) offers supercomputer resources on the highest level (Tier-0) to European researchers. Jülich, as a member of GCS and involved in shaping PRACE

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

as well as hosting the only European Tier-0 supercomputer currently available, is dedicating a 35 % share of the IBM Blue Gene/P system JUGENE to PRACE within the framework of its commitments.

The first regular PRACE call for proposals is currently open until 15 August 2010 for the granting period 1 November 2010 - 31 October 2011 with a total available capacity of about 360 million compute core hours. For full details of the call see *http://www.fz-juelich.de/jsc/news/prace-call*.

The PRACE peer review process for the proposals is headed by Prof. Richard Kenway, EPCC. Jülich invites all interested European scientists to participate in this call provided they can meet the scientific and technical criteria.
(Contact: Dr. Walter Nadler, ext. 2324)

QPACE – Still No. 1 on the GREEN500

The latest list of the most energy-efficient supercomputers GREEN500 is headed again by the German QPACE supercomputer (QCD Parallel Computing on the Cell). QPACE was developed by an academic consortium of universities and research centres together with the German IBM Research and Development Centre in Böblingen as part of a government-funded research collaboration. One 4-rack QPACE system is installed at JSC with an aggregate peak performance of more than 100 Tflop/s; a similar system is currently running at the University of Wuppertal.
(Contact: Willi Homberg, ext. 2424)

Improved Parallel Application Support in UNICORE 6.3.0

The latest release 6.3.0 of the UNICORE Grid middleware brings many enhancements targetted at further improving the support for HPC applications and typical usage scenarios. UNICORE allows users to easily run parallel applications without having to know the site-specific invocation and configuration of the parallel environment. Advanced users now can use a GUI to select and configure the parallel environment specifically for their application. As a second major improvement, UNICORE now offers flexible definitions of the available resource and batch system settings, thus allowing the user to make ready use of these settings. One example for this would be the network topology on the JUGENE system. (Contact: Dr. Bernd Schuller, ext. 8736)

Rescue Disks for Malware-Infected PCs

Computer viruses, Trojan horses and backdoors are a permanent threat to all types of interconnected computer systems. JSC has revised its range of supported rescue discs for checking potentially malware-infected PCs of Forschungszentrum Jülich personnel: Now AVG Rescue CD, Avira Antivir Rescue CD and Kaspersky Rescue Disc enable novice and advanced users to examine and heal all common types of malware on Microsoft Windows systems for both professional and personal use. Avira Antivir can also handle Linux-based systems. All rescue disc products previously in use are no longer supported by JSC. How to use these three solutions is described in the Technical Short Note TKI-0411, which is available at
http://www.fz-juelich.de/jsc/files/docs/tki/tki-0411.pdf.
(Contact: FZJ CERT Team at JSC, ext. 6440)

Vacancies at JSC

JSC is seeking several scientists in physics, chemistry, mathematics, informatics or a related field at the earliest opportunity. The positions are available in various areas:

- Technology development of future supercomputer architectures in collaboration with renowned hardware and software vendors in the supercomputing domain
- IT system administration of supercomputers
- Central IT security tasks on campus und for the supercomputers
- Community-oriented application support in the fields of plasma physics, climate modelling and molecular physics
- Optimization of application codes on parallel high-performance supercomputers
- Java programming for software tools on high-performance supercomputers
- Management tasks in major European supercomputing projects, e.g. PRACE

The qualifications and skills required are:

- a university degree in physics, chemistry, mathematics, informatics or a related field of study;
- appropriate experiences and knowledge in at least one of the above-mentioned fields;
- good command of written and spoken English;
- structured and systematic functioning;
- professional skills, cooperative team work and a high degree of commitment.

The official advertisement will be published at
http://www.fz-juelich.de/jsc/news/jobs.

Events

Introduction to parallel programming with MPI and OpenMP
Speakers: M.-A. Hermanns, GRS; Chr. Rössel, JSC
Date: 3 - 6 August 2010, 9:00 - 16:30
Venue: Ausbildungsraum 1, Jülich Supercomputing Centre
Registration: *M.A.Hermanns@grs-sim.de*

WE Heraeus Summer School "Fast Methods for Long-Range Interactions in Complex Systems"
Date: 6 - 10 September 2010
Venue: Rotunda, Jülich Supercomputing Centre
Application: *http://www.fz-juelich.de/wehss*

Editor: Dr. Sabine Höfler-Thierfeldt, ext. 6765