## First PRACE Petascale Summer School

The first PRACE Petascale Summer School organized by the Center for Parallel Computers, Sweden, the IT Center for Science (CSC), Finland, and the Jülich Supercomputing Centre took place in Stockholm from 26 - 29 August 2008. The goal of this four-day event was the training of young computational scientists on future petascale architectures. The summer school attracted 31 participants from 16 different countries, including all 14 PRACE member states.

The school was divided into lectures on advanced parallel programming in the morning and hands-on exercises in the afternoon. The participants were offered advice on porting and running their own applications on the Jülich Blue Gene/P system and the Cray XT4 at CSC. More than half the participants took the opportunity to try out their applications on JUGENE and to scale and analyse them on at least 2048 Blue Gene/P cores.

Tools for the performance analysis of massively parallel programs like Scalasca, developed at JSC and University of Tennessee, proved very popular for identifying bottlenecks and improving application scalability. Some students were able to run multi-rack jobs on the third day. One group from CERFACS, France, achieved a remarkable scale-up of 65,536 cores with their code, solving the Helmholtz equation used in geophysical seismic imaging. Jülich provided a total computing time of 360,000 CPU hours for the school.

This school will be followed by a PRACE winter school in Greece in February 2009, see: *http://www.prace-project.eu/events* (Contact: Wolfgang Frings, ext. 2435)

## New Master's Course in Technomathematics

In winter semester 2008, 26 students who graduated with a bachelor's degree in "Scientific Programming" (or equivalent) continued their studies in a following master's course in technomathematics. The new master's course is a cooperation between Aachen University of Applied Sciences and Forschungszentrum Jülich.

The curriculum has three major fields: applied mathematics, scientific computing and engineering. It contributes to the mathematical and computational know-how needed in the research activities at Forschungszentrum Jülich, especially for modelling and simulation. The teaching is done by professors from Aachen University of Applied Sciences and scientists from Jülich Supercomputing Centre. Five lecture courses take place at JSC.

The two-year master's in technomathematics with a research-oriented final master's project is designed for 30 - 40 students per year. Applications are accepted for the winter and also the summer semester. Admission requirements include a bachelor's degree with a grade significantly above average. Most of the students work in various institutes at Forschungszentrum Jülich or at local partner companies. Here they gain work experience in computational science

or engineering projects in order to complete their master's thesis. (Contact: Prof. Dr. Johannes Grotendorst, ext. 6585)

## More Software Packages Available on JUMP and JUGENE

A number of software packages for simulations in materials science, soft matter physics, biophysics and many-particle physics have been updated or newly installed on the IBM Power6 system JUMP and the IBM Blue Gene/P system JUGENE at Jülich Supercomputing Centre.

Updated/new software packages available on JUMP and JUGENE:

- CPMD version 3.13.1-02, Car-Parrinello molecular dynamic simulations (user must apply for licence)
- VASP version 4.6.35, ab initio quantum-mechanical molecular dynamic simulations using pseudopotentials and a plane wave basis set (user must apply for licence)
- LAMMPS version 21 May 2008, Large-scale Atomic/Molecular Massively Parallel Simulator

Updated/new software packages available on JUGENE:

- NAMD version 2.6, Nanoscale Molecular Dynamics software package
- GROMACS version 4.0, classical molecular dynamic simulations

Updated/new software package available on JUMP:

- CP2K version 25 April 2008, general framework for different methods such as density functional theory (DFT) and classical pair and many-body potentials

For further information concerning licence issues and a complete list of software packages for these research fields available at JSC, please see:
*http://www.fz-juelich.de/jsc/mathsoft/chem/*
(Contact: Dr. Florian Janetzko, ext. 1446)

## First PRACE Industry Seminar

PRACE, the Partnership for Advanced Computing in Europe, organized a one-day seminar titled "Industrial Competitiveness: Europe goes HPC" on 3 September 2008 in Amsterdam. The seminar had close to 100 invited attendees comprising CEOs, CIOs, CTOs and high-level decision makers from different industrial domains as well as academic participants, scientific software developers and representatives from the European Commission. The attendees represented 13 European countries.

One of PRACE's targets is to increase interest in high-end computing in industry and its potential for competitiveness as well as to raise awareness of the creation of a world-class computing infrastructure in Europe for HPC applications. The participants enjoyed a rich and varied programme highlighting the ideas for a European HPC infrastructure and presenting numerous examples of the benefits of HPC for

industry. As a result of the seminar, industrial pilot applications suitable for petaflop/s scalability are planned to be run on the PRACE prototype systems. PRACE also collected information on needs and expectations from the attendees during discussions and will arrange follow-up meetings.

PRACE is also organizing two scientific seminars; the first one will take place on 26 November in Lyon, France. These scientific seminars are aimed at potential academic HPC users. (Contact: Dr. Florian Berberich, ext. 2547)

## UNICORE Course at GridKa 2008

The UNICORE course at the International GridKa School in Karlsruhe on 11 September 2008 was organised by JSC. The course started with a general introduction to the UNICORE Grid technology, an overview of the available clients and a brief summary of the server architecture. In the practical part of the session, the participants installed the UNICORE server components and workflow services on their laptops. They learnt how to configure the UNICORE command line client and the Eclipse-based graphical client to use with their own installation. With both clients, the participants created and submitted single jobs as well as workflow jobs, learnt to transfer files and monitor their jobs. The agenda and accompanying material can be found at:
*http://gks08.fzk.de/Agenda.html*
(Contact: Rebecca Breu, ext. 2294).

## A-WARE Project Successfully Completed

On 27 June 2008, the A-WARE project (An easy Way to Access grid REsources) successfully passed its final review, marking the completion of this 2-year EU-funded project. Together with partners in Italy (CINECA, NICE), France (Airbus) and the UK (Fujitsu), A-WARE developed a solution providing user-friendly, Web-based access to UNICORE 6. Focussing on workflow functionality, the approach was validated with a real-world CFD use case provided by Airbus. Going further, exploitable results of the project include commercialization of the A-WARE software by NICE and various follow-on activities: for example, the portal activities in DEISA and at JSC further research expanding on the concept of the Grid as a Web application. Additional information can be found at: *http://www.a-ware-project.eu/*
(Contact: Roger Menday, ext. 1588)

## Events

**Einführung in die parallele Programmierung mit MPI und OpenMP**
Speaker: Dr. Rolf Rabenseifner, HLRS Stuttgart
Date: 26 - 28 November 2008, 8:30 - 18:00
Venue: Ausbildungsraum 1, Jülich Supercomputing Centre
Registration: Please use the application form at
*http://www.fz-juelich.de/jsc/neues/termine/mpi-openmp*

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