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Winter School 2009

From 2 – 6 March 2009, the Winter School "Multiscale Simulation Methods in Molecular Sciences" was held at Jülich Supercomputing Centre. It continued the successful series of biennial Winter Schools organized by JSC. The focus of this year's school was on simulation methods for materials, soft matter and biomatter covering various length and time scales. The programme was complemented by lectures on methodological foundations (molecular dynamics, Monte Carlo techniques, DFT and electronic structure theory, embedding methods), mathematical aspects of multiscale approaches, as well as practical sessions on parallel computing. The scientific programme was drawn up by Johannes Grotendorst, Norbert Attig, Stefan Blügel (Forschungszentrum Jülich), and Dominik Marx (Ruhr-Universität Bochum). Leading scientists in computational physics, chemistry, biology and mathematics presented stimulating lectures for 50 PhD students and young postdocs from 20 different countries. In two poster sessions the young scientists presented topics from their own research.

Highlights of the meeting were the keynote lectures of Aiichiro Nakano, University of Southern California, on "Large spatio-temporal-scale materials simulations on petaflop computers" and Klaus Schulten, University of Illinois at Urbana-Champaign, on "Application of residue-based and shape-based coarse graining to biomolecular simulations".

The lecture notes are published as volume 42 in the NIC series and are available online at: *http://www.fz-juelich.de/nic-series/volume42/*
(Contact: Prof. Dr. Johannes Grotendorst, ext. 6585)

Call for Large-Scale Projects

The Gauss Centre for Supercomputing (GCS) has issued its first call for large-scale projects. This call applies to the petaflop supercomputer JUGENE, which will be operational at JSC from July. Proposals from publicly funded German academic and research institutions are eligible. Projects are classified as "large-scale" if they require more than 5 % of the potentially available CPU cycles on a member centre's high-end system, for example more than about 60 million core hours or 20 rack months on JUGENE. Requests for resources below these limits will still be reviewed by the individual member centres. Requests above these limits will be handed over to GCS, processed according to the joint procedures, and will be reviewed in the national context. It is expected that two or three high-profile projects will be selected.

Projects should fulfil particular requirements of scientific excellence, i.e. challenging scientific problems, clear scientific goals, verifiable milestones, and scalability of programs. Further details can be found at: *http://www.gauss-centre.eu/computing-time/call*.

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The electronic application forms can be accessed through: *http://www.gauss-centre.eu/computing-time/jugene*. Applications should be submitted at the latest by 28 April 2009.

This deadline also applies to applications for regular projects on JUGENE and on the new general-purpose supercomputer, JUROPA. For more information see: *http://www.fz-juelich.de/jsc/computing-time*.
(Contact: Dr. Walter Nadler, ext. 2324)

DEISA Extreme Computing Initiative – Call for Proposals 2009

The DEISA Extreme Computing Initiative (DECI) offers European researchers a chance to obtain access to the most powerful computing resources in Europe, regardless of their country of origin or work. The latest DECI-5 call for proposals 2009 was opened on 1 March 2009 and will close on 4 May 2009. Proposed projects should deal with complex, demanding and innovative simulations, which can only be realised using the DEISA infrastructure and will benefit from the unique services and exceptional resources available in the consortium. The following application profiles are particularly suited to DECI:

- Large, highly scalable parallel applications requiring exceptional computational resources
- Data-intensive applications requiring access to distributed data repositories
- Workflow simulations managing simulation chains that access more than one computing platform
- Distributed parallel applications that need to run on more than one platform (excluding metacomputing)

DEISA offers project assistance for porting and optimizing applications on the appropriate platforms of the DEISA consortium through experts at the leading European HPC centres in DEISA. Projects selected under this call will be given access to the DEISA infrastructure for application enabling from 1 October 2009 and for production runs from 1 November 2009 to 30 September 2010. For more information see: *http://www.deisa.eu/science/deci/*
(Contact: Dr. Florian Janetzko, *deisa-support@fz-juelich.de*, ext. 1446).

Successful UNICORE and Supercomputing Workshop 2009

On 18 March 2009, the UNICORE and Supercomputing Workshop took place at the Deutscher Wetterdienst (DWD) in Offenbach near Frankfurt, Germany. The objective of the workshop was to present and demonstrate interesting results of UNICORE usage in supercomputing to major stakeholders in supercomputing from Germany and Europe, as well as to members of the UNICORE Forum (*http://www.unicore.eu/forum*). About 40 people participated in the workshop and listened to the seven speakers. The workshop opened with an overview of UNICORE 6 followed by presentations from the life-sciences domain, the exploitation of DEISA – the European Supercomputing Grid e-infrastructure – and presentations from the French Commissariat à l'Énergie Atomique (CEA) and T-Systems SfR about the usage and adaptation of UNICORE in industrial environments. The detailed programme and all presentations can be found at: *http://www.unicore.eu/events/supercomputing-workshop-2009/*
(Contact: Dr. Achim Streit, ext. 6576)

First Master's Degrees in Technomathematics

At the end of winter semester 2008/09, the first students in the master's course "Technomathematics" graduated from Aachen University of Applied Sciences (FH Aachen). Since 2007, this new course has been offered jointly by FH Aachen and Forschungszentrum Jülich. Nine students at Jülich passed their exams and were awarded their master's degrees. They worked on computational science and engineering projects at various institutes, reflecting the broad spectrum of technomathematics at Jülich, namely applied mathematics, modelling, simulation, and computer science. At JSC, six master's students graduated: Stephan Graf, Andrea Portz, Stefanie Meier, Marc Keldenich, Annika Schiller, and Lidia Westphal. Congratulations!

Detailed information can be found at:
http://www.fz-juelich.de/jsc/tm/
(Contact: Prof. Dr. Johannes Grotendorst, ext. 6585)

Joint DEISA PRACE Symposium 2009

DEISA and PRACE are merging their annual science symposia into a single European HPC event for the first time: the DEISA PRACE Symposium 2009 – HPC Infrastructures for Petascale Applications. The symposium will take place from 11 May to 13 May in Amsterdam, the Netherlands, and will be hosted by SARA and NCF at the Royal Tropical Institute. Presentations will be given by representatives of funding agencies, HPC infrastructure providers and scientific users from Europe and around the world, addressing a broad audience of users, HPC technology experts, vendors, government representatives and industry partners. More information and registration:
http://www.deisa.eu or *http://www.prace-project.eu*
(Contact: Dr. Thomas Eickermann, ext. 6596)

Events

Guest Student Programme
Date: 3 August - 9 October 2009
Info: *http://www.fz-juelich.de/jsc/gaststudenten/*
Application deadline: 30 April 2009

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