

JSCNews

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1st CHANGES Workshop

New and highly scalable algorithms, performance tools and performance modelling were the topics of the first CHANGES workshop on high-performance computing, which took place from 3 to 5 September 2012 at JSC. The workshop was initiated by the Computer Network Information Center (CNIC) of the Chinese Academy of Sciences (CAS), the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign (UIUC), and the Jülich Supercomputing Centre at Forschungszentrum Jülich. These global players in supercomputing together with the organizations to which they belong joined forces and agreed to co-sponsor a CHinese-American-German E-Science and cyberinfrastructure workshop series (CHANGES) with local organization of the workshops alternating between the three partners each year. In the past, the three institutions had organized several bilateral cooperations and workshops, such as the US-American-Chinese series ACCESS and the German-Chinese Workshop on Supercomputing CHSC11. CHANGES, however, is the first trilateral cooperation and will not only consider the issues of the partner institutions but will also take national topics into account.

The first CHANGES workshop was a high-level platform dealing with the latest trends in supercomputing, sophisticated information techniques and interdisciplinary applications. About 40 well-known experts came together by invitation, and presented and discussed the latest results in their re-

search fields. The workshop focussed on the above-mentioned topics but also covered several fields in supercomputing, as well as e-science and its applications in China, Germany and the United States. In addition to the presentations, the workshop provided a forum for trilateral cooperations on student exchanges and mutual research projects. The first promising cooperation ideas were developed and will be launched in the near future.

(Contact: Dr. Norbert Attig, n.attig@fz-juelich.de)

News from PRACE Implementation Projects

From 5 to 7 September 2012, more than 180 participants from the 24 PRACE member countries and the Brussels Office met at the Institut de Physique du Globe de Paris for a three-day project meeting of PRACE-2IP and PRACE-3IP, the second and third implementation phase projects for the PRACE Research Infrastructure. The European Commission is providing funding worth € 18 million and € 19 million for both two-year projects, respectively. The preceding project, the first implementation phase project PRACE-1IP, just passed its second periodic review very successfully. The reviewers attested excellent progress as the overall result. All three projects support and accelerate the implementation of the pan-European high-end computing research infrastructure created and operated by PRACE (Partnership for Advanced Computing in Europe). JSC is the coordinator of all three PRACE implementation projects.

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At the project meeting, the current status and future work of PRACE-2IP, which started in September 2011, was discussed in an all-hands meeting, covering the first one and a half days. This was followed by the kick-off of PRACE-3IP and the welcoming of Denmark and Israel as the latest partner countries in the PRACE projects. PRACE-3IP continues the work of the PRACE-1IP project. It will also undertake a pilot joint pre-commercial procurement (PCP), focusing on whole system design for energy-efficient HPC. PCP is a new instrument for R&D procurements by public procurers in Europe. Thus, the project complements PRACE-2IP, which puts special emphasis on providing access to national HPC resources (Tier-1), building on the former DEISA projects. Application-enabling and scaling support in partnership with scientific communities, support for industrial users and the operation of the recently created PRACE Advanced Training Centres (PATC) are further important activities. Dr. Florian Berberich from JSC was appointed project manager of PRACE-3IP.

(Contact: Dr. Florian Berberich, f.berberich@fz-juelich.de)

Workshop on Hybrid Particle-Continuum Methods in Computational Materials Physics

One of the main purposes of computational materials physics is to establish a fundamental link between atomic-scale processes and the macroscopic behaviour of condensed matter, including composite materials, complex fluids, and materials of technological interest. A common characteristic of these systems is the existence of important features at multiple time or length scales. Typical examples are crack propagation in solids or protein folding in solution. Modelling such systems is challenging because the small and large scales have to be incorporated simultaneously and their underlying constitutive equations differ.

There has been much progress on coupling different descriptions and levels of resolution in the communities interested in complex fluids and complex solids. However, there has been surprisingly little exchange between them. In the tradition of previous workshops organized by research groups of the John von Neumann Institute for Computing (NIC) at Jülich fostering the exchange between various scientific communities, a workshop on "Hybrid Particle-Continuum Methods in Computational Materials Physics" will be held at Forschungszentrum Jülich from 4 to 7 March 2013. The two main topics will be: continuum-mediated interactions between particles, as well as adaptive and non-adaptive coupling between particle-based and continuum-based descriptions. More details can be found at: <http://www.fz-juelich.de/ias/jsc/HYBRID2013>.

(Contact: Prof. Dr. Martin Müser, m.mueser@fz-juelich.de)

MATSE: Exams Passed, New Course Started

At the end of August 2012, 28 MATSE trainees (mathematical technical software developers) prepared by the JSC education team passed their final examinations. During a ceremony on 10 September 2012, they proudly received congratulations from representatives of Forschungszentrum Jülich, the Chamber of Commerce Aachen (IHK), and Aachen University of Applied Science (FH Aachen). More than 60 percent of the trainees achieved an overall grade of at least "good"; a grade of "excellent" was achieved by Martin Vieten (IEK), Sarah Haas (IEK), Marcel Huysegoms (INM), Ingo Heimbach (PGI) and Florian Rhiem (PGI). The last two scored 96 percent and are the best among the 127 examinees in the district of Aachen.

On 3 September 2012, 34 new students started the bachelor's course in Scientific Programming at FH Aachen in combination with the training course as a MATSE at Forschungszentrum Jülich. Of these students, 25 will receive their practical training in various institutes at Forschungszentrum Jülich, while nine students are with external partners (six industrial companies). Both the vocational training and academic studies are designed to take three years. The curriculum and further information can be found at: <http://www.fz-juelich.de/matse>.

(Contact: Prof. Paul Jansen, p.jansen@fz-juelich.de)

Events

Introduction to the Density Functional Theory Program ADF and its Usage on the JUROPA Supercomputer

Instructor: Dr. Fedor Goumans, SCM, Amsterdam

Date: 22-23 October 2012, 09:30-16:30

Venue: Ausbildungsraum 2, Jülich Supercomputing Centre

Info: <http://www.fz-juelich.de/ias/jsc/events/adf>

Registration: f.janetzko@fz-juelich.de

Workshop: Cooperative Quantum Dynamics and Its Control

Date: 29-31 October 2012

Venue: Rotunda, Jülich Supercomputing Centre

Info: <http://www.fz-juelich.de/ias/jsc/events/cqdc12>

UNICORE - uniform access to the supercomputer systems

Instructor: Michael Rambadt, JSC

Date: 5 November 2012, 09:00-12:00

Venue: Ausbildungsraum 1, Jülich Supercomputing Centre

Registration: unicore-info@fz-juelich.de

If you would like to receive regular information on our events, please send an e-mail to jsc-events-join@fz-juelich.de.

Further events, talks, and training courses:

<http://www.fz-juelich.de/ias/jsc/events>