

1st CHANGES Workshop

New and highly scalable algorithms, performance tools, and performance modelling have been 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 University of Illinois, Urbana-Champaign (UIUC) and the Jülich Supercomputing Centre at Forschungszentrum Jülich. These global players in supercomputing together with their mother organizations joined forces and reached an agreement about co-sponsoring a CHinese-AmericaN-German E-Science and cyberinfrastructure workshop series (CHANGES), where the three sites will be local organizers alternately every year. In the past, the three institutions already had a couple of bilateral cooperations and workshops, like 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 into account national topics.

The first CHANGES workshop was a high-level platform dealing with latest trends in supercomputing, sophisticated information techniques and interdisciplinary applications. About 45 well-known experts, among them 21 speakers, came together by invitation and discussed latest results of their research fields. The workshop focussed on the above mentioned topics but covered also several fields in supercomputing, e-Science and its applications in China, Germany and the United States. Besides the presentations the workshop provided a forum for trilateral cooperations on student exchange and mutual research projects. First promising cooperation ideas were developed and are foreseen to be launched in the near future.

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Workshop on Hybrid Particle-Continuum Methods

A main purpose of computational materials physics is to establish a fundamental link between atomic-scale processes and the macroscopic behavior 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 e.g. crack propagation in solids or protein folding in solution. A precise description of interatomic interactions is needed at the crack tip or when two side chains of the protein come close to each other. However, stress boundary conditions or local electrostatic fields in these examples are strongly affected by long-range interactions. The latter are conveyed by a medium that can be described in terms of continuous fields. Modeling such systems is challenging because the small and the large scale have to be incorporated simultaneously and their underlying constitutive equations differ. This is why sequential multi-scale modeling is not an option, despite its success in the bottom-up development of field theoretical approaches to homogeneous media.

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 the Forschungszentrum Jülich from 4 to 7 March 2013. In order to narrow down the focus of the workshop, we will concentrate on methods that couple particles, or discrete degrees of freedom, to continuum fields. The two main topics are:

- Continuum-mediated interactions between particles
- Adaptive and non-adaptive coupling between particle-based and continuum-based descriptions of materials.

So far, 16 internationally recognized scientists have accepted our invitation to present their research. We will also allow for a limited number of contributed talks and give everybody attending the workshop the possibility to present a poster. More details can be found at <http://www.fz-juelich.de/jsc/HYBRID2013>

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