

IAS Winter School: Hierarchical Methods for Dynamics in Complex Molecular Systems

From March 5 to 9, 2012, the IAS Winter School and CECAM tutorial "Hierarchical Methods for Dynamics in Complex Molecular Systems" was held at Jülich Supercomputing Centre (JSC). It was organized by the Jülich CECAM node and continued the successful series of biennial Winter Schools at JSC. The focus of this year's School was on hierarchical methods for dynamics in hard and soft materials, biomolecular systems, flow simulation and transport. The programme was complemented by lectures on advanced methods (fast algorithms for DFT on modern HPC, multigrid QM/MM approaches, accelerated MD methods), numerical software for supercomputers and an introduction to parallel computing followed by a hands-on programming session.

The scientific programme was compiled by Johannes Grotendorst, Godehard Sutmann, Gerhard Gompper (Forschungszentrum Jülich), and Dominik Marx (Ruhr-Universität Bochum). Leading scientists in computational physics, chemistry, biology and mathematics presented lectures for 50 PhD students and young postdocs from eleven different countries. During poster sessions the young scientists were encouraged to present their own research in short oral presentations and to discuss methods and results at the poster.

The lecture notes of the school have been published as volume 10 of the IAS series. The volume is available either as hard copy or as PDF files on the web <http://hdl.handle.net/2128/4545>



• Johannes Grotendorst

Jülich Supercomputing Centre

International Workshop on SMQS-IP2011

The "International Workshop on Simulation and Manipulation of Quantum Systems for Information Processing (SMQS-IP2011)" took place from 17 to 19 October 2011 in the rotunda of the Jülich Supercomputing Centre. The goal of the workshop was to discuss methods to simulate and manipulate quantum systems for pure scientific as well as for more applied purposes.

More than 50 researchers from Germany, France, Poland, the Netherlands, the United States and Japan participated in the workshop. Recent developments in quantum annealing, open quantum systems, quantum computer hardware, optical lattices, equilibration and thermalization of quantum systems, quantum biology, and related topics were highlighted in talks and posters.

The exploitation of quantum effects, requiring coherent control of dissipative dynamics and entanglement control, is

expected to have profound implications for future emerging technologies including nanotechnology, biotechnology and information technology. The magnetic moments of nuclei, atoms and molecules can exhibit strong quantum behaviour. Studying the dynamics of these systems is of great importance for quantum information processing.

Managing and designing complex quantum systems with specified behaviour for quantum information processing requires a deep understanding of the cooperative behaviour of their components. Unravelling this behaviour necessitates an intensive collaboration between theoreticians and experimenters. The workshop successfully presented an overview of the current research on a broad spectrum of topics related to quantum information processing. A follow-up workshop will take place in Jülich in October 2012.



• Kristel Michielsen

Jülich Supercomputing Centre