

# CECAM – Jülich Summer School on Fast Methods for Long-Range Interactions in Complex Systems

After the successful tutorial on “Methods for Coulomb Solvers” in 2010, the Jülich-CECAM node organized a Summer School on “Fast Methods for Long-Range Interactions in Complex Systems”, which is one of various CECAM events organized by the Jülich node (cmp. [www2.fz-juelich.de/jsc/cecam](http://www2.fz-juelich.de/jsc/cecam)). The school took place from September 12 to 16, 2011 at JSC and consisted of morning lectures and afternoon practical sessions.

About 30 participants from various countries (France, Germany, Greece, Italy, Slovenia, Spain, Sweden, UK, USA) came to Jülich to learn about modern algorithms which efficiently solve the Coulomb problem and reduce the numerical complexity from  $O(N^2)$  to  $O(N \log(N))$  or  $O(N)$ . Lecturers from Universities of Bielefeld, Chemnitz, Mainz, Stuttgart, Wuppertal and the Forschungszentrum Jülich presented state-of-the-art methods, algorithms and implementations of various approaches to tackle the long-range interactions in many-particle systems.

The motivation for organizing this Summer School arose from the BMBF funded network project ScaFaCoS (Scalable Fast Coulomb Solver), which aims at developing a scalable library for various fast methods solving the long-

range interactions between particles in complex systems. The spectrum of presentations ranged from simple cut-off methods to Fourier-based methods (P3M), hierarchical tree methods, multigrid techniques, the fast multipole method (FMM) and a grid-based Maxwell solver. In addition an introduction into parallel sorting methods was given, which are required by various hierarchical implementations. For each method, emphasis was given to the theoretical foundation, the error control of approximations and parallelization algorithms.

To get participants acquainted with parallel computing, the first day included a special introduction to MPI followed by a hands-on programming session. Practical afternoon sessions focused on an introduction to the parallel interface of the ScaFaCoS library. This was included into various test programs, thereby integrating methods like multigrid, tree-methods or the fast multipole method. Participants were also encouraged to integrate the library into their own codes.

During a poster session, participants were encouraged to present their own research in short oral presentations and to discuss methods and results at the poster.

## NIC Symposium 2012

The John von Neumann Institute for Computing (NIC), formed by the contract partners Forschungszentrum Jülich, Deutsches Elektronen-Synchrotron DESY and GSI Helmholtzzentrum für Schwerionenforschung, will hold its sixth Symposium at Forschungszentrum Jülich on February 7 to 8, 2012. Every two years the NIC organizes this symposium to report on the activities and results obtained by the NIC projects and research groups in the last two years. It will provide an overview on a broad spectrum of computational science, with projects from Astrophysics, Chemistry,

Elementary Particle Physics, Materials Science, Condensed Matter Physics, Polymers, Earth and Environment, Computer Science, and further topical research areas. To accompany the conference, an extended proceedings volume will be published.

### Activities

• Godehard Sutmann

Jülich  
Supercomputing  
Centre

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• Walter Nadler

Jülich  
Supercomputing  
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