Summer School on fast Methods for Long-Range Interactions in complex Systems

From September 6 - 10, 2010 Jülich Supercomputing Centre organized a Summer School on Fast Methods for Long-Range Interactions in Complex Systems, which was financially supported by the Wilhelm and Else Heraeus Foundation.

About 30 participants from five countries 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 $O(N)$. Ten lecturers from Universities of Bielefeld, Chemnitz, Stuttgart, Wuppertal and the Forschungszentrum Jülich presented state-of-the-art methods, algorithms and implementations of various approaches to tackle the long-range interactions between particles.

The motivation for organizing this Summer School arose from the BMBF funded network project ScaFaCoS (Scalable Fast Coulomb Solver), which aims to develop a scalable library for various fast methods solving the long-range interactions between particles in complex systems. Since different physical problems have different requirements the school covered a variety of algorithms. The spectrum of presentations ranged from simple cutoff methods to Fourier-based methods (P3M), hierarchical tree methods, multigrid techniques and the fast multipole method (FMM). For each method, emphasis was given to the theoretical foundation and derivation, the error control of the approximations and the parallelization.

To get participants acquainted with parallel computing, the first day included a special introduction to MPI followed by a hands-on programming session. Further practical sessions complemented the talks on theoretical foundations and implementation issues of different algorithms in the afternoons, where specific program packages, e.g. the Soft Matter Code ESPResSo or the plasma physics code PEPC were introduced.