INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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Friday, May 18, 10.30 am
ICAMS lecture room UHW 11/1102

Fast Methods for Long Range Interactions in Particle Simulations

The simulation of classical particle systems by means of molecular dynamics, requires the evaluation of mutual interactions between particles in order to explore the phase- or configuration space of the system. The interactions may be classified into short-range and long-range contributions. While short-range potentials may be evaluated very efficiently by means of neighbour list techniques, which reduce the computational complexity to O(N), the long range interactions must be evaluated over all particle pair contributions in the system, which increases the complexity to O(N2), limiting very often the tractable system size to a few thousand particles.

A typical long range contribution for molecular systems is the electrostatic interaction between particles carrying partial charges - a situation which appears e.g. in polar liquids, biological molecules or solids. Progress has been made to reduce the computational work by methods, which decompose the system hierarchically and solving Poisson's equation very efficiently.

An overview will be given for different methods, which were further developed or optimised at JSC and which are based on multipole-, multigrid- and treemethods, which reduce the complexity to O(N) or O(N logN). The interaction between colloids or polymers in solution is often strongly affected by hydrodynamic interactions, which also have long range character. A particle based method (the multi-particle collision dynamics method) of complexity O(N) is discussed, which operates locally but captures the essential hydrodynamic effects. Progress on parallelization for massively parallel architectures will be reported and an outlook is given for the inclusion of the presented methods into existing complex simulation codes.