Implementation of Advanced Electrostatic Solvers for kinetic Monte-Carlo Simulations

Bachelor's thesis, Master's thesis

Motivation:

In simulations based on the kinetic Monte-Carlo (kMC) method, Coulomb interactions between different types of particles play a crucial role for the temporal evolution of the considered system. This requires the dynamic and in particular efficient solution of Poisson equation for suitable boundary conditions in every kMC step. To obtain feasible simulation times even for large numbers of involved particles N, the computational effort should scale linearly with N.

Our group developed a generalized kMC framework for charge transport in organic materials. So far, Coulomb interactions are either treated by a spherical cut-off or the classic Ewald summation. These methods scale as $\mathcal{O}(N^2)$ and $\mathcal{O}(N^{3/2})$, respectively. For a few hundreds of particles, the computational effort is bearable. However, for several thousands of particles the treatment of electrostatic interactions becomes a bottleneck for kMC simulations.

Our goal is the implementation of advanced electrostatic solvers with more favorable computational scaling (e.g. $\mathcal{O}(N \ln N)$, $\mathcal{O}(N)$, $\mathcal{O}(\ln N)$). Thus, simulations with larger numbers of particles become attainable.

Objectives:

The central task of this thesis is the implementation and testing of advanced electrostatic solvers.

- (Bachelor's thesis) Implementation of Particle-Particle Particle-Mesh ($\mathrm{P^3M}$) as an extension of the pre-implemented Ewald summation. Computational effort: $\mathcal{O}(N \ln N)$
- (Master's thesis) Implementation of the Fast Multipole Method (FMM) for kMC simulations with thousands of particles. Computational effort: $\mathcal{O}(N) - \mathcal{O}(\ln N)$.
- Testing of the implemented solvers for consistency and comparison to pre-implemented solvers ("benchmarking").

Requirements:

- Interest in physical modeling and programming.
- Either adequate knowledge in MATLAB or Object Oriented Programming with C++

Duration:

The duration of this Bachelor's thesis 3 months. The project can be extended to a Master's thesis with a duration of 6 months.

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