

# DEVELOPMENT OF A LARGE SCALE *ab initio* ELECTRON TRANSPORT SIMULATION PROGRAM

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## Abstract

The aim of this project is the development and implementation of computational algorithms for *ab initio* electron transport calculations for large scale systems. The Hamiltonian matrix is obtained from density functional theory (DFT) based codes, such as SIESTA and OpenMX. All these codes are very efficient and scale linearly with system size for the calculation of the Hamiltonian. The charge density for the given Hamiltonian is calculated using the non-equilibrium Green's functions (NEGF) method. We then iterate until self-consistency is achieved between the Hamiltonian and the charge density. This method is implemented in the SMEAGOL code, which is currently however limited to rather small systems (up to about  $10^3$  atoms in the simulation cell). The main reason for this limitation is that the current algorithm scales cubically with system size, whereas to be able to handle large systems a linear scaling algorithm is needed. Moreover scalability of the method to a large number of processors is required. Further extensions to the code that will be implemented are the inclusion of inelastic- and coherence-breaking effects on a mean field level, the possibility to use an arbitrary number of electrodes, and consequently also a solver for the Poisson equation that can treat arbitrary mixed boundary conditions. This is mainly a development project, the goal is to develop the SMEAGOL program to a linear scaling code, with which it is possible to run a small Si based transistor, with up to about  $10^4 - 10^5$  atoms in the simulation cell. Moreover this should make it possible to include the gate terminal in the calculation from first principles, and to investigate the transition of a device from the fully quantum limit to the diffusive limit. Calculations for a carbon-nanotube based transistor, as well as for a Si based transistor will be performed in the second part of this project in order to test the new code developments for real systems.