Self-consistent Monte Carlo Solution of Wigner and Poisson Equations Using an Efficient Multigrid Approach

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An accurate self-consistent solution of the coupled Wigner and Poisson equations is of high importance in the analysis of semiconductor devices. The solver proposed in this paper has two main components; a Wigner solver which treats the Wigner potential as a generating mechanism and is responsible for the generation and annihilation of signed particles, and a Poisson solver which uses an efficient multigrid approach to take the charge density distribution, and update the value of the potential in each time step.
As illustrated in Fig. 1, the Monte Carlo simulation starts with an initialization step in which geometrical aspects and physical quantities such as density and potential are fed to the simulator by input files or internal functions. Some other simulation parameters and the boundary conditions are set and the properties of the particles to be injected in the region are also decided. The Wigner potential is then calculated which in turn determines the statistics of generation mechanisms. The Poisson solver is called in each time step to use the current value of the charge density and update the value of the potential for the next time step. A charge redistribution scheme is then used to map charges in the neighboring cells in a more efficient way for the next round. The Monte Carlo evolution of particles is then performed using the Signed Particle Monte Carlo approach.

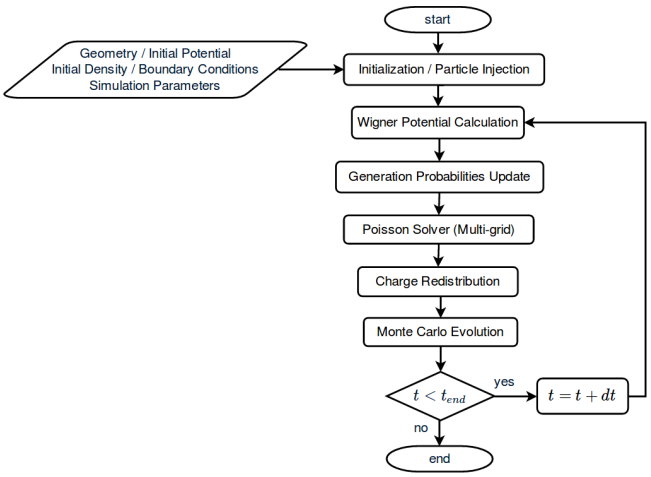

Figure 1: Flowchart for the self-consistent solution of Poisson and Wigner equations

The Poisson block receives the updated density in each time step and provides the updated potential which is then used to calculate the new Wigner potential, and hence the new statistics for the generation of new pairs of particles. Special considerations are taken into account in order to provide the solver with a compatible and consistent set of boundary constraints,

including Dirichlet and von Neumann conditions. Since the physical domain of interest is discretized in space, an efficient multigrid algorithm replaces the problem, which is on an initial fine grid, by an approximation on a coarser grid and uses the corresponding solution as a starting guess for the problem on the fine grid, which is then iteratively updated. The coarse grid problem is solved recursively, i.e. by using a still coarser grid approximation, etc. In this approach, efficiency depends on the coarse grid solution being a good approximation to the fine grid.
Results for density, potential and the electrostatic force calculated as the gradient of the potential energy are presented for a Cartesian xy-region which is not charged by any external doping or other sources of fixed charge in the beginning. However, wavepackets representing electrons are constantly injected from the bottom edge into the region every femtosecond, which results in a different distribution of charges in each time step. Fig. 2 shows the carrier density in two cases, namely, obtained without the application of the Poisson equation and with the Poisson equation, respectively, and illustrates the repulsion of wavepackets in the latter using the vectors of the force.

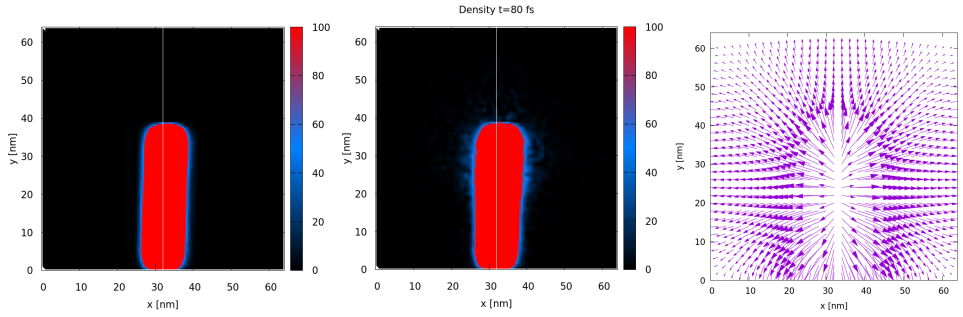

Figure 2: The carrier density without solving the Poisson equation (left), the carrier density with solving the Poisson equation (middle), and the force corresponding to the case with solving the Poisson equation (right) after 80 femtoseconds.

Note that the spread of the density is not due to the force acting on the particles, but entirely due to generation/annihilation of unaccelerated particles affected by the Wigner potential which is recalculated in every step based on the current position-dependent potential energy obtained from the solution of the Poisson equation. The Multigrid Poisson solver also allows for the selection of a position-dependent relative permittivity in the region in case one needs to model two or more materials next to each other in the same region.

Acknowledgements. This research is partially supported by the Austrian Science Fund through the project FWF-P29406-N30.