Improved Sampling Algorithms for Monte Carlo Device Simulation

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Monte Carlo (MC) is a widely used method to statistically estimate integrals and the solution of integral equations. In semiconductor physics, the method is often used to estimate the solution of the Boltzmann transport equation (BTE) [1] [2].
In stationary simulations, statistical averages can be obtained by the so-called before-scattering method. This method, however, becomes ineffective when applied to small devices where the mean-free-path is larger than the average size of the mesh cells. We present a new method which is better suited for small devices and which can even be applied in the quasi-ballistic transport regime.

Estimation of Non-Equilibrium Averages

Before scattering method - Trajectories are sampled before a scattering event takes place. The sample values are weighted with the reciprocal of total scattering rate $\Gamma(\vec{k})$[1][4][5]. When the simulation domain is decomposed into Voronoi volumes V_j, averages of local attributes can be built for every discretization volume V_j separately [6][7].

Boundary method - Particle states are sampled whenever a particle crosses an interface between two Voronoi volumes. The sample values have to be weighted with the reciprocal of the velocity component perpendicular to the interface $|v_\perp(\vec{k})|$ [3]. The benefit of this method is that the number of sampling points now depends on the surface of a Voronoi box, and not on the volume. With mesh refinement the surface of a cell scales more favorably than the volume.

Combination of methods - The samples obtained by the before-scattering method and from the boundary method can be combined. This combination of samples gives a smaller statistical error than the ones of each method individually.

Generation of an Equilibrium Distribution

In a MC simulation, particles are injected at a contact from an equilibrium distribution. Especially in the backward MC method, one can employ different variants of a weighted equilibrium distribution. Here, two methods for generating such distributions in a full-band simulation are shown. To obtain an equilibrium distribution, the electric field is set to zero.

Box Method - A single-particle MC simulation is performed for a uniform semiconductor with a finite length in one dimension, the so-called box. Perfectly reflecting boundary conditions are assumed. Every time the carrier hits a boundary and gets reflected, its state is added to the sample. The distribution of the generated sample represents a velocity weighted Maxwellian distribution [3] $f_v(\vec{k}) = |v_\perp(\vec{k})|\, f(\vec{k})$ where $|v_\perp(\vec{k})|$ is the velocity component perpendicular to the boundary.

Bulk Method - A single-particle MC simulation is performed for a uniform semiconductor with no boundaries. In this case the trajectory is sampled before a scattering event occurs (*before scattering method*). The distribution of the generated sample is a Maxwellian weighted with the total scattering rate, $f_\Gamma(\vec{k}) = \Gamma(\vec{k})\, f(\vec{k})$ [4][5].

Constant Time Step Method - Sampling the equilibrium trajectory with a constant time step yields the equilibrium distribution $f(\vec{k})$ directly.

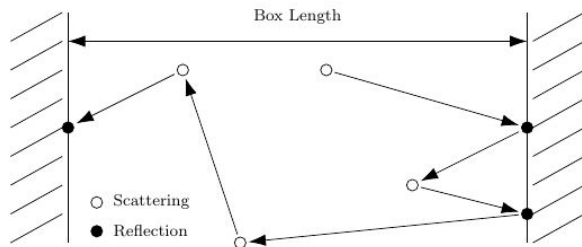


Fig. 1: Generating an equilibrium sample using the box method.

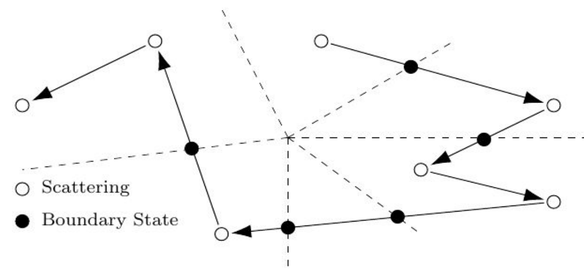
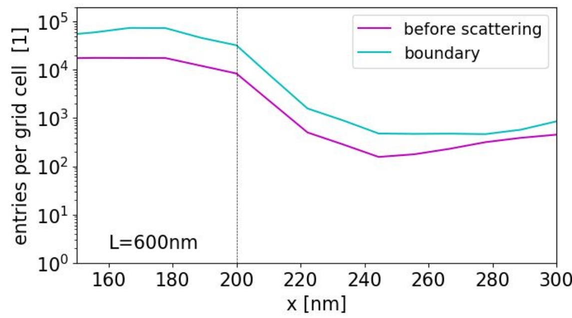


Fig. 2: Boundary and before-scattering method sampling in a device. The dashed lines are the boundaries between the Voronoi volumes.



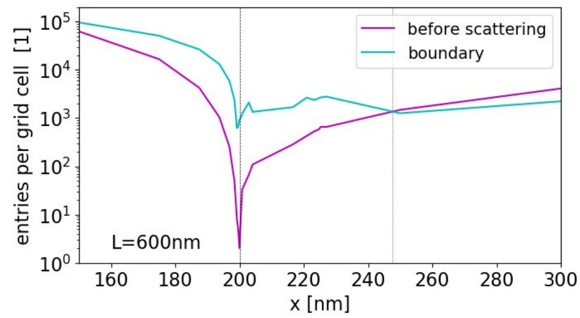
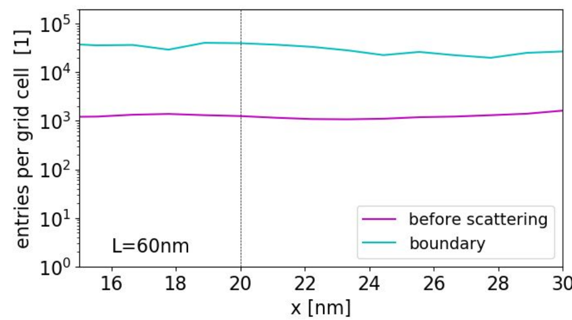


Fig. 3: Comparison of two different averaging methods in an silicon **600nm** $n^+n^-n^+$ diode with constant (a) and variable (b) grid size. Both images show the region around the n^+n^- junction at $200nm$.



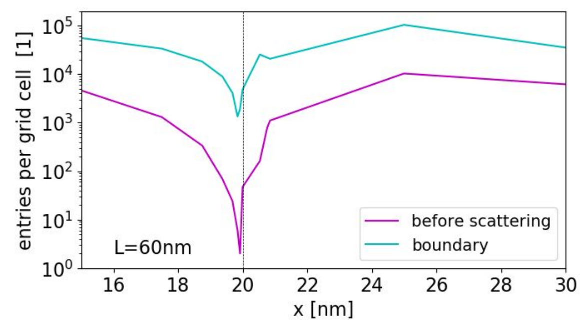


Fig. 4: Comparison of two different averaging methods in an silicon **60nm** $n^+n^-n^+$ diode with constant (a) and variable (b) grid size. Both images show the region around the n^+n^- junction at $20nm$. The box method yield a considerably higher number of sampling points and thus higher accuracy.

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