Efficient Stochastic Algorithms for Semiconductor Device Modeling

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Final Report

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1 Introduction

Carrier transport in modern, highly down-scaled semiconductor devices is well described by the semi-classical Boltzmann equation. The Monte Carlo algorithms, which are used to date to solve the Boltzmann equation, are imitating the real transport process by calculating physical carrier trajectories. With these algorithms severe problems are encountered when scarcely populated phase space regions are to be considered. This is virtually always the case in applications to semiconductor devices, where transport is controlled by means of energy barriers. In such cases the computational expense of the Monte Carlo method dramatically increases due to the high variance in the scarcely populated regions. Statistical enhancement and variance reduction techniques are therefore required in Monte Carlo device simulation, aiming at simulation time reduction and extension of the operating conditions in which the Monte Carlo method can be applied. In the last decade new Monte Carlo algorithms have been reported in the literature, however, they are applicable only to the initial value problem. Since a semiconductor device is represented by a bounded simulation domain, a rigorous treatment of the boundary value problem is required. This is the subject of the project. Only the stationary case is considered.

2 Aims

A theory of the stationary Monte Carlo method has to be developed. The integral form of the Boltzmann equation in presence of boundary conditions has to be formulated, which requires analysis of:

- the properties introduced by stationarity,
- uniqueness of the solution, which is determined by the boundary conditions,
- application of the iteration approach, which has been used successfully in the transient theory, to the stationary formulation of the equation.

The first tasks is to obtain the existing, stationary algorithms in a formal way. In particular, the probability densities for trajectory construction, the before-scattering and time-recording methods for average recording, and the trajectory splitting method, a widely used variance reduction technique, have to be recovered. The second task is to derive new stationary algorithms, namely the weighted forward method, which relies on event biasing, and the backward method. The new algorithms have to be implemented in an existing Monte Carlo simulator and tested. In this way the efficiency and the regions of applicability can be determined. Finally, the algorithms are applied to real devices and structures under conditions in which the performance of the common stationary algorithms become very poor.

3 Results and Applications

The integral formulation of the stationary Boltzmann equation has been derived and its properties have been analyzed. It has been shown that the distribution function at the boundary of the simulation domain is sufficient to determine the free term of the integral equation and hence to ensure uniqueness of the solution. Convergence of the Neumann series has been proved.

Evaluating the elements of the Neumann series by means of Monte Carlo integration leads to the stationary Monte Carlo backward algorithm, which is completely novel. There exists two versions, one to determine the distribution function in a given point and one to obtain averages in some phase space subdomain. Variants of the before-scattering and the time-integration schemes for average recording, which are known from the forward algorithm, are available also in the backward algorithm.

Stationary forward Monte Carlo algorithms have been derived from the Neumann series of the conjugate integral equation. First, the well known one-particle Monte Carlo algorithm has been derived in a formal way, including the before-scattering and the time-integration schemes for average recording. From the consistent treatment of the boundary condition it follows that the initial points of trajectories are to be generated from the velocity-weighted boundary distribution.

A weighted one-particle algorithm based on event biasing, which offers a number of options in the construction of the numerical trajectories, has been developed. To enhance statistics in scarcely populated regions the probabilities of phonon emission and absorption as well as the distribution of the scattering angle are biased in a favorable way. As a by-product of the theoretical treatment a new method for variance estimation of the simulated quantities has been found.

The discussed algorithms have been implemented on a Monte Carlo simulator, which can handle Silicon, various compound semiconductors and semiconductor alloys. The code implements the common, the backward and the weighted one-particle algorithms, which can be selected in a user-friendly input deck. The method for variance estimation has been included.

As a starting point, the weighted forward and the backward algorithms for the transient case have been tested for a bulk semiconductor. In a remarkable example it is shown that the backward algorithm can resolve thirty orders of magnitude of the distribution function, a resolution out of reach with the commonly used forward algorithms.

The weighted forward algorithm has been applied to one-dimensional semiconductor devices. As a typical example an npn-bipolar transistor has been chosen. Transport over barriers of 1eV can be simulated using event biasing as a statistical enhancement method. For a 0.8eV barrier the variance of the weighted Monte Carlo method is evaluated as 1/170 of that of a common trajectory split method, which amounts to an estimated performance gain of 170.

The obtained results have been presented in an invited [1] and a contributed conference talk[2], and in three journal publications [3][4][5].

4 Description of the Method

The integro-differential form of the stationary Boltzmann equation is transformed into an integral equation of the second kind:

$$f(x) = \int K(x, x') f(x') \, dx' + f_0(x) \; . \tag{1}$$

The free term f_0 contains the given boundary distribution. Successive approximation of the solution leads to the Neumann series. All the elements of that series are multi-dimensional integrals, which can be evaluated by means of Monte Carlo integration. Such an approach yields the backward Monte Carlo algorithm, since the trajectories evolve back in time. To derive forward algorithms the conjugate equation of (1) has to be used. In the involved transformations the sign of the time variable is changed and integration over before-scattering states is replaced by integration over after-scattering states.

5 Unexpected Results

The formal approach described above has been applied to a variant of the Boltzmann equation which arises from linear small signal analysis. The frequency dependence of transport coefficients can be determined by newly developed Monte Carlo algorithms. A carrier system is supposed to be in a steady state with respect to a stationary electric field. The linear response of the carrier system to a field impulse, superimposed on the stationary field, is the quantity of interest. The governing equation appears to be a derivate of the Boltzmann equation with an initial condition containing a delta function in time. The first step is to transform the equation into an integral equation. From the obtained integral form several Monte Carlo algorithms have been deduced.

A module for small-signal analysis has bee incorporated in the Monte Carlo simulator. The frequency-dependent differential mobility of electrons in Silicon has been calculated and the Transit Time Resonance effect occurring in Gallium Arsenide at low temperature has been investigated. The results are presented in [6][7][8].

References

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