

# Theory of the Monte Carlo Method for Semiconductor Device Simulation

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**Abstract**—A brief review of the semiclassical Monte Carlo (MC) method for semiconductor device simulation is given, covering the standard MC algorithms, variance reduction techniques, the self-consistent solution, and the physical semiconductor model. A link between physically based MC methods and the numerical method of MC integration is established. The integral representations the transient and the steady-state Boltzmann equations are presented as well as the corresponding conjugate equations. The structure of the iteration terms of the Neumann series and their evaluation by MC integration is discussed. Using this formal mathematical approach, the standard algorithms and variety of new algorithms are derived. The basic ideas of the weighted ensemble MC and the MC backward algorithms are explained.

**Index Terms**—Boltzmann transport equation, event biasing, Monte Carlo algorithms, semiconductor device simulation, small signal analysis.

## I. INTRODUCTION

**O**VER the last three decades the Monte Carlo (MC) method has evolved to a reliable and frequently used tool that has been successfully employed to investigate a great variety of transport phenomena in semiconductors and semiconductor devices.

The method consists of a simulation of the motion of charge carriers in the six-dimensional (6-D) phase space formed by the position and wave vectors. Subjected to the action of an external force, the pointlike carriers follow trajectories determined by Newton's law and the carrier's dispersion relation. Due to imperfections of the crystal lattice, the drift process is interrupted by scattering events, which are considered to be local in space and instantaneous in time. The duration of a drift process and the type of scattering mechanism are selected randomly according to given probabilities that describe the microscopic process.

In principle, such a procedure yields the carrier distribution in phase space. Integrating the distribution function over some phase space volume gives a measure for the relative number of carriers in that volume. Macroscopic quantities are obtained as mean values of the corresponding single-particle quantities. Moreover, the distribution function satisfies a Boltzmann equation (BE).

The method of generating sequences of drift and scattering appears so transparent from a physical point of view that it is frequently interpreted as a direct emulation of the physical process

rather than as a numerical method. The main MC algorithms used to date were originally devised from merely physical considerations, viewing an MC simulation as a simulated experiment. The proof that the used algorithms implicitly solve the BE was carried out later.

The alternative way to use the BE explicitly and to formulate MC algorithms for its solution was reported only one decade ago in the literature [1], [2]. New MC algorithms are derived which typically differ from the common ones by the fact that additional statistical variables appear, such as weights, that do not have a counterpart in the real statistical process.

## II. APPLICATION OF THE MC METHOD TO SEMICONDUCTOR DEVICES

Based upon the physical picture of the MC technique, it has been possible to apply the method to the simulation of a great variety of semiconductor devices. When the need for variance reduction techniques emerged, these have again been devised from physical considerations, such as splitting a particle into light ones by conserving the charge. For the MC simulation of devices, there are two algorithms generally employed, known as the *ensemble MC* (EMC) and the *one-particle MC* (OPMC) algorithms.

### A. MC Algorithms

For a systematic description of the MC algorithms, let us begin with the homogeneous case. Transient phenomena occur when the carrier system evolves from an initial to some final distribution. Accordingly, the evolution of an ensemble of test particles is simulated starting from a given initial condition. The physical characteristics are obtained in terms of ensemble averages, giving rise to the name "ensemble" MC [3], [4]. For example, the distribution function in a given phase space point at a given time is estimated by the relative number of particles in a small volume around the point.

The EMC algorithm can also be applied under stationary conditions. In this situation, for large evolution times the final distribution approaches a steady state, and the information introduced by the initial condition is lost entirely. Alternatively, the ergodicity of the process can be exploited to replace the ensemble average by a time average. Since it is sufficient to simulate one test particle for a long period of time, the algorithm is called "one-particle" MC. The effect of the particle's initial state vanishes for long simulation times. The distribution function in a given phase space point is estimated by the time spent by the particle in a fixed, small volume around the point divided by the total time the trajectory was followed. Another method of obtaining steady-state averages has been introduced by Price [5]. With the

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