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TITLE

Monte Carlo Algorithms for Stationary Device Simulation

ABSTRACT

The Monte Carlo (MC) method for simulation of semi-classical transport in semiconductors evolved for more than three decades to meet the challenges in the research and development of new semiconductor devices. The main MC algorithms used to date were initially devised from merely physical considerations, viewing the method as a direct emulation of the elementary events underlying the transport process. Later it has been proved that these algorithms implicitly solve the equation governing semi-classical transport, namely the Boltzmann equation (BE). The ensemble MC algorithm (EMC) simulates an ensemble of test particles assuming physically-based probability distributions. The ensemble is simulated starting from a given initial distribution until some final distribution is reached at the selected evolution time. The physical quantities are obtained as ensemble averages taken at the end of the simulation so that the algorithm is appropriate for transient phenomena.

Especially designed for stationary simulations is the single-particle MC algorithm (SPMC), which is the subject this work. The algorithm relies on the ergodicity of the stationary process allowing to replace the ensemble average by a time average. Then a single test particle can be followed and the averages are recorded during the whole time of simulation. The time recording technique estimates the distribution in a phase space domain Ω by the relative time spent by the particle in Ω. Using the before-scattering technique, averages are formed by sampling the trajectory at the end of each free flight.

The alternative way to use the BE explicitly and to formulate stochastic algorithms for its solution initiated one decade ago [1][2]. The integral form of the transient BE and its conjugate equation have been approached by numerical MC methods for solving integrals and integral equations. As applied to the BE, the approach yields a MC backward algorithm. The simulation follows the natural evolution back in time until the initial time is reached. The conjugate equation gives rise to the EMC and the weighted EMC algorithms. In the latter the probabilities of the natural events are biased to guide the particles towards the region of interest, making numerical trajectories differ from the natural ones [2]. Each test particle gives a single realization of the random variable θ which samples a desired physical quantity.

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This work addresses the extension of the approach to stationary transport, formulated as a stationary boundary value problem [3]. The boundary conditions provide not only the free term of the integral form of the BE, but also affect the kernel. It is proved that the boundary conditions guarantee a unique solution. A backward stationary MC algorithm is derived in analogy with its transient counterpart, with the difference being that the backward simulation continues in a variable time interval, until the boundary is reached. The forward stationary MC algorithm offers more peculiar results. The derivation of the conjugate equation gives an additional time integration in the iteration terms as compared to the transient case. The extra time integral allows to derive both the before-scattering and time integration methods for average recording. Moreover, it proves the ergodicity of the stationary transport process. In the iteration terms a velocity weighted boundary distribution appears. Injection from the boundaries must be chosen according the product of the velocity and the distribution function imposed on the boundaries.

An independent realization of the random variable θ is related to a complete numerical trajectory that starts and terminates at the boundary. Therefore, the SPMC algorithm can interpreted to simulate a regenerative stationary process [5]. A new variance estimation method is proposed [4], which avoids the commonly assumed separation of the particle's history into sub-histories with artificially predefined duration.

A weighted SPMC algorithm has been developed, which biases the probabilities for phonon emission and absorption to create artificial carrier heating and the scattering angle to introduce artificial carrier diffusion. The experiments show that event biasing is a competitive statistical enhancement technique. It can be applied by its own or in combination with other variance reduction techniques.

Finally, an application of the approach to small signal analysis is discussed. Both existing and a variety of new stationary MC algorithms are obtained in a unified way and the physical explanation of the algorithms is supported [6].

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