Hans Kosina [1]
Mihail Nedjalkov
Siegfried Selberherr
Institute for Microelectronics
TU-Vienna
Gußhausstraße 27-29/E360
A-1040 Vienna, Austria
e-mail: `Kosina@TUWien.ac.at`
`http://www.iue.tuwien.ac.at`

TITLE

An Event Bias Technique for Monte Carlo Device Simulation

ABSTRACT

Monte Carlo (MC) simulation of semiconductor devices requires measures to enhance the statistics in phase space regions of interest that are sparsely populated. There are two general classes of statistical enhancement techniques, namely population control techniques and event bias techniques [1]. To date virtually all MC device simulation codes utilize population control techniques, whereas the event bias technique, introduced in the field of semiconductor transport only one decade ago, [2][3], has found no application.

This work deals with the MC method for stationary carrier transport, known as the Single-Particle MC method. It gives a solution to the stationary boundary value problem defined by the semi-classical Boltzmann equation. A theoretical analysis of this MC algorithm begins with the transformation of the stationary Boltzmann equation into an integral equation [4]. Because the obtained equation describes the evolution back in time and we are aiming at a forward MC algorithm, the conjugate equation needs to be formulated. The elements of the Neumann series of the conjugate equation are finally evaluated by means of MC integration [4]. Using this mathematically-based approach the Single-Particle MC method is derived in a formal way. For the first time, the independent, identically distributed random variables of the simulated process are identified, allowing to supplement this MC method with the natural stochastic error estimate. Furthermore, the extension of the MC estimators to the case of biased events is derived.

The kernel of the conjugate equation yields the natural probability distributions which are used for the construction of the particle trajectory. However, it is possible to choose other than the natural probabilities for the MC integration of the terms of the Neumann series. In that case one constructs numerical trajectories that differ from the physical ones. The motivation for using arbitrary probabilities is the possibility to guide particles towards a phase space regions of interest to enhance statistics. In this work we increase carrier diffusion against a retarding electric field by introducing artificial carrier heating. The probability for phonon absorption is increased at the expense of phonon emission, a measure which increases the probability of a numerical particle to surmount an energy barrier. In regions with small field, where transport is diffusion dominated, the distribution of the scattering

---

[1] This work has been partly supported by the IST program, project NANOTCAD, IST-1999-10828.

angle is biased so as to induce artificial carrier diffusion. Furthermore, the distribution at the boundaries has been modified, injecting test particles at much higher temperature than the lattice temperature.

Changing probability distributions requires compensatory changes in the estimators. The event bias technique can be summarized by a simple rule. Whenever in the course of numerical trajectory construction a random variable, for example, a free flight time or an after scattering state, is selected from a numerical density rather than from a physical density, the weight of the test particle changes by the ratio of the physical over the numerical density. As a consequence, the weight of a test particle evolves randomly. Individual particle weights can evolve to extremely different values, predominantly to very small ones.

Optimal values of the parameters which control the bias are not known a priori. If the bias is chosen too small, not enough particles will, for example, surmount an barrier, rendering statistical enhancement inefficient. On the other hand, by choosing the bias too large numerous numerical trajectories will pass through the low concentration region. However, due to the aggressive biasing the spreading of the particle weights will be very large, and the recorded averages will again show a large variance. To find some optimum between these two extreme cases a careful tuning of the bias parameters is necessary.

The described behavior of the event bias scheme suggests the usage of additional variance reduction techniques [5]. In the presented simulation study evolution of the particle weight is governed predominantly by the event bias technique, and explicit measures are taken only to prevent particle weights from getting extremely high or low [6].

The formal approach, which is based on Monte Carlo integration of the terms of the Neumann series, clearly shows what the independent, identically distributed random variables are. A realization of such random variable is a complete numerical trajectory that starts and terminates at the domain boundary. Only complete numerical trajectories can be considered independent from each other, whereas particle states generated on one trajectory are statistically dependent. Knowing these random variables standard textbook formulae can be applied to estimate the variance of the MC estimates [7].

References

[1] M. Gray, T. Booth, T. Kwan, and C. Snell, “A Multicomb Variance Reduction Scheme for Monte Carlo Semiconductor Simulators,” *IEEE Trans.Electron Devices*, vol. 45, no. 4, pp. 918–924, 1998.

[2] C. Jacoboni, “A New Approach to Monte Carlo Simulation,” in *Int.Electron Devices Meeting*, (Washington, D.C.), pp. 469–472, IEEE Electron Devices Society, 1989.

[3] M. Nedjalkov and P. Vitanov, “Application of the Iteration Approach to the Ensemble Monte Carlo Technique,” *Solid-State Electron.*, vol. 33, no. 4, pp. 407–410, 1990.

[4] H. Kosina, M. Nedjalkov, and S. Selberherr, “Theory of the Monte Carlo Method for Semiconductor Device Simulation,” *IEEE Trans.Electron Devices*, vol. 47, no. 10, pp. 1898–1908, 2000.

[5] C. Wordelman, T. Kwan, and C. Snell, “Comparison of Statistical Enhancement Methods for Monte Carlo Semiconductor Simulation,” *IEEE Trans.Computer-Aided Design*, vol. 17, no. 12, pp. 1230–1235, 1998.

[6] H. Kosina, M. Nedjalkov, and S. Selberherr, “Variance Reduction in Monte Carlo Device Simulation by Means of Event Biasing,” in *Proc. Modeling and Simulation of Microsystems, MSM 2001* (M. Laudon and B. Romanowicz, eds.), pp. 11–14, Computational Publications, Mar. 2001.

[7] H. Kosina, M. Nedjalkov, and S. Selberherr, “Variance and Covariance Estimation in Stationary Monte Carlo Device Simulation,” in *Proc. Simulation of Semiconductor Processes and Devices*, (Athens, Greece), Sept. 2001.