



ELSEVIER

Mathematics and Computers in Simulation 62 (2003) 367–375



MATHEMATICS  
AND  
COMPUTERS  
IN SIMULATION

www.elsevier.com/locate/matcom

# An event bias technique for Monte Carlo device simulation

H. Kosina\*, M. Nedjalkov, S. Selberherr

*Institute for Microelectronics, TU Wien, Gusshausstrasse 27–29, A-1040 Vienna, Austria*

---

## Abstract

In Monte Carlo (MC) simulations of semiconductor devices it is necessary to enhance the statistics in sparsely populated regions of interest. In this work the Monte Carlo method for stationary carrier transport, known as the Single-Particle MC method, is considered. It gives a solution to the stationary boundary value problem defined by the semi-classical Boltzmann equation (BE). Using a formal approach which employs the integral form of the problem and the Neumann series expansion of the solution, the Single-Particle MC method is derived in a formal way. The independent, identically distributed random variables of the simulated process are identified. Estimates of the stochastic error are given. Furthermore, the extension of the MC estimators to the case of biased events is derived. An event bias technique for particle transport across an energy barrier is developed and simulation results are discussed.

© 2002 IMACS. Published by Elsevier Science B.V. All rights reserved.

PACS: 02.30.Rz; 02.50.-r; 02.70.Lg; 72.10.-d

Keywords: Monte Carlo method; Event bias technique; Variance reduction; Device simulation; Boltzmann equation

---

## 1. Introduction

In the Monte Carlo (MC) simulation of semiconductor devices measures have to be taken to enhance the statistics in interesting phase space regions that are sparsely populated. The purpose of statistical enhancement is to reduce the variance of the MC estimates in those regions. Such a reduction comes at the expense of increased variance in other, less interesting regions [1]. There are two general classes of statistical enhancement techniques, namely population control techniques and event biasing techniques. To date, virtually all MC device simulation codes utilize population control techniques. On the other hand, the event biasing technique has been introduced in the field of semiconductor transport only one decade ago, when the *Weighted Ensemble* MC method has been proposed [2,3]. However, this method has not been used in MC device simulation yet. The present work focuses on the steady state, and consequently a *Weighted Single-Particle* MC method is presented. It is applied to npn-structures and the suitability for variance reduction is studied.

---

\* Corresponding author. Tel.: +43-1-58801-36013.

E-mail address: hans.kosina+e360@tuwien.ac.at (H. Kosina).

## 2. The Monte Carlo method

The kinetic equation considered is the stationary Boltzmann equation (BE), supplemented by boundary conditions. MC algorithms for the solution of the stationary boundary value problem can be constructed formally as outlined in the following.

In a first step, the stationary BE is transformed into an integral equation of the second kind,

$$f(x) = \int f(x')K(x', x) dx' + f_0(x), \quad (1)$$

where the six-dimensional variable  $x$  stands for  $(\mathbf{k}, \mathbf{r})$ . The kernel  $K$  describes the propagation of the particles, while the free term,  $f_0$  contains the boundary condition. Since the integral form of the BE represents a backward equation, and we are aiming at a forward MC algorithm, the conjugate equation needs to be formulated. Its kernel is given by  $K^\dagger(x, x') = K(x', x)$ ,

$$g(x') = \int g(x)K^\dagger(x, x') dx + A(x'). \quad (2)$$

The two integral equations are stated explicitly in [4]. With a forward method, only mean values of some quantity  $A(x)$  can be evaluated, which is due to the necessity of employing the following equality.

$$\int A(x)f(x) dx = \int f_0(x)g(x) dx. \quad (3)$$

Note that usage of this equation precludes a pointwise evaluation of the distribution function  $f$ , because the choice  $A(x) = \delta(x)$  can not be treated by the MC method.

Substituting the conjugate equation recursively into the right hand side of (3) yields an iteration series, the elements of which are finally evaluated by means of MC integration. Using this procedure, the Single-Particle MC algorithm is obtained in a formal way. In particular, recovered are the well-known probability densities for trajectory construction, and both the *time averaging* and the *before-scattering* methods for mean value calculation [5,6].

In addition, the random variable can be identified whose realizations are statistically independent. Knowledge of the independent random variables form the basis for determination of the variance of the MC estimators and thus for stating error estimates. In the Single-Particle MC algorithm, a realization of this random variable, say  $X$ , is given by a complete numerical trajectory that starts and terminates at the domain boundary. The  $i$ -th realization consists of all generated random variables for the  $i$ -th trajectory, such as the initial state at the domain boundary,  $\mathbf{k}_0, \mathbf{r}_0$ , the free flight times,  $t_j$ , and the after-scattering states,  $\mathbf{k}_j^a$ ,

$$x_i = \{\mathbf{k}_0, \mathbf{r}_0, t_0, \mathbf{k}_1^a, t_1, \dots, \mathbf{k}_j^a, t_j, \dots\} \quad j \leq N_i, \quad (4)$$

where  $N_i + 1$  is the number of free flight segments for the considered trajectory. Another random variable  $Y(X)$  needed below is defined by its realizations:

$$y_i = \{\mathbf{k}_1^b, \mathbf{r}_1, \dots, \mathbf{k}_j^b, \mathbf{r}_j, \dots\} \quad j \leq N_i, \quad (5)$$

which contain all before-scattering states  $\mathbf{k}_b^j$  and the particle locations at the times of scattering,  $\mathbf{r}_j$ . Then, with any quantity of interest,  $A(\mathbf{k}, \mathbf{r})$ , a random variable  $\Psi_A(Y)$  is associated. Using the before-scattering

method, a realization of  $\Psi_A$  is of the form:

$$\psi_{Ai} = \sum_{j=1}^{N_i} \frac{A(\mathbf{k}_j^b, \mathbf{r}_j)}{\lambda(\mathbf{k}_j^b, \mathbf{r}_j)}, \tag{6}$$

with  $\lambda$  being the total scattering rate. Summation in (6) is over one complete trajectory.

### 3. The event bias method

The kernel  $K^\dagger$  of the conjugate Eq. (2) yields the natural probability distributions that can be 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 iteration series. In that case one constructs numerical trajectories that are different from the physical ones.

Changing probability distributions requires compensatory changes of random variables. 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, evaluated at the selected value. Introducing  $w_j$ , the weight of the particle constructed by this rule, the estimator (6) gets extended to:

$$\psi_{Ai} = \sum_{j=1}^{N_i} w_j \frac{A(\mathbf{k}_j^b, \mathbf{r}_j)}{\lambda(\mathbf{k}_j^b, \mathbf{r}_j)}. \tag{7}$$

The weight of each injected particle is set to  $w_1 = 1$ , the subsequent weights evolve randomly. This gives rise to increasing variance in the MC estimates with increasing time cumulated by a trajectory. However, since the particle weight is reset whenever a particle leaves and reenters the domain, the variance stays bounded.

The motivation for using arbitrary probabilities is the possibility to guide particles towards a region of interest [7]. Such situation occurs when carrier transport is controlled by an energy barrier. On the rising edge of such a barrier, we increase carrier diffusion by introducing artificial carrier heating. Controlled by a parameter  $M_1 \geq 1$ , the probability for phonon absorption is increased at the expense of phonon emission,

$$\lambda'_a = \lambda_a + \lambda_e \left(1 - \frac{1}{M_1}\right), \quad \lambda'_e = \frac{\lambda_e}{M_1}. \tag{8}$$

If in the MC simulation phonon absorption is selected, the particle weight is to be multiplied by  $\lambda_a/\lambda'_a$ , otherwise by  $\lambda_e/\lambda'_e = M_1$ . The distribution of the flight time is not affected, because the sum of emission and absorption rate are not changed.

Carrier diffusion can be enhanced by modifying the distribution of the scattering angle. The event bias technique is applied only to isotropic processes. For these the distribution of  $\chi = \cos \theta$  is constant:  $p(\chi) = 1/2$  for  $\chi \in (-1, 1)$ . Here,  $\theta$  is defined as the angle between the after-scattering momentum and the field direction. The following modified probability density is assumed:

$$p'(\chi) = \begin{cases} \frac{1}{2M_2}, & -1 \leq \chi < \chi_0 \\ \frac{M_2}{2}, & \chi_0 \leq \chi < 1 \end{cases}, \tag{9}$$

where  $M_2 \geq 1$  is a given parameter,  $\chi_0$  is determined from the normalization. The cumulative probability at this point evaluates to  $P'(\chi_0) = (1 + M_2)^{-1}$ . With a random number,  $r$ , evenly distributed between 0 and 1, one obtains for  $r < P'(\chi_0)$

$$\chi_r = 2M_2r - 1, \quad \frac{p}{p'} = M_2,$$

and otherwise

$$\chi_r = 1 - \frac{2(r - 1)}{M_2}, \quad \frac{p}{p'} = \frac{1}{M_2}.$$

This means that the particle weight is either reduced or increased by the factor  $M_2$  whenever  $\chi$  is generated from the density (9).

#### 4. Variance estimation

The result of a stationary MC device simulation can be expressed most generally as a ratio of statistical averages,

$$C = \frac{\langle\langle A \rangle\rangle}{\langle\langle B \rangle\rangle}, \quad (10)$$

with the definition  $\langle\langle x \rangle\rangle = \int_D d\mathbf{r} \int d\mathbf{k} x(\mathbf{k}, \mathbf{r}) f(\mathbf{k}, \mathbf{r})$ . Here,  $D$  denotes the simulation domain. The function,  $A$  is typically a product of some  $\mathbf{k}$ -dependent function and an  $\mathbf{r}$ -dependent charge assignment function [8], whereas the denominator accounts for the normalization.

The random variable to be considered now is given by  $\Psi_C = \Psi_A/\Psi_B$ . In the MC simulation one has to generate the samples  $\psi_{Ai}$  and  $\psi_{Bi}$  using estimators of the form (7). The so-called classical estimator of  $C$  is given by the ratio of the sample means.

$$\bar{C} = \frac{\bar{\psi}_A}{\bar{\psi}_B}, \quad \bar{\psi}_\alpha = \frac{1}{N} \sum_{i=1}^N \psi_{\alpha i}, \quad \alpha = A, B. \quad (11)$$

Additionally, the sample variances,  $s_A^2$  and  $s_B^2$ , and the sample covariance  $s_{AB}^2$  have to be evaluated from the following definitions.

$$s_\alpha^2 = \frac{1}{N-1} \left[ \sum_{i=1}^N \psi_{\alpha i}^2 - \frac{1}{N} \left( \sum_{i=1}^N \psi_{\alpha i} \right)^2 \right], \quad \alpha = A, B, \quad (12)$$

$$s_{AB}^2 = \frac{1}{N-1} \left[ \sum_{i=1}^N \psi_{Ai} \psi_{Bi} - \frac{1}{N} \sum_{i=1}^N \psi_{Ai} \sum_{i=1}^N \psi_{Bi} \right], \quad (13)$$

$N$  is the number of trajectories constructed in the simulation. From these inputs the variance of the random variable  $\Psi_C$  can be estimated [9].

$$s_C^2 = s_A^2 - 2\bar{C}s_{AB}^2 + \bar{C}^2s_B^2. \quad (14)$$

The error estimate for the result  $\bar{C}$  is finally given by the standard deviation

$$\sigma\{\bar{C}\} = \frac{s_C}{\bar{\psi}_B \sqrt{N}}. \tag{15}$$

### 5. Application and discussion

The following example demonstrates how the presented method of error estimation can be applied. As a first example an  $n + /n/n +$  silicon structure with a 0.2 eV energy barrier has been simulated using an unbiased MC method. In all,  $5 \times 10^8$  scattering events have been processed, which resulted in the simulation of  $N = 5.48 \times 10^7$  trajectories.

When computing the mean velocity using (10),  $\langle\langle A \rangle\rangle$  represents the particle current density and  $\langle\langle B \rangle\rangle$  the particle density. The correlation factor  $r_{AB} = s_{AB}^2 / (s_A s_B)$  of the MC estimate of the two densities is plotted in Fig. 1. An important result is the high positive correlation of the energy density and the particle density, which gives a significant reduction in standard deviation according to (14). A consequence of positive correlation is that a mean value per carrier has less variance than a mean value per unit volume (Fig. 2) [10].

As a second example, the modified probabilities described in Section 3 have been used to simulate electron transport through the npn-structure with a 0.8 eV energy barrier. To enhance statistics in the emitter–base barrier region artificial carrier heating is introduced. In the barrier and the base region the distribution of the scattering angle is biased so as to induce artificial carrier diffusion towards the collector. Optimal values for the parameters  $M_1$  and  $M_2$  controlling the bias are not known a priori. For instance, if  $M_1$  is chosen too small, not enough particles will surmount the barrier, rendering statistical enhancement inefficient. On the other hand, choosing  $M_1$  and  $M_2$  too large, plenty of numerical trajectories will pass through the low concentration region. However, due to the aggressive biasing the individual particle weights will evolve to extremely different values, predominantly to extreme small ones. Because

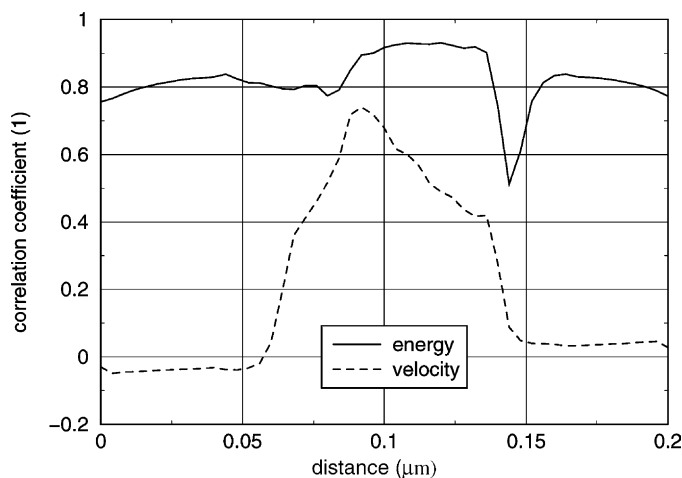


Fig. 1. Correlation coefficients of the energy density  $n(\epsilon)$  and the particle density  $n$ , and of the particle current  $n\langle v_x \rangle$  and  $n$ .

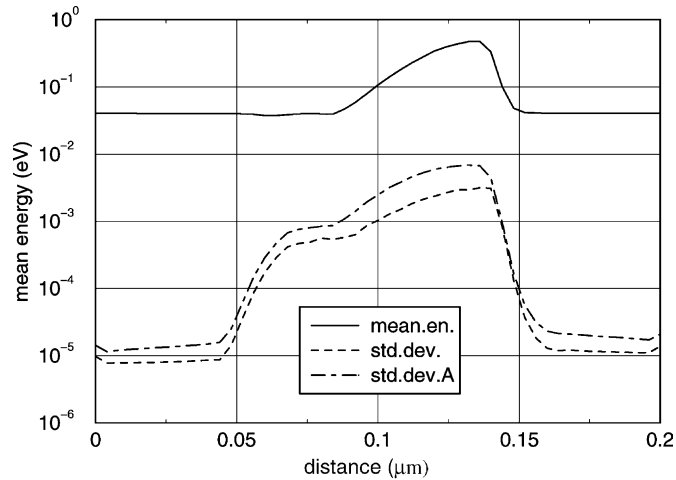


Fig. 2. Mean energy and its standard deviation, including the fluctuations of energy density and particle density (std.dev.), and neglecting the fluctuation of particle density (std.dev.A).

of the large spreading of the particle weights the recorded averages will again show a large variance. Reasonable values found for the considered structure are  $M_1 = 2$  and  $M_2 = 2$ .

The described behavior of the event biasing scheme suggests the usage of additional variance reduction techniques [11]. The general goal must be a reduction of the spreading of the weights. Such techniques are not used in this study. Instead, the evolution of the particle weight is governed predominantly by the event bias algorithm. Explicit measures are taken only to prevent weights from getting extremely high or low.

The event bias method has been compared with a simple particle split method. To first order such comparison is fair since the light-weight particles generated with either method are not further recycled.

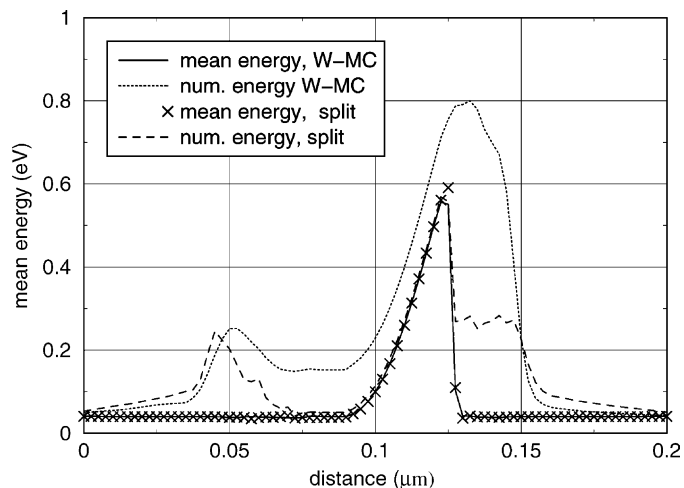


Fig. 3. Mean energy of the physical system (mean) and of the simulated carriers (num.) in the npn-structure with 0.8 eV barrier height. Comparison of the event bias method (W-MC) and a particle split method is shown.

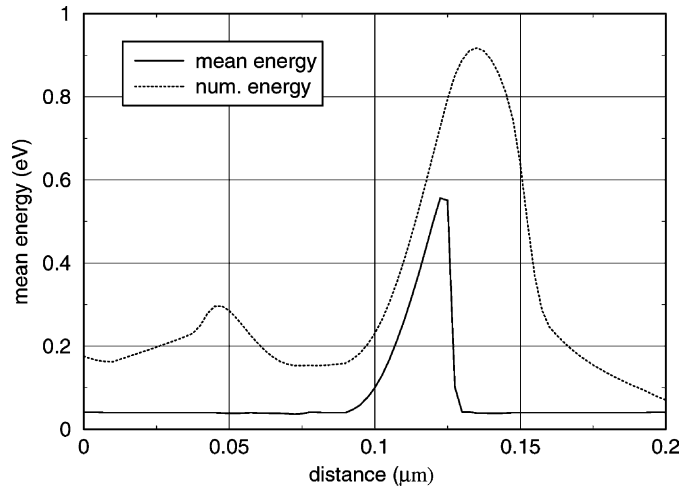


Fig. 4. Mean energy in the 0.8 eV structure. In addition to Fig. 3, electrons are injected at the left contact at 1500 K, whereas at the right contact a Maxwellian at 300 K is assumed.

Fig. 3 demonstrates that with event biasing the correct physical mean energy is reproduced. The mean energy of the simulated particles is considerably higher than the physical mean energy.

In the simulation shown in Fig. 4, a biased boundary distribution is assumed in addition. Electrons are injected from the emitter contact with a Maxwellian distribution at five times the lattice temperature. Again the correct physical mean energy is obtained. In Fig. 5, the electron concentration and the standard deviations of the two MC methods are depicted. In the quasi-neutral base region (75–90 nm) event biasing gives a standard deviation reduced by more than one order of magnitude. Fig. 6 shows the superior

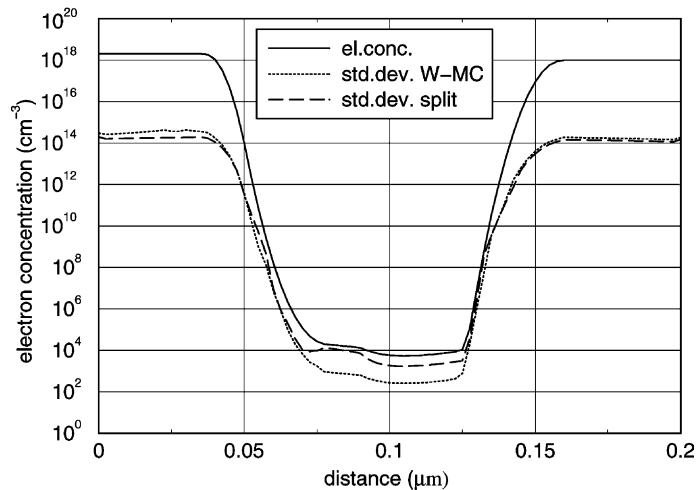


Fig. 5. The electron concentration varies by more than 14 orders. In the base region the event bias method gives significantly less variance than the split method.

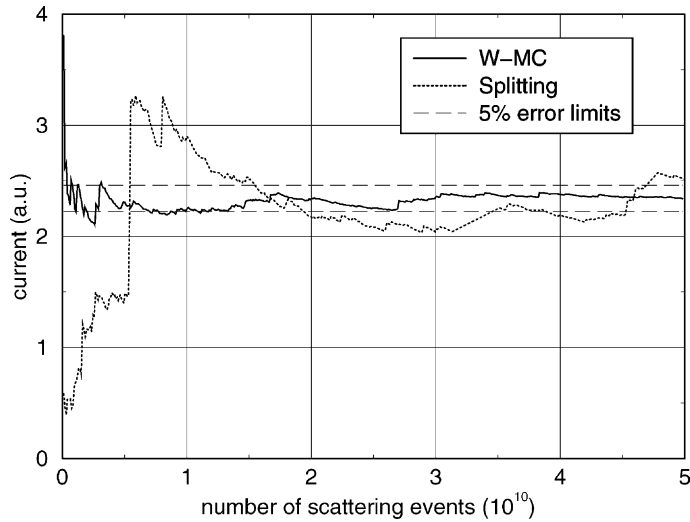


Fig. 6. Evolution of the device current for extremely long simulation times, evaluated every  $10^8$  scattering events. W-MC converges faster and shows better stability than the split method.

convergence of the event bias method. Because of the poor convergence of the split method for the 0.8 eV barrier structure  $1.5 \times 10^{10}$  scattering events needed to be processed to permit realistic comparisons [12].

## 6. Conclusion

For the Single-Particle MC method it has been demonstrated that event biasing is a competitive statistical enhancement technique. It can be used on its own or in combination with other, presently used variance reduction techniques. Implementation of the method does not require structural changes of an existing code. The independent, identically distributed random variables underlying the Single-Particle MC method have been identified. Based on these random variables the stochastic error is estimated. Without variance estimation, the statistics can be collected after each free flight of the test particle, whereas variance estimation requires that over one particle trajectory a sub-statistics is collected, which is added to the total statistics when the trajectory terminates at the domain boundary. If mean values per particle on a mesh are to be computed, correlation of the mean value per volume and the particle number per volume has to be taken into account, which leads to partial cancellation of statistical fluctuations.

## Acknowledgements

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

## References

- [1] M. Gray, T. Booth, T. Kwan, C. Snell, A multicomponent variance reduction Scheme for Monte Carlo semiconductor simulators, IEEE Trans. Electron Devices 45 (4) (1998) 918–924.



- [2] C. Jacoboni, A new approach to Monte Carlo simulation, in: International Meeting on Electron Devices of IEEE Electron Devices Society, Washington, DC, 1989, pp. 469–472.
- [3] M. Nedjalkov, P. Vitanov, Application of the iteration approach to the ensemble Monte Carlo technique, *Solid-State Electron* 33 (4) (1990) 407–410.
- [4] H. Kosina, M. Nedjalkov, S. Selberherr, Theory of the Monte Carlo method for semiconductor device simulation, *IEEE Trans. Electron Devices* 47 (10) (2000) 1898–1908.
- [5] P. Price, Calculation of hot electron phenomena, *Solid-State Electron* 21 (1978) 9–16.
- [6] C. Jacoboni, L. Reggiani, The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials, *Rev. Mod. Phys.* 55 (1983) 645–705.
- [7] P. Poli, L. Rota, C. Jacoboni, Weighted Monte Carlo for electron transport in semiconductors, *Appl. Phys. Lett.* 55 (10) (1989) 1026–1028.
- [8] R. Hockney, J. Eastwood, *Computer Simulation Using Particles*, Adam Hilger, Bristol, 1988.
- [9] R. Rubinstein, *Simulation and the Monte Carlo Method*, Wiley, New York, 1981.
- [10] H. Kosina, M. Nedjalkov, S. Selberherr, Variance and covariance estimation in stationary Monte Carlo device simulation, in: *Proceedings of Simulation of Semiconductor Processes and Devices*, Athens, Greece, 2001, pp. 140–143.
- [11] C. Wordelman, T. Kwan, C. Snell, Comparison of statistical enhancement methods for Monte Carlo semiconductor simulation, *IEEE Trans. Computer-Aided Design* 17 (12) (1998) 1230–1235.
- [12] H. Kosina, M. Nedjalkov, S. Selberherr, Variance reduction in Monte Carlo device simulation by means of event biasing, in: M. Laudon, B. Romanowicz (Eds.), *Proceedings of Modeling and Simulation of Microsystems, MSM 2001*, Computational Publications, 2001, pp. 11–14.