Variance and Covariance Estimation in Stationary Monte Carlo Device Simulation

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Abstract

This work deals with the Monte Carlo method for stationary device simulation, known as the Single-Particle Monte Carlo method. A thorough mathematical analysis of this method clearly identifies the independent, identically distributed random variables of the simulated process. Knowledge of these random variables allows usage of straight-forward estimates of the stochastic error. The presented method of error estimation is applicable to both distributed quantities and integrated quantities such as terminal currents.

1 Introduction

To assess the accuracy of Monte Carlo (MC) simulation it is necessary to estimate the probabilistic error bounds of the results. In the field of MC device simulation this problem has received renewed attention [1]. We present a new method of estimating the variance of the stationary MC method. The method is based on the identification of those random variables whose realizations are statistically independent. Knowing these random variables standard textbook formulae can be applied to estimate the variance.

2 Variance Estimation

In a thorough mathematical analysis of the single-particle MC method, outlined in [2][3], the Neumann series of the related integral equation is derived. Each term of that series describes the propagation of a carrier from the point of injection to the exit point at some contact. From this fact follows that only a complete numerical trajectory, that starts and terminates at the domain boundary, can be considered an independent realization of some random variable. In contrast, particle states generated on one trajectory are statistically dependent. The i-th realization of this random variable, say X, 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, $\mathbf{k}_j^a$.

$$x_i = \{\mathbf{k}_0, \mathbf{r}_0, t_0, \mathbf{k}_1^a, t_1, \ldots \mathbf{k}_j^a, t_j, \ldots\} \qquad j \leq N_i \tag{1}$$

The considered trajectory consists of $N_i + 1$ free flight segments. Another random variable $Y(X)$ needed in the following is defined by its realizations

$$y_i = \{\mathbf{k}_1^b, \mathbf{r}_1, \ldots \mathbf{k}_j^b, \mathbf{r}_j, \ldots\} \qquad j \leq N_i, \tag{2}$$

which contain all before-scattering states $\mathbf{k}_b^j$ and the particle locations at the times of scattering, $\mathbf{r}_j$.

With any quantity of interest, $A(\mathbf{k}, \mathbf{r})$, a random variable $\Psi_A(Y)$ is associated. Assuming the before-scattering method for average recording, the i-th realization of Ψ_A is of the form

$$\psi_{Ai} = \sum_{j=1}^{N_i} w_j \frac{A(\mathbf{k}_j^b, \mathbf{r}_j)}{\lambda(\mathbf{k}_j^b, \mathbf{r}_j)} \tag{3}$$

with λ being the total scattering rate. Summation is again over one complete trajectory starting and terminating at the domain boundary. If a statistical enhancement technique is used, the particle weighs w_j has to be accounted for, otherwise all weights equal one.

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

$$C = \frac{\langle\langle \mathrm{A} \rangle\rangle}{\langle\langle \mathrm{B} \rangle\rangle} \tag{4}$$

with the definition $\langle\langle \, . \, \rangle\rangle = \int_D \mathrm{d}\mathbf{r} \int \mathrm{d}\mathbf{k} \; . \; f(\mathbf{k}, \mathbf{r})$. 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 [4], whereas the denominator accounts for the normalization (cf. Table 1).

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 ψ_{Ai} and ψ_{Bi} using the rule (3). The so-called classical estimator of C is given by the ratio of the sample means.

$$\overline{C} = \frac{\overline{\psi}_A}{\overline{\psi}_B}, \qquad \overline{\psi}_\alpha = \frac{1}{N} \sum_{i=1}^{N} \psi_{\alpha i}, \qquad \alpha = A, B \tag{5}$$

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.

$$s_\alpha^2 = \frac{1}{N-1} \left[\sum_{i=1}^{N} \psi_{\alpha i}^2 - \frac{1}{N} \left(\sum_{i=1}^{N} \psi_{\alpha i} \right)^2 \right], \qquad \alpha = A, B \tag{6}$$

$$s_{AB}^2 = \frac{1}{N-1} \left[\sum_{i=1}^{N} \psi_{Ai} \psi_{Bi} - \frac{1}{N} \sum_{i=1}^{N} \psi_{Ai} \sum_{i=1}^{N} \psi_{Bi} \right] \tag{7}$$

N is the number of trajectories constructed in the simulation. From these inputs the variance of the random variable Ψ_C can be estimated [5].

$$s_C^2 = s_A^2 - 2\overline{C} s_{AB}^2 + \overline{C}^2 s_B^2 \tag{8}$$

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

$$\sigma\{\overline{C}\} = \frac{s_C}{\overline{\psi}_B \sqrt{N}}. \tag{9}$$

3 Application and Discussion

The following example demonstrates how the presented method of error estimation can be applied to both distributed quantities and integrated quantities such as terminal currents. As an example an n+nn+ silicon diode has been simulated, processing $5 \cdot 10^8$ scattering events, which resulted in the simulation of $N = 5.48 \cdot 10^7$ trajectories. The variances of the physical quantities collected in Table 1 have been calculated.

In Table 1 the number of physical particles in the simulation domain is denoted by N_D, $W_p(\mathbf{r})$ is the charge assignment function for grid point $\mathbf{r}_p$ and $V_p = \int W_p(\mathbf{r}) \mathrm{d}\mathbf{r}$. The

quantity	C	A	B
carrier concentration	n	$(N_D/V_p)W_p(\mathbf{r})$	1
current density	$\mathbf{j}$	$(qN_D/V_p)\mathbf{v}(\mathbf{k})W_p(\mathbf{r})$	1
terminal current	I_l	$(qN_D/V_p)\mathbf{v}(\mathbf{k})\cdot\nabla h_l(\mathbf{r})$	1
mean velocity	$\langle\mathbf{v}\rangle$	$\mathbf{v}(\mathbf{k})W_p(\mathbf{r})$	$W_p(\mathbf{r})$
mean energy	$\langle\epsilon\rangle$	$\epsilon(\mathbf{k})W_p(\mathbf{r})$	$W_p(\mathbf{r})$

Table 1: Examples of physical quantities used in (4).

current calculation employs the weight function method with $h_l(\mathbf{r})$ being the weight function for contact l.

Fig. 1 shows the electron concentration and the distribution of the standard deviation. In Fig. 2 the current density is depicted, which exhibits large fluctuations in the left and right contact region. Consistent with the observed fluctuation is the estimated standard deviation which is considerably higher in the contact regions than in the n-region.

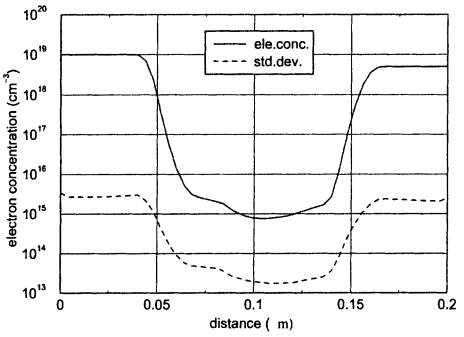

Fig. 1: Electron concentration and standard deviation in an n+nn+ diode with a 0.2 eV built-in barrier.

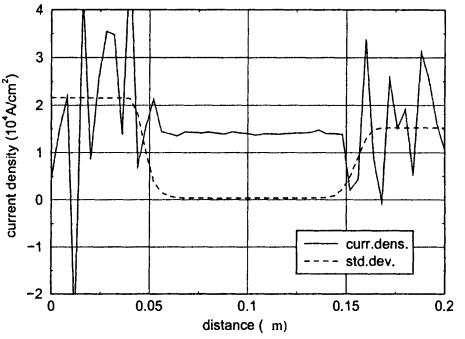

Fig. 2: Current density and standard deviation.

When computing the mean velocity using (4), $\langle\langle \mathrm{A} \rangle\rangle$ represents the particle current density and $\langle\langle \mathrm{B} \rangle\rangle$ 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. 3 (dashed line). An interesting result is the high positive correlation of the energy density and the particle density (solid line), which gives a significant reduction in standard deviation according to (8). A consequence of positive correlation is that a mean value per carrier has less variance than a mean value per unit volume, This is demonstrated in Fig. 4. Accounting for the fluctuations of both the energy density and the particle density gives the lower standard deviation (curve std.dev), while by neglecting the fluctuation of the particle density the standard deviation is clearly increased (curve std.dev.A).

The presented method has been used in conjunction with two statistical enhancement methods, the trajectory repetition scheme due to Philips and Price [6], and the recently investigated method of event biasing [3]. The presented method is parameter free in the sense that neither an unknown parameter of a stochastic process such as the correlation time needs to be estimated, nor the particle's history needs to be divided into sub-histories of some artificially predefined length.Instead, the total history is divided naturally into independent sub-histories at the times when the particle reenters the sim-

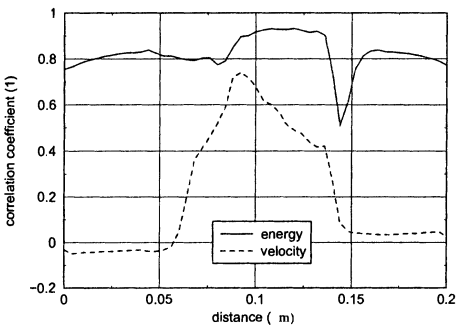

Fig. 3: Correlation coefficients of the the energy density $n\langle\epsilon\rangle$ and n, and of the particle current $n\langle v_x\rangle$ and n.

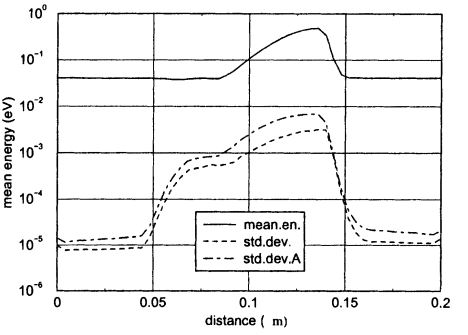

Fig. 4: Mean energy and its standard deviation, including the fluctuations of energy density and particle density (std.dev), and neglecting the fluctuation of particle density (std.dev.A).

ulation domain. A process with such property is referred to as regenerative stochastic process [5].

4 Conclusion

For the first time the independent, identically distributed random variables underlying the Single-Particle Monte Carlo method for device simulation have been identified. Knowing these random variables allows this Monte Carlo method to be supplemented with the natural stochastic error estimate. 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. Variance estimation of both distributed and integrated quantities is demonstrated. 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.

Acknowledgment

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[1] C. Jungemann and B. Meinerzhagen, "Efficiency and Stochastic Error of Monte Carlo Device Simulations," in *Int.Electron Devices Meeting*, pp. 109–112, 2000.

[2] 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.

[3] 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.

[4] R. Hockney and J. Eastwood, *Computer Simulation Using Particles.* Bristol and Philadelphia: Adam Hilger, 1988.

[5] R. Rubinstein, *Simulation and the Monte Carlo Method.* John Wiley and Sons, 1981.

[6] A. Phillips and P. Price, "Monte Carlo Calculations on Hot Electron Tails," *Applied Physics Letters*, vol. 30, pp. 528–530, May 1977.