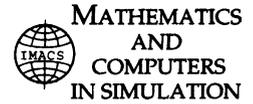




ELSEVIER

Mathematics and Computers in Simulation 62 (2003) 453–461



www.elsevier.com/locate/matcom

Monte Carlo algorithms for stationary device simulations

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

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

Abstract

The stochastic method used to simulate the stationary transport in semiconductor devices is revised in terms of the numerical Monte Carlo theory. A mathematically based approach has been used to derive the basic simulation algorithms, previously devised from physical considerations. The approach reveals novel properties of the method. It is shown that the method can be interpreted as a regenerative stationary process. The ergodicity of the process is proved and the random variable whose realizations are independent is identified.

© 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 algorithms; Semiconductor devices; Simulation

1. Outline of the mathematical method

In the semi-classical transport theory, the distribution function f is determined by a Fredholm integral equation of the second kind.

$$f(x) = \int f(x')K(x', x) dx' + f_0(x) \tag{1}$$

where the kernel K describes the propagation of the particles in the phase space of momentum \mathbf{k} and position \mathbf{r} , while the free term f_0 accounts for boundary and initial conditions. The variable x stands for (\mathbf{k}, \mathbf{r}) in the steady-state case. Substituting (1) recursively into itself presents the solution as an iteration series, known as the Neumann series.

$$f = \sum_i f^{(i)}; \quad f^{(n+1)}(x) = \int f^{(n)}(x')K(x', x) dx'; \quad f^{(0)}(x) = f_0(x) \tag{2}$$

Instead of a direct evaluation of f a weak formulation can be used, defining an inner product: $(f, A) = \int f(x)A(x) dx$, where A is some physical quantity. The inner product can be calculated by either by using

* Corresponding author. Fax: +43-1-58801-36099.

E-mail address: nedjalkov@iue.tuwien.ac.at (M. Nedjalkov).

(1) or alternatively by the conjugate equation:

$$g(x') = \int g(x)K(x', x) dx + A(x') \quad (3)$$

Multiplying (1) by $g(x)$ and (3) by $f(x')$, and integrating over x and x' , respectively results in the equality $(f, A) = (g, f_0)$. In this way the task has been reformulated in evaluation of the inner product of g with the free term of (1). The given function A has to be used as the free term of the conjugate equation. In the framework of the stochastic approach, the terms of the Neumann series are evaluated by numerical methods for Monte Carlo (MC) integration. In the basic idea of MC methods, integration is briefly reviewed [1] in the following. A way of computing the integral

$$I = \int_a^b \phi(x) dx = \int_a^b p(x)\theta(x) dx \quad (4)$$

is to represent it as an expected value of some random variable. Consider a factorization $\phi = p\theta$, where p is a density function, that is, p is non-negative and satisfies $\int_a^b p(x) dx = 1$. Integral (4) becomes the expected value of the random variable θ : $I = E\{\theta\}$. From the density p , a sample x_1, \dots, x_N of the random variable is generated and the sample mean is computed which is an estimate of the expected value.

$$I \simeq \bar{\theta} = \frac{1}{N} \sum_{i=1}^N \theta(x_i) \quad (5)$$

In addition to the result I , the MC method gives an estimate for the error, which is obtained via the sample variance. Since the factorization is not unique, different random variables can be introduced depending on the choice of the density p . All of them have the same expectation value, but different variance and higher moments.

2. Integral form of the transport equation

Under steady-state conditions, when the electric field \mathbf{E} and all material properties are independent of time, the carrier transport is governed by the stationary Boltzmann equation:

$$[\mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{r}} + \mathbf{F}(\mathbf{r}) \cdot \nabla_{\mathbf{k}}]f(\mathbf{k}, \mathbf{r}) = Q[f](\mathbf{k}, \mathbf{r}) \quad (6)$$

where $\mathbf{F} = q\mathbf{E}/\hbar$ and $\mathbf{r} \in D$. This equation which is posed in the simulation domain D , is supplemented by boundary conditions modeling the interaction of the device with the environment. The present approach relies on the assumption for a linear scattering operator Q , when many-body effects such as carrier–carrier scattering and degeneracy are neglected

$$Q[f](\mathbf{k}, \mathbf{r}) = \int f(\mathbf{k}', \mathbf{r})S(\mathbf{k}', \mathbf{k}, \mathbf{r}) d\mathbf{k}' - \lambda(\mathbf{k}, \mathbf{r})f(\mathbf{k}, \mathbf{r}) \quad (7)$$

where $\lambda(\mathbf{k}, \mathbf{r}) = \int S(\mathbf{k}, \mathbf{k}', \mathbf{r}) d\mathbf{k}'$ denotes the total scattering rate. The integral form of the equation is obtained by using the method of characteristics.

Characteristics of the differential operator in (6) are the classical trajectories. A trajectory is initialized by a phase space point (\mathbf{k}, \mathbf{r}) and a time t_0

$$\mathbf{K}(t; t_0, \mathbf{k}, \mathbf{r}) = \mathbf{k} + \int_{t_0}^t \mathbf{F}(\mathbf{R}(y; \cdot)) \, dy; \quad \mathbf{R}(t; t_0, \mathbf{k}, \mathbf{r}) = \mathbf{r} + \int_{t_0}^t \mathbf{v}(\mathbf{K}(y; \cdot)) \, dy \quad (8)$$

Eq. (8) can be read as the phase space position of a particle at time t , that passes through \mathbf{k} and \mathbf{r} at time t_0 . The order of t_0 and t is irrelevant. Provisionary, a trajectory is called forward if the evolution time is greater than the initialization time: $t > t_0$. Otherwise, the trajectory is called backward. Then the limits of the time integration in (8) can be exchanged by changing the sign of the integrals. To describe a time-invariant system, an absolute time scale is not needed. Only the time difference between two consecutive events is important. Invariance under time translation can be proven

$$\mathbf{K}(t + \tau; t_0 + \tau, \mathbf{k}, \mathbf{r}) = \mathbf{K}(t; t_0, \mathbf{k}, \mathbf{r}); \quad \mathbf{R}(t + \tau; t_0 + \tau, \mathbf{k}, \mathbf{r}) = \mathbf{R}(t; t_0, \mathbf{k}, \mathbf{r}) \quad (9)$$

This property will be used to adjust conveniently the time reference $t_0 = 0$ for each trajectory. A short-cut notation $\mathbf{K}(t) = \mathbf{K}(t; 0, \mathbf{k}, \mathbf{r})$ and $\mathbf{R}(t) = \mathbf{R}(t; 0, \mathbf{k}, \mathbf{r})$ can be introduced. A particularly useful relation can be obtained from (9)

$$\int d\mathbf{k} \, d\mathbf{r} \int_{-T}^0 dt \phi(\mathbf{k}, \mathbf{r}, \mathbf{K}(t), \mathbf{R}(t)) = \int d\mathbf{k}' \, d\mathbf{r}' \int_0^T dt \phi(\mathbf{K}'(t), \mathbf{R}'(t), \mathbf{k}', \mathbf{r}') \quad (10)$$

where $\mathbf{K}(t), \mathbf{R}(t)$ is a backward trajectory initialized by \mathbf{k}, \mathbf{r} , while $\mathbf{K}'(t), \mathbf{R}'(t)$ is a forward trajectory initialized by \mathbf{k}', \mathbf{r}' . The relation is proved by introducing new integration variables $\mathbf{k}' = \mathbf{K}(t; 0, \mathbf{k}, \mathbf{r})$ $\mathbf{r}' = \mathbf{R}(t; 0, \mathbf{k}, \mathbf{r})$. Then,

$$\mathbf{k} = \mathbf{K}(0; t, \mathbf{k}', \mathbf{r}') = \mathbf{K}(-t; 0, \mathbf{k}', \mathbf{r}'); \quad \mathbf{r} = \mathbf{R}(0; t, \mathbf{k}', \mathbf{r}') = \mathbf{R}(-t; 0, \mathbf{k}', \mathbf{r}')$$

According to the Liouville theorem, the phase volume is invariant under this transformation: $d\mathbf{k}' \, d\mathbf{r}' = d\mathbf{k} \, d\mathbf{r}$. The last step is to reverse the time by switching the sign of t .

To obtain the integral form of the stationary Boltzmann equation, we consider a given phase space point \mathbf{k}, \mathbf{r} . This point determines uniquely a phase space trajectory, $\mathbf{K}(t)$ and $\mathbf{R}(t)$ in backward parametrization. The left hand side of (6) represents the total time derivative of $\hat{f}(t) = f(\mathbf{K}(t), \mathbf{R}(t))$. The Boltzmann equation can be multiplied by an integrating factor $\exp(\int_0^t \hat{\lambda}(y) \, dy)$ and rewritten as an ordinary differential equation of first order

$$\frac{d}{dt} \left(\exp \left(\int_0^t \hat{\lambda}(y) \, dy \right) \hat{f}(t) \right) = \exp \left(\int_0^t \hat{\lambda}(y) \, dy \right) \hat{Q}_g[f](t) \quad (11)$$

This equation can be integrated straight forwardly. The upper bound of integration should be $t = 0$ to obtain $\hat{f}(0) = f(\mathbf{k}, \mathbf{r})$, the value of f at the given phase space point. The lower time bound has to be chosen such that the functions $\mathbf{K}(t)$ and $\mathbf{R}(t)$ take on values at which the distribution function is known. In the steady state, the distribution function is known only at the domain boundary. An appropriate lower time bound is therefore the time, say t_b^- , at which the trajectory crosses the simulation domain boundary. Apparently, this time depends on the point \mathbf{k}, \mathbf{r} under consideration. For trajectories closed in D , the time t_b is $-\infty$. Integration of (11) in the time bounds discussed above results in the integral form of the

stationary Boltzmann equation,

$$\begin{aligned}
 f(\mathbf{k}, \mathbf{r}) &= \int dt' d\mathbf{k}' \int_{t_b^-(\mathbf{k}, \mathbf{r})}^0 f(\mathbf{k}', \mathbf{R}(t')) S(\mathbf{k}', \mathbf{K}(t'), \mathbf{R}(t')) \\
 &\quad \times \exp\left(-\int_{t'}^0 \lambda(\mathbf{K}(y), \mathbf{R}(y)) dy\right) + f_0(\mathbf{k}, \mathbf{r}) \\
 f_0(\mathbf{k}, \mathbf{r}) &= f_b(\mathbf{K}(t_b^-(\mathbf{k}, \mathbf{r})), \mathbf{R}(t_b^-(\mathbf{k}, \mathbf{r}))) \exp\left(-\int_{t_b^-(\mathbf{k}, \mathbf{r})}^0 \lambda(\mathbf{K}(y), \mathbf{R}(y)) dy\right)
 \end{aligned} \tag{12}$$

where f_b denotes the boundary distribution.

Using the notation of Section 1, the conjugate equation has the same kernel as the integral equation, but integration is carried out over the unprimed variables. To apply this rule, the integral form of the BE first has to be transformed into the standard form

$$f(\mathbf{k}, \mathbf{r}) = \int d\mathbf{k}' \int d\mathbf{r}' f(\mathbf{k}', \mathbf{r}') K(\mathbf{k}', \mathbf{r}', \mathbf{k}, \mathbf{r}) + f_0(\mathbf{k}, \mathbf{r}) \tag{13}$$

The required \mathbf{r}' integration is introduced by augmenting the kernel to

$$K(\mathbf{k}', \mathbf{r}', \mathbf{k}, \mathbf{r}) = \int_{-\infty}^0 dt' S(\mathbf{k}', \mathbf{K}(t'), \mathbf{r}') \times \exp\left(-\int_{t'}^0 \lambda(\mathbf{K}(y), \mathbf{R}(y)) dy\right) \delta(\mathbf{r}' - \mathbf{R}(t')) \theta_D(\mathbf{r}') \tag{14}$$

The indicator function of the simulation domain θ_D ensures the proper lower bound $t_b^-(\mathbf{k}, \mathbf{r})$ of the time integral. In the obtained equation, the integration variables are changed from \mathbf{k} to $\mathbf{k}^a = \mathbf{K}(t'; 0, \mathbf{k}, \mathbf{r})$ and from \mathbf{r} to $\mathbf{r}'' = \mathbf{R}(t'; 0, \mathbf{k}, \mathbf{r})$. Using the steps leading to (10), the conjugate equation can be stated explicitly

$$\begin{aligned}
 g(\mathbf{k}', \mathbf{r}') &= \int d\mathbf{k}_a \int_0^\infty d\tau S(\mathbf{k}', \mathbf{k}_a, \mathbf{r}') \\
 &\quad \times \exp\left(-\int_0^\tau \lambda(\mathbf{K}(y), \mathbf{R}(y)) dy\right) g(\mathbf{K}(\tau), \mathbf{R}(\tau)) \theta_D(\mathbf{r}') + A(\mathbf{k}', \mathbf{r}')
 \end{aligned} \tag{15}$$

The forward trajectory $(\mathbf{K}(t), \mathbf{R}(t))$ is initialized by $\mathbf{k}_a, \mathbf{r}'$. The equation has the desired property that integration is carried out over final states and that the time variable is positive. The iteration series of (15) will be used to obtain forward MC algorithms.

The mean value $\langle A \rangle$ of a physical quantity A is defined as an integral in the simulation domain.

$$\langle A \rangle = \int_D d\mathbf{r} \int d\mathbf{k} A(\mathbf{k}, \mathbf{r}) f(\mathbf{k}, \mathbf{r}) \tag{16}$$

It is transformed into (f_0, g) by means of the equality $(f, A) = (g, f_0)$

$$\langle A \rangle = \int_D d\mathbf{r}' \int d\mathbf{k}' f_b(\mathbf{K}(t_b^-), \mathbf{R}(t_b^-)) \exp\left(-\int_{t_b^-}^0 \lambda(\mathbf{K}(y), \mathbf{R}(y)) dy\right) g(\mathbf{k}', \mathbf{r}') \tag{17}$$

where t_b^- and the backward trajectory $\mathbf{K}(t)$ and $\mathbf{R}(t)$ are initialized by \mathbf{k}', \mathbf{r}' . Since f_b is defined only at the boundary ∂D , a transformation is needed that leads from a volume to a boundary integral. A phase

space point $(\mathbf{k}', \mathbf{r}')$ is bijectively mapped onto $(\mathbf{K}(t_b), \mathbf{r}_b = \mathbf{R}(t_b), t_b)$, where $\mathbf{r}_b \in \partial D$, if $t_b > -\infty$. This prompts that the transformation must replace one of the space integrals by a time integral. We consider the subspace Φ_b of points $(\mathbf{k}', \mathbf{r}')$ having finite t_b . Fortunately this is the relevant subdomain for the integral (17), since in the complementary subspace the integrand vanishes. The required time integral is introduced as follows. The domain boundary can be defined implicitly by $B(\mathbf{r}) = 0$. This gives an implicit definition of the boundary time as a root of $B(\mathbf{R}(t')) = 0$. Then the equality

$$\delta(t' - t_b) = \delta(B(\mathbf{R}(t')))|\nabla_{\mathbf{r}} B(\mathbf{r}_b)||\mathbf{v}_{\perp}(\mathbf{K}(t_b))|$$

can be used to augment (17) by a time integral on t' in the limits $(0, -\infty)$. Here, \mathbf{v}_{\perp} is the velocity component normal to the domain boundary in the crossing point with the trajectory. The obtained equation can be processed using the same steps leading to (15). The variables $(\mathbf{k}', \mathbf{r}')$ are changed to $(\mathbf{k}_b = \mathbf{K}(t'; 0, \mathbf{k}', \mathbf{r}'), \mathbf{r}'' = \mathbf{R}(t'; 0, \mathbf{k}', \mathbf{r}'))$. The \mathbf{r}'' integral is transformed with the aid of the delta function

$$\int_D \delta(B(\mathbf{r}''))\phi(\mathbf{r}'') d\mathbf{r}'' = \oint \frac{\phi(\mathbf{r}_b)}{|\nabla_{\mathbf{r}} B(\mathbf{r}_b)|} d\sigma(\mathbf{r}_b)$$

where ϕ is a test function. Eq. (17) is transformed into

$$\begin{aligned} \langle A \rangle &= \oint_{\partial D} d\sigma(\mathbf{r}_b) \int_{K_+(\mathbf{r}_b)} \int_0^{\infty} dt_0 |\mathbf{v}_{\perp}(\mathbf{k}_b)| f_b(\mathbf{k}_b, \mathbf{r}_b) \\ &\times \exp\left(-\int_0^{t_0} \lambda(\mathbf{K}_b(y), \mathbf{R}_b(y)) dy\right) g(\mathbf{K}_b(t_0), \mathbf{R}_b(t_0)) \end{aligned} \tag{18}$$

The accomplished change from volume to boundary integration is a key step in the treatment of the boundary value problem. It proves that knowledge of the boundary distribution is sufficient to determine arbitrary volume integrals defined by (16) and therefore to determine f uniquely. Note that only the subspace K_+ of boundary states \mathbf{k}_b having inward directed velocity component \mathbf{v}_{\perp} appear in (18) and thus determine the boundary condition. The complementary part is unknown and comes out as a result of the simulation. Introduced for the purpose of normalization are the integrals

$$j_{\perp}(\mathbf{r}_b) = \int_{K_+(\mathbf{r})} d\mathbf{k} |\mathbf{v}_{\perp}(\mathbf{k})| f_b(\mathbf{k}, \mathbf{r}_b), \quad \Gamma_D = \oint_{\partial D} j_{\perp}(\mathbf{r}) d\sigma(\mathbf{r}) \tag{19}$$

which represent the normal component of the incident particle current density and the total incident particle current.

3. The Monte Carlo method

Substituting the Neumann series of the conjugate equation, $g = \sum_0^{\infty} g^{(i)}$, into (18) results in a series for the mean value

$$\langle A \rangle = \sum_{i=0}^{\infty} \langle A \rangle_i \tag{20}$$

As an instructive example, the term of second order is discussed. An explicite decomposition into a probability density p_2 and a random variable θ_2 according to (4) is pursued in (21). The density p_2 appears

as a product of conditional probability densities, which are enclosed in curly brackets. The normalization is ensured by factors which are additionally introduced. They cancel each other so that the mean value $\langle A \rangle_2$ remains unchanged.

$$\begin{aligned} \langle A \rangle_2 = & \Gamma_D \oint_{\partial D} d\sigma \int_{K_+} d\mathbf{k}_b \int_0^\infty dt_0 \int d\mathbf{k}_1 \int_0^\infty dt_1 \int d\mathbf{k}_2 \int_0^\infty dt_2 \times \left\{ \frac{j_\perp(\mathbf{r}_b)}{\Gamma_D} \right\} \left\{ \frac{|v_\perp(\mathbf{k}_b)| f_b(\mathbf{k}_b, \mathbf{r}_b)}{j_\perp(\mathbf{r}_b)} \right\} \\ & \times \left\{ \lambda(\mathbf{K}_b(t_0), \mathbf{R}_b(t_0)) \exp \left(- \int_0^{t_0} \lambda(\mathbf{K}_b(y), \mathbf{R}_b(y)) dy \right) \right\} \left\{ \frac{S(\mathbf{K}_b(t_0), \mathbf{k}_1, \mathbf{R}_b(t_0))}{\lambda(\mathbf{K}_b(t_0), \mathbf{R}_b(t_0))} \right\} \\ & \times \left\{ \lambda(\mathbf{K}_1(t_1), \mathbf{R}_1(t_1)) \exp \left(- \int_0^{t_1} \lambda(\mathbf{K}_1(y), \mathbf{R}_1(y)) dy \right) \right\} \left\{ \frac{S(\mathbf{K}_1(t_1), \mathbf{k}_2, \mathbf{R}_1(t_1))}{\lambda(\mathbf{K}_1(t_1), \mathbf{R}_1(t_1))} \right\} \\ & \times \exp \left(- \int_0^{t_2} \lambda(\mathbf{K}_2(y), \mathbf{R}_2(y)) dy \right) \theta_D(\mathbf{R}_b(t_0)) \theta_D(\mathbf{R}_1(t_1)) \theta_D(\mathbf{R}_2(t_2)) A(\mathbf{K}_2(t_2), \mathbf{R}_2(t_2)) \end{aligned} \tag{21}$$

The density p determines a numerical trajectory which is built up by pieces of classical trajectories. The probability densities in the first two curly brackets select the boundary state $\mathbf{k}_b, \mathbf{r}_b$ which initializes the first classical trajectory $\mathbf{K}_b(y), \mathbf{R}_b(y)$. The next two terms are the well-known densities used in the MC transport simulation, namely the distribution of the free flight time $p_t = \lambda \exp(-\int \lambda)$ and that of the after-scattering state $p_k = S/\lambda$ [2]. After being selected, t_0 and \mathbf{k}_1 determine the initialization point $\mathbf{k}_1, \mathbf{R}_b(t_0)$ of the next piece of classical trajectory $\mathbf{K}_1(y), \mathbf{R}_1(y)$. The real space part of the numerical trajectory is continuous, $\mathbf{R}_b(t_0) = \mathbf{R}_1(0)$. Similarly, the next two terms initialize $\mathbf{K}_2(y), \mathbf{R}_2(y)$. The integrand in the last line denoted by L is separated into two parts. The first part is assigned to p_2 while the second is the random variable θ_2 . This can be done in two different ways, leading to either the *synchronous ensemble* method or the *time-integration* method of average recording.

The first option is to multiply and divide L by λ to obtain a product of p_t and θ_2

$$\begin{aligned} L = & \left\{ \lambda(\mathbf{K}_2(t_2), \mathbf{R}_2(t_2)) \exp \left(- \int_0^{t_2} \lambda(\mathbf{K}_2(y), \mathbf{R}_2(y)) dy \right) \right\} \\ & \times H(t_{b_0}^+ - t_0) H(t_{b_1}^+ - t_1) H(t_{b_2}^+ - t_2) \frac{A(\mathbf{K}_2(t_2), \mathbf{R}_2(t_2))}{\lambda(\mathbf{K}_2(t_2), \mathbf{R}_2(t_2))} \end{aligned} \tag{22}$$

A new piece of classical trajectory with end point $\mathbf{K}_2(t_2), \mathbf{R}_2(t_2)$ is added to the numerical trajectory by the third free flight probability density p_t . The last line displays the random variable θ_2 . An equivalent formulation of θ_2 is used by substituting the domain indicators $\theta_D(\mathbf{R}_i(t_i))$ by unit step functions $H(t_{bi}^+ - t_i)$, where t_{bi}^+ is the forward boundary time of the i -th trajectory. If the numerical trajectory lies entirely in D , θ_2 takes value A/λ evaluated at the third free flight end point.

A second option is to process the t_2 -integral in (21) by integration by parts. L becomes a product of a free flight density p_t , the same as in (22), and a random variable θ_2

$$\begin{aligned} L = & \left\{ \lambda(\mathbf{K}_2(t_2), \mathbf{R}_2(t_2)) \exp \left(- \int_0^{t_2} \lambda(\mathbf{K}_2(y), \mathbf{R}_2(y)) dy \right) \right\} \\ & \times H(t_{b_0}^+ - t_0) H(t_{b_1}^+ - t_1) \int_0^{t_2} H(t_{b_2}^+ - \tau) A(\mathbf{K}_2(\tau), \mathbf{R}_2(\tau)) d\tau \end{aligned} \tag{23}$$

The value of θ_2 in this expression is identified as the path integral over τ . If $t_2 < t_{b2}^+$, the τ -integration is performed until the next scattering event occurs, otherwise until the boundary is reached. Assume A to be the domain indicator of some subdomain Ω : $A = \theta_\Omega(\mathbf{k}, \mathbf{r})$. According to (16), $\langle A \rangle$ is the mean particle number in Ω . The path integral then records the time spent in Ω during the third free flight.

In principle, one can obtain the mean value $\langle A \rangle$ by evaluating the separate terms in the series (20) by means of (5). One peculiarity of the single-particle MC (SPMC) method is that the sample for the iteration term of order i is not generated independently from that for the term of order $i - 1$. Instead, a realization of p_i is generated by adding to the realization of p_{i-1} another after-scattering state \mathbf{k}_i and another free flight time t_i . The following considerations aim at obtaining the single-particle MC algorithm and to find that random variable whose realization is independent from each other. In (21), we designate the multi-dimensional integration variable as x_2 , the probability density as p_2 , and random variable as θ_2 , such that $\langle A \rangle_2 = \int dx_2 p_2(x_2) \theta_2(x_2)$, where

$$x_2 = (\mathbf{r}_b, \mathbf{k}_b, t_0, \mathbf{k}_1, t_1, \mathbf{k}_2, t_2) \tag{24}$$

$$p_2(x_2) = \{j_\perp / \Gamma_D\} \{v_\perp f_b / j_\perp\} \{p_t\} \{p_k\} \{p_t\} \{p_k\} \{p_t\} \tag{25}$$

$$\theta_2(x_2) = H_0 H_1 H_2 A / \lambda \quad \text{or} \quad \theta_2(x_2) = H_0 H_1 \int H_2 A \tag{26}$$

If $\theta_2(x_2)$ is replaced by $\theta_1(x_1) = H_0 H_1 A / \lambda$ (or $\theta_1(x_1) = H_0 \int H_1 A$) in (21), the equation recovers the mean value for $\langle A \rangle_1$ since the integrals over \mathbf{k}_2 and t_2 give unity. Thus, the trajectory generated by p_2 can be used for evaluation of $\langle A \rangle_1$ and in the same way of $\langle A \rangle_0$. This result can be utilized to express $\langle A \rangle$ as one multiple integral of infinite order

$$\langle A \rangle = \lim_{n \rightarrow \infty} \int p_n(x_n) \theta^{[n]}(x_n) dx_n \tag{27}$$

using the label $\mathbf{k}_i^b = \mathbf{K}_i(t_i)$ for the i -th before-scattering state and the recursive definitions

$$x_n = (x_{n-1}, \mathbf{k}_n, t_n) \tag{28}$$

$$p_n = p_{n-1} \times \left\{ \frac{S(\mathbf{k}_{n-1}^b, \mathbf{k}_n)}{\lambda(\mathbf{k}_{n-1}^b)} \right\} \left\{ \lambda(\mathbf{K}_n(t_n)) \exp \left(- \int_0^{t_n} \lambda(\mathbf{K}_n(y)) dy \right) \right\} \tag{29}$$

$$\theta^{[n]} = \theta^{[n-1]} + \prod_{j=0}^n H(t_{bj}^+ - t_j) \frac{A(\mathbf{k}_n^b, \mathbf{r}_n)}{\lambda(\mathbf{k}_n^b)} \tag{30}$$

or

$$\theta^{[n]} = \theta^{[n-1]} + \prod_{j=0}^{n-1} H(t_{bj}^+ - t_j) \int_0^{t_n} H(t_{bn}^+ - \tau) A(\mathbf{K}_n(\tau), \mathbf{R}_n(\tau)) d\tau, \tag{31}$$

To evaluate (27) by MC integration one has to generate N realizations of the random variable x_∞ . Each realization comprises a trajectory construction, which begins as described above and continues by consecutive use of the scattering and free flight densities. In principle, this process should be infinite.

However, if in the course of numerical trajectory construction a time $t_l > t_{bl}^+$ is generated, the unit step function in (31) evaluates to zero. The random variable keeps its value

$$\theta_j = \sum_{j=0}^{l-1} \frac{A(\mathbf{k}_j^b, \mathbf{r}_j)}{\lambda(\mathbf{k}_j^b)} \quad \text{or} \quad \theta_j = \sum_{j=0}^{l-1} \int_0^{t_j} A \, d\tau + \int_0^{t_{bl}^+} A \, d\tau, \quad (32)$$

and the construction process can be terminated. This value is the output of one realization of the random variable x_∞ . The θ_i given by the sum (32) are summed up in the sample mean (5). This gives a double sum which can be replaced by one sum over all free flights (aff) that have been generated in the simulation.

$$\langle A \rangle \simeq \Gamma_D \frac{1}{N} \sum_{i=1}^N \theta_i = \Gamma_D \frac{1}{N} \sum_{\text{aff}} \frac{A(\mathbf{k}^b, \mathbf{r}^b)}{\lambda(\mathbf{k}^b)} = \Gamma_D \frac{1}{N} \sum_{\text{aff}} \int A(\mathbf{K}(\tau), \mathbf{R}(\tau)) \, d\tau \quad (33)$$

The normalization constant Γ_D need not be evaluated from the theoretical definition (19). Instead, by setting $A = 1$, a relation between Γ_D and the total number of particles N_D is obtained. N_D is usually known, for instance from the constraint of total charge neutrality in the device.

$$4\pi^3 N_D = \Gamma_D \frac{1}{N} \sum_{\text{aff}} \lambda(\mathbf{k}^b)^{-1} = \Gamma_D \frac{1}{N} T \quad (34)$$

where T is the total time the particle has been followed during the simulation.

4. Discussions and conclusions

The described procedure contains all basic steps known from single-particle MC (SPMC) algorithm. The initial state is generated from a velocity-weighted boundary distribution, $v_\perp f_b$. This state is the starting point of a numerical trajectory which is built up according to the semi-classical model for carrier transport in semiconductors. The free flight time and the after-scattering state are generated from the densities p_l and p_k . In this sense, the constructed numerical trajectories coincide with the real trajectories of the semiconductor carriers. The two SPMC methods for average recording are recovered. The well-known formula $\sum_{\text{aff}} A \lambda^{-1} / \sum_{\text{aff}} \lambda^{-1}$ for computing the mean value per particle can be obtained from (33) and (34). The physics-based way of deriving the SPMC assumes ergodicity of the transport process in order to replace the ensemble average by a time average. Here, the ergodicity of the transport process as implied by the time averaging method comes out as a result of the numerical approach. Particularly, the mean of the distribution function in a subdomain Ω is obtained from the simulation time spent in Ω divided by the total simulation time T .

The SPMC method can be interpreted to simulate a regenerative stationary process [3]. After a trajectory leaves the domain the process is renewed by the next trajectory starting from the boundaries. An independent realization of the random variable θ is identified as a complete numerical trajectory that starts and terminates at the boundary. This allows to supplement the SPMC method with event biasing schemes [4] and variance estimates of the numerical Monte Carlo theory. The variance estimates are considered in another contribution to this issue.

Acknowledgements

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

References

- [1] I. Sobol, Numerical Methods Monte Carlo, Nauka, Moscow, 1973.
- [2] C. Jacoboni, L. Reggiani, The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials, *Rev. Modern Phys.* 55 (1983) 3.
- [3] R. Rubinstein, Simulation and the Monte Carlo Method, Wiley, New York, 1981.
- [4] H. Kosina, M. Nedjalkov, S. Selberherr, Variance reduction in Monte Carlo device simulation by means of event biasing, in: Proceedings of the Conference on Modeling and Simulation of Microsystems, MSM 2001, 2001.