IMPROVED ALGORITHMS IN MONTE CARLO DEVICE SIMULATION

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Abstract

Algorithms are presented which advance the state of the art in Monte Carlo device simulation in two ways. Firstly, a method of free-flight time calculation using a new self-scattering algorithm is described. A piecewise linear total scattering rate allows for an efficient reduction of self-scattering events. Secondly, a unique Monte Carlo–Poisson coupling scheme is adopted, which converges faster than presently known schemes do. It is based on so-called Monte Carlo–Drift Diffusion coupling, a method which can be rigorously justified within the semiclassical Boltzmann transport theory.

1 INTRODUCTION

When developing a Monte Carlo code, an ever valid requirement is the reduction of the solution times. Due to the computational burden the use of the Monte Carlo technique has until now been restricted to research purposes. However, thanks to both the continuing increase of the power of modern computers and the development of more efficient Monte Carlo algorithms, this situation is likely to change in the near future. Monte Carlo device simulation will then also become feasible as an engineering tool. The topics presented below are intended to be a step in this direction.

In the one-particle Monte Carlo method, the steady state average of a quantity can be calculated just by sampling the electron trajectory immediately before the scattering events. When self-scattering is introduced, the trajectory is sampled much more frequently than it is actually required. This increases the computational effort, since for each instance of a self-scattering event the electrons state has to be evaluated. A method for reducing the number of self-scatterings and thus produce increased free-flight durations is presented in the next section. In section 3 a new, self-consistent iteration method is introduced, and simulation results of submicron MOSFETs are discussed in detail.

2 SELF-SCATTERING

In a Monte Carlo simulation a stochastic sequence of a free-flight times must be generated according to a given probability distribution. Using the direct technique [5] one obtains for the free-flight time t_f the following integral equation,

$$\int_0^{t_f} \lambda(\mathrm{k}_{(t)}, \mathrm{r}_{(t)})\, dt = -\ln(r)\,, \tag{1}$$

where r is a random number evenly distributed between 0 and 1, and $\lambda(\mathrm{k}, \mathrm{r})$ denotes the momentum- and space-dependent total scattering rate. However, in order to solve (1) the trajectory $\mathrm{k}(t), \mathrm{r}(t)$ of the particle must be known. In order to accomplish this, one has to tackle a coupled system of

equations consisting of (1) and the equations of motion, $\hbar\,\dot{\mathbf{k}} = -e\,\mathbf{E}(\mathbf{r})$ and $\dot{\mathbf{r}} = \mathbf{v}(\mathbf{k})$. This system can be solved either numerically or analytically. A numerical solution requires a discretization of time with timesteps $\Delta t \ll \lambda^{-1}(\mathbf{k},\mathbf{r})$. This technique is not well suited for efficient implementation on scalar computers. Pursuing an analytic solution which is continuous in time one can simplify the integral equation (1) by the introduction of a virtual scattering mechanism called self-scattering [10]. With the associated self-scattering rate $\lambda_{ss}(\mathbf{k})$ the total scattering rate becomes

$$\Gamma(\mathbf{k},\mathbf{r}) = \lambda(\mathbf{k},\mathbf{r}) + \lambda_{ss}(\mathbf{k},\mathbf{r}) \tag{2}$$

The self-scattering does not affect the state of a particle, so, whenever it occurs the trajectory of the particle continues unperturbed. In the so called constant Γ technique the self-scattering rate is chosen so that Γ becomes independent from $\mathbf{k}$ and $\mathbf{r}$. Then (1) simplifies to a first-order algebraic equation

$$\Gamma \cdot t_f + \ln(r) = 0\,. \tag{3}$$

Although the solution for t_f is quite trivial, this technique has computational drawbacks. Since the total scattering rate is kept artificially high, a high percentage of self-scattering events occurs. Improvements of the constant Γ technique are the piecewise-constant Γ technique [11] and those techniques, which try to optimize a constant Γ level with respect to the current particle's state [6] [9]. All the methods outlined above share the assumption that self-scattering can only be used to simplify (1) into (3). An equation of intermediate complexity, yet analytically soluble, is presented below.

Our Ansatz starts with the equation of motion in $\mathbf{k}$ space, which we solve analytically under the constraint that the electric field is constant within one mesh-cell,

$$\dot{\mathbf{k}} = -\xi = \text{const} \quad \Rightarrow \quad \mathbf{k}(t) = \mathbf{k}_0 - \xi \cdot t\,. \tag{4}$$

Here ξ is related to the electric field, $\xi = -e\mathbf{E}/\hbar$, and $\mathbf{k}_0$ denotes the wave vector at the beginning of the free flight. Now we deviate from the constant Γ and allow a linear dependence from k^2,

$$\Gamma(\mathbf{k}) = a\,k^2 + b\,. \tag{5}$$

Inserting in (5) the wave vector $\mathbf{k}(t)$, which evolves according to (4) linearly in time, it becomes obvious, that $\Gamma(\mathbf{k}(t))$ is a second-order polynomial in time. Integration of $\Gamma(\mathbf{k}(t))$ yields a cubic polynomial. Inserting this polynomial in (1), we end up with a third-order algebraic equation in the free-flight time,

$$t_f^3 - 3\,T_0\,t_f^2 + S\,t_f + T = 0\,. \tag{6}$$

Here the coefficients are defined as

$$T_0 = \frac{(\mathbf{k}_0 \cdot \xi)}{\xi^2}\,, \quad S = \frac{3\Gamma_0}{a\xi^2}\,, \quad T = \frac{3\ln(r)}{a\xi^2}\,, \tag{7}$$

where Γ_0 is the total scattering rate at the beginning of the free flight according to (5), $\Gamma_0 = a\,k_0^2 + b$. The free-flight time can be obtained analytically from (6), since for third-order algebraic equations a closed solution always exists.

Furthermore we can show, that the conditions $a > 0$ and $b \geq 0$ are sufficient to make the discriminant in (6) positive. In other words, if both the slope a and the offset b of the linear total scattering rate (5) are positive, one real and two complex solutions always exist. Thus, the free flight time is uniquely given by Cardano's formula. For non-parabolic bands one can see in Fig. 1 that advantageous linear scattering rates after (5) fulfill the condition for a positive discriminant.

Therefore, during the Monte Carlo simulation, checking the discriminant or the free-flight time for poitive sign can be omitted. In a situation where straight lines with a negative slope are used, three real solutions may occur and checks in order to find out the physical one are necessary.

We have implemented the piecewise linear Γ technique using three different linear segments. The amount of self-scattering lies typically below 5%.

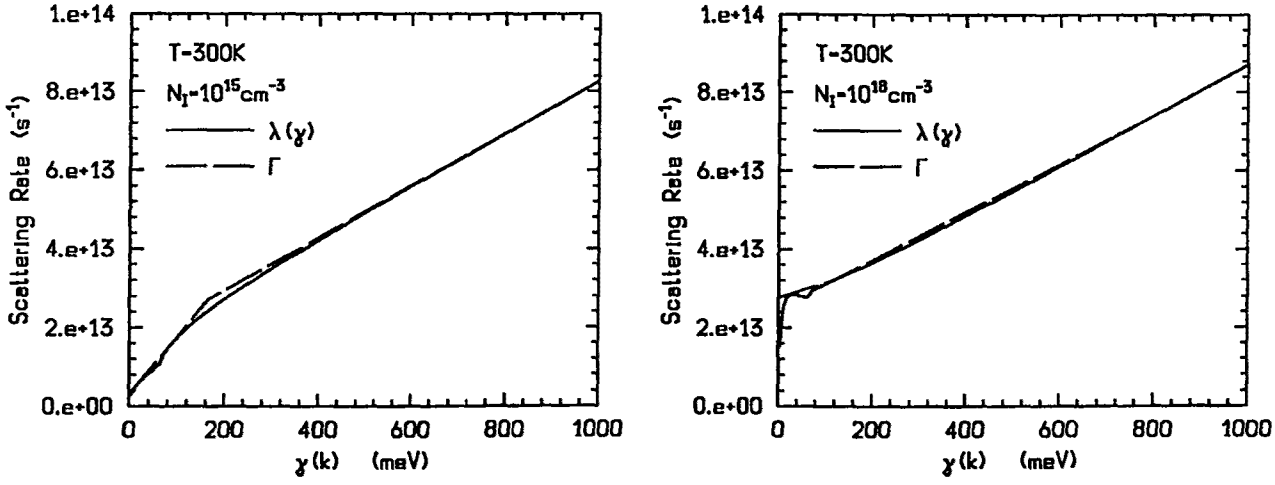

Figure 1: Use of self-scattering to set up a piecewise linear envelope function for the total scattering rate. The scattering rates are represented as functions of γ, which is defined as $\gamma = \hbar^2 k^2 / 2m_0$.

3 MONTE CARLO–POISSON COUPLING

Monte Carlo simulations of submicron MOSFETs employing the potential distribution of a conventional Drift-Diffusion simulation may lead to unrealistic results. Velocity overshoot phenomena can be clearly observed in such small devices. In particular we noted that at high gate biases a non-self-consistent treatment tends to overestimate the influence of these phenomena on the drain current. Therefore realistic results can only be expected by applying some sort of self-consistent technique. Previously published algorithms couple the Boltzmann transport equation, solved by the Monte Carlo-method, with either the linear [4] or the nonlinear [12] Poisson equation. In the latter method stability problems can be avoided and the convergence rate can be improved. In [8] we have described a one-dimensional implementation of a self-consistent algorithm, which is based on the so called Monte Carlo–Drift-Diffusion coupling technique.

3.1 Monte Carlo–Drift-Diffusion Coupling

Monte Carlo–Drift-Diffusion coupling is based upon an extended Drift-Diffusion like current relation, which is motivated by the first moment of the Boltzmann transport equation,

$$j_i = q\, n\, \mu_{ij} \left(E_j + \frac{1}{n} \frac{\partial\, n U_{T,jk}}{\partial r_k} \right). \tag{8}$$

The basic idea is that (8) exactly reproduces the Monte Carlo current density $j_i = -en < v_i >$, provided that the coefficients μ_{ij} and $U_{T,ij}$ are calculated in an appropriate way by the Monte

Carlo method. In the original work of Bandyopadhyay [1] the first three moments of the distribution function, $n(\mathbf{r})$, $<v_i>$ and $<\hbar k_i \cdot v_j>$ are calculated, and related to the required coupling coefficients by

$$\mu_{ij}\left(E_j + \frac{1}{en}\cdot\frac{\partial\left(n\ <\hbar k_j \cdot v_k>\right)}{\partial r_k}\right) = -<v_i>\ , \tag{9}$$

$$U_{T,ij} = \frac{1}{e}\ <\hbar k_i \cdot v_j>\ . \tag{10}$$

However, difficulties arise when the non-local mobility (9) is evaluated by the MC-method. In particular a spatial derivative of Monte Carlo quantities must be calculated. Due to the noise associated with such quantities, this treatment will lead to inaccurate results. Using the equation for the first moment the mobility definition (9) can also be written as [1]

$$\mu_{ij}\left(\frac{dp_j}{dt}\right)_c = <v_i>\ . \tag{11}$$

Our approach is to evaluate the average momentum loss rate at the left hand side of (11) directly by means of the Monte Carlo method, thus circumventing any problems arising from spatial derivatives [7]. The average momentum loss rate can be expressed in terms of the energy-dependent momentum relaxation time $\tau_m(\epsilon)$ as

$$\left(\frac{dp}{dt}\right)_c = <\hbar \mathbf{k} \cdot \tau_m(\epsilon)^{-1}>\ . \tag{12}$$

Finally, it should be mentioned that approaching thermal equilibrium, the extended current relation (8) simplifies to the conventional Drift-Diffusion current relation and the Monte Carlo–Drift-Diffusion coupling coefficients (10) and (11) approach the equilibrium temperature voltage and the ohmic mobility, respectively.

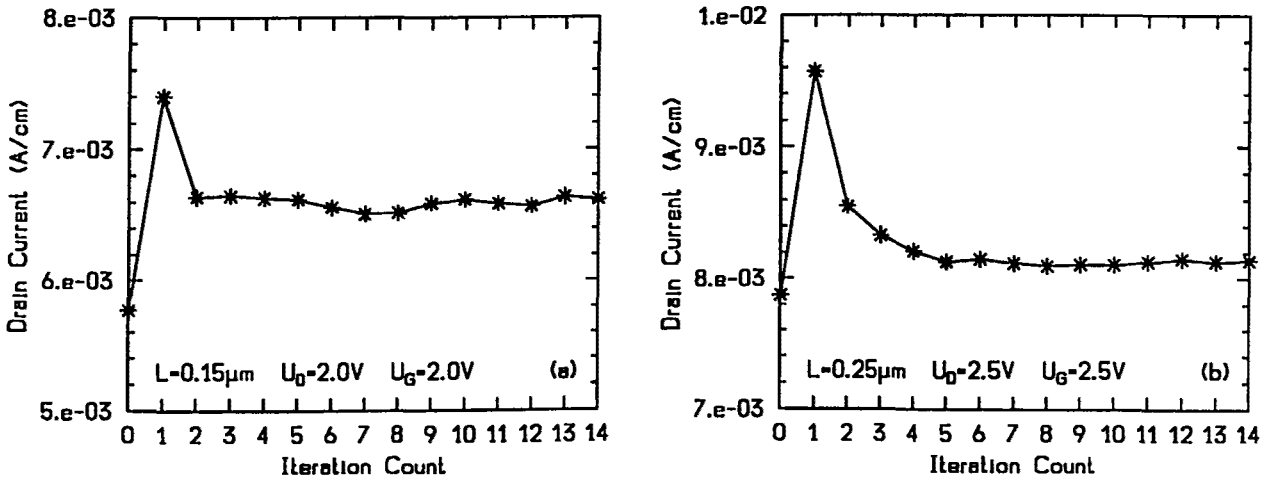

Figure 2: Drain current as a function of the number of iterations for two different submicron MOSFETs.

3.2 Self-Consistent Iteration Technique

Monte Carlo–Poisson coupling can be done by including the continuity equation and the extended current relation in the iteration loop,

$$\mathrm{div}(\epsilon\ \mathrm{grad}\,\psi) = e\ (n - p - N_C)\ , \tag{13}$$

$$\operatorname{div} \mathbf{j} = 0 \,, \tag{14}$$

$$\mathbf{j} = e\,\mu_{MC}\; n\Big(-\operatorname{grad}\psi + \frac{1}{n}\;\operatorname{grad}(n\;U_{T,MC})\Big)\;. \tag{15}$$

Each Monte Carlo step performs an update of the Monte Carlo–Drift-Diffusion coupling coefficients μ_{MC} and $U_{T,MC}$.

In MINIMOS [3] a two-dimensional version of the Monte Carlo–Poisson coupling algorithm has been implemented. The Figures 2 (a)(b) and 3 (a)(b) show the evolution of the drain current with the number of iterations for different submicron MOSFETs. Figure 3 (c) and (d) additionally show the relative norms of the increments of carrier concentration and electrostatic potential as a function of the number of iterations. The norms first decrease rapidly but then are limited due the statistical noise inherent in the MC-method. In no one of the examples we have shown an iteration count larger than 5 was required to obtain the final drain current. The norms also do not exhibit any systematic change after 5 iterations. The number of costly Monte Carlo-Poisson iterations is therefore reduced drastically compared to other self-consistent coupling schemes reported in the literature [2] [4] [12].

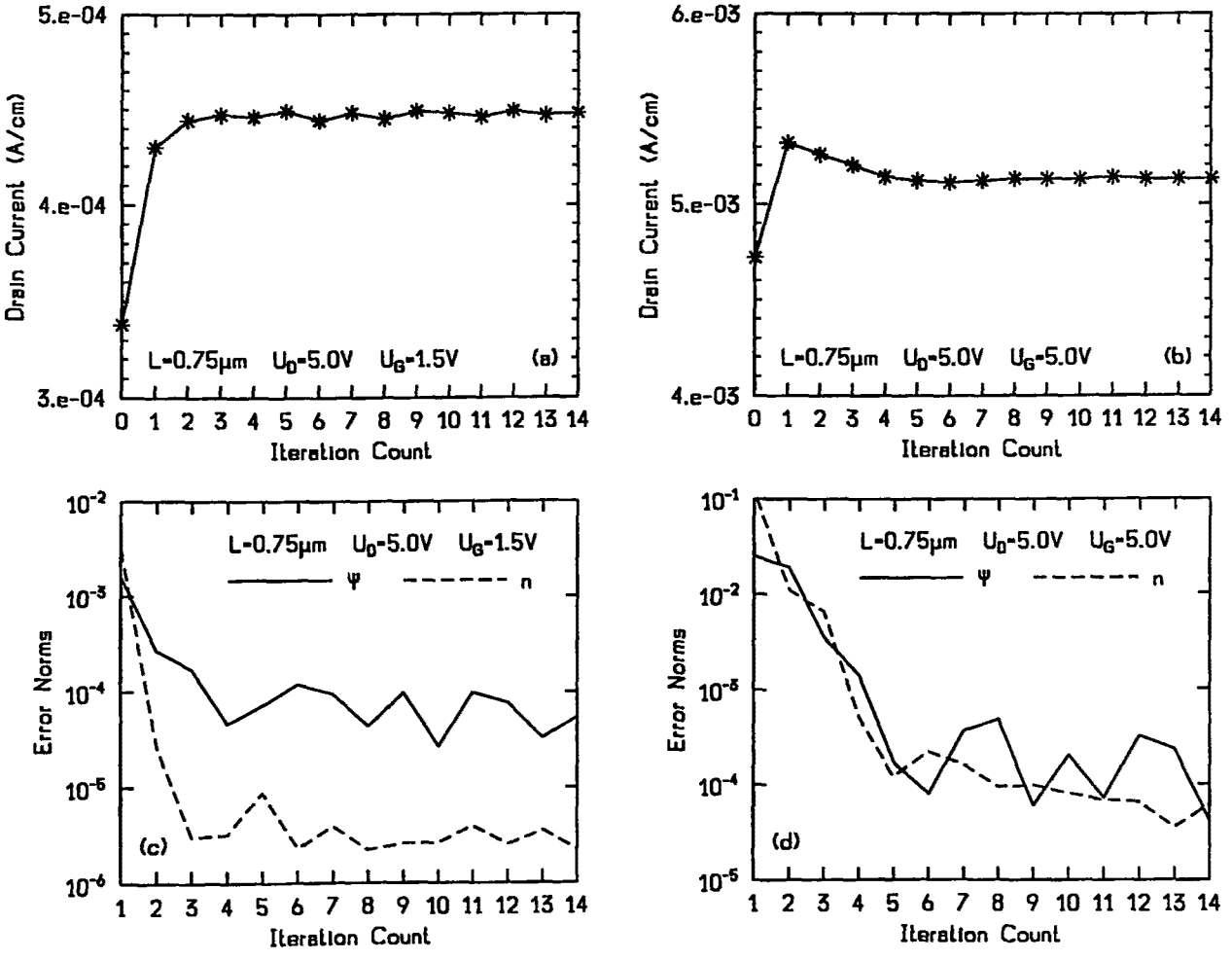

Figure 3: Drain current and relative norm of the n- and ψ-increments as a function of the number of iterations for a $0.75\mu m$-transistor at two different gate biases.

5 CONCLUSION

A self-scattering algorithm using a piecewise linear total scattering rate has been proposed. The efficiency of the reduction of self-scattering events has been demonstrated. A Monte Carlo—Poisson coupling method, which is based on Monte Carlo–Drift-Diffusion coupling, has been implemented in a two-dimensional device simulator for the first time. The expectation of a high convergence rate has been validated. Application to submicron MOSFETs has demonstrated the applicability of the new algorithm as well as the necessity of self-consistent simulation for such small devices.

References

[1] BANDYOPADHYAY, S., KLAUSMEIER-BROWN, M.E., MAZIAR, C.M., DATTA, S., AND LUNDSTROM, M. A Rigorous Technique to Couple Monte Carlo and Drift-Diffusion Models for Computationally Efficient Device Simulation. *IEEE Transactions on Electron Devices ED-34*, 2 (Feb. 1987), 392–399.

[2] FISCHETTI, M.V., AND LAUX, S.E. Monte Carlo Analysis of Electron Transport in Small Semiconductor Devices Including Band-Structure and Space-Charge Effects. *Physical Review B 38*, 14 (Nov. 1988), 9721–9745.

[3] HÄNSCH, W., AND SELBERHERR, S. MINIMOS 3: A MOSFET Simulator that Includes Energy Balance. *IEEE Transactions on Electron Devices ED-34*, 5 (Mai 1987), 1074–1078.

[4] HOCKNEY, R.W., AND EASTWOOD, J. W. *Computer Simulation Using Particles.* Adam Hilger, Bristol and Philadelphia, 1988.

[5] JACOBONI, C., AND REGGIANI, L. The Monte Carlo Method for the Solution of Charge Transport in Semiconductors with Applications to Covalent Materials. *Review of Modern Physics 55*, 3 (Juli 1983), 645–705.

[6] KATO, K. Hot-Carrier Simulation for MOSFET's Using a High-Speed Monte Carlo Method. *IEEE Transactions on Electron Devices 35*, 8 (Aug. 1988), 1344–1350.

[7] KOSINA, H., AND SELBERHERR, S. Coupling of Monte Carlo and Drift Diffusion Method with Applications to Metal Oxide Semiconductor Field Effect Transistors. *Japanese Journal of Applied Physics 29*, 12 (Dez. 1990), L2283–L2385.

[8] KOSINA, H., LINDORFER, PH., AND SELBERHERR, S. Monte-Carlo – Poisson Coupling Using Transport Coefficients. In Proc: *21st European Solid State Device Research Conference* (Montreux, Sep. 1991), M. Illegems and M. Dutoit, Eds., Elsevier, pp. 53–56.

[9] MOGLESTUE, C. A Self-Consistent Monte Carlo Particle Model to Analyze Semiconductor Microcomponents of Any Geometry. *IEEE Transactions on Computer-Aided Design CAD-5*, 2 (Apr. 1986), 326–354.

[10] REES, H.D. Calculation of Distribution Functions by Exploiting the Stability of the Steady State. *J. Phys. Chem. Solids 30* (1969), 643–655.

[11] SANGIORGI, E., RICCO, B., AND VENTURI, F. *MOS*^{2}: An Efficient Monte Carlo Simulator for MOS Devices. *IEEE Transactions on Computer-Aided Design 7*, 2 (Feb. 1988), 259–271.

[12] VENTURI, F., SMITH, R.K., SANGIORGI, E.C., PINTO, M.R., AND RICCO, B. A General Purpose Device Simulator Coupling Poisson and Monte Carlo Transport with Applications to Deep Submicron MOSFET's. *IEEE Transactions on Computer-Aided Design 8*, 4 (Apr. 1989), 360–369.