Evaluation of Solenoidal and Statistically Enhanced Total Current Densities in Multi-Particle Monte Carlo Device Simulators

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***Abstract*—For noise analysis and transient Monte Carlo simulations the evaluation not only of the conduction current but also of the displacement current is necessary. The simulated total terminal currents should be solenoidal, but this basic property is often lost in the discretization process. Here a consistent discretization of the conduction current densities and Poisson's equation is presented which yields solenoidal currents. The new method does not require more CPU time than previous methods, but yields terminal currents with a considerably better signal to noise ratio than former methods. Results are shown for stationary and transient simulations and discussed.**

I. Introduction

A new method for the evaluation of conduction current densities $\vec{j}_c$ (electrons and holes) and displacement current densities

$$\vec{j}_d = \epsilon \frac{\partial}{\partial t} \vec{E} \tag{1}$$

in ensemble Monte Carlo (EMC) device simulators is presented which yields a (discrete) field of total current densities

$$\vec{j}_t = \vec{j}_d + \vec{j}_c \ , \tag{2}$$

that is statistically enhanced and fulfills the discrete analogue of $\nabla \cdot \vec{j}_t = 0$ exactly. Due to this property simulated terminal currents of multi-terminal devices not only fulfill Kirchhoff's current law exactly, but they can be calculated in a straight forward manner by just integrating $\vec{j}_t$ along the boundary of the device terminals. As a consequence this new method allows the direct computation of transient terminal currents of advanced devices by EMC device simulation with a quality of time resolution and noise level that at least to our best knowledge has never been demonstrated before.

In principle the field of total current densities $\vec{j}_t$ is solenoidal in all electronic devices [1]. However this property is easily lost in numerical device models, where $\vec{j}_c$, $\vec{j}_d$ are only available in discrete form. As a consequence

$$\nabla \cdot \vec{j}_t = 0 \tag{3}$$

and Kirchhoff's current law are often valid only when the grid intervals in space and time are infinitesimal and/or the number of particles goes to infinity. This problem occurs for example, when the standard method of evaluating conduction currents in EMC device simulators, which consists of just counting particles crossing a given surface element per time interval, is used in conjunction with the standard cloud in cell method [2] and box integration [3] for the discretization of Poisson's equation. Therefore special care during the development of our new discretization for $\vec{j}_c$ was given to this problem in order to ensure that $\vec{j}_c$, $\vec{j}_d$ in discrete form sum up to a field $\vec{j}_t$, which is solenoidal in the discrete sense. The numerical effort for our new discretization of $\vec{j}_c$ is comparable to the standard method. Moreover, since (3) is exactly valid, it can be shown that the terminal currents calculated by our new method cannot be further improved concerning their statistical properties by the method published in [4]. This means that a simple integration of $\vec{j}_t$ along the terminal boundaries is sufficient and the substantial effort of evaluating optimal test functions [4] can be avoided.

II. Discretization Method

To preserve property (3) during the discretization process it is necessary to evaluate the discretized conduction current densities in a way which is consistent with the discretization of the electric field *and* the mapping of the particle charge onto the grid points. In the eddy current free approximation the quasi-stationary electric field can be determined with Poisson's equation [5]. Here Poisson's equation is discretized using the box integration method [3] and finite differences for the electric field along the grid lines of a nonuniform tensor product grid (Fig. 1):

$$\begin{aligned} E_{x,i,j} &= \frac{\Psi_{i,j} - \Psi_{i+1,j}}{x_{i+1} - x_i} \\ E_{y,i,j} &= \frac{\Psi_{i,j} - \Psi_{i,j+1}}{y_{j+1} - y_j} \ , \end{aligned} \tag{4}$$

where $\Psi_{i,j}$ is the discrete electric potential at the grid point (x_i, y_j). The derivative in time of the electric field for the displacement current (1) is calculated with finite differences:

$$\frac{\partial}{\partial t} E_{x/y,i,j} \approx \frac{E_{x/y,i,j}(t+T) - E_{x/y,i,j}(t)}{T} \ . \tag{5}$$

T is the time step length of the MC simulation in the self-consistent iteration loop of the MC method and Poisson's equation [2].

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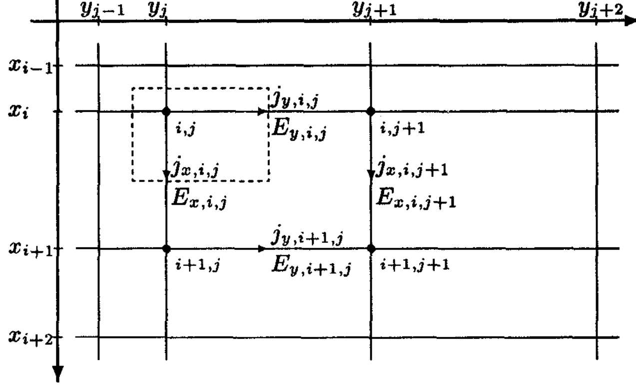

Fig. 1. The nonuniform tensor product grid. The box of the grid point i, j is shown with a dashed line.

Equation (3) is also discretized with the box integration method on the same grid as Poisson's equation. Thus the conduction current densities $j_{c,x,i,j}$, $j_{c,y,i,j}$ along the grid lines are required. The particle charge at the grid points is evaluated with bilinear mapping (cloud in cell method) [2], [6], [7]. The nodal charges $Q_{i,j}$ of a particle at (x, y) with $x_i < x \leq x_{i+1}$ and $y_j < y \leq y_{j+1}$ are:

$$\begin{aligned} Q_{i,j} &= \frac{q}{A}(x_{i+1} - x)(y_{j+1} - y) \\ Q_{i+1,j} &= \frac{q}{A}(x - x_i)(y_{j+1} - y) \\ Q_{i,j+1} &= \frac{q}{A}(x_{i+1} - x)(y - y_j) \\ Q_{i+1,j+1} &= \frac{q}{A}(x - x_i)(y - y_j) \ , \end{aligned} \tag{6}$$

where q is the particle charge and $A = (x_{i+1} - x_i)(y_{j+1} - y_j)$ is the cell size. Assuming that the mapped particle charge flows from one node to another along the grid lines the current densities $j_{c,x,i,j}$, $j_{c,y,i,j}$ can be calculated:

$$\begin{aligned} j_{c,x,i,j} &= \frac{q}{TA}(x(t+T) - x(T)) \\ &\quad (y_{j+1} - \frac{1}{2}(y(t+T) + y(t))) \\ j_{c,y,i,j} &= \frac{q}{TA}(x_{i+1} - \frac{1}{2}(x(t+T) + x(t))) \\ &\quad (y(t+T) - y(t)) \\ j_{c,x,i,j+1} &= \frac{q}{TA}(x(t+T) - x(T)) \\ &\quad (\frac{1}{2}(y(t+T) + y(t)) - y_j) \\ j_{c,y,i+1,j} &= \frac{q}{TA}(\frac{1}{2}(x(t+T) + x(t)) - x_i) \\ &\quad (y(t+T) - y(t)) \ . \end{aligned} \tag{7}$$

$x(t), y(t)$ is the position of the particle at the beginning of the time step and $x(t+T), y(t+T)$ at the end. If the particle moves from one cell to another during the time step, the current densities (7) have to be evaluated for each cell and the respective position at the beginning and at the end has to be replaced by the boundary crossing point. For the deduction of (7) it has been assumed that the particle moves from its position at the beginning of the time step to the position at the end of the time step with

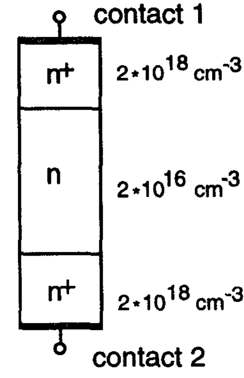

Fig. 2. n^+nn^+-structure ($100nm \times 400nm$).

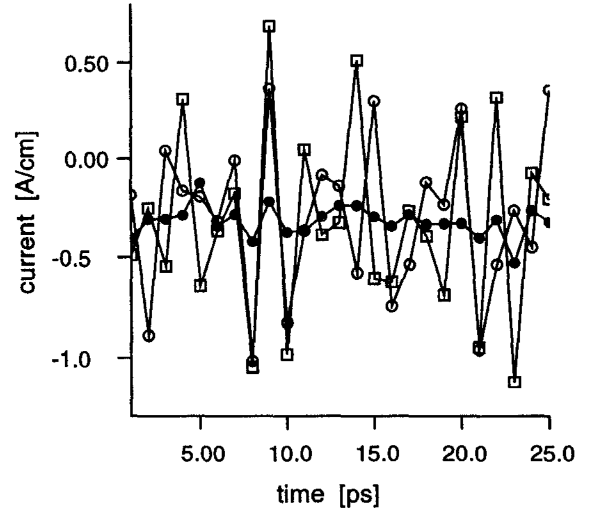

Fig. 3. Terminal currents of the n^+nn^+-structure for a bias of $0.2V$.

a constant velocity vector. This has been done to simplify the evaluation of (7). This simplification of the particle path is possible, because only the particle position at the beginning and at the end of the time step enter Poisson's equation and not the particle path itself. It would have also been possible to solve the path integrals along the real particle path, but that is not only CPU intensive but also unnecessary. The current densities evaluated for a cell by path integration differ from (7) only by a mesh current. The resulting total current densities are in both cases solenoidal.

III. Results

The advantages of our new method are demonstrated for two examples. The first one is a simulation of an n^+nn^+-structure (see Fig. 2) in stationary state with an applied bias of $0.2\,V$.

In Fig. 3 the terminal currents evaluated by our new method and the standard method as a function of time

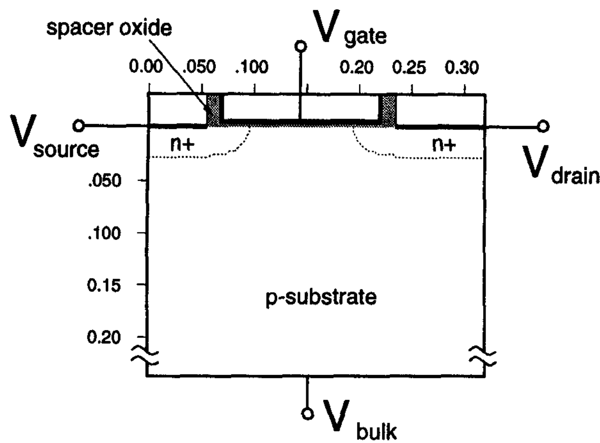

Fig. 4. Silicon n-MOSFET test structure. The coordinates are given in μm.

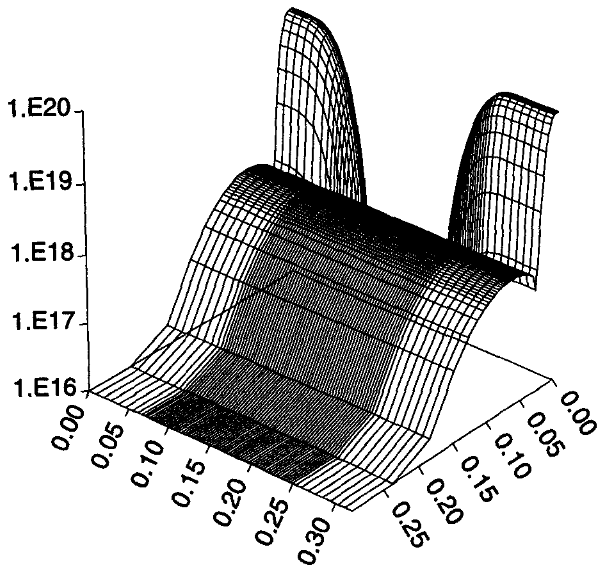

Fig. 5. Spatial doping distribution of the n-MOSFET.

are compared. In both cases the terminal currents were calculated directly at the device terminals and the data shown in Fig. 3 were evaluated by averaging the raw data resulting at every time step over $1ps$.

The simulation was carried out employing a weighted particle ensemble with about 6 particles per mesh cell resulting in a total number of 2200 particles. Please note that for the new method the current evaluated at contact 1 is identical to the one at contact 2. Moreover it should be pointed out that the fluctuations of the terminal current around the mean value are much smaller for the new method. In terms of standard deviation the new method is five times better than the standard one for this example. This demonstrates clearly the large statistical enhancement that is achieved by our new method.

In order to push the capabilities of our new method to the limit we have simulated the transient behavior of the terminal currents for the ultrashort Silicon n-MOSFET shown in Fig. 4 [8]. The oxide thickness of this device is $4nm$ and the doping density at the source and drain terminals reaches a value of about $7{\cdot}10^{19}cm^{-3}$ (see Fig. 5).

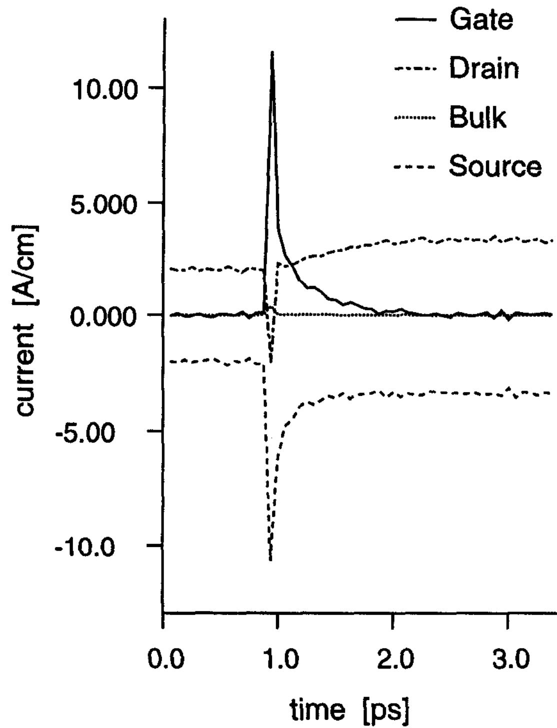

Fig. 6. Transient terminal currents of the n-MOSFET for an abrupt gate voltage step of $0.25V$ at $t = 0.875ps$.

Starting from a stationary state in strong inversion with $V_{GS} = 1.0V, V_{DS} = 1.5V, V_{BS} = 0V$ the gate voltage is increased at $t = 0.875ps$ to $V_{GS} = 1.25V$ in an abrupt manner. Fig. 6 shows the resulting transients of the source, drain, gate, and bulk currents that have been evaluated by our new method by direct integration along the terminal boundaries. The shown current values have been generated by averaging the raw data over $62.5fs$. Please note that the new method allows to resolve the fast transient switching behavior of this device with time constants in the sub picosecond range with a noise level that is sufficiently low for most applications. In fact the noise level is so low that the MC results can now be used for a direct comparison with terminal transients from classical drift-diffusion or hydrodynamic device simulators in order to study the limitations of these classical simulation methods. In comparison to previous papers which show the transient behavior of terminal currents evaluated by the MC method (e.g. [9], [10]) the terminals currents in Fig. 6 have been evaluated directly without employing any noise reducing steps involving fit functions, so that they fulfill Kirchhoff's current law exactly. Moreover in comparison to [9], [10] the doping at the device terminals is much higher for our n-MOS test device, which makes it very difficult to evaluate terminal currents with standard methods. Therefore at least for ultrashort n-MOSFETs with realistic doping densities at the source and drain terminals the results shown in Fig. 6 are probably the best results for terminal transients computed so far by EMC in a direct manner without noise reduction besides simple

time averaging.

IV. Conclusions

Consistent discretization of the conduction current densities and Poisson's equation has led to a formulation of the total current densities which is solenoidal in the discrete sense. The new method is efficient, because it does not consume more CPU time than standard methods and because terminal currents can be evaluated by simply integrating the total current density along the terminal boundaries. Moreover the estimator for the terminal currents is optimal and unbiased. Therefore the new method is not only well suited for terminal current evaluation in stationary or transient MC simulations, but also well suited for noise analysis.

Acknowledgment

This work was supported in part by the Bundesministerium für Bildung, Wissenschaft, Forschung und Technologie under contract no. 01 M 2416 A. The authors thank Dr. C. Jungemann (University of Bremen) for support during the preparation of the manuscript.

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