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DSMC versus WENO-BTE: A double gate MOSFET example

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Abstract Time-dependent solutions to the Boltzmann-Poisson system in two spatial dimensions and three-dimensional velocity space are obtained by using a recently developed high order WENO scheme. The collision operator of the Boltzmann equation models the scattering processes between electrons and phonons which are assumed to be in thermal equilibrium. In this paper, the deterministic numerical solutions for a double gate silicon MOSFET are compared with Monte Carlo simulations. The main aim of this investigation is to show how direct solutions of the Boltzmann transport equation coupled with the Poisson equation can, through comparisons, suggest improvements of the DSMC algorithms such as, in particular, the charge assignment to the mesh, the treatment of the boundary conditions and the free flight duration.

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1 Introduction

In modern highly integrated devices, a consistent description of the dynamics of carriers is essential for a deeper understanding of the observed transport properties. The semiclassical Boltzmann equation

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon \cdot \nabla_{\mathbf{x}} f - \frac{q}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f = Q(f) \tag{1}$$

coupled with the Poisson equation

$$\nabla_{\mathbf{x}}\left[\epsilon_r(\mathbf{x})\mathbf{E}\right] = -\frac{q}{\epsilon_0}\left[\rho(t,\mathbf{x}) - N_D(\mathbf{x})\right] \tag{2}$$

provides a general theoretical framework for modeling electron transport, whose solutions contain all the information on the evolution of the carrier distribution. In Eq. (1), f represents the electron probability density function with wave number $\mathbf{k}$ at location $\mathbf{x}$ and time t. $\mathbf{E}$ is the electric field, $Q(f)$ denotes the collision operator, which describes electron-phonon interactions, ε is the energy-band function and $\hbar$ and q are the Planck constant divided by 2π and the positive electric charge, respectively. In Eq. (2), ϵ_0 is the dielectric

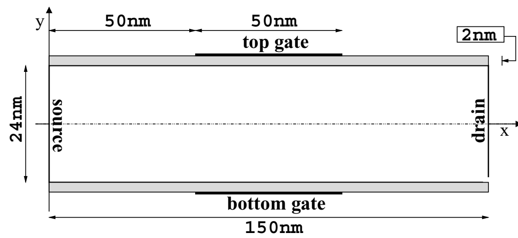


Fig. 1 A double gate MOSFET structure

constant in vacuum, $\epsilon_r(\mathbf{x})$ labels the relative dielectric function, $\rho(t, \mathbf{x})$ is the electron density and $N_D(\mathbf{x})$ is the doping. Deterministic solvers to the Boltzmann-Poisson system (1)–(2) for two-dimensional devices have been proposed in [1–4]. These methods provide accurate results which, in general, agree well with those obtained from Monte Carlo simulations.

2 The double gate MOSFET

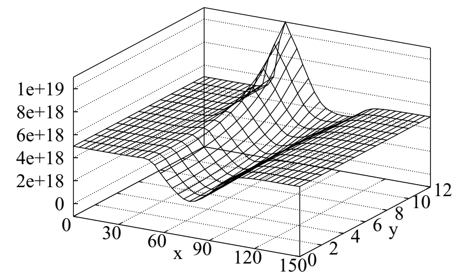
In this paper, we simulate and compare the results of WENO schemes, applied to Eqs. (1)–(2), and DSMC approximations of a two dimensional silicon device. The complete description of the deterministic finite difference numerical scheme can be found in [5]. We show simulations for a DG-MOSFET, widely used by electronic engineers, where its structure is described in Fig. 1: two bands of oxide of thickness 2 nm sandwich a band of Si of 24 nm where electrons transit. Two gates (top and bottom) with 50 nm of length are considered at 50 nm of the source.

Let V_s, V_d and V_g be the applied voltages at the source, drain and gate, respectively. Let d_M be the maximum value of the doping concentration, we consider three different cases, denoted by A, B and C, respectively (see Table 1).

Following [6], a "V"-shaped doping profile function $N_D(x, y)$ was taken into account. Here, $N_D(x, y) = d_M$ for $0 \le x \le 50$ or $100 \le x \le 150$, and $N_D(x, y) = (d_M - d_m)\frac{|x-75|}{25} + d_m - N_a$ for $50 < x < 100$, where $d_m = 10^{15}\,\text{cm}^{-3}$ and the acceptors concentration $N_a = 10^{10}\,\text{cm}^{-3}$. Figure 2 shows the stationary charge density and electrical potential from the deterministic scheme. Symmetry considerations allow us to compute only the $y \ge 0$ domain.

Table 1 Doping and voltage parameters

Case	d_M	$V_d - V_s$	$V_g - V_s$
A	$5 \times 10^{18}\,\text{cm}^{-3}$	$1.0\,V$	$0.53646\,V$
B	$5 \times 10^{19}\,\text{cm}^{-3}$	$1.0\,V$	$0.53646\,V$
C	$5 \times 10^{18}\,\text{cm}^{-3}$	$0.5\,V$	$0.25\,V$



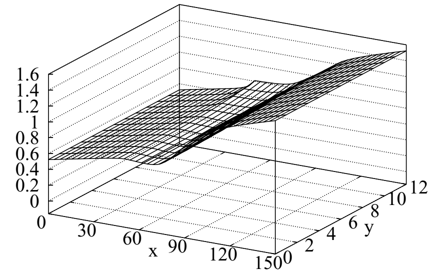


Fig. 2 Charge density and electric potential; case A. Units: x (nm), y (nm), density (cm^{-3}), potential (Volt)

3 Deterministic and stochastic results

In order to make meaningful comparisons, we adopt the same scattering rates: acoustic and non-polar optical phonons with a single frequency [5]. Moreover, the boundary conditions are chosen in agreement trivially in all boundaries except for source and drain that we discuss. We now describe the boundary conditions for the Boltzmann equation and the DSMC in the source zone (corresponding to $x = 0$). The drain boundary is treated analogously. For the BTE, we impose that

$$f(t, -\Delta x, y, \mathbf{k}) = \frac{N_D(0, y)}{\rho(t, 0, y)} f(t, 0, y, \mathbf{k}), \qquad (3)$$

where Δx is the mesh size of the x variable. With this boundary condition, the distribution function f at each point outside the device is proportional to f evaluated in the nearest point inside the device. The proportionality factor in Eq. (3) guarantees the charge neutrality in highly doped regions. The use of ghost points for $x < 0$ is necessary to describe the particle flux correctly. In the DSMC case, we add some cells outside the device, where particles can be created or destroyed, so that charge neutrality holds. Since the method of cloud in cell is used to get the charge density, a suitable number of electrons in the cells outside allows us to have the correct charge density at the source. We do not create particles inside. When we must create some electrons, say n, in an exterior cell, we choose n random electrons in real cells very near the exterior cell and use the values of their wavevector for creating electrons. They are placed in the exterior cell randomly. This approach is very similar to Eq. (3). Figure 3 shows the averaged x-momentum over y direction for

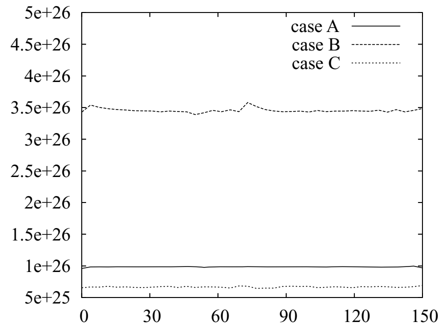


Fig. 3 Averaged x-momentum over vertical direction for DSMC results

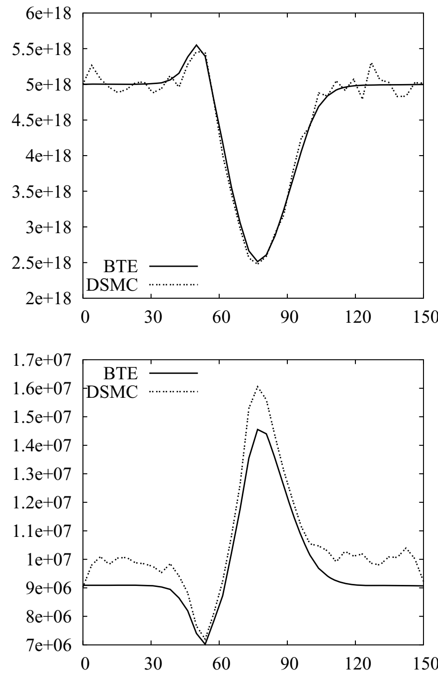
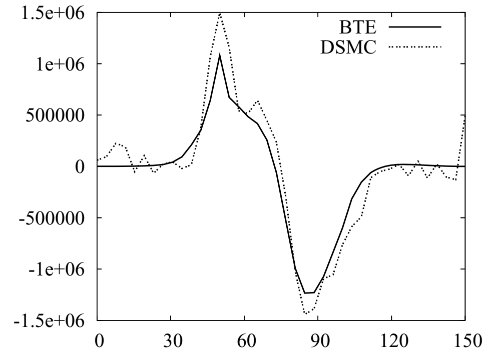


Fig. 4 Charge density and x-velocity at $y = 6$; case A

DSMC results. We use the following units: x (nm), density (cm^{-3}), velocity (cm/s), energy (eV).

In the next figures, we show comparisons between deterministic BTE and DSMC results in the three cases. To make the differences clear, we consider hydrodynamical quantities in the stationary regime, for a fixed value (6 nm) of the variable y. The main differences concern the x-component of the velocity and the electron energy. In case A the low doping value at the contacts allows very high velocity close to the saturation velocity (Fig. 4), hence many electrons leave or enter the device. In the other cases this effect decreases and the agreement is better than that for case A. In our opinion, the deterministic solutions might improve the algorithm of DSMC, such as, in particular, the charge assignment to the mesh, the treatment of the boundary conditions and the free flight duration. A compelling numerical evidence and



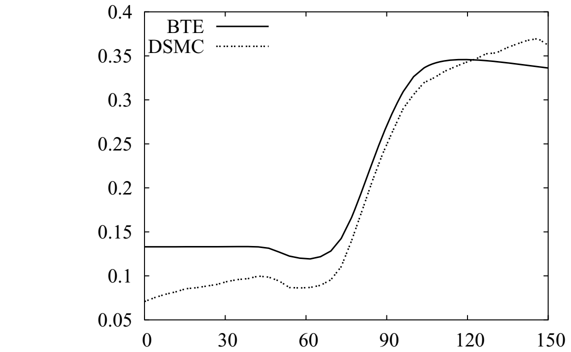
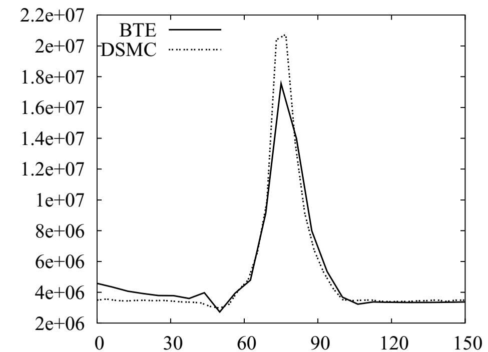


Fig. 5 y-velocity and electron energy at $y = 6$; case A



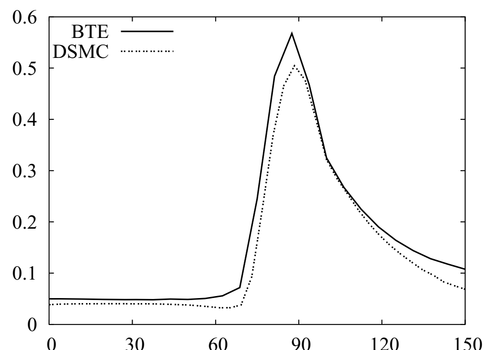


Fig. 6 x-velocity and electron energy at $y = 6$; case B

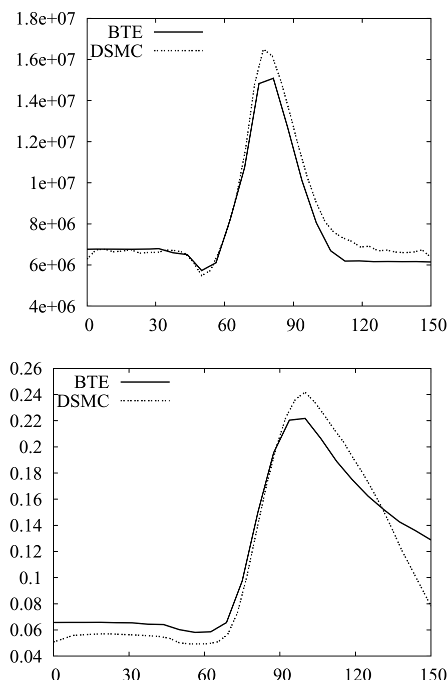


Fig. 7 x-velocity and electron energy at $y = 6$; case C

argument of this boundary correction in these three cases is the disappearance of boundary layers for the BTE simulation, which is in accordance to the realization of homogeneous states in the highly doped neutrally charged region and their corresponding Ohmic contacts.

4 Conclusions

WENO methods lead to high-order accurate solutions of the BTE for different materials and geometries. They actually represent benchmarks for hydrodynamic or drift-diffusion solvers that can be tested against them fairly. These deterministic methods, at their birth stage and far from optimal computational tools, provide an alternative to DSMC solvers for mesoscopic scale models and aid the visualization of the evolution of computed probabilities as well as provide a criteria to resolve boundary data issues for their corresponding DSMC counterparts.

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