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Galerkin methods for Boltzmann–Poisson transport with reflection conditions on rough boundaries

José A. Morales Escalante [a,*], Irene M. Gamba [b]

[a] TU Wien – Institute for Analysis and Scientific Computing, Austria
[b] The University of Texas at Austin – Institute for Computational Engineering and Sciences & Department of Mathematics, United States

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ABSTRACT

We consider in this paper the mathematical and numerical modeling of reflective boundary conditions (BC) associated to Boltzmann–Poisson systems, including diffusive reflection in addition to specularity, in the context of electron transport in semiconductor device modeling at nano scales, and their implementation in Discontinuous Galerkin (DG) schemes. We study these BC on the physical boundaries of the device and develop a numerical approximation to model an insulating boundary condition, or equivalently, a pointwise zero flux mathematical condition for the electron transport equation. Such condition balances the incident and reflective momentum flux at the microscopic level, pointwise at the boundary, in the case of a more general mixed reflection with momentum dependant specularity probability $p(\vec{k})$. We compare the computational prediction of physical observables given by the numerical implementation of these different reflection conditions in our DG scheme for BP models, and observe that the diffusive condition influences the kinetic moments over the whole domain in position space.

1. Introduction

The dynamics of electronic transport in modern semiconductor devices can be described by the semiclassical Boltzmann–Poisson (BP) model

$$\frac{\partial f_i}{\partial t} + \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon_i \cdot \nabla_{\vec{x}} f_i - \frac{q_i}{\hbar}\vec{E}\cdot\nabla_{\vec{k}} f_i = \sum_j Q_{i,j}, \tag{1.1}$$

$$\nabla_{\vec{x}}\cdot(\epsilon\,\nabla_{\vec{x}} V) = \sum_i q_i\rho_i - N(\vec{x}), \quad \vec{E} = -\nabla_{\vec{x}} V, \tag{1.2}$$

where $f_i(\vec{x},\vec{k},t)$ is the probability density function (pdf) over phase space $(\vec{x},\vec{k})$ of a carrier in the i-th energy band in position $\vec{x}$, with crystal momentum $\hbar\vec{k}$ at time t. The collision operators $Q_{i,j}(f_i, f_j)$ model i-th and j-th carrier recombinations, collisions with phonons or generation effects. $\vec{E}(\vec{x},t)$ is the electric field, $V(\vec{x},t)$ is the electric potential, $\varepsilon_i(\vec{k})$ is the i-th energy band surface, the i-th charge density $\rho_i(t,\vec{x})$ is the k-average of f_i, $-q_i$ is the electric charge of the i-th carrier, $N(\vec{x})$ is the doping profile, and ϵ is the electric permittivity of the material.

* Corresponding author.
E-mail addresses: jose.morales.escalante@tuwien.ac.at (J.A. Morales Escalante), gamba@math.utexas.edu (I.M. Gamba).

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The BP model for electron transport on a single conduction energy band for electrons has the form

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k})\cdot\nabla_{\vec{x}} f - \frac{q}{\hbar}\vec{E}(\vec{x},t)\cdot\nabla_{\vec{k}} f = Q(f), \tag{1.3}$$

$$\nabla_{\vec{x}}\cdot(\epsilon\,\nabla_{\vec{x}} V) = q\left[\rho(\vec{x},t) - N(\vec{x})\right], \quad \vec{E} = -\nabla_{\vec{x}} V, \tag{1.4}$$

with the quantum mechanical electron group velocity $\frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k})$, and the electron density $\rho(\vec{x},t) = \int_{\Omega_{\vec{k}}} f(\vec{x},\vec{k},t)\,d\vec{k}$. The collision integral operator $Q(f)$ describes the scattering over the electrons, where several mechanisms of quantum nature can be taken into account. In the low density regime, the collisional integral operator can be approximated as linear in f, having the form

$$Q(f) = \int_{\Omega_{\vec{k}}} \left[S(\vec{k}',\vec{k})\,f(t,\vec{x},\vec{k}') - S(\vec{k},\vec{k}')\,f(t,\vec{x},\vec{k})\right] d\vec{k}', \tag{1.5}$$

where $S(\vec{k},\vec{k}')$ is the scattering kernel, representing non-local interactions of electrons with a background density distribution. For example, in the case of silicon, one of the most important collision mechanisms are electron–phonon scatterings due to lattice vibrations of the crystal, which are modeled by acoustic (assumed elastic) and optical (non-elastic) non-polar modes, the latter with a single frequency ω_p, given by

$$\begin{aligned} S(\vec{k},\vec{k}') = {} & (n_q+1)\,K\,\delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) + \hbar\omega_p) \\ & + n_q\,K\,\delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) - \hbar\omega_p) + K_0\,\delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}))\,, \end{aligned} \tag{1.6}$$

with K, K_0 constants for silicon. The symbol δ indicates the usual Dirac delta distribution corresponding to the well known Fermi's Golden Rule [13]. The constant n_q is related to the phonon occupation factor

$$n_q = \left[\exp\left(\frac{\hbar\omega_p}{K_B T_L}\right) - 1\right]^{-1},$$

where K_B is the Boltzmann constant and $T_L = 300$ K is the lattice temperature.

The semi-classical Boltzmann description of electron transport in semiconductors is, for a truly 3-D device, an equation in six dimensions plus time when the device is not in steady state. The heavy computational cost is the main reason why the BP system had been traditionally solved numerically by means of Direct Simulation Monte Carlo (DSMC) methods [14]. However, after the pioneer work [15], in recent years, deterministic solvers to the BP system were proposed in [16–22]. These methods provide accurate results which, in general, agree well with those obtained from Monte Carlo (DSMC) simulations, often at a fractional computational time. Moreover, these type of solvers can resolve transient details for the electron probability density function f, which are difficult to compute with DSMC simulators.

The initial methods proposed in [18–21] using weighted essentially non-oscillatory (WENO) finite difference schemes to solve the Boltzmann–Poisson system, had the advantage that the scheme is relatively simple to code and very stable even on coarse meshes for solutions containing sharp gradient regions. However, a disadvantage of the WENO methods is that it requires smooth meshes to achieve high order accuracy, hence it is not very flexible for adaptive meshes.

Motivated by the easy *hp*-adaptivity and the simple communication pattern of the discontinuous Galerkin (DG) methods for macroscopic (fluid level) models [23–26], it was proposed in [27,28] to implement a DG solver to the full Boltzmann equation, that is capable of capturing transients of the probability density function.

In the previous work [27,28], the first DG solver for (1.1)–(1.2) was proposed, and some numerical calculations were shown for one and two-dimensional devices. In [29], the DG-LDG scheme for the Boltzmann–Poisson system was carefully formulated, and extensive numerical studies were performed to validate the calculations. Such scheme models electron transport along the conduction band for 1D diodes and 2D double gate MOSFET devices with an analytic Kane energy band model.

A DG method for full conduction bands BP models was proposed in [30], following the lines of the schemes in [27–29], generalizing the solver that uses the Kane non-parabolic band and adapting it to treat the full energy band case. A preliminary benchmark of numerical results shows that the direct evaluation of the Dirac delta function can be avoided, and so an accurate high-order simulation with comparable computational cost to the analytic band cases is possible. It would be more difficult or even unpractical to produce the full band computation with other transport scheme. It is worth to notice that a high-order positivity-preserving DG scheme for linear Vlasov–Boltzmann transport equations, under the action of quadratically confined electrostatic potentials, independent of the electron distribution, has been developed in [31]. The authors there show that these DG schemes conserve mass and preserve the positivity of the solution without sacrificing accuracy. In addition, the standard semi-discrete schemes were studied showing stability and error estimates.

The type of DG method discussed in this paper, as was done in [29], belongs to a class of finite element methods originally devised to solve hyperbolic conservation laws containing only first order spatial derivatives, e.g. [32–36]. Using a piecewise polynomial space for both the test and trial functions in the spatial variables, and coupled with explicit and