A fast approach to Discontinuous Galerkin solvers to Boltzmann-Poisson transport systems for full electronic bands and phonon scattering

Irene M. Gamba*, Armando Majorana†, Jose A. Morales* and Chi-Wang Shu‡
* ICES, The University of Texas at Austin, Austin, TX 78712
†Dipartimento di Matematica e Informatica, Università di Catania, Catania, Italy
‡Division of Applied Mathematics, Brown University, Providence, RI 02912
e-mail: gamba@math.utexas.edu, majorana@dmi.unict.it, jmorales@ices.utexas.edu, shu@dam.brown.edu

INTRODUCTION

The semi-classical Boltzmann-Poisson system guarantees a good description of the dynamics of electrons in modern semiconductor devices. The equations of this model are given by

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

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

In Eq. (1), f represents the electron probability density function (*pdf*) in phase space $\mathbf{k}$ at the physical location $\mathbf{x}$ and time t. $\mathbf{E}$ is the electric field, $Q(f)$ denotes the collision operator, which describes electron-phonon interactions and ε is the energy-band function. Physical constants $\hbar$ and q are the Planck constant divided by 2π and the positive electric charge, respectively. In Eq. (2), ϵ_0 is the dielectric constant in a vacuum, $\epsilon_r(\mathbf{x})$ labels the relative dielectric function depending on the material, $\rho(t,\mathbf{x})$ is the electron density, and $N_D(\mathbf{x})$ is the doping. The kinetic equation (1) is an equation in six dimensions (plus time if the device is not in steady state) for a truly 3-D device. This high dimensionality has been a motivation for the BP system to be solved by the Direct Simulation Monte Carlo (DSMC) methods [1]. Yet we have proposed in [2] a deterministic approach based discontinuous Galerkin (DG) method for solving Eqs. (1)-(2) that can be competitive. We refer to this reference for a detailed description of DG and examples of applications of the DG scheme to 1D diode and 2D double gate MOSFET devices.

Our current work is mainly motivated by the development of a DG based deterministic solver for the extension of the BTE to a system of transport Boltzmann equations for full electronic multi-band transport with intra-band scattering mechanisms. However, in this short abstract, we restrict our presentation to the single band as the proposed method described next will be also valid in the multi-band system as well. It mainly consists in finding scattering effects of high complexity (such as numerically computed full electronic bands) by simply using the standard routines of a suitable Monte Carlo approach only once.

THE PROPOSED METHOD

We denote by $\Omega_{\mathbf{k}}$ the bounded domain of the $\mathbf{k}$-vector variable, and introduce a partition by means of a family of N open cells C_α such that, for every α and β,

$$C_\alpha \subseteq \Omega_{\mathbf{k}},\ C_\alpha \cap C_\beta = \emptyset\ (\alpha \neq \beta),\ \bigcup_{\alpha=1}^{N} \overline{C_\alpha} = \Omega_{\mathbf{k}}\,.$$

Any Galerkin method at the lowest order for the $\mathbf{k}$-vector variable, given by a piecewise constant approximation, assumes that in every cell C_α and for fixed $\mathbf{x}$ and time t, f can be approximated by an unknown $f_\alpha(t,\mathbf{x})$ representing the approximated probability density function of finding an electron at physical position $\mathbf{x}$ and time t, with its wave-vector $\mathbf{k}$ belonging to the cell C_α.

The main difficulty in applying DG method to Eq. (1) is to calculate the constant numerical parameters arising from the collision operator, which is

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

where the numerical parameters are

$$K_{\alpha\beta} = \int_{C_\alpha} d\mathbf{k} \int_{C_\beta} d\mathbf{k}'\, S(\mathbf{k}',\mathbf{k})\,.$$

We show that the resulting $K_{\alpha\beta}$ is proportional to the number of electrons, with $\mathbf{k}$-vector belonging to the cell C_β before one scattering process, have $\mathbf{k}$-vector belonging to the cell C_α after the scattering. Such balance anzat allows to find the value of the parameters $K_{\alpha\beta}$ by simply using the standard routines, to determine the scattering process, of a DSMC (Monte Carlo) solver **only once**. In particular we take these computed parameters as the elements of the coefficient matrix of the corresponding DG scheme for the Boltzmann transport equation. Thanks to this new approach, we can easily introduce scattering terms also having high complexity, such as anisotropic electronic bands, or full band calculations.

PRELIMINARY NUMERICAL RESULTS

For the one dimensional silicon $n^+ - n - n^+$ 400nm channel diode, where the doping $N_D = 5 \times 10^{17}$ cm^{-3} in the n$^+$ and $N_D = 2 \times 10^{15}$ cm^{-3} in the n region, we use 1440 cells in k-space and N_x intervals in space. The applied potential is $2\,V$. We consider Kane model for the energy band, and we show some quantities at time $t = 0.5ps$ (a transient state).

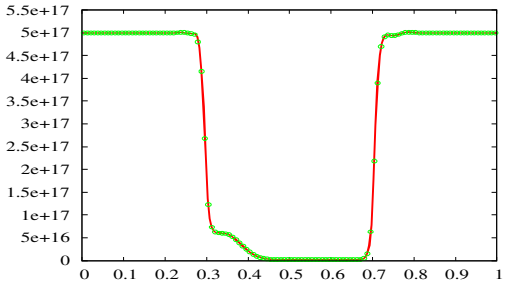

Fig. 1. Density of charge in cm^{-3} at $t = 0.5$ ps. Continuous line ($N_x = 200$), points ($N_x = 120$).

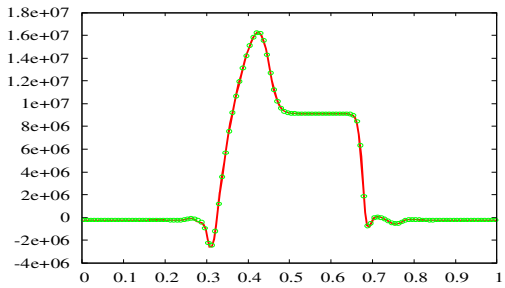

Fig. 2. Velocity in cm/s at $t = 0.5$ ps. Continuous line ($N_x = 200$), points ($N_x = 120$).

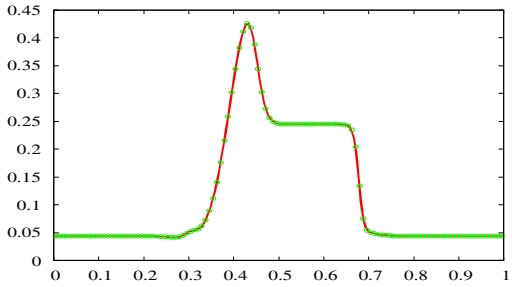

Fig. 3. Mean energy in eV at $t = 0.5$ ps. Continuous line ($N_x = 200$), points ($N_x = 120$).

nx	minimum	maximum
120	$1.0517e-14$	$7.133e-04$
150	$1.0517e-14$	$7.223e-04$
180	$1.0520e-14$	$7.350e-04$
200	$1.0519e-14$	$7.389e-04$

Minimum and maximum of *pdf* multiplied a fixed function of $\mathbf{k}$ at 0.5ps (a.u.)

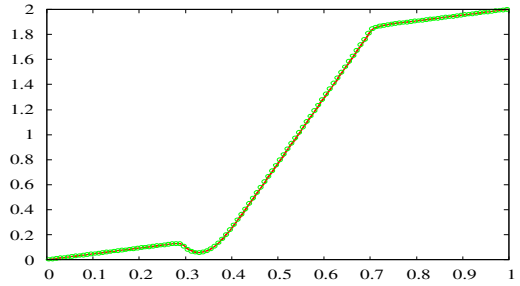

Fig. 4. Electric potential in V at $t = 0.5$ ps. Continuous line ($N_x = 200$), points ($N_x = 120$).

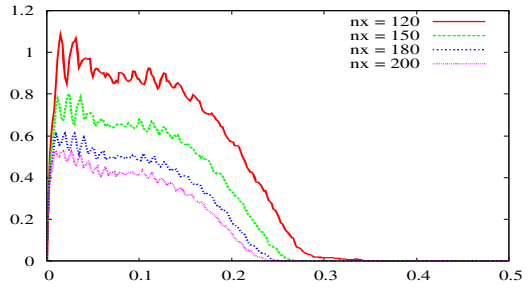

Fig. 5. The ratio, multiplies by 100, of the number of cells in phase space where *pdf* is negative to the total numbers of cells versus time (in ps) for different N_x

$particles$	maximum error	mean value error
10^6	0.06291	0.0044408
10^7	0.01403	0.0014447
10^8	0.00906	0.0004225
$5 \cdot 10^8$	0.00271	0.0002024
10^9	0.00145	0.0001313

Errors of the numerical coefficients $K_{\alpha\beta}$ using DSMC with respect to *exact* values.

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