Parallelization of Collision Integrals on DG solvers for Full Band Boltzmann-Poisson models of Electron Transport

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INTRODUCTION

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

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

$$\nabla_{\vec{x}}\cdot(\epsilon\,\nabla_{\vec{x}}V)=q\left[\rho(\vec{x},t)-N(\vec{x})\right],\ \vec{E}=-\nabla_{\vec{x}}V \quad (2)$$

$f(\vec{x},\vec{k},t)$ is the probability density function (pdf) over the phase space $(\vec{x},\vec{k})$ of a carrier in the conduction band being in position $\vec{x}$, with crystal momentum $\hbar\vec{k}$ at time t. The collision operator $Q(f)$ models different scattering mechanisms; for example, in the case of silicon devices, it can model electron - phonon collisions. $\vec{E}(\vec{x},t)$ is the electric field, $\varepsilon(\vec{k})$ is the conduction energy band surface, the electron density $\rho(\vec{x},t)=\int_{\Omega_{\vec{k}}} f\,d\vec{k}$ is given by the $\vec{k}$-average of f, where $\Omega_{\vec{k}}$ is the $\vec{k}$-space domain, and $N(\vec{x})$ is the doping profile.

$Q(f)$ is related to integral (non-local) operators in $\vec{k}$-space, given by the difference of a gain minus a loss operator:

$$\begin{aligned} Q(f) &= \int_{\Omega_{\vec{k}}} S(\vec{k}'\to\vec{k})f(\vec{x},\vec{k}',t)\,d\vec{k}' \\ &- f(\vec{x},\vec{k},t)\int_{\Omega_{\vec{k}}} S(\vec{k}\to\vec{k}')\,d\vec{k}' \end{aligned}$$

The form of the collision kernel $S(\vec{k}\to\vec{k}')$ depends on the particular device considered in the modeling. For example, for the case of a silicon device, the main collisional mechanisms are acoustic and optical electron - phonon scattering, so

$$S(\vec{k}\to\vec{k}')=\sum_{i=-1}^{1} c_i\delta(\varepsilon(\vec{k}')-\varepsilon(\vec{k})+i\hbar w_p), \quad (3)$$

with $\delta(\cdot)$ the Dirac Delta distribution due to the Fermi's golden rule, w_p the phonon frequency (assumed constant), $c_1=(n_q+1)c$, $c_{-1}=n_q c$, with c and c_0 constants related to optical and acoustic electron-phonon scattering in silicon respectively, and $n_q=(\exp(\hbar w_p/K_BT_L)-1)^{-1}$ the occupation number of phonons, with K_B the Boltzmann constant and T_L the lattice temperature.

The specific form of the collisional operator for silicon devices is, in this case:

$$\begin{aligned} Q(f) &= \sum_{i=-1}^{1} c_i\int_{\Omega_{\vec{k}}}\delta(\varepsilon(\vec{k})-\varepsilon(\vec{k}')+i\hbar w_p)f'\,d\vec{k}' \\ &- f\sum_{i=-1}^{1} c_i\int_{\Omega_{\vec{k}}}\delta(\varepsilon(\vec{k}')-\varepsilon(\vec{k})+i\hbar w_p)\,d\vec{k}' \end{aligned}$$

Deterministic solvers for the BP system using Discontinuous Galerkin (DG) FEM have been proposed in [1], [2] to model electron transport along the conduction band for 1D diodes and 2D double gate MOSFET devices. In [1], the energy band $\varepsilon(\vec{k})$ model used was the nonparabolic Kane band model. These solvers are shown to be competitive with Direct Simulation Monte Carlo methods [1]. The energy band models used in [2] were the Kane and Brunetti, $\varepsilon(|\vec{k}|)$ analytical models, but implemented numerically for benchmark tests.

PROPOSED METHOD

When using deterministic solvers to model the BP system, most of the computational cost of the numerical scheme is related to the collision integral. In the case of DG solvers for BP, the functions under study are projected in a space of piecewise continuous polynomials across the cells of the domain.

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In this work we will study the reduction of the computational cost associated to the collision integrals by means of parallelization of the computation of the collisional sums approximating these operators.

We work with a coordinate description of $\vec{k}(k_1, k_2, k_3)$ in which the energy is one of the coordinates, say, $k_1 = \varepsilon$. We could have, for example, $k_2 = k_x/|\vec{k}|$ the polar component and $k_3 = \varphi$ the azimuthal angle, but we could choose other coordinates k_2, k_3 too. We decompose the $\vec{k}$-domain in cells $K_{kmn} = [k_{1_k}^-, k_{1_k}^+] \times [k_{2_m}^-, k_{2_m}^+] \times [k_{3_n}^-, k_{3_n}^+]$. The collisional sums are then given by:

$$Q(f) = \sum_{i=-1}^{1} c_i \sum_{k,m,n} \left[\int_{K_{kmn}} \delta(\varepsilon - \varepsilon' + i\hbar w_p) f' \, d\vec{k}' - f \int_{K_{kmn}} \delta(\varepsilon' - \varepsilon + i\hbar w_p) \, d\vec{k}' \right]$$

Computing analytically the integrals just over the energy variable involving Dirac deltas:

$$Q(f)(\vec{x}, \varepsilon, k_2, k_3) = \sum_{i=-1}^{+1} c_i \left[\sum_k \chi_{[\varepsilon_k^-, \varepsilon_k^+]}(\varepsilon + i\hbar w_p) \times \right.$$
$$\times \sum_m \sum_n \int_{k_{2_m}^-}^{k_{2_m}^+} \int_{k_{3_n}^-}^{k_{3_n}^+} f' \frac{\partial \vec{k}'}{\partial(\varepsilon', k_2', k_3')}\bigg|_{\varepsilon' = \varepsilon + i\hbar w_p} dk_2' dk_3'$$
$$- f(\vec{x}, \vec{k}(\varepsilon, k_2, k_3)) \sum_k \chi_{[\varepsilon_k^-, \varepsilon_k^+]}(\varepsilon - i\hbar w_p) \times$$
$$\left. \times \sum_m \sum_n \int_{k_{2_m}^-}^{k_{2_m}^+} \int_{k_{3_n}^-}^{k_{3_n}^+} \frac{\partial \vec{k}'}{\partial(\varepsilon', k_2', k_3')}\bigg|_{\varepsilon' = \varepsilon - i\hbar w_p} dk_2' dk_3' \right]$$

The computation of these collisional sums will be parallelized by means of OpenMP and MPI for two different silicon devices: the benchmark $n^+ - n - n^+$ diode problem and the double gated MOSFET. We will find the scaling of computational time versus the number of compute nodes on TACC high performance computing resources.

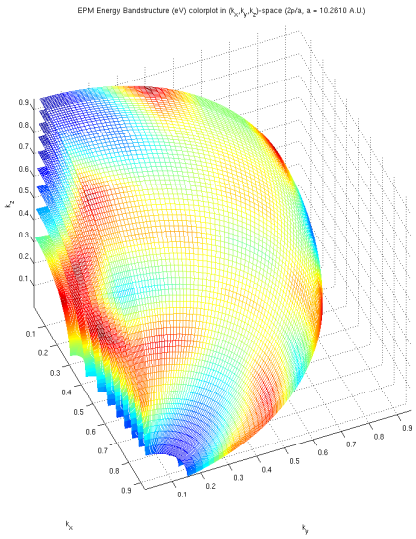

Fig. 1. Piecewise Linear Approximation of the Silicon conduction energy full band structure (ε) color plot in $\vec{k}$-space (1st octant Brillouin Zone) obtained by Local EPM.

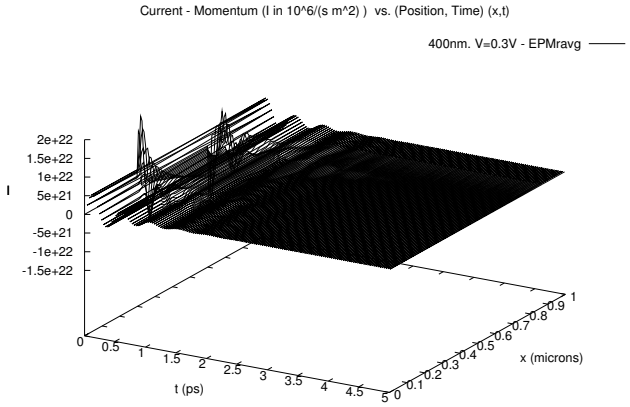

Fig. 2. Current (Momentum) vs. (t, x) for a $n^+ - n - n^+$ Si diode with a 400nm n-channel, using an EPM radial average band. From initial time to t = 5.0ps. 0.3 Volts bias.

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