Deterministic DG Solvers for EPM-Boltzmann-Poisson Transport

Jose A. Morales Escalante*, Irene M. Gamba*, Armando Majorana†,
Yingda Cheng‡, Chi-Wang Shu§, and James R. Chelikowsky*
*ICES, The University of Texas at Austin, USA. e-mail: jmorales@ices.utexas.edu
† Dipartamento di Matematica e Informatica, Universitá degli Studi di Catania, Italy.
‡ Department of Mathematics, Michigan State University, USA.
§ Division of Applied Mathematics, Brown University, USA.

INTRODUCTION

The purpose of this work is to incorporate full electronic band structure computed by Empirical Pseudopotential Methods (EPM) in Discontinuous Galerkin (DG) transport schemes in order to solve the Boltzman-Poisson transport along numerical energy surfaces generated by EPM.

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

$$\frac{\partial f_i}{\partial t} + \frac{1}{\hbar}\nabla_k \varepsilon_i \cdot \nabla_x f_i - \frac{q_i}{\hbar} E \cdot \nabla_k f_i = \sum_j Q_{i,j} \quad (1)$$

$$\nabla_x \cdot (\epsilon \nabla_x V) = \sum_i q_i \rho_i - N(x), E = -\nabla_x V \quad (2)$$

where $f_i(x,k,t)$ is the probability density function over phase space (x,k) of a carrier in the i-th energy band in position x, with crystal momentum $\hbar k$ 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. $E(x,t)$ is the electric field, $\varepsilon_i(k)$ is the i-th energy band surface, the i-th charge density $\rho_i(t,\mathbf{x})$ is the k-average of f_i, and $N(\mathbf{x})$ is the doping profile. Deterministic solvers using the Discontinuous Galerkin (DG) method have been proposed in [1], [2] to model electron transport along the conduction band for 1D diodes and 2D double gate MOSFET devices with the energy band $\varepsilon(k)$ given by analytical models valid close to a local minimum, such as the parabolic or the Kane models. These solvers are shown to be competitive with Direct Simulation Monte Carlo methods.

This preliminary work is focused on simulations for electron transport along a single conduction band for Si computed by EPM, which gives a full band structure spectral approximation in k-space [3] for a crystal lattice model as the sum of potentials due to individual atoms and associated electrons, with few parameters fitting empirical data such as optical gaps, absorption rates, etc.

WORK & PRELIMINARY RESULTS

When the approximation $\varepsilon(k) = \varepsilon(|k|)$ for the conduction band is assumed (as in the parabolic or Kane band approximations), computations for collision terms using Fermi's Golden Rule are significantly reduced. However, this assumption simplifies band structure details and hinders the application to transport of electrons in relative strong Electric fields which induce a flow in phase space that requires values of the band structure that not only are far from the conduction band minimum, but where also the band structure becomes anisotropic (Fig. 1). In this preliminary work, we calculated the EPM-Boltzmann-Poisson transport with a spherically averaged EPM calculated energy surface and compared the output to the classical analytical band models. We observed a significant correction in moments, exhibiting a computational strategy as a midpoint in between an analytical radial and full conduction band model.

To this end, the calculated EPM band structure was averaged by means of Gaussian quadrature on angular space over k-spheres around the local energy minimum $k_0 = (0.8562, 0, 0)2\pi/a$. In this way we obtain a band model that not only represents the variation of the conduction band in the k-space, but also has radial dependence $\varepsilon(|k|)$, retaining then desired advantages. These EPM spherical averages

978-3-901578-26-7

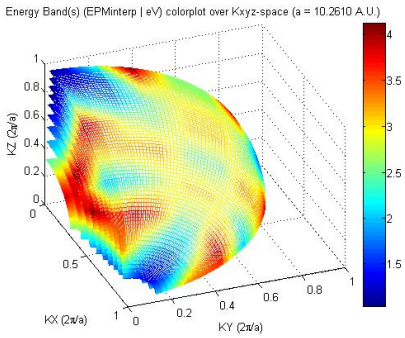

Fig. 1. Conduction Band (CB) for Si (E) Color Plot in k-space by Local EPM. First Quadrant Si Brillioun Zone. CB Min: $k_o = (0.8562, 0, 0)(2\pi/a)$

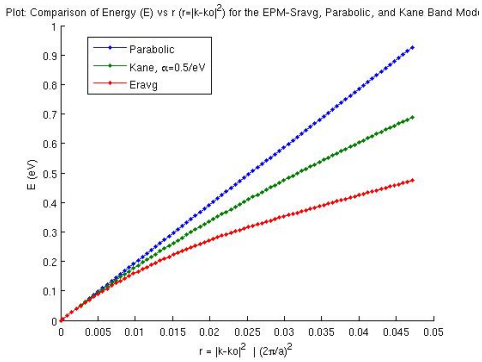

Fig. 2. Energy (E) vs. $r = |k - k_o|^2$ for the Parabolic, Kane, and EPM Radial Average Band Models. $\frac{dE}{dr}$ at the center-point of each k-cell calculated by cubic splines

of the first conduction band are shown in Fig. 2 vs $r = |k - k_0|^2$ for Si (in red), along with the parabolic (blue) and Kane (green) conduction band models. Following the computational strategy in [2], a spherical coordinate transformation over k is applied to (1). In this work we consider 1D $n^+ - n - n^+$ $1\mu m$ Si diodes with either a $400nm$ or a $50nm$ channel in the middle, with doping of $5\times10^{23}/m^3$ in the $n+$ region and $2\times10^{21}/m^3$ in the n region. Since for the approximated $\varepsilon(k) = \varepsilon(|k|)$, then, when the initial condition also depends on $|k|$, the problem retains azimuthal symmetry in k-space, which is suitable for dimensionality reduction for one dimensional x-space transport.

We compare the transport calculated on three different conduction band models: the EPM spherical average, parabolic, and Kane (Fig. 2). The derivative for the EPM average is interpolated by splines. Plots of average kinetic energy (Fig. 3) and momentum (current, Fig. 4) (moments of f) are shown for a $400nm$ channel with a 0.3 V potential bias at $t = 5.0ps$. There is a clear quantitative difference particularly for these moments, calculated as $\varepsilon(k)$-weighted averages in k-space between the different used band models.

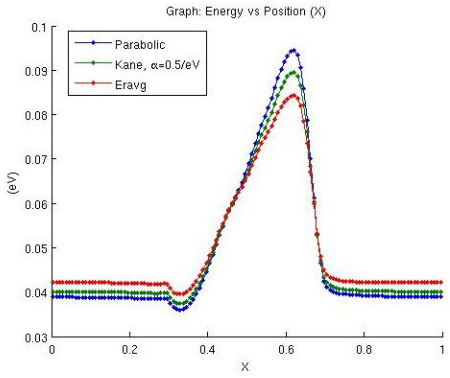

Fig. 3. Comparison of Average Energy (ε) vs. Position (x) for different Conduction Band Models: Parabolic, Kane, EPM Average. Bias: 0.3 Volt. $t = 5.0ps$.

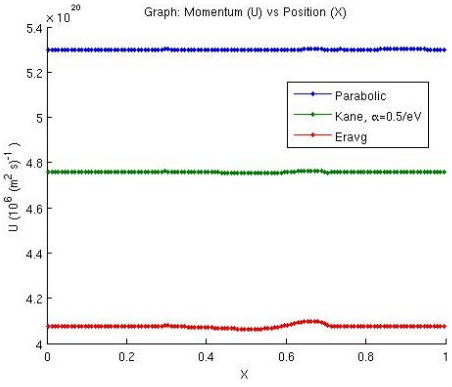

Fig. 4. Comparison of Current (Momentum) vs. (x, t) plots for different Conduction Band Models: Parabolic, Kane, EPM Average. Bias: 0.3 Volt. $t = 5.0ps$.

REFERENCES

[1] Y. Cheng, I. M. Gamba, A. Majorana, and C.W. Shu *A Discontinous Galerkin solver for Boltzmann-Poisson systems in nano-devices*, CMAME **198**, 3130-3150 (2009).

[2] Y. Cheng, I. M. Gamba, A. Majorana and C.-W. Shu, *A discontinuous Galerkin solver for full-band Boltzmann-Poisson models*, IWCE13 Proceedings (2009).

[3] J. Chelikowsky, and M. Cohen, *Electronic Structure of Silicon*, Physical Review B **10**, 12 (1974).