Discontinuous Galerkin Solver for the Semiconductor Boltzmann Equation

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Abstract

We present preliminary results of a discontinuous Galerkin scheme applied to deterministic computations of the transients for the Boltzmann-Poisson system describing electron transport in semiconductor devices. The collisional term models optical-phonon interactions which become dominant under strong energetic conditions corresponding to nanoscale active regions under applied bias. The proposed numerical technique, that is a finite element method which uses discontinuous piecewise polynomials as basis functions, is applied for investigating the carrier transport in bulk silicon and in a silicon $n^+ - n - n^+$ diode. Additionally, the obtained results are compared to those of a high order WENO scheme solver.

1 Basic Equations

In modern highly integrated devices, a consistent description of the dynamics of carriers is essential for a deeper understanding of the observed transport properties. For this purpose the semi-classical Boltzmann-Poisson system is used and given by

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon \cdot \nabla_{\mathbf{x}} f - \frac{q}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}} f = Q(f),\ \nabla_{\mathbf{x}}\left[\varepsilon_r(\mathbf{x})\mathbf{E}\right] = -\frac{q}{\varepsilon_0}\left[\rho(t,\mathbf{x}) - N_D(\mathbf{x})\right], \quad (1)$$

which provides a general theoretical framework for modeling electron transport. Time-dependent solutions of the Boltzmann-Poisson system contain all the information on the evolution of the carrier distribution. 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 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. The parameter ε_0 is the dielectric constant in a vacuum, $\varepsilon_r(\mathbf{x})$ 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 collision operator $Q(f)$ describes electron-phonon interactions where most

important ones in Si are due to scattering with lattice vibrations of the crystal, which are modeled by acoustic and optical non-polar modes with a single frequency ω_p, i.e.

$$Q(f)(t,\mathbf{x},\mathbf{k}) = \int_{\mathbb{R}^3} \left[S(\mathbf{k}',\mathbf{k})f(t,\mathbf{x},\mathbf{k}') - S(\mathbf{k},\mathbf{k}')f(t,\mathbf{x},\mathbf{k})\right]\, d\mathbf{k}', \tag{2}$$

where the kernel S is defined by

$$\begin{aligned} S(\mathbf{k},\mathbf{k}') &= K_0(\mathbf{k},\mathbf{k}')\,\delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})) + K(\mathbf{k},\mathbf{k}') \\ &\quad \left[(\mathsf{n}_q+1)\,\delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})+\hbar\omega_p) + \mathsf{n}_q\,\delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})-\hbar\omega_p)\right]. \end{aligned} \tag{3}$$

The phonon occupation factor is $\mathsf{n}_q = [\exp\left(\frac{\hbar\omega_p}{k_B T_L}\right) - 1]^{-1}$ where k_B is the Boltzmann constant and $T_L = 300^\circ K$ is the constant lattice temperature. The symbol δ indicates the usual Dirac distribution.

2 Numerical Method

Very recently, deterministic solvers to the Boltzmann-Poisson system (1)-(2)-(3) for two-dimensional devices were proposed [1, 2, 3, 6, 7]. These methods provide accurate results which, in general, agree well with those obtained from Monte Carlo (DSMC) simulations, often at a fractional computational time. These methods can resolve transient details for the *pdf*, which are difficult to compute with DSMC simulators. The methods proposed in [1, 2] used weighted essentially non-oscillatory (WENO) finite difference scheme to solve the Boltzmann-Poisson system. The advantage of the WENO scheme is that it is relatively simple to code and very stable even on coarse meshes for solutions containing sharp gradient regions. A disadvantage of the WENO finite difference method is that it requires smooth meshes to achieve high order accuracy, hence it is not very flexible for adaptive meshes. We propose here a discontinuous Galerkin (DG) method for solving the Boltzmann-Poisson system. The DG method is a finite element method using discontinuous piecewise polynomial basis functions and relies on an adequate choice of numerical fluxes, which handle effectively the interactions across element boundaries. See for example the review paper [5] and references therein. Recent development of the locally discontinuous Galerkin methodology allows us to adopt a unified discretization strategy to handle all spatial derivatives in semiconductor device models including the Boltzmann-Poisson system [4, 8, 9, 10], with an L^2 stable and locally conservative scheme having the potential for full *h-p* adaptivity.

3 Transformed equations and computational results

The transport equation (1) is written in energy based coordinates that can handle the singular energy masses in the scattering terms [11]. In fact, we perform a coordinate transformation for $\mathbf{k}$ according to

$$\mathbf{k} = \frac{\sqrt{2m^* k_B T_L}}{\hbar}\sqrt{w(1+k_B T_L \alpha w)}\left(\mu, \sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi\right), \tag{4}$$

where the new independent variables are the dimensionless energy w, the cosine of the polar angle μ, and the azimuth angle φ. The physical parameter α is related to the

crystal conduction band. The new unknown charge distribution is

$$\Phi(t,x,y,z,w,\mu,\phi) = s(w)\tilde{f}(t,x,y,z,w,\mu,\phi) \ ,$$

where $s(w) = \sqrt{w(1+\alpha_\kappa w)}(1+2\alpha_\kappa w)$ is related to the density of the states, and $\tilde{f}$ corresponds to f in the new variables. The corresponding transformed dimensionless Boltzmann equation remains in conservative form [1]. We point out that the corresponding free streaming operator depends on the electric field $\mathbf{E}$. In particular, the numerical fluxes for the DG approximation should be taken carefully in an upwind fashion. For other details and physical constants we refer to [1, 2]. The transient behavior for a

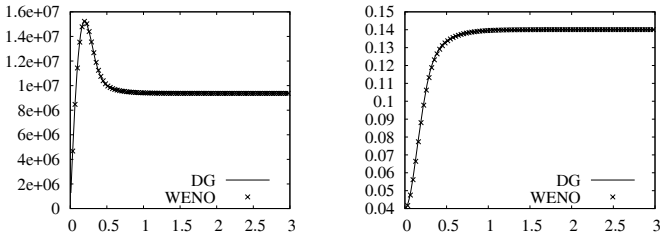

Figure 1: Mean velocity (cm/s) and mean energy (eV) versus time (ps).

simple bulk device with a constant electric field $(30KV/cm)$ is shown in Fig. 1, where the numerical DG and WENO solutions are compared. For the one dimensional silicon $n^+ - n - n^+$ diode, where the doping $N_D(x) = 5 \times 10^{23} m^{-3}$ in the n^+ region [0, 0.3] and [0.7, 1] (unit: micron) and $N_D(x) = 2 \times 10^{21} m^{-3}$ in the channel [0.3, 0.7], the simulation result at the steady state $(t = 5ps)$ is shown in Fig. 2, where the numerical DG and WENO solutions are compared. The applied voltage is $1V$. In all the simulations

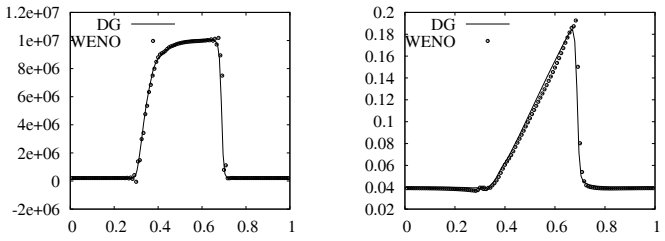

Figure 2: Mean velocity (cm/s) and mean energy (eV) at the steady state $t = 5ps$.

we use $120 \times 60 \times 24$ cells in the x-w-μ space. Figure 3 shows the *pdf* at the location $x = 0.5$ micron in the computational stationary state, both in the scaled energy-polar and cartesian coordinates in the velocity space.

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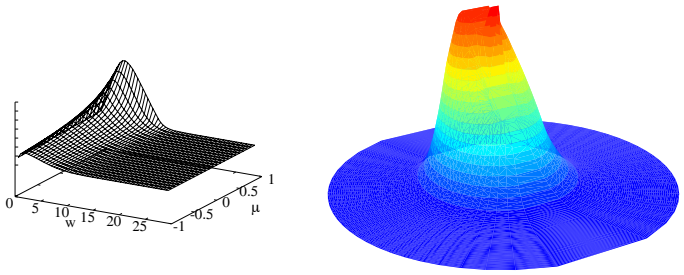

Figure 3: *pdf* in the stationary regime at the center of the device. Left: the scaled pdf Φ in the (w,μ) coordinates; right: the pdf f in the $(k_1, \sqrt{k_2^2+k_3^2})$ coordinates.

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