



A Direct Solver for 2D Non-Stationary Boltzmann-Poisson Systems for Semiconductor Devices: A MESFET Simulation by WENO-Boltzmann Schemes

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Abstract. We present preliminary results of a high order WENO scheme applied to deterministic computations for two dimensional formulation 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. We treat the Boltzmann Transport equation in a spherical coordinate system for the wave-vector space. The problem is three dimensional in the wave-vector space and two dimensional in the physical space, plus the time variable driving to steady states. The new formulation avoids the singularity due to the spherical coordinate system.

Keywords: Boltzmann-Poisson system for semiconductors, WENO scheme, spherical coordinate system

The Boltzmann equation (BTE) describes electron transport in semiconductor devices. Solving it numerically is not an easy task because the BTE is an integro-differential equation with six dimensions in position-wave-vector and one in time. Though one of the most popular methods to simulate charge transport in such devices is the Monte Carlo method, it is very noisy at high energy regimes and inefficient for simulations of transients.

We consider the two-space, three wave-vector dimensional single-band Boltzmann equation describing electron flow in a MESFET device. The collision operator models scattering processes between free electrons and phonons in thermal equilibrium, including terms modeling phonon absorption and emission rates. The doping profile and the self-consistent electric field are related by the Poisson equation relating the potential to total space charges under strong applied bias.

In this work we extend our recent one-dimensional simulation [1,2] using a simple numerical scheme based on a method of lines where the advection part is treated with the high order non-oscillatory finite difference WENO approximation and the time discretization by Runge-Kutta method [3], after a spherical coordinate transformation is performed in order to deal with the singular nature of the phonon-scattering processes. The resulting numerical deterministic solver is high order accurate regardless of the irregularity of the distribution function near the junctions of the device.

In addition, our direct computational method produces a natural way to visualize the kinetic probability distribution function in strong anisotropic equilibrium regions induced by relatively strong bias. Also, the method allows for direct computation and visualization of transients.

1. Basic Equations

We consider an electron gas, which interacts with a bath of phonons assumed to be in thermal equilibrium. In this case the Boltzmann equation is

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon \cdot \nabla_{\mathbf{x}} f - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f = Q(f). \quad (1.1)$$

The unknown f is the electron distribution function, which depends on time t , space coordinates \mathbf{x} and wave-vector vector \mathbf{k} . The parameters \hbar and e are the Planck constant divided by 2π and the positive electric charge, respectively. The symbol $\nabla_{\mathbf{k}}$ stands for the gradient with respect to the variables \mathbf{k} and $\nabla_{\mathbf{x}}$ that with respect to the space coordinates \mathbf{x} . The particle energy ε is an assigned nonnegative continuous function of \mathbf{k} . If the Kane model is assumed, then

$$\varepsilon(\mathbf{k}) = \frac{1}{1 + \sqrt{1 + 2 \frac{\tilde{\alpha}}{m^*} \hbar^2 |\mathbf{k}|^2}} \frac{\hbar^2}{m^*} |\mathbf{k}|^2, \quad (1.2)$$

where m^* is the effective mass and $\tilde{\alpha}$ is the nonparabolicity factor. The widely used parabolic approximation is obtained from Eq. (1.2) by putting $\tilde{\alpha} = 0$.

In Eq. (1.1) the electric field \mathbf{E} satisfies the Poisson equation

$$\nabla_{\mathbf{x}}(\epsilon \nabla_{\mathbf{x}} V) = e[n(t, \mathbf{x}) - N_D(\mathbf{x})], \quad (1.3)$$

$$\mathbf{E} = -\nabla_{\mathbf{x}} V, \quad (1.4)$$

where ϵ is the permittivity, $n(t, \mathbf{x}) = \int_{\mathbb{R}^3} f(t, \mathbf{x}, \mathbf{k}) d\mathbf{k}$ is the electron density, $N_D(\mathbf{x})$ is the doping and V is the electric potential. Equations (1.1)–(1.3) and (1.4) give the Boltzmann-Poisson system.

We follow a semi-classical approach for the collision term $Q(f)$, so that, in the low density regime, it is

$$Q(f)(t, \mathbf{x}, \mathbf{k}) = \int_{\mathbb{R}^3} [S(\mathbf{k}', \mathbf{k}) f(t, \mathbf{x}, \mathbf{k}') - S(\mathbf{k}, \mathbf{k}') f(t, \mathbf{x}, \mathbf{k})]. \quad (1.5)$$

The kernel S , which takes into account the scattering processes between electrons and phonons, is defined by

$$S(\mathbf{k}, \mathbf{k}') = K_0(\mathbf{k}, \mathbf{k}') \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k})) + K(\mathbf{k}, \mathbf{k}') \times [(\eta_q + 1) \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) + \hbar\omega_p) + \eta_q \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) - \hbar\omega_p)]. \quad (1.6)$$

incorporating intra-valley acoustic phonon scattering in the elastic approximation and intra-valley optical non-polar phonon scattering with one frequency. These scattering mechanisms are chosen because of their importance in Si. The constant η_q is the occupation number of phonons and is given by

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

where ω_p is the constant phonon frequency, k_B is the Boltzmann constant and T_L is the lattice temperature. The symbol δ indicates the usual Dirac distribution.

As in [1,2,4], we introduce dimensionless equations, and use the following coordinate transformation for the wave-vector \mathbf{k}

$$\mathbf{k} = \frac{\sqrt{2 m^* k_B T_L}}{\hbar} \sqrt{\omega} \sqrt{1 + \alpha_K \omega} \times (\mu, \sqrt{1 - \mu^2} \cos \phi, \sqrt{1 - \mu^2} \sin \phi) \quad (1.7)$$

where $\alpha_K = k_B T_L \tilde{\alpha}$, $\omega \geq 0$ is a dimensionless energy, $\mu \in [-1, 1]$ is the cosine of the angle with respect to x -axis and $\phi \in [0, 2\pi]$ the azimuthal angle respectively. We consider a two dimensional problem in the physical space. Let

$$\Phi(t, x, y, \omega, \mu, \phi) = s(\omega) f(t, x, y, \omega, \mu, \phi),$$

where $s(\omega) = \sqrt{\omega(1 + \alpha_K \omega)}(1 + 2\alpha_K \omega)$ is, apart from a dimensional constant factor, the Jacobian of

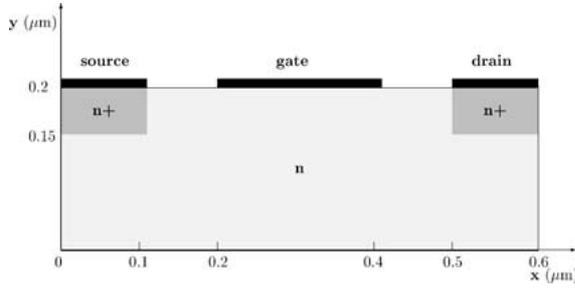


Figure 1. Schematic representation of a bidimensional MESFET.

the transformation of coordinates (1.7). The use of the dimensionless unknown Φ instead of the distribution function f allows us to write the dimensionless Boltzmann equation in the following conservative form:

$$\begin{aligned} \frac{\partial \Phi}{\partial t} + \frac{\partial}{\partial x}(a_1 \Phi) + \frac{\partial}{\partial y}(a_2 \Phi) + \frac{\partial}{\partial \omega}(a_3 \Phi) \\ + \frac{\partial}{\partial \mu}(a_4 \Phi) + \frac{\partial}{\partial \phi}(a_5 \Phi) = s(\omega)C(\Phi) \end{aligned} \quad (1.8)$$

where the coefficients for the flux terms are

$$\begin{aligned} a_1(\omega) &= \frac{1}{t_*} \frac{\mu s(\omega)}{(1 + 2\alpha_\kappa \omega)^2} \\ a_2(\omega, \mu, \phi) &= \frac{1}{t_*} \frac{\sqrt{1 - \mu^2} s(\omega) \cos \phi}{(1 + 2\alpha_\kappa \omega)^2} \\ a_3(t, x, y, \omega, \mu, \phi) &= -\frac{1}{t_*} \frac{2s(\omega)}{(1 + 2\alpha_\kappa \omega)^2} \\ &\times [E_x(t, x, y)\mu + E_y(t, x, y)\sqrt{1 - \mu^2} \cos \phi] \end{aligned}$$

$$\begin{aligned} a_4(t, x, y, \omega, \mu, \phi) &= -\frac{1}{t_*} \frac{1 + 2\alpha_\kappa \omega}{s(\omega)} \sqrt{1 - \mu^2} \\ &\times [E_x(t, x, y)\sqrt{1 - \mu^2} - E_y(t, x, y)\mu \cos \phi] \\ a_5(t, x, y, \omega, \mu, \phi) &= \frac{E_y(t, x, y)}{t_*} \frac{\sin \phi}{\sqrt{1 - \mu^2}} \frac{1 + 2\alpha_\kappa \omega}{s(\omega)}, \end{aligned}$$

and the dimensionless collision operator $t^* C(\Phi)$ is given by

$$\begin{aligned} C(\Phi)(t, x, y, \omega, \mu, \phi) \\ = \frac{1}{2\pi t^*} \int_0^\pi \int_{-1}^1 [\beta \Phi(t, x, y, \omega, \mu', \phi') \\ + a \Phi(t, x, y, \omega + \alpha, \mu', \phi') \\ + \Phi(t, x, y, \omega - \alpha, \mu', \phi')] d\phi' d\mu' \\ - \frac{1}{s(\omega) t^*} [\beta s(\omega) + a s(\omega - \alpha) \\ + s(\omega + \alpha)] \Phi(t, x, y, \omega, \mu, \phi). \end{aligned} \quad (1.9)$$

The constant parameters t_* , α , a and β depend on scattering mechanisms. They are the same physical constants introduced in 1-D case (see [1] for details).

2. Numerical Results

We simulate a MESFET geometry (Fig. 1) [5] with size of $0.6 \mu\text{m}$ by $0.2 \mu\text{m}$. We observe high accurate non-oscillatory behavior near junctions and expected high channel anisotropic energy near the gate and drain region, where the two-dimensional effects are important.

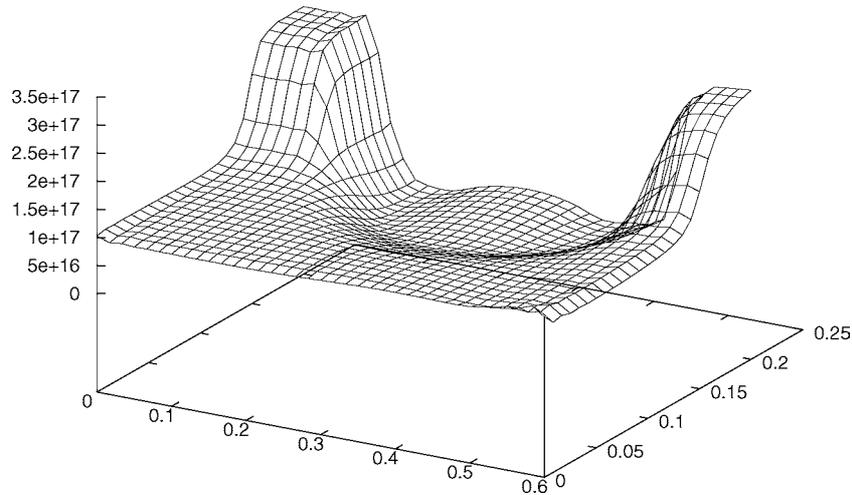


Figure 2. Concentration in cm^{-3} at 5 ps.

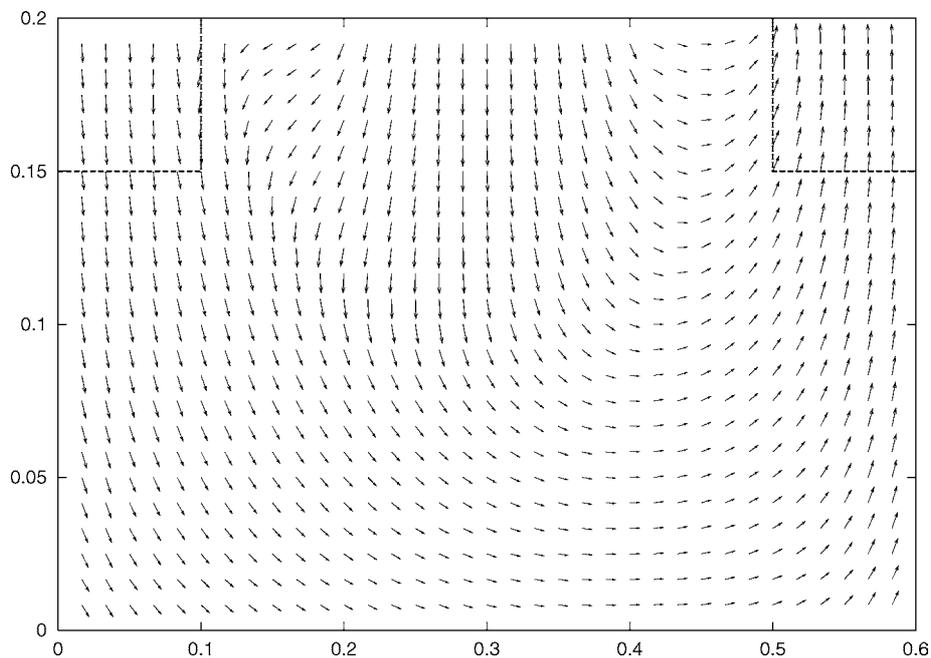


Figure 3. Velocity field at 5 ps.

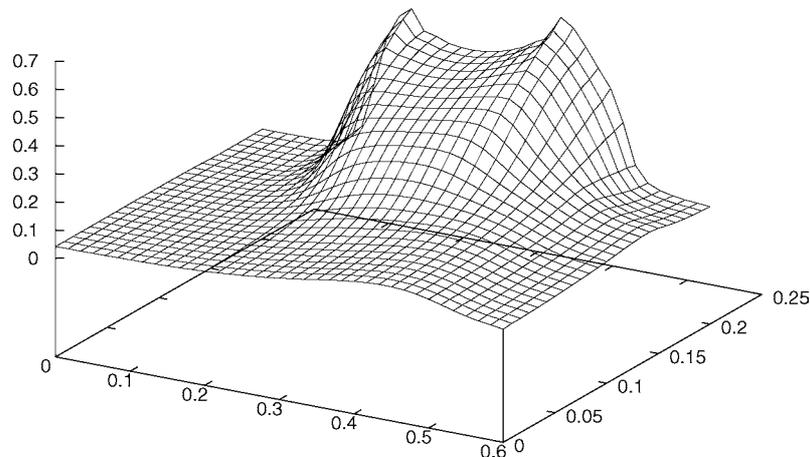


Figure 4. Mean energy in eV at 5 ps.

Following [6], mirror boundary condition (specular reflection) for the particle dynamics assumes perfectly reflecting boundaries, where the velocity component normal to the surface is reversed when particles collide against the surface. From the analysis of the Poisson equation, the Neumann condition (zero electric field in the direction normal to the surface) is applied on those boundary regions where there are no contacts (insulating boundaries).

The source and drain contacts act as particle reservoirs. Particles may exit or enter through the contacts.

The gate Schottky contact is assumed to be an absorbing boundary for particles. For the solution of the Poisson equation, the source, drain, and gate contacts are treated as Dirichlet boundaries where the bias voltages are applied.

The dimensional doping is given by $N_D = 3 \times 10^{17} \text{ cm}^{-3}$ in the n^+ region and $N_D = 10^{17} \text{ cm}^{-3}$ in the n region. The electric potential is assigned at the gate (-0.8 V), drain (0 V) and drain (1 V).

In the following sequel we include the plots of the first thermodynamic quantities of f , namely the

concentration n (Fig. 2), the velocity field (Fig. 3), the kinetic energy (Fig. 4), the electric potential V (Fig. 5) and the electric field \mathbf{E} (Fig. 6). The vectors in Figs. 3 and 6 are suitably rescaled. In this simulation we use $37 \times 25 \times 45 \times 12 \times 8$ grid points of the $(x, y, \omega, \mu, \phi)$ domain.

We apply the fifth order weighted ENO (WENO) schemes developed in [3] for non-linear systems of conservation laws. WENO schemes are designed for hyperbolic conservation laws or other problems containing

either discontinuous solutions or solutions with sharp gradients. The guiding principle is an adaptive usage of a nonlinear convex combination of contributions from local stencils, so that contributions from stencils containing a possible discontinuity or other unpleasant features (e.g., a high gradient) are assigned a nearly zero weight (hence the term weighted essentially non-oscillatory, or WENO). In doing this, uniform high order accuracy can be achieved without introducing any oscillations near discontinuities or sharp gradient

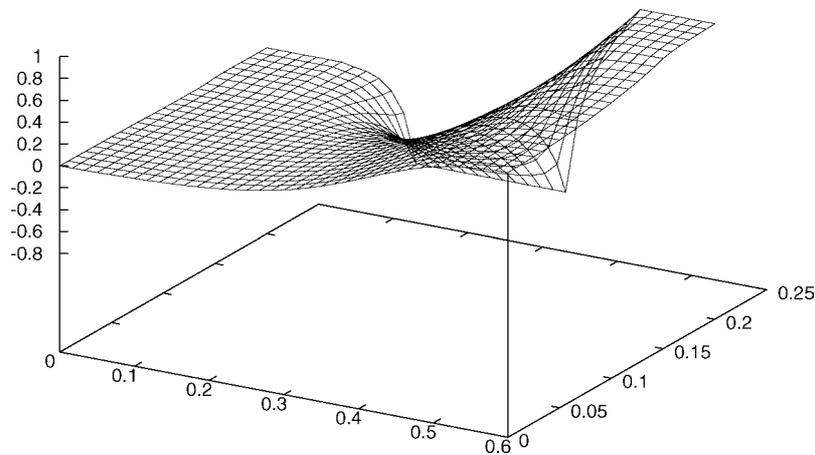


Figure 5. Electric potential in V at 5 ps.

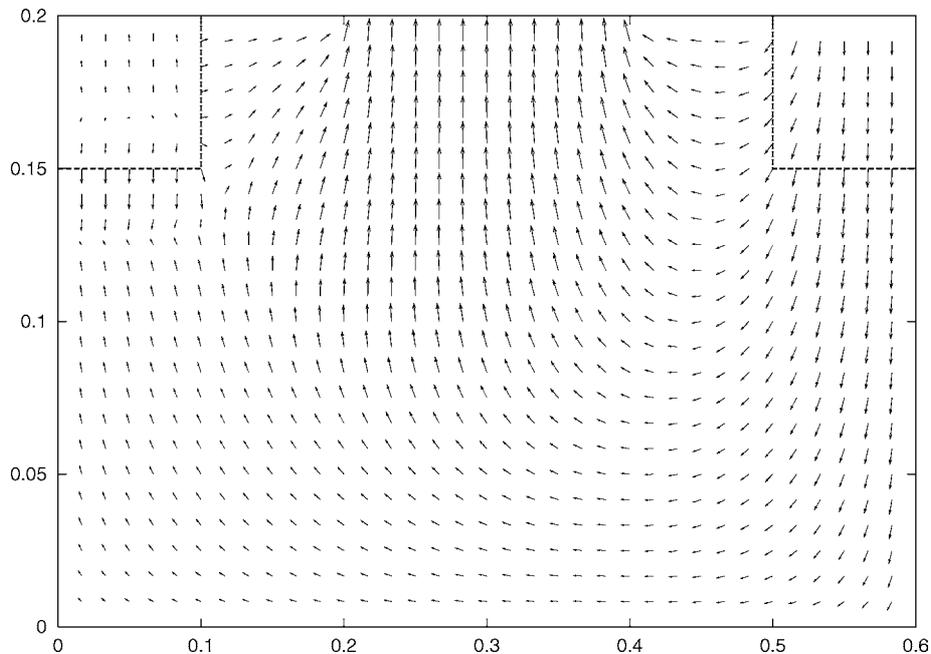


Figure 6. Electric field at 5 ps.

regions. Steady state is achieved by a time accurate marching, allowing us to use the same code to simulate time accurate solutions.

3. Conclusions

Our work is a follow up on the development of direct solvers, as an alternative to DSMC methods, initiated by Fatemi and Odeh [7], recently re-taken by Majorana and Pidotella [4] and the authors [1,2].

Our computational method provides a direct deterministic simulation for the higher dimension electron distribution function that is accurate and considerably computationally efficient for channel geometries. Also, since our code is time accurate, it can be used to capture transients in time dependent devices. The high order accuracy of these algorithms allows us to use relatively coarse grids and still get very accurate results.

In our preliminary numerical simulation, we have observed the formation of significant anisotropies in the channel drain junctions. Comparisons with Monte Carlo simulations and with various moment models such as hydrodynamic and energy transport models, and experiments on other devices are under way, and will be presented in future work.

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References

1. J.A. Carrillo, I.M. Gamba, A. Majorana, and C.-W. Shu, "A WENO-solver for the 1D non-stationary Boltzmann-Poisson system for semiconductor devices," *Journal of Computational Electronics*, **1**, 365 (2002).
2. J.A. Carrillo, I.M. Gamba, A. Majorana, and C.-W. Shu, "A WENO-solver for the transients of Boltzmann-Poisson system for semiconductor devices. Performance and comparisons with Monte Carlo methods," *Journal of Computational Physics*, **184**, 498 (2003).
3. G. Jiang and C.-W. Shu, "Efficient implementation of weighted ENO schemes," *Journal of Computational Physics*, **126**, 202 (1996).
4. A. Majorana and R.M. Pidotella, "A finite difference scheme solving the Boltzmann-Poisson system for semiconductor devices," *Journal of Computational Physics*, **174**, 649 (2001).
5. J. Jerome and C.-W. Shu, "Energy models for one-carrier transport in semiconductor devices," in *IMA Volumes in Mathematics and Its Applications*, edited by W. Coughran, J. Cole, P. Lloyd, and J. White (Springer-Verlag, 1994), vol. 59, p. 185.
6. K. Tomizawa, *Numerical Simulation of Submicron Semiconductor Devices* (Artech House, Boston, 1993).
7. E. Fatemi and F. Odeh, "Upwind finite difference solution of Boltzmann equation applied to electron transport in semiconductor devices," *Journal of Computational Physics*, **108**, 209 (1993).