Comparison of Monte Carlo and deterministic simulations of a silicon diode

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Abstract

Electron transport models in Si transistors with channel length of 0.4 microns and 50 nanometers are examined and compared between classical Direct Monte Carlo Simulations and deterministic WENO solvers for a self-consistent kinetic field-relaxation Poisson model. This model is a well accepted low density reduction of the full non-equilibrium transport phenomena. In this comparison we control the calibration of the field dependent, saturated mobility. Our computations show that, at channel length of order 0.4 microns, the relaxation model captures the the first two moments of the particle distribution function inside the channel. In particular a domain decomposition technique that implements classical drift diffusion in the high density regions and augmented drift diffusion inside the channel region gives a correction to the classical drift diffusion simulations, and produces similar qualitative results to the Monte Carlo simulations with a 0.002 CPU time reduction factor. However, we show that in the case of a 50 nanometer channel, the kinetic field-relaxation model fails to approximate well even the first moment, and in particular it does not approximate well the current voltage curve output from Monte Carlo simulations, making it necessary to incorporate high energy effects into the collision operator.

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1 Introduction

We report a computational comparison between a full one space-three velocity dimensional Boltzmann Transport Equation (BTE) solved by a Direct Simulation Monte Carlo (DSMC) method and recent deterministic computations corresponding to a one dimensional kinetic field-relaxation model using Weighted Essentially Non-Oscillatory (WENO) schemes, with a field dependent relaxation time approximation for electron transport, both for a 0.4 microns and a 50 nanometers channel of a n^+-n-n^+ Si diode.

This comparison is motivated in order to show the validation of this kinetic relaxation model as a good approximation for moderate quasi-ballistic regimes [1, 2] in the channel region up to orders of .3 microns for relative high energies.

In addition, we show that computations corresponding to a shorter Si nanodevice with a channel length of 0.05 micron, are not well modeled by the one dimensional field-dependent kinetic relaxation system, for two-parameter, field dependent mobilities, when compared with DSMC for the full BTE. This is also considered to be quasi-ballistic [11].

The longer channel asymptotics correspond to a length scale that balances the strength of collisions with the drift strength. As a result, the density and currents are well captured by the deterministic computation at 10^{-2} fraction of the computational time when using a domain decomposition technique that incorporates a multi-scale analysis.

As a consequence, for these quasi-ballistic regimes, we are able to obtain a multi-scale computational algorithm for current-voltage characteristics (IV-curves) which agree with Monte Carlo IV curves at a higher order of the relative error. This multi-scale computational algorithm has been presented in [4] and compared with the same one dimensional field dependent kinetic relaxation model for which we perform the comparisons in this paper. In fact, when comparing the relative errors between both drift-diffusion and the multi-scale algorithm output for IV-curves with Monte Carlo, the latter improves in a factor of 2 with respect to the former one.

We see that for shorter (or "faster") devices the relaxation model fails to capture the high energy effects coming from stronger scattering rates. This means that the full acoustic and non-polar optical phonon scattering collision operators must be modeled. As a consequence, most classical hydrodynamical closures based on collisional models that fail to incorporate high energy effects will not reproduce a good fitting of Monte Carlo simulations, even for the lower moments.

For completeness of this paper, we recall the models that are computed, with the exception of the classical Drift Diffusion Poisson (DDP) system with field dependent mobility.

The classical kinetic relaxation model for charged transport is derived from a low density approximation of the semi classical Boltzmann-Poisson system, taking into account only collisions with background impurities. Though this system is posed in the three dimensional velocity space, a one dimensional model recovers the important features of the charge transport that are given in the direction parallel to

the force field. Such a configuration is a correct description of a channel-like flow, as in the modeling of diodes, due to the simple geometry of the device. Therefore this equation reads [10]

$$\frac{\partial f}{\partial t} + v f_x - \frac{e}{m} E(t,x) f_v = \frac{1}{\tau}(M_{\Theta_o}\rho(f) - f) \tag{1.1}$$

$f = f(t,x,v)$ is the density function for an electron at position $x \in [0,L]$ and velocity $v \in I\!R$ at time $t \geq 0$, where L is the device channel length. The constants e and m represent the unit charge and effective electron mass, respectively. The electric field $E = E(t,x)$ is self-consistently produced by the electrons moving in a fixed ion background with density $C(x)$, called doping profile. E is determined by the Poisson equation

$$\begin{aligned} \varepsilon_o \Phi_{xx} &= e(\rho(f) - C(x)) \\ E(t,x) &= -\Phi_x \end{aligned} \tag{1.2}$$

where ε_o is the permittivity of the material and

$$\rho(t,x) = \int_{I\!R} f(t,x,v)dv, \quad j(t,x) = \int_{I\!R} v f(t,x,v)dv, \quad x \in [0,L],\ t \geq 0 \tag{1.3}$$

are, respectively, the charge and current densities of the electrons. M_{Θ_o} is the absolute Maxwellian given by

$$M_{\Theta_o} = (2\pi\Theta_o)^{-1/2} \ \exp\left(-\frac{v^2}{2\Theta_o}\right),$$

where Θ_o is the lattice temperature, that is, $\Theta_o = \frac{k_B}{m} T_o$ with the Boltzmann constant k_B and the lattice temperature T_o in Kelvin.

Here, the relaxation time τ depends on the absolute value of the force field in such a way that the mobility $\mu = \frac{e}{m}\tau E$ is linear for small values of $|E|$ with slope μ_0 and has a horizontal asymptote v_d as $|E|$ becomes large. We have chosen the following formula for describing the mobility,

$$\mu(E) = \frac{e}{m}\tau(E) = \frac{2\mu_0}{1 + \sqrt{1 + 4\left(\frac{\mu_0}{v_d}E\right)^2}} \tag{1.4}$$

where the parameters μ_0 (low-field mobility) and v_d (saturation speed) are adjusted for calibrating the drift speed μE in the bulk Si with respect to the DSMC data obtained by the `Damocles` code [8]. In this way, we make sure that both models in our comparison refer to the same physical device.

The calibration can be performed by means of different procedures. Here, the calibration has been made by using the tool `Exemplar` [9], where the minimum of the residual function (i.e. the square of the difference of the Monte Carlo data and the data obtained by Formula (1.4) is obtained by the simplex algorithm. Accordingly, we take μ_0=1799 $\frac{cm^2}{V sec}$ and v_d=1.5117×$10^7 \frac{cm}{sec}$. In Figure 1 we have

plotted the drift speed of the Monte Carlo run compared to the plot of the function in (1.4) given by the above procedure.

There are different choices to calibrate the relaxation model, for instance, to find numerically, by using the mobility results from `Damocles`, an approximation to the limit at infinity v_d and the initial slope μ_0. Another possible choice would be to use an interpolation of the data from `Damocles` as input for the mobility in the relaxation code. These other two different calibrations have been tested numerically and they give very similar results to the `Exemplar` calibration and it seems the results qualitatively are not very sensitive to the calibration procedure.

We shall see that the transport regime corresponding to the larger channel device ($0.4\mu m$) is well modeled by the field dependent relaxation-Poisson system (1.1)-(1.2)-(1.4). As it was worked out in [4], such a device model can, in fact, be modeled by a hybrid domain decomposition technique consisting of the computation of classical drift-diffusion-Poisson (DDP) models in the n^+ regions which correspond to dominant collision processes, and augmented-drift-diffusion-Poisson (ADDP) models in the n-channel region which corresponds to drift-collision balance processes that take over the channel for this quasi-ballistic regime. The (ADDP) system in its dimensionalized form reads [6]

$$\rho_t + \partial_x (J) = 0 \tag{1.5}$$

$$J = -\mu\rho E + \tau\mu \left(\frac{e}{\varepsilon_o}\right) \rho(-\mu\rho E + \omega) - \tau[\rho(\Theta_o + 2\mu^2 E^2)]_x + \tau\mu E(\mu\rho E)_x \tag{1.6}$$

$$E = -\Phi_x, \qquad \text{and} \qquad \varepsilon_o \Phi_{xx} = e(\rho(f) - C(x)). \tag{1.7}$$

The constant ω is fixed as

$$\omega = (\mu\rho E)|_{x=x_\omega}, \tag{1.8}$$

where x_ω is some point in the computational region. The total current $j(t,x)$, as defined in (1.3), is approximated by $J(t,x)$ solution of (1.5)-(1.8). We refer to [6] and the references therein for a deeper discussion of this system and the role of ω.

The density $\rho(t,x)$ and current $J(t,x)$ that solve the hybrid DDP and ADDP system, with the latter given by (1.5)-(1.8), are Chapman-Enskog asymptotic approximations of the first and second moments of $f(t,x,v)$ solution of the kinetic system (1.1)-(1.2)-(1.4) in the $n+$ and n-channel regions respectively.

2 Numerical comparisons

We solve numerically the full BTE by using `Damocles`, the Monte Carlo code developed in IBM [8]: the spherical parabolic band approximation is used and acoustic and non-polar optical phonon scattering mechanisms are considered. We compared the results with respect to the deterministic simulation of the one dimensional relaxation-Poisson system (1.1)-(1.2)-(1.4). We shall call the numerical

output corresponding to these computations (1-D BTE). We used WENO finite-difference method [7] to solve in a deterministic way the (1-D BTE) as introduced in [5]. WENO methods are high order accurate yet non-linearly stable (essentially non-oscillatory) in the presence of sharp gradients or shocks in the solution.

It is important to notice that we are comparing 24 hour running time for a DSMC simulation versus a 45 minute computation for a WENO simulation of the (1-D BTE) and a 3.5 minute computation of the hybrid domain decomposition method (DDP-ADDP) used in the longer channel case.

Next, we make the comparison for two different devices. The main difference between them is the length scale. The second device is much shorter than the first one. We refer to these two devices as *longer* and *shorter* channel in this sequel. The shorter device has been studied also in [3].

Units are $1/cm^3$ for density, $10^7 cm/sec$ for mean velocity, V for potential, V/cm for force field, eV for energy and $10^2 A/cm^2$ for current. The values of the parameters, common to both Si devices, are given by $m = 0.26 \times 0.9109$ $(10^{-30} kg)$, $e = 0.1602$ $(10^{-18} C)$, $k_b = 0.138046 \times 10^{-4}$ $(10^{-18} J/K)$, $\varepsilon_o = 11.7 \times 8.85418$ $(10^{-18} F/\mu m)$, $T_o = 300K$ and background density $n_i = 1.45 \times 10^{10}/cm^3$.

2.1 Longer channel

Here, we consider a one dimensional Si n^+-n-n^+ structure of length $0.6\mu m$ with a channel length of $0.4\mu m$. Thus, the domain of the device model is $\Omega = [0, 0.6]$, and the doping profile, given by $C(x)$, is a sharp step function with density values $5 \times 10^{17}/cm^3$ in $0 \leq x \leq 0.1$ and in $0.5 \leq x \leq 0.6$ corresponding to the n^+ regions; and $2 \times 10^{15}/cm^3$ in $0.1 < x < 0.4$ corresponding to the n-channel region. The numerical results are shown in Figure 2 with the `Exemplar` approximation of the mobility.

We observe a remarkable coincidence of the results of the 1-D velocity relaxation-time model with respect to the full BTE when comparing density, force field and potential. For comparisons between (1-D BTE) and the hybrid (DDP)-(ADDP) computations the first three moments, potential and forced field see [4]. We also show the comparison of electron energies for both simulations. In order to compare the energies for the 1-D velocity model we need to assume that the corresponding pdf in 3-D corresponds to the 1-D pdf multiplied by a Maxwellian with zero mean velocity and background temperature in the orthogonal directions. As observed, the comparison of the energy is much worse than the one for the mean velocity. As a consequence the 1-D relaxation-time model fails in capturing the energy of the full BTE.

Despite of the discrepancy with the mean velocity and energy (Figure 2), we see that the 1-D model with the `Exemplar` approximation is fairly accurate in capturing the IV-curves (Figure 2, lower right corner). We have also plotted there the IV curves of the drift-diffusion-Poisson (DDP) system and the hybrid domain decomposition using drift-diffusion-Poisson and augmented-drift-diffusion-Poisson (DDP-ADDP) system with field-dependent mobility given by (1.4). Recall that it requires only approximately 3 minutes to numerically solve the (DDP-ADDP)

system, compared with a 24-hour DSMC simulation.

2.2 Shorter channel

Now, we consider a shorter one dimensional Si n^+-n-n^+ structure of length $250nm$ with a n-channel of $50nm$. Here, the doping profile given by $C(x)$ is a sharp step function with density values $5 \times 10^{18}/cm^3$ in $0 \le x \le 100$ and in $150 \le x \le 250$; and $1 \times 10^{15}/cm^3$ in $100 < x < 150$. The rest of the parameters and units remain the same. The numerical results are shown in Figure 3.

Here, the deterministic computations of the kinetic relaxation system clearly underestimate the mean velocity and overestimate the density with respect to the DSMC computations of the full BTE. As a consequence the IV-curves (Figure 3, lower right corner) are not well captured by the kinetic computation of the one dimensional field dependent relaxation (1D-BTE). Notice that the computed IV-curve of the hybrid (DDP-ADDP), being an asymptotic approximation to the field dependent relaxation (1D-BTE), can only approximate well that of the (1D-BTE), not that of the DSMC computations of the full BTE.

In addition the (1D-BTE) computation of the energy grossly underestimates that computed with the DSMC for the full BTE, making this kinetic approximating model unreliable.

3 Conclusions

We have compared two Si diode models, a longer one with a $0.4\mu m$ channel length, and a shorter nano-device with a $0.05\mu m$ channel length, using the DSMC `Damocles` for the full BTE and the deterministic WENO scheme for the 1-D field dependent relaxation approximation to the full BTE. We show that the density, IV-curves, force field and potential corresponding to the longer device is well modeled by the 1-D kinetic relaxation model and its corresponding hybrid DDP-ADDP macroscopic simulation, both computed with a deterministic WENO scheme, reducing the computational time from 24 hours to about 3 minutes for the similar IV-curves. In particular the IV-curve produced by the hybrid DDP-ADDP model approaches the one with Monte Carlo simulation by a factor of 2 when compared with the corresponding DDP solver. This factor does not depend sensitively on the mobility approximation or the calibration procedure. The computational cost of the Drift-Diffusion-Poisson solver and the hybrid DDP-ADDP one are of the same order. However the energy is not well modeled and the mean velocity is fairly approximated by the 1D kinetic relaxation model when compared with the Monte Carlo simulation of the full BTE.

For the nano-device, the the 1D-kinetic field dependent relaxation model fails to produce a good approximation for any of the moments. The comparisons for the IV-curves show the need of better approximations and asymptotics for the full BTE for high energetic processes in order to improve the agreement with Monte Carlo simulations.

Even though the correct collision mechanism should include optical phonon collisions, at larger devices with relatively low voltage bias the levels of energy injection are low enough, so that the the dominant collisions are acoustical, explaining the agreement of the relaxation and Damocles for 0.4μ and voltage drops from 0.4 to 0.7 V. Beyond that bias, the field-relaxation model and Monte Carlo differ significantly. This regime can be identified as the quasi-ballistic one [3].

This fact brings up the need to compare the diode computation with a deterministic acoustical-optical phonon collision solver. This is part of a work in progress.

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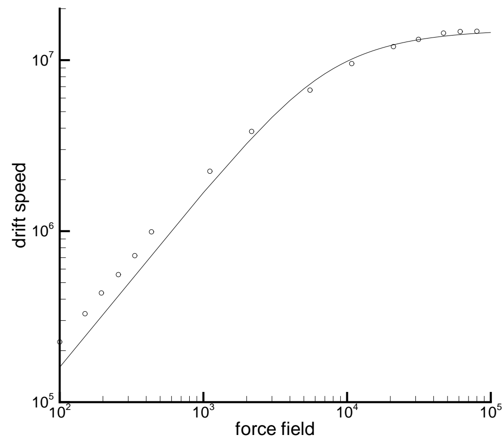

Figure 1: Drift speed for bulk Si. Solid line: Formula (1.4) with `Exemplar` values; circle symbols: the BTE system result by DSMC `Damocles`.

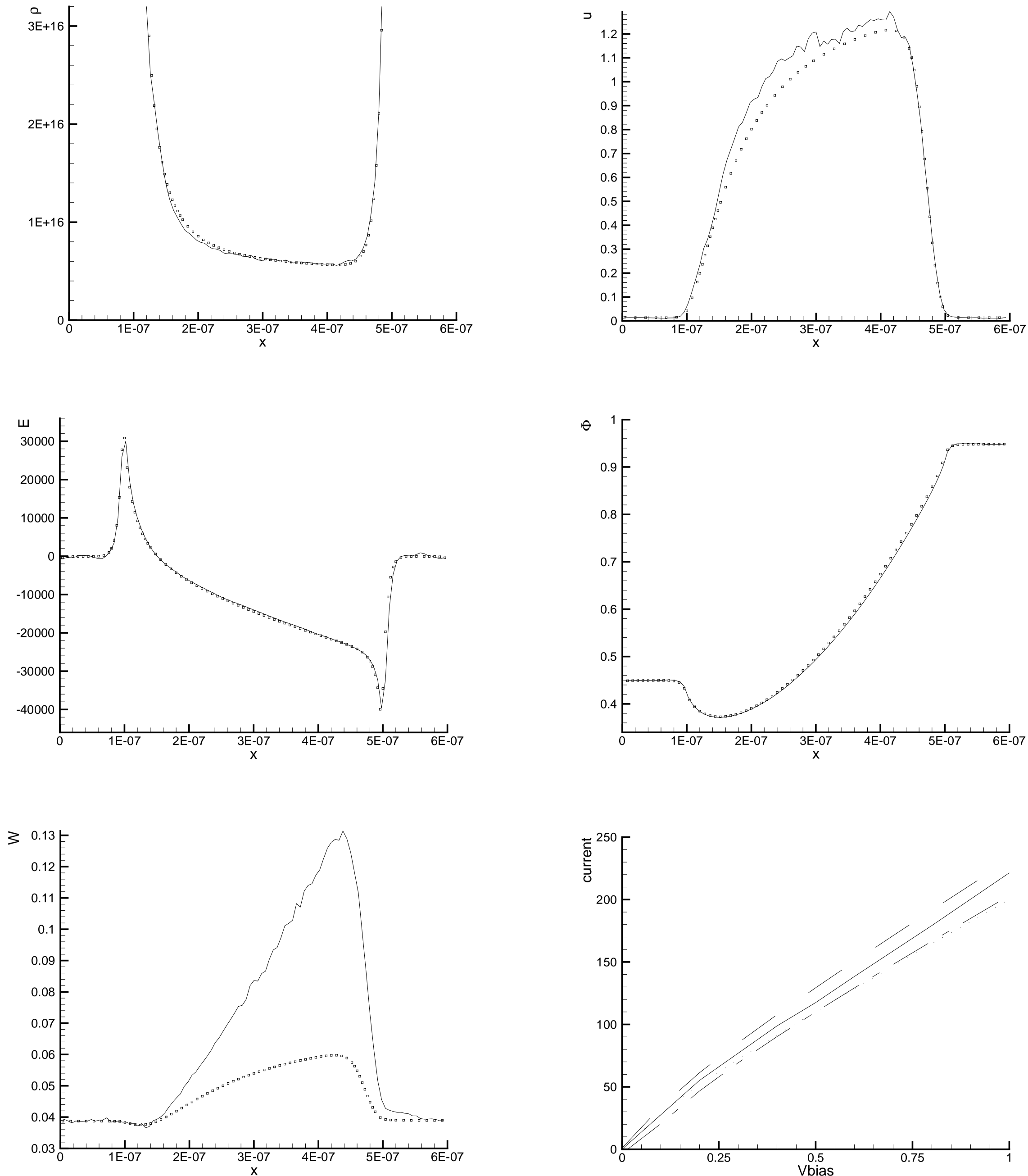

Figure 2: Numerical comparison of density (top left), mean velocity (top right), force field (middle left), potential (middle right), energy (bottom left) and IV-curves (bottom right) for the Si n$^+$-n-n$^+$ device with a $0.4\mu m$ channel at $V_{bias} = 0.5$V. Relaxation 1-D BTE by WENO (square symbols and dotted line); BTE system by DSMC `Damocles` (solid line); DDP system (dashed line) and the hybrid DDP-ADDP system (dash-dotted line).

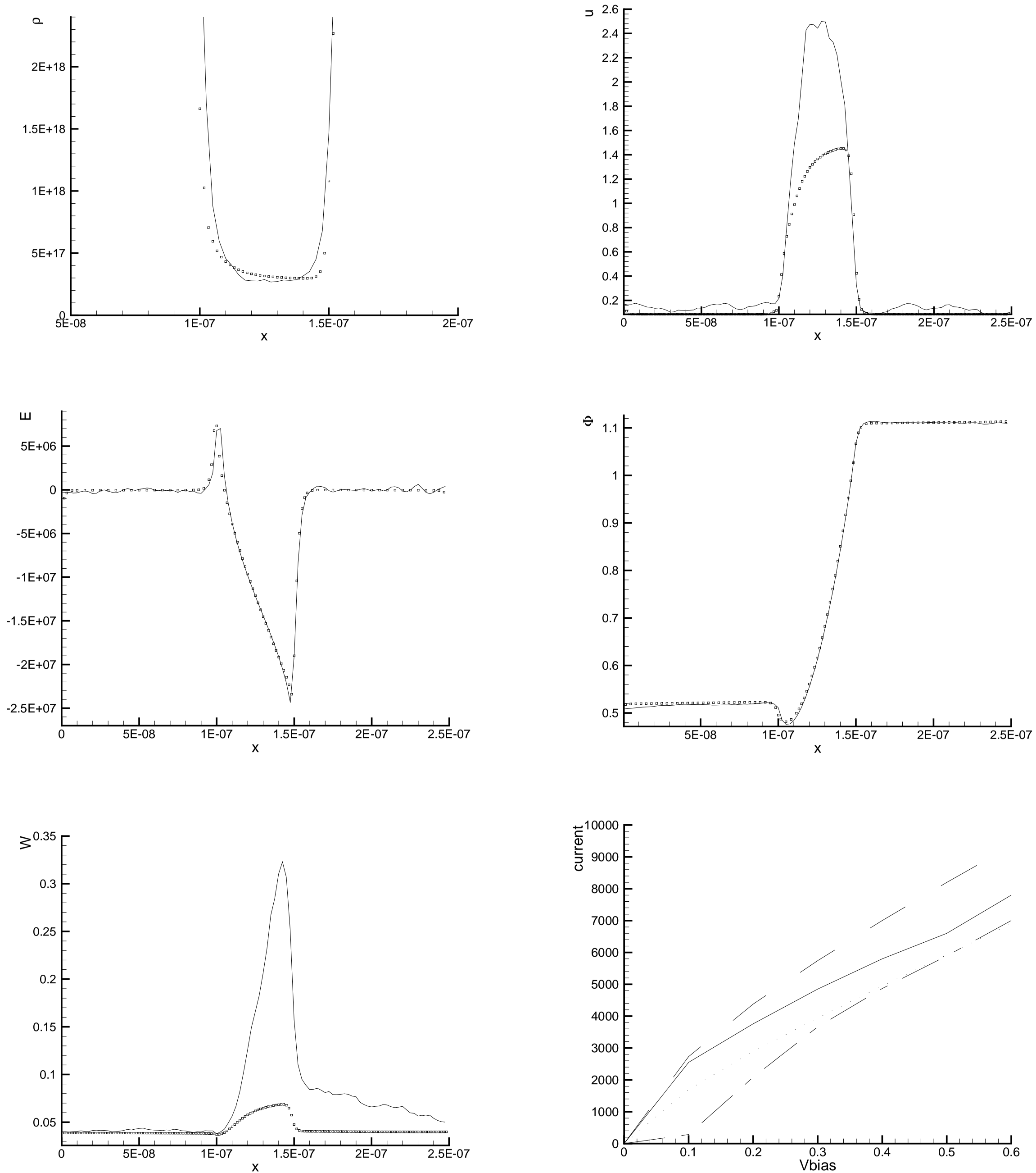

Figure 3: Numerical comparison of density (top left), mean velocity (top right), force field (middle left), potential (middle right), energy (bottom left) and IV-curves (bottom right) for the Si n$^+$-n-n$^+$ device with a $0.05\mu m$ channel at $V_{bias} = 0.6$V. Relaxation 1-D BTE by WENO (square symbols and dotted line); BTE system by DSMC `Damocles` (solid line); DDP system (dashed line) and the hybrid DDP-ADDP system (dash-dotted line).