Numerical solution for hydrodynamical models of semiconductors

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Abstract

Numerical solutions of recent hydrodynamical models of semiconductors are computed in one space dimension. Such models describe charge transport in semiconductor devices. Two models are taken into consideration. The first one has been developed by Blotekjaer, Baccarani et al., and the second one by Anile et al. In both cases the system of equations can be written as a convection-diffusion type system, with a right hand side describing relaxation effects and interaction with a self consistent electric field. The numerical scheme is a splitting scheme based on the Nessyahu-Tadmor scheme for the hyperbolic step, and a Crank-Nicolson scheme for the relaxation step. The numerical results are compared to detailed Monte Carlo simulation.

1 Indroduction

Charge transport in semiconductors has recently become an interesting research field in applied mathematics.

The model that has been used in engineering applications is the so called *Drift-Diffusion* model [1, 2]. Such model, however, is not accurate enough for submicron devices, and several relevant physical effects, such as inertial effects, are not captured by this model.

For devices with channel length of some tenths of micron, when direct quantum effects are negligible, an accurate physical description is given by semiclassical kinetic models. The carriers are described by a density function in phase space, satisfying a Boltzmann-like equation. The most effective technique for the numerical solution of such equation is Monte Carlo simulation. However, computational times required for an accurate solution are too large for a widespread use of Monte Carlo simulation as a practical CAD tool of semiconductor devices. It is therefore desirable to approximate the transport equation with simpler models

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which are accurate enough to maintain relevant physical effects of charge transport in submicron devices, and much faster to solve than kinetic models.

The Drift-Diffusion model can be derived from the kinetic equation by the Chapman-Enskog expansion [3]. These models are commonly used for device simulations. They provide a reasonable approximation when the channel length is large enough (say more than a few microns) with applied voltage of the order of one Volt. The evolution of the carriers is described by a balance equation, where the current is assumed a function of the density and density gradient.

With the reduction of the size of the devices, and the increase in electric field, the Drift-Diffusion approximation is no longer satisfying, and more sophisticated models are necessary, which are able to describe carrier evolution under the effect of high electric field.

Blotekjaer [4], Baccarani and Wordeman [5] proposed a model which is the analogue of the classical Navier-Stokes-Fourier model for dissipative fluids.

In BBW model, electrons are treated as an inviscid, thermal conducting, monoatomic gas. Heat flux is given by an empirical Fourier law, with a thermal conductivity that contains a fitting parameter. The latter is chosen to fit experimental data or Monte Carlo simulations. This expression for the heat flux has been recently criticized by Stettler [6] and Tang [7], who suggest to add an empirical convective term in the heat flux.

Anile et al. [8] (which we denote by AP) proposed a model based on *Extended Thermodynamics* [9, 10]. They obtain in a consistent way, an expression for the heat flux which contains a convective term, and has no fitting parameter, because all transport coefficients are obtained from the theory.

In the present paper we perform a numerical integration of the equations of AP and BBW models. As a test problem we consider the simulation of a $n^+ - n - n^+$ diode in 1D. The time dependent problem is solved. The stationary solution is obtained as a limit of the time dependent solution, for large enough time. The numerical solutions are then compared with detailed Monte Carlo simulations obtained by the DAMOCLES code developed by IBM [11, 12]

The mathematical structure of the system of equations is the same for both models. The differential part of the system can be written as a sum of a hyperbolic and parabolic term. The right hand side contains a relaxation term, which describes the interaction with the lattice, and a drift term due to the electric field. The latter is self-consistently computed via Poisson's equation.

The numerical scheme used is based on a splitting scheme. In the first step the hyperbolic part is solved, and in the second step diffusion, relaxation, and drift terms are computed. The hyperbolic step is solved by a variant of second order *shock-capturing* TVD scheme, recently developed by Nessyahu and Tadmor [13]. A Uniformly Non Oscillatory reconstruction from cell averages is used.

A similar problem was consider in [14] by using ENO schemes. The choice of the NT scheme is motivated by the following considerations. First we observe that, because of the convective term in the heat flux for AP model, the hyperbolic part of the equations is different from that of Euler's equations and there is no simple analytical expression of the characteristic speeds. The second reason is that more complex models can be derived by extended thermodynamics. They are described by hyperbolic systems with relaxation, and also in this case there is no simple expression for the characteristic speeds, therefore it is not practical to use upwind-based methods. NT scheme does not require the computation of the eigenvalues of the system, since the building block is Lax-Friedrichs scheme.

The plan of the paper is the following: in Section 2 we briefly recall the kinetic formulation, the Drift-Diffusion model, and the two hydrodynmical models (BBW and AP). In the third section we describe the numerical method used in the computation and the last section is devoted to the numerical results.

2 Mathematical models for semiconductors

In a doped semiconductor, the carriers (electrons and holes) move under the influence of the electric field, and interact with phonons and impurities of the crystal.

Energy transport in crystal is mainly carried by phonons [15]. A detailed physical description of transport phenomena requires a three component model, electrons, phonons, and holes, each of which satisfies a quantum transport equation coupled with Maxwell's equations for the electromagnetic field.

Carrier speed is at least three orders of magnitude smaller than light speed, and therefore it is justified to neglect effect of the magnetic field induced by the currents. A quasistatic approximation is assumed, where the self consistent electric field $\mathbf{E}$ is coupled to the system through the Poisson equation.

Furthermore, we shall neglect generation-recombination effects, whose characteristic time is of the order of nanoseconds. The relaxation of our system, in fact, takes place in times of the order of few picoseconds.

From now on we consider only one family of carriers, namely electrons. We shall assume that phonons are in thermodynamical equilibrium, and neglect the effect of the heating of the crystal. Therefore the phonons are described by an equilibrium distribution at temperature T_0.

In a semiclassical kinetic description, the electron dynamics is described by a transport equation for a one particle distribution function $f(\mathbf{x}, t, \mathbf{k})$, which represents the probability density to find a particle at time t at position $\mathbf{x}$ and with momentum $\mathbf{k}$,

$$\frac{\partial f}{\partial t} + v^i(\mathbf{k})\frac{\partial f}{\partial x^i} - eE^i\frac{\partial f}{\partial k^i} = \mathcal{C}[f]. \tag{1}$$

Here e represents the (positive) electron charge, $\mathbf{E}$ the electric field, $\mathbf{k}$ the electron impulse, belonging to the first Brillouin zone[1] [2].

$\mathcal{C}[f]$ is the collision term that describes the scattering with acoustical and optical phonons (see [16]). It is given by

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[1] Einstein summation over repeated indices is assumed. Physical units are such that $\hbar = 1$

$$\mathcal{C}[f] = \int d\mathbf{k}' \left[s(\mathbf{x}, \mathbf{k}', \mathbf{k}) f'(1-f) - s(\mathbf{x}, \mathbf{k}, \mathbf{k}') f(1-f') \right]. \tag{2}$$

The first term (gain) represents the probability that an electron in $\mathbf{x}$ and with momentum $\mathbf{k}'$ is scattered into an electron of momentum $\mathbf{k}$, while the second term (loss) represents the probability an electron is scattered from state $(\mathbf{x}, \mathbf{k})$ into state $(\mathbf{x}, \mathbf{k}')$.

The terms $1-f$ and $1-f'$ describe the effect of Pauli exclusion principle. Electron velocity $v(\mathbf{k})$ depends on the energy of the conduction band via the dispersion relation,

$$v(\mathbf{k}) = \nabla_{\mathbf{k}} \mathcal{E}.$$

In general, the band structure may be very complicated, and depends on the type and doping of the semiconductor. We shall consider a single band with parabolic approximation. The energy is therefore given by

$$\mathcal{E} = \frac{k^2}{m^*},$$

where m^* is electron effective mass. In this approximation, electron velocity is given by

$$v^i = \frac{k^i}{m^*}.$$

Consistently, the first Brillouin zone is extended to $\mathbf{R^3}$.

Equation (1) is a non linear integrodifferential equation in 7 variables. In actual devices the density in the conduction band is low enough that Pauli effect can be neglected.

By considering only elastic scattering, and neglecting Pauli correction, a good approximation of the collision term (2) is given by [1, 2]

$$\mathcal{C}[f] = -\frac{f - f_{eq}}{\tau(\mathcal{E}(\mathbf{k}))},$$

where τ rapresents the relaxation time, and f_{eq} is the Maxwell-Boltzmann limit of Fermi-Dirac distribution

$$f_{eq} = \exp\left(-\frac{\mathcal{E}(\mathbf{k}) - e(\phi - \mathcal{E}_F)}{k_B T_0} \right),$$

where T_0 is the lattice temperature, k_B the Boltzmann constant, ϕ the electrostatic potential, $(E = -\nabla\phi)$ and $\mathcal{E}_F$ the Fermi energy.

Let us consider the formal Hilbert expansion of density function f in power of the relaxation time τ

$$f = f_0 + \tau f_1 + \tau^2 f_2 + \cdots,$$

with $f_{eq} = f_0$. We assume that if $h = O(\tau^n)$ then $\nabla h = O(\tau^{n+1})$. Substituting the formal expansion in (1), one obtains, to first order in τ:

$$f = f_{eq} - \tau(\mathcal{E}(\mathbf{k}))\frac{f_{eq}}{k_B T_0}\left[\frac{\mathcal{E}(\mathbf{k}) - e(\phi - \mathcal{E}_F)}{k_B T_0}\mathbf{v}(\mathbf{k}) \cdot \nabla T_0 - e\mathbf{v}(\mathbf{k}) \cdot \nabla \mathcal{E}_F\right].$$

By introducing electron number density n and flux $\mathbf{F}$ by

$$n = \int d\mathbf{k} f \qquad \text{and} \qquad \mathbf{F} = \int d\mathbf{k}\frac{\mathbf{k}f}{m^*},$$

and integrating Eq.(1) with respect to $\mathbf{k}$ one obtains the balance equation for the density

$$\frac{\partial n}{\partial t} + \frac{\partial F^i}{\partial x^i} = R - G, \tag{3}$$

where $R - G$ is the electron-hole generation-recombination term (which we shall neglect).

Under the assumption that the electron temperature is equal to the (constant) lattice temperature T_0, and by introducing the mobility

$$\mu_n = \frac{(4\pi)^2 e}{3m^* k_b T_0 n}\int dk\, f_{eq} k^4 \tau(\mathcal{E}(\mathbf{k})),$$

one obtains

$$\mathbf{F} = \mu_n n \nabla\phi - D_n \nabla n, \tag{4}$$

where the diffusion coefficient is given by $D_n = \mu_n k_B T_0 / e$.

Equation (4), coupled with the analogue equation for holes and with the Poisson equation, constitute the well-known Drift-Diffusion model [1, 2].

For submicron devices, with electric potential of the order of 1 Volt, the assumption of constant electron temperature is no longer valid, since the electric field is strong enough to prevent thermodynamical equilibrium. It is therefore necessary a more detailed description of transport phenomena. Modified versions of the classical Drift-Diffusion model have been proposed, which include some effects related to temperature gradients, but hydrodynamical models seem more suitable to describe non equilibrium effects [17]. In BBW model, electrons are treated as an inviscid, thermal conducting fluid. The system is described by continuity equation, momentum balance equation, and energy balance equation,

$$\frac{\partial}{\partial t}n + \frac{\partial}{\partial x^i}(nv_i) = 0, \tag{5}$$

$$\frac{\partial}{\partial t}(nv_i) + \frac{\partial}{\partial x^j}\left(nv_iv_j + \frac{p}{m^*}\delta_{ij}\right) = -\frac{nv_i}{\tau_p} - neE_i, \tag{6}$$

$$\frac{\partial}{\partial t}\left(\frac{nv^2}{2} + \frac{3}{2}\frac{p}{m^*}\right) + \frac{\partial}{\partial x^i}\left[\left(\frac{nv^2}{2} + \frac{5p}{2m^*}\right)v_i + \frac{q_i}{m^*}\right] = -\frac{W - W_0}{m^*\tau_W} - \frac{nev_iE^i}{m^*} \tag{7}$$

coupled to the Poisson's equation

$$\epsilon \Delta \phi = -e(N_D - N_A - n).$$

Here N_A is the acceptor density, N_D the donor density , ϵ the dielectric constant, $W_0 = \frac{3}{2} n k_B T_0$. W is the energy density given by

$$W = \frac{1}{2} n m^* v^2 + \frac{3}{2} n k_B T,$$

where T is the electron temperature, which is related to the pressure p by ideal gas law

$$p = n k_B T.$$

The heat flux satisfies Fourier's law

$$q_i = -kn \frac{\partial T}{\partial x^i},$$

where

$$k = \left(\frac{5}{2} + c \right) k_B^2 \frac{T \tau_p}{m^*}.$$

c is a free parameter, whose value is chosen in order to fit experimental or Monte Carlo simulations.

Relaxation times are given by the following phenomenological expressions

$$\begin{aligned} \tau_p &= \frac{m^* \mu_n T_0}{eT}, \\ \tau_W &= \mu_n T_0 \left(\frac{m^*}{2eT} + \frac{3T}{2 e v_S^2 (T + T_0)} \right), \end{aligned}$$

where μ_n is low field mobility, $v_S = 1.03 \times 10^7$cm/sec is saturation velocity.

BBW equations have been solved numerically, both in the stationary [18, 19] and nonstationary case [14]. This model, however, does not have the correct limit near thermodynamical equilibrium [20], since it does not satisfy Onsager's reciprocity conditions [21].

A recent formulation of constitutive equations, in better agreement with the linear theory of irreversible process, has been obtained for the heat flux by Anile et al. [8]. The formulation is based on the theory of Extended Thermodynamics [9, 10]. The same derivation can be obtained by the moment method approach of Levermore [22].

If we define the moments,

$$F_{i_1 i_2 \cdots i_n} = \frac{1}{(m^*)^n} \int d\mathbf{k} f k_{i_1} k_{i_2} \cdots k_{i_n},$$

the transport equation (1) can be replaced by the infinite system for the moments, obtained by multiplying Eq.(1) by $k^{i_1} k^{i_2} \cdots k^{i_n}$ and integrating in $\mathbf{k}$ space. The generic equation is of the form:

$$\frac{\partial}{\partial t}F_{i_1 i_2 \cdots i_n} + \frac{1}{m^*}\frac{\partial}{\partial x^k}F_{i_1 i_2 \cdots i_n k} = Q_{i_1 i_2 \cdots i_n} - eE^i \int d\mathbf{k}\frac{f}{(m^*)^n}\frac{\partial}{\partial k^i}k_{i_1}k_{i_2}\cdots k_{i_n} \tag{8}$$

where $Q_{i_1 i_2 \cdots i_n}$ are the moments of the collision term

$$Q_{i_1 i_2 \cdots i_n k} = \frac{1}{(m^*)^n}\int d\mathbf{k}\mathcal{C}[f]k^{i_1}k^{i_2}\cdots k^{i_n}.$$

In this way the number of independent variables is reduced to four, but it is necessary to find a way to truncate the infinite system of equations. The equation for moment of order N, in fact, contains the moment of order $N+1$, an therefore the system is never closed.

Because of the analogy with standard hydrodynamics, we shall consider a model whose moments have an immediate physical interpretation.

We introduce from a kinetic point of view particle numerical density, $n = F$, flux F_i, energy density for unit mass,

$$\frac{1}{2}F_{ii} = \frac{1}{2}\int \frac{d\mathbf{k} f k^2}{(m^*)^2},$$

flux momentum density,

$$F_{ij} = \int \frac{d\mathbf{k} f k_i k_j}{(m^*)^2},$$

flux energy density,

$$\frac{1}{2}F_{ill} = \frac{1}{2}\int \frac{d\mathbf{k} f k_i k^2}{(m^*)^3},$$

and neglect generation-recombination effects. The balance equations for the first thirteen moments take the form

$$\begin{aligned}
\frac{\partial F}{\partial t} + \frac{\partial}{\partial x^k}F_k &= 0, && (9)\\
\frac{\partial F_i}{\partial t} + \frac{\partial}{\partial x^k}F_{ik} &= Q_i - \frac{neE_i}{m^*}, && (10)\\
\frac{\partial F_{ll}}{\partial t} + \frac{\partial}{\partial x^k}F_{llk} &= Q - \frac{2ne}{m^*}\mathbf{v}\cdot\mathbf{E}, && (11)\\
\frac{\partial F_{<ij>}}{\partial t} + \frac{\partial}{\partial x^k}F_{<ij>k} &= Q_{<ij>} - \frac{2ne}{m^*}E_{<i}v_{j>}, && (12)\\
\frac{\partial F_{ill}}{\partial t} + \frac{\partial}{\partial x^k}F_{ikll} &= \hat{Q}_i - \frac{e}{m^*}\left(2F_{il}E^l + F^{ll}E_i\right), && (13)
\end{aligned}$$

where Q_i, Q, $Q_{<ij>}$, $\hat{Q}_i$ are production terms for momentum, energy, the deviatoric part of the stress tensor[2], energy flux. By introducing the notation

$$F^A = (F, F_i, F_{ll}, F_{<ij>}, F_{ill}), \qquad \mathrm{A} = 1, 2, \cdots, 13$$

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[2] The deviatoric part of a tensor is given by the symmetric trace-free part. For example $A_{<ij>} = \frac{1}{2}(A_{ij} + A_{ji}) - \frac{1}{3}A_{ll}\delta_{ij}$

$$\begin{aligned}
F^{Aj} &= (F_i, F_{ij}, F_{ill}, F_{<ij>k}, F_{ijll}),\\
P^A &= (0, Q^i - \frac{neE_i}{m^*}, Q - \frac{2ne}{m^*}\mathbf{v}\cdot\mathbf{E},\\
&\qquad Q_{<ij>} - \frac{2ne}{m^*}E_{<i}v_{j>}, \hat{Q}_i - \frac{e}{m^*}\left(2F_{il}E^l + F^{ll}E_i\right)),
\end{aligned}$$

the balance equations can be written in a compact form

$$\frac{\partial F^A}{\partial t} + \frac{\partial F^{Aj}}{\partial x^j} = P^A. \tag{14}$$

In order to close system (14), it is necessary to express F_{ijk}, F_{ijll} and the production terms P^A as function of the components of F^A. By following the principles of Extended Thermodynamics , we assume that there exists a supplementary balance law

$$\frac{\partial S(F^A)}{\partial t} + \frac{\partial S^i(F^A)}{\partial x^i} = g(F^A) \geq 0 \tag{15}$$

which is valid for any solution of system (14). In the previous equation, S, S^i and g represents entropy, entropy flux, and entropy production.

In the deduction of constitutive equations, the electric field is assumed to be external and therefore it does not contribute to entropy production.

By applying Liu's theorem [23], it is possible to take into account Eq.(15) by introducing Lagrange multipliers Λ_A and by imposing that for arbitrary values of the fields F^A and their derivative, the following relation holds

$$\frac{\partial S(F^A)}{\partial t} + \frac{\partial S^i(F^A)}{\partial x^i} - \sum_A \Lambda_A \left(\frac{\partial F^A}{\partial t} + \frac{\partial F^{Aj}}{\partial x^j} - P^A\right) \geq 0. \tag{16}$$

From this inequality it follows

$$\begin{aligned}
&\frac{\partial S(F^A)}{\partial t} + \frac{\partial S^i(F^A)}{\partial x^i} - \sum_A \Lambda_A \left(\frac{\partial F^A}{\partial t} + \frac{\partial F^{Aj}}{\partial x^j}\right) = 0,\\
&\sum_A \Lambda_A P^A \geq 0.
\end{aligned}$$

In principle, from Eq.(16) it is possible to deduce the required constitutive laws. However, because of the nonlinear terms, an explicit analytical representation is not possible.

For our purposes it is sufficient to obtain a linearized version of constitutive relations. This is obtained by inverting relation (16) near partial thermodynamical equilibrium, characterized by $T = T_0$, and zero velocity, heat flux and stress tensor. In this way, first order deviations from partial thermodynamical equilibrium are obtained

$$F_{ijk} = nv_iv_jv_k + \frac{1}{m^*}\left[3v_{(i}\sigma_{jk)} + 3pv_{(i}\delta_{jk)} + \frac{6}{5}q_{(i}\delta_{jk)}\right],$$

$$
\begin{aligned}
F_{ijll} &= nv_iv_jv^2 + \frac{1}{m^*}\left[5\frac{p^2}{nm^*}\delta_{ij} + 3pv_iv_j + v^2\sigma_{ij} + pv^2\delta_{ij} + \right. \\
& \left. \frac{7p}{nm^*}\sigma_{ij} + 4v^kv_{(j}(\sigma_{ki)} + p\delta_{ki)}) + 4v_{(i}q_{j)} + \frac{6}{5}q_{(i}\delta_{jk)}v^k\right],
\end{aligned}
$$

where q^i is the heat flux, and σ_{ij} the stress tensor[3]. Substituting the closure relations into system (14), one obtains a closed system for the thirteen unknowns F^A. The properties of this system will be investigated in a forthcoming paper. Here we shall consider a simplified model that can be derived from system (14), which is similar to the Navier-Stokes model for dissipative fluids: the evolution equations are the usual balance law for density, momentum and energy, while the constitutive relations for shear and heat flux are deduced from the corresponding balance equations (11), (12) by performing the so called *Maxwellian iteration* [24, 20]. This procedure is similar to the Chapman-Enskog expansion of the Boltzmann equation. The field is written as a formal expansion in terms of a small parameter representing, in the case of semiconductors, deviation from *partial thermal equilibrium* [20], and derivatives are assumed to be of higher order in this parameter.

If we rewrite the components of F^A in the more familiar form

$$
\begin{aligned}
F_{ij} &= nv_iv_j + \frac{1}{m^*}(\sigma_{ij} + p\delta_{ij}), \\
F_{ll} &= nv^2 + \frac{3p}{m^*}, \\
F_{ill} &= nv^2v^i + \frac{1}{m^*}\left(5pv^i + 2q^i + 2\sigma_{ij}v^j\right),
\end{aligned}
$$

to first order one obtain the following constitutive equations [8]

$$
\begin{aligned}
\sigma_{ij} &= 0, && (17) \\
q_i &= -\frac{5nk_B^2T\tau_q}{2m^*}\frac{\partial T}{\partial x^i} + \frac{5}{2}nk_BTv_i\left(\frac{1}{\tau_p} - \frac{1}{\tau_q}\right)\tau_q. && (18)
\end{aligned}
$$

At variance with BBW model, Eq. (18) does not contain free parameters. Moreover, due to the presence of the convective term in the constitutive equation for the heat flux, Onsager relations for small deviations from thermodynamical equilibrium are satisfied [20].

About production terms, we shall use the same approximation used in BBW, but with relaxation times given by Monte Carlo simulation.

3 Numerical method

Let us write the 1D version of the equations of the two models

$$
\frac{\partial}{\partial t}n + \frac{\partial}{\partial x}(nv) = 0, \qquad (19)
$$

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[3] Parenthesis around indices mean symmetrization. For example $A_{(ij)} = 1/2(A_{ij} + A_{ji})$

$$\frac{\partial}{\partial t}(nv) + \frac{\partial}{\partial x}\left(nv^2 + \frac{p}{m^*}\right) = -\frac{nv}{\tau_p} - neE, \tag{20}$$

$$\begin{aligned}&\frac{\partial}{\partial t}\left(nv^2 + 3\frac{p}{m^*}\right) + \frac{\partial}{\partial x}\left(nv^3 + \frac{5pv}{m^*} + \frac{2q}{m^*}\right) = \\ &-2\frac{W - W_0}{m^*\tau_W} - \frac{2nevE}{m^*}.\end{aligned} \tag{21}$$

Heat flux q is given by

$$q = -\frac{5nk_B^2 T\tau_q}{2m^*}\frac{\partial T}{\partial x} + \frac{5}{2}nk_B Tv\left(\frac{\tau_q}{\tau_p} - 1\right) \tag{22}$$

for AP model, and by

$$q = -\left(\frac{5}{2} + c\right)k_B^2\frac{T\tau_p}{m^*}$$

for BBW model. The equations must be supplemented with Poisson's equation.

For future reference it is better to write the previous equations in a more compact form. Let us define the following vector fields

$$\begin{aligned}\mathbf{U} &= (n, nv, 2W), \\ \mathbf{f_{BBW}} &= \left(nv, nv^2 + \frac{p}{m^*}, nv^3 + \frac{5pv}{m^*}\right), \\ \mathbf{f_{AP}} &= \left(nv, nv^2 + 3p, nv^3 + 5\frac{pv}{m^*}\frac{\tau_q}{\tau_p}\right), \\ \mathbf{g_{BBW}} &= \left(0, -\frac{nv}{\tau_p} - nE, -2\frac{W - W_0}{\tau_w} - 2nvE + 2\frac{\partial}{\partial x}\left(kn\frac{\partial T}{\partial x}\right)\right), \\ \mathbf{g_{AP}} &= \left(0, -\frac{nv}{\tau_p} - nE, -2\frac{W - W_0}{\tau_w} - 2nvE + \frac{\partial}{\partial x}\left(\frac{5nk_B^2 T\tau_q}{m^*}\frac{\partial T}{\partial x}\right)\right).\end{aligned}$$

The system are then written as

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{f_{BBW}}}{\partial x} = \mathbf{g_{BBW}} \tag{23}$$

for BBW model, and

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{f_{AP}}}{\partial x} = \mathbf{g_{AP}}, \tag{24}$$

for AP model.

The left hand side of Eqs.(23) and (24) represents a quasilinear hyperbolic operator, while the right hand side contains relaxation, diffusion and drift terms. We make use of a splitting scheme, based on the following decomposition. Let us consider a system of the form

$$\mathcal{U}_t + \mathcal{A}(\mathcal{U})\mathcal{U}_x = \mathcal{B}(\mathcal{U}), \tag{25}$$

where $\mathcal{U} = (u_1, \cdots, u_N)$ is the unknown vector, $\mathcal{A}$ and $\mathcal{B}$ are matrix functions of $\mathcal{U}$.

Let A and B be two operators that represent the finite difference approximation of $\mathcal{A}\mathcal{U}_x$ and $\mathcal{B}\mathcal{U}$. For simplifying the analysis we assume that A and B are represented by constant coefficient matrices.

The solution of

$$\mathcal{U}_t + A\mathcal{U} = 0,$$

with

$$\mathcal{U}(t) = \mathcal{U}_0$$

is given by

$$\mathcal{U}_1(t + \Delta t) = \exp(-\Delta t A)\mathcal{U}_0 = \mathcal{U}_0 - \Delta t A\mathcal{U}_0 + o(\Delta t). \tag{26}$$

The solution of

$$\mathcal{U}_t = B\mathcal{U},$$

with

$$\mathcal{U}(t) = \mathcal{U}_1(t + \Delta t)$$

is given by

$$\mathcal{U}_2(t) = \exp(\Delta t B)\mathcal{U}_1(t + \Delta t). \tag{27}$$

On the other hand, the solution of (25) is given by

$$\mathcal{U} = \exp[(B - A)\Delta t]\mathcal{U}_0. \tag{28}$$

By comparing the formal expansion of (26) and (27) it appears that solution (27) agrees with (28) to first order in Δt, therefore if A and B are consistent discretization of the corresponding differential operators, the simple splitting constitutes a first order consistent method.

The splitting scheme that we use is therefore

$$\mathcal{U}_t + A\mathcal{U} = 0, \tag{29}$$

(convection step)

$$\mathcal{U}_t = B\mathcal{U}, \tag{30}$$

(relaxation step) with initial data given by the solution of (27).

We shall call this scheme *simple splitting* (SP). Note that this scheme is only first order in time, independently of the accuracy of the solution of the two steps.

A better scheme is obtained by a more sophisticated splitting strategy, as shown at the end of the section.

3.1 Convection step

During the convection step one integrates the quasilinear hyperbolic system

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{U})}{\partial x} = \mathbf{0}. \tag{31}$$

It is well known that the solutions of such systems suffer loss of regularity and may develop discontinuities. There is a wide literature on shock capturing schemes for hyperbolic systems of conservation laws, which are second order accurate in space in the region of regularity, and give sharp shock profile. A recent account on numerical methods for conservation laws is given in [25]. Higher order methods have been developed, and used for solving problems in semiconductor device simulation, such as ENO schemes (see [14]). Such schemes, however, require an exact or approximate Riemann solver, or at least the knowledge of the characteristic structure of the Jacobian matrix. For systems similar to gas dynamics, an approximate Riemann solver based on the Roe matrix is used. Such approach is suitable in the case of BBW model, since the hyperbolic operator is the same as the one in gas dynamics, and therefore the analytical expression for the eigenvalues and eigenvectors is explicitly known. In AP model, the presence of the term τ_q/τ_p does not allow us to write down a simple analytical expression for the eigenvalues of the system (see next section). Therefore it is desirable to use a shock-capturing scheme that does not require the explicit knowledge of the characteristic structure of the system. The scheme proposed by H. Nessyahu e E. Tadmor (NT) [13] has these properties. Its building block is Lax-Friedrichs scheme, corrected by a MUSCL type interpolation that guarantees second order in smooth regions and TVD property [26].

For sake of completeness, we report the derivation of NT scheme and UNO reconstrution. For more details, see [13, 27].

Let us consider a system of the form

$$\frac{\partial v}{\partial t} + \frac{\partial F(v)}{\partial x} = 0, \tag{32}$$

where $v \in \mathbf{R}^m$ and $F : \mathbf{R}^m \to \mathbf{R}^m$. We introduce a uniform grid in x, x_1, x_2, $\cdots$, x_N, and in t, t_1, t_2, $\cdots$.

By integrating Eq.(32) on a cell $[x_j, x_{j+1}] \times [t_n, t_{n+1}]$, one obtains

$$\overline{v}_{j+\frac{1}{2}}(t_n+\Delta t) = \overline{v}_{j+\frac{1}{2}}(t_n) - \frac{1}{\Delta x}\left[\int_{t_n}^{t_n+\Delta t} F(v(x_{j+1},\tau))d\tau - \int_{t_n}^{t_n+\Delta t} F(v(x_j,\tau))d\tau\right], \tag{33}$$

where

$$\overline{v}_{j+\frac{1}{2}}(t_n) = \frac{1}{\Delta x}\int_{x_j}^{x_{j+1}} v(y,t_n)dy$$

represents the cell average of $v(x,t)$ in $[x_j, x_{j+1}]$ for $t = t_n$. The integral of the flux $F(v(x,t))$ is computed by the midpoint quadrature rule:

$$\int_{t_n}^{t_n+\Delta t} F(v(x_j,\tau))d\tau = \Delta t\, F\left(v(x_j, t_n + \frac{\Delta t}{2}\right) + O(\Delta t^3). \tag{34}$$

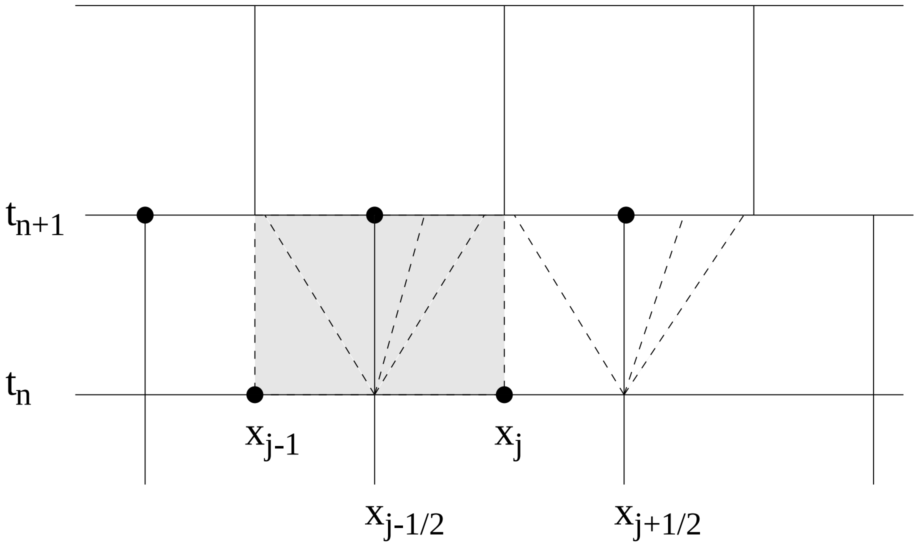

Figure 1: NT scheme on a staggered grid

The quantity $v(x_j, t_n + \Delta t/2)$, is computed according to Lax-Wendroff approach, by using Taylor's formula:

$$v(x_j, t + \frac{\Delta t}{2}) = v_j(t) - \frac{1}{2}\lambda F'_j + O(\Delta t^2),$$

where $F'_j/\Delta x$ is an approximation of the derivative of the flux (yet to be specified), and $\lambda = \frac{\Delta t}{\Delta x}$. In order to obtain a second order scheme we require that

$$\frac{1}{\Delta x} F'_j = \frac{\partial}{\partial x} F(v(x,t)) + O(\Delta x).$$

By substituting (34) into (33), one has a relation that involves both cell averages and point values of the solution.

By introducing a MUSCL interpolation, we approximate $v(x,t)$ by a piecewise linear polynomial

$$L_j(x,t) = v_j(t) + (x - x_j)\frac{1}{\Delta x} v'_j, \qquad x_{j-\frac{1}{2}} \leq x \leq x_{j+\frac{1}{2}}.$$

and in order to ensure a second order accuracy we require that

$$\frac{1}{\Delta x} v'_j = \frac{\partial}{\partial x} v(x_j, t) + O(\Delta x). \tag{35}$$

Therefore, Eq. (35) gives

$$v_{j+\frac{1}{2}}(t + \Delta t) = \frac{1}{2}\left[v_j(t) + v_{j+1}(t)\right] + \frac{1}{8}\left[v'_j - v'_{j+1}\right] +$$
$$-\lambda \left[F(v_{j+1}(t_n) - \frac{1}{2}\lambda F'_{j+1}) - F(v_j(t_n) - \frac{1}{2}\lambda F'_j)\right] + O(\Delta t^3).$$

Because the initial state at $t = t_n$ is given by the piecewise linear function $L_j(x, t_n)$, the fluxes remain regular functions if the solution to the corresponding generalized Riemann problems between adjacent cells do not interact.

This is obtained by imposing the following CFL condition

$$\lambda \cdot \max \rho(A(v(x,t)) < \frac{1}{2} \tag{36}$$

where $\rho(A(v(x,t))$ is the spectral radius of the Jacobian matrix,

$$A = \frac{\partial F}{\partial v}.$$

In this way a family of predictor-corrector schemes is obtained:

$$v_j^{n+\frac{1}{2}} = v_j^n - \frac{1}{2}\lambda F_j',$$

$$v_{j+\frac{1}{2}}^{n+1} = \frac{1}{2}\left[v_j^n + v_{j+1}^n\right] - \lambda\left[g_{j+1} - g_j\right],$$

where

$$g_j = F(v_j^{n+\frac{1}{2}}) + \frac{1}{8\lambda} v_j'.$$

Such schemes are conservative and consistent, which is a necessary requirement for correct shock capturing.

In order to determine the expression of v_j' and F_j', we make use of a Uniform Non Oscillatory reconstruction [27], which guarantees uniform second order accuracy (even near local extrema) for smooth solutions.

Starting from cell average of $v(x,t)$, one constructs a piecewise quadratic polynomial $Q(x,t)$, such that

$$\begin{aligned} Q(x_j, t) &= v(x_j, t) + O(\Delta x^3), \\ \frac{d}{dx} Q(x \pm 0, t) &= \frac{dv(x,t)}{dx} + O(\Delta x^2), \end{aligned}$$

when $v(x,t)$ is a regular function.

The required condition on $Q(x,t)$ is to be non oscillatory, in the sense that its number of local extrema is not larger than that of $v(x,t)$. This is obtained with an appropriate choice of the stencil.

For $x_j \le x \le x_{j+1}$, the two candidates to $Q(x,t)$ are the polynomial interpolating the function on the nodes x_{j-1}, x_j, x_{j+1}, and the one interpolating the function on the nodes x_j, x_{j+1}, x_{j+2}. The one which is closer to the line through points $(x_j, v(x_j,t))$ e $(x_{j+1}, v(x_{J+1}, t))$ is chosen.

In the interval $x_j \le x \le x_{j+1}$ we write

$$Q(x, \cdot) = v_j + d_{j+\frac{1}{2}} v \frac{x - x_j}{\Delta x} + \frac{1}{2} D_{j+\frac{1}{2}} v \frac{(x - x_j)(x - x_{j+1})}{(\Delta x)^2},$$

with

$$d_{j+\frac{1}{2}}v = v_{j+1} - v_j.$$

Then one has

$$D_{j+\frac{1}{2}}v = v_{j+1} - 2v_j + v_{j-1}$$

if we choose x_{j-1}, x_j, x_{j+1}, and

$$D_{j+\frac{1}{2}}v = v_{j+2} - 2v_{j+1} + v_j$$

if we choose x_j, x_{j+1}, x_{j+2}.

This choice can be expressed in the form

$$D_{j+\frac{1}{2}}v = MM(v_{j+2} - 2v_{j+1} + v_j, v_{j+1} - 2v_j + v_{j-1}) \tag{37}$$

where $MM(x,y)$ is the min mod function, defined by

$$MM(x,y) = \begin{cases} sgn(x) \cdot \min(|x|, |y|) & \text{if} sgn(x) = sgn(y) \\ 0 & \text{otherwise.} \end{cases}$$

We can compute the slope of $L_j(x,t)$ by

$$\frac{v_j'}{\Delta x} = MM\left(\frac{d}{dx}Q(x_j - 0, t), \frac{d}{dx}Q(x_j + 0), t)\right).$$

that is by

$$v_j' = MM\left(d_{j-\frac{1}{2}}v + \frac{1}{2}MM(D_{j-1}, D_j), d_{j+\frac{1}{2}}v - \frac{1}{2}MM(D_j, D_{j+1})\right) \tag{38}$$

where

$$D_j = v_{j+1} - 2v_j + v_{j-1}.$$

The computation of F_j' can be obtained by a similar reconstruction, from the values of $F(\overline{v}_j^n)$. or by the Jacobian matrix

$$F_j' = \frac{\partial F}{\partial v}(v_j)v_j'.$$

Because of the staggered grid, we perform the convection step by two NT steps, so that the field for the relaxation step is computed on a non staggered grid.

3.2 Relaxation step

The relaxation step has been solved by a semi-implicit Euler scheme, in order to avoid stability restriction on the time step Δt. In the case of AP model the equations are

$$\begin{aligned} \frac{dn}{dt} &= 0, \qquad (39) \\ \frac{dm}{dt} &= -\frac{m}{\tau_p} - \frac{neE}{m^*}, \qquad (40) \\ \frac{d2W}{dt} &= -2\frac{W-W_0}{\tau_W} - 2meE - 2\frac{\partial q}{\partial x} \qquad (41) \end{aligned}$$

with $m = nv$. During the relaxation step from t_n to t_{n+1} we approximate the relaxation times, τ_p, τ_W and τ_q, to the value that they assume at time t_n.

From Eq. (39) we have

$$n_j^{n+1} = n_j^n, \qquad (42)$$

therefore during the relaxation step the electric field E is constant. The electric potential is obtained by solving the tridiagonal system

$$\epsilon(\phi_{j+1} - 2\phi_j + \phi_{j-1}) = -(\Delta x)^2 \left(N_D - N_A - n_i^n\right)$$

by standard procedure.

The electric field is computed from the potential by centered differences.

From Eq. (40) one has

$$m_j^{n+1} = \left(m_j^n + \frac{n_j e E_j^n \tau_{pj}^n}{m^*}\right) \exp(-\frac{\Delta t}{\tau_{pj}^n}) - \frac{n_j^n e E_j^n}{m^*}\tau_{pj}^n.$$

It is more convenient to integrate an equation for the temperature T, rather that Eq. (41),

$$\frac{dT}{dt} = \frac{1}{3}\frac{m^*}{k_B}\left(\frac{2}{\tau_p} - \frac{1}{\tau_W}\right) v^2 - \frac{T - T_0}{\tau_W} + \frac{5k_B}{3nm^*}\frac{\partial}{\partial x}\left[n\tau_q T \frac{\partial T}{\partial x}\right]. \qquad (43)$$

Let

$$\begin{aligned} A &= \frac{5k_B}{3nm^*}, \\ H &= \frac{1}{3}\frac{m^*}{k_B}\left(\frac{2}{\tau_p} - \frac{1}{\tau_W}\right) v^2 + \frac{T_0}{\tau_W}, \\ G &= n\tau_q, \end{aligned}$$

Then Eq. (43) is discretized as

$$\frac{T_j^{n+1} - T_j^n}{\Delta t} = -\frac{T_j^{n+1}}{\tau_{Wj}} +$$
$$\frac{A_j}{(\Delta x)^2}\left[G_{j+\frac{1}{2}}^n T_{j+\frac{1}{2}}^n (T_{j+1}^{n+1} - T_j^{n+1}) - G_{j-\frac{1}{2}}^n T_{j-\frac{1}{2}}^n (T_j^{n+1} - T_{j-1}^{n+1})\right] + H_j,$$

with

$$G_{j+\frac{1}{2}} = \frac{G_{j+1} + G_{j-1}}{2}$$

A similar equation can be written for $T^n_{j+\frac{1}{2}}$.

Once more we obtain a tridiagonal system for T_j^{n+1} which can be solved by standard technique.

A similar procedure has been used in order to integrate the BBW equations.

3.3 Second order splitting

Because of the splitting, scheme SP is not second order accurate even for the computation of steady state solutions.

Accuracy can be improved by using a better splitting strategy.

A second order scheme, uniformly accurate in the relaxation times, has been developed in [28] for a first order convection step, and in [29] for NT-convection step.

The latter scheme, generalized to the case where an electric field is present, is given by the following steps: given the fields at time t_n, (U^n, E^n), the fields at time t_{n+1} are obtained as

$$\begin{aligned}
U_1 &= U^n - R(U_1, E^n, \Delta t), \\
U_2 &= \frac{3}{2}U^n - \frac{1}{2}U_1, \\
U_3 &= U_2 - R(U_3, E^n, \Delta t), \\
U_4 &= \mathcal{C}_\Delta t U_3, \\
E^{n+1} &= \mathcal{P}(U_4), \\
U^{n+1} &= U_4 - R(U^{n+1}, E^{n+1}, \Delta t/2)
\end{aligned}$$

where R represents the numerical operator corresponding to relaxation step, $\mathcal{C}_\Delta t$ represents the numerical convection operator corresponding to two steps of NT scheme, $\mathcal{P}(U)$ gives the solution of Poisson's equation.

4 Numerical results

As test problem we consider the numerical solution of a balistic diode $n^+ - n - n^+$, which models the channel of a MOSFET. The device is made of silicon and its temperature is 300 K. The n^+ regions are $0.1 \mu m$ long, and the n region is 0.4 μm long. In n^+ regions the doping density is $n_0 = 10^{18}$ cm^{-3}, and in the n region the doping density is $n_0 = 10^{16}$ cm^{-3}.

The effective electron mass, in the approximation of parabolic band, is $m^* = 0.32\ m_e$ where m_e is the electron mass [30]. The dielectric constant of silicon is $\epsilon = \epsilon_r \epsilon_0$, where ϵ_r =11.7 is the relative dielectric constant and $\epsilon_0 = 8.85 \times 10^{-18} C/V \mu m$ is the dielectric constant of vacuum.

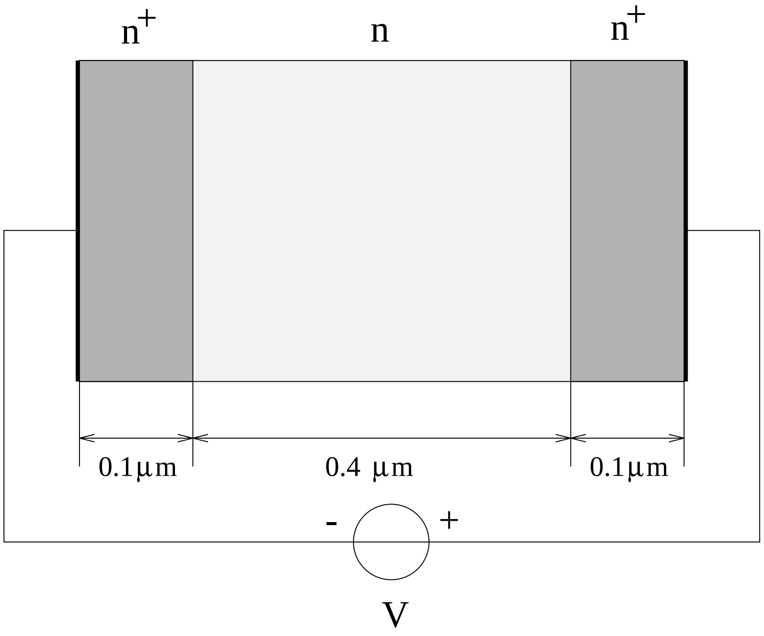

Figure 2: $n^+ - n - n^+$ diode

Relaxation times τ_W, τ_p τ_q, respectively of energy, momentum, and energy flux, have been obtained by a fitting of the results of Monte Carlo simulations [12]. They can be expressed as function of the total energy per electron, by the following formulas

$$\tau_A = a + b(\mathcal{E} - 1) + c \exp(-d(\mathcal{E} - 1)),$$

where $\tau_A = \tau_p, \tau_w, \tau_q$, with

$$\mathcal{E} = \frac{\text{energy per electron in eV}}{0.025\text{eV}}$$

Coefficients a, b, c, d are reported in Tables 1 and 2.

Table 1: Coefficients for the fitting of relaxation times

	τ_p	τ_W	τ_q
a	0.0681	0.1731	0.0471
b	-0.0023	0.0313	-0.0007
c	0.2051	0.2382	0.1330
d	0.9547	0.5167	0.6911

In Fig. 3 we report the values of the relaxation times that have been used in the calculations, for a channel length of 0.4 μm. It appears that $\tau_q/\tau_p \neq 1$, and

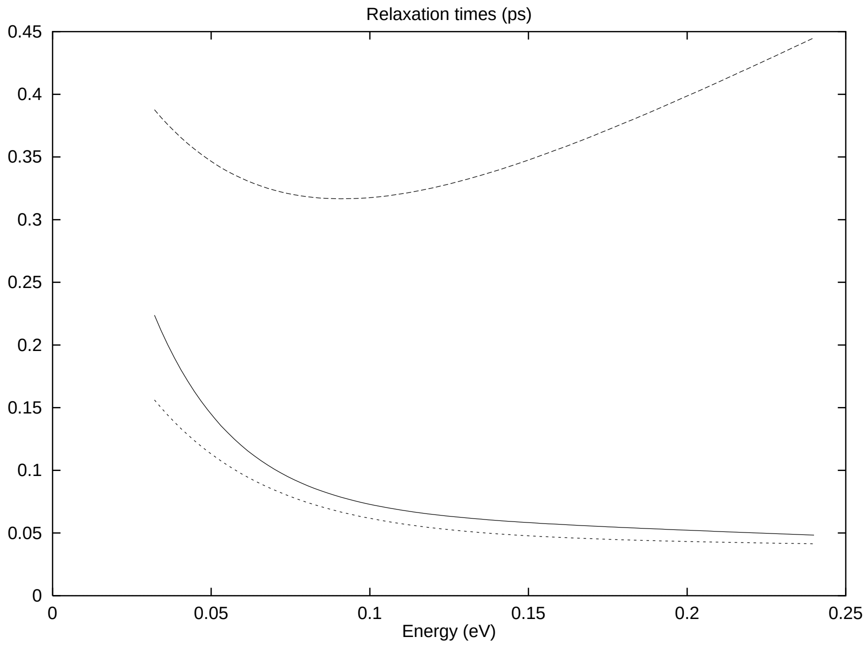

Figure 3: Relaxation times fitted from Monte Carlo calculations: τ_W (dashed line), τ_p (continuous line), and τ_q (dotted line)

therefore it is not justified to neglect the convective term in the expression for the heat flux.

Initially the temperature is uniform at 300 K, and the charges do not move. Then an external voltage of $1V$ is applied, that causes a flux of charges in the semiconductor.

The following initial conditions are assumed

$$n(x,0) = n_0(x), \qquad T(x,0) = 300K, \qquad v(x,0) = 0, \qquad q(x,0) = 0. \quad (44)$$

The initial values for n_0 have been obtained by smoothing the discontinuities in the doping profile by a hyperbolic tangent:

$$n_0(x) = n_0 - d_0 \left(\tanh \frac{x - x_1}{s} - \tanh \frac{x - x_2}{s} \right).$$

We have: $n_0 = n_0(0)$, $d_0 = n_0(1 - 10^{-2})/2$, $s = 0.02\mu\text{m}$, $x_1 = 0.1\mu\text{m}$ e $x_2 = 0.5\mu\text{m}$ (see Fig. 4).

We now discuss the boundary conditions. The number of independent boundary conditions for a hyperbolic system on each boundary should be equal to the number of characteristics entering the domain on that portion of the boundary. The other boundary conditions should be given consistent to the field equations. Following [14], we set

$$n(0,t) = n(L,t) = 10^{18}\text{cm}^{-3}, \qquad (45)$$

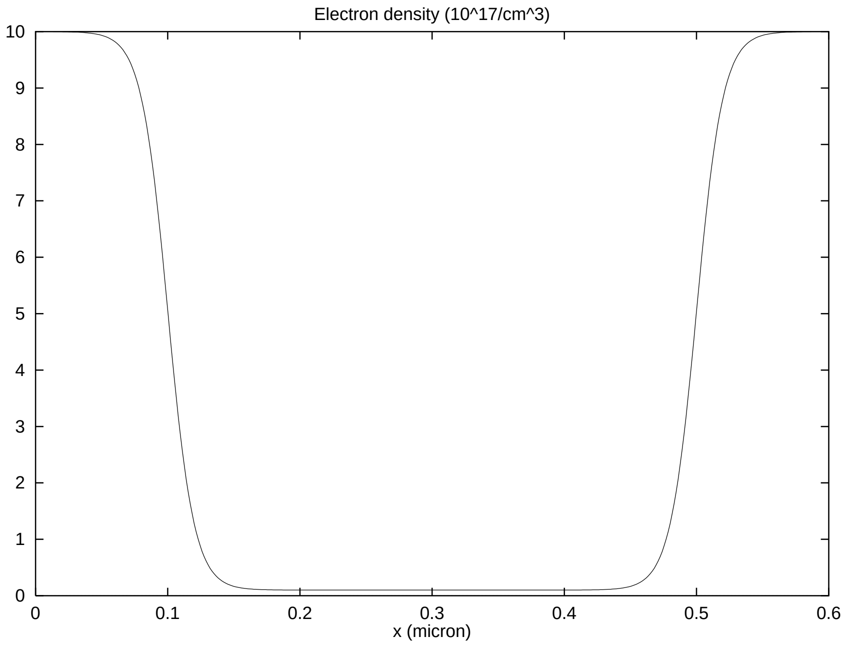

Figure 4: Doping profile

$$\frac{\partial}{\partial x}T(0,t) = \frac{\partial}{\partial x}T(L,t) = 0, \tag{46}$$

$$\frac{\partial}{\partial x}v(0,t) = \frac{\partial}{\partial x}v(L,t) = 0, \tag{47}$$

$$e\phi(0) = T\ln\left(\frac{n(0)}{n_i}\right), \qquad e\phi(L) = T\ln\left(\frac{n(L)}{n_i}\right) + eV_b, \tag{48}$$

where n_i =1.4×10^{10} cm^{-3} is the intrinsic electron concentration, and V_b is the applied bias voltage. The assignement of a redundant number of boundary conditions is justified by the fact that in the n^+ regions the profiles of the field variables are quite flat. The compatibility with the equations is observed *a posteriori* by the lack of spurious oscillations or reflected waves on the boundary.

Because an implicit scheme has been used in the relaxation step, the only stability limitation is given by the CFL condition on the convection step.

In all the simulations, condition $\Delta t = \Delta x/2c_s$, $c_s \equiv \sqrt{k_B T_0/m^*}$ has been used. Note that the largest eigenvalue of the hyperbolic matrix is always less than c_s, and therefore condition (36) is always satisfied.

The accuracy study is performed by comparing computations with 200, 400, and 800 grid points. The results for simple splitting are reported in Table 2. 200 grid points give a solution with an L^∞ relative error in velocity less than 5 %. Convergence results for the second order splitting are presented in Table 3. As expected, the latter scheme works better than simple splitting, confirming almost second order accuracy.

In the expression of the heat flux in BBW model, the values $c = -1$ [14, 19]

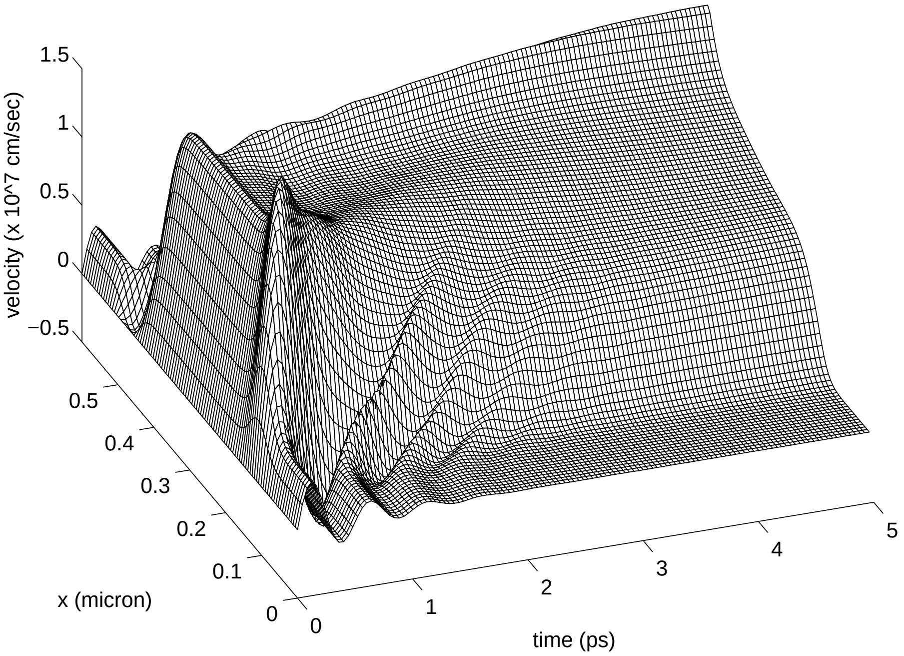

Figure 5: Time evolution of electron velocity for AP model. Second order scheme with 200 points

Table 2: Numerical convergence study for the simple splitting scheme. Stationary solution AP model. L^1 and L^∞ norms of relative errors

		200–400 points	400–800 points	convergence rate
L^1	velocity	0.0044	0.0018	1.275
Norm	energy	0.0027	0.0010	1.392
L^∞	velocity	0.0433	0.0140	1.631
Norm	energy	0.0199	0.0059	1.751

and $c = -2.1$ [14, 31] have been used. The latter provides a better agreement with Monte Carlo . We remark, however, that those values are not deduced by thermodynamical principles, but are treated as fitting parameters, which may be different for a different device.

In all our simulations, about 5 picoseconds are enough to reach steady state. In Fig. 5 we report the time evolution of the velocity field. After a rapid transient, steady state regime is approcahed.

In Figures 6 and 7 we compare velocity and energy profiles for AP, Monte Carlo results obtained by the code DAMOCLES [11], and BBW models for $c = -1$ and $c = -2.1$, for a channel of length 0.4 μm. If $c = -1$ the two models have roughly the same agreement with Monte Carlo , while for $c = -2.1$, BBW model shows a better agreement. For both models, the results on energy are more accurate

Table 3: Numerical convergence study for the second order splitting scheme. Stationary solution AP model. L^1 and L^∞ norms of relative errors

		200–400 points	400–800 points	convergence rate
L^1	velocity	0.0040	0.0011	1.814
Norm	energy	0.0016	0.0005	1.506
L^∞	velocity	0.0224	0.0056	1.993
Norm	energy	0.0112	0.0023	2.265

than those on electron velocity. The region with the poorest agreement is near the second junction, because of the peak in the velocity profiles for AP model and for BBW model with $c = -1$.

The two models show a very different behavior when we consider the heat flux. In the AP model, the convective term constitutes the dominant part (see Fig. 8), and shows a good agreement with Monte Carlo calculations, except near the second junction. BBW model overestimates the heat flux for both values of c, and the location of the maximum is different. This result is in accordance with what has been observed in [6], where it was suggested to introduce a convective term in the heat flux, in order to improve the agreement between Monte Carlo and BBW model.

Conclusions

Stationary and non-stationary numerical solutions of recent hydrodynamical models for semiconductors are presented. A numerical scheme has been suitable developed for the purpose. At variance with ENO schemes already used in [14], our scheme is only second order in space, but accuracy is maintained in time by a suitable splitting technique. The scheme is quite simple to implement, and it does not require neither exact or approximate Riemann solvers nor the eigenvalues and eigenvectors of the Jacobian matrix of the hyperbolic part of the system. Such property is desirable, since for one of the models there is no simple expression of the characteristic fields.

Two models have been considered: BBW, and AP.

A comparison between numerical results and Monte Carlo simulations show that BBW model gives satisfactory results for electron velocity and energy, provided a suitable value is chosen for a fitting parameter contained in the expression for the heat conductivity. A bad agreement is observed with Monte Carlo about the heat flux.

AP model, on the contrary, is derived in a systematic way from a kinetic formulation, by using techniques proper of Extended Thermodynamics . The model gives a reasonable agreement with Monte Carlo for the heat flux, but the agreement of velocity and energy profiles is similar to that obtained by BBW model with $c = -1$.

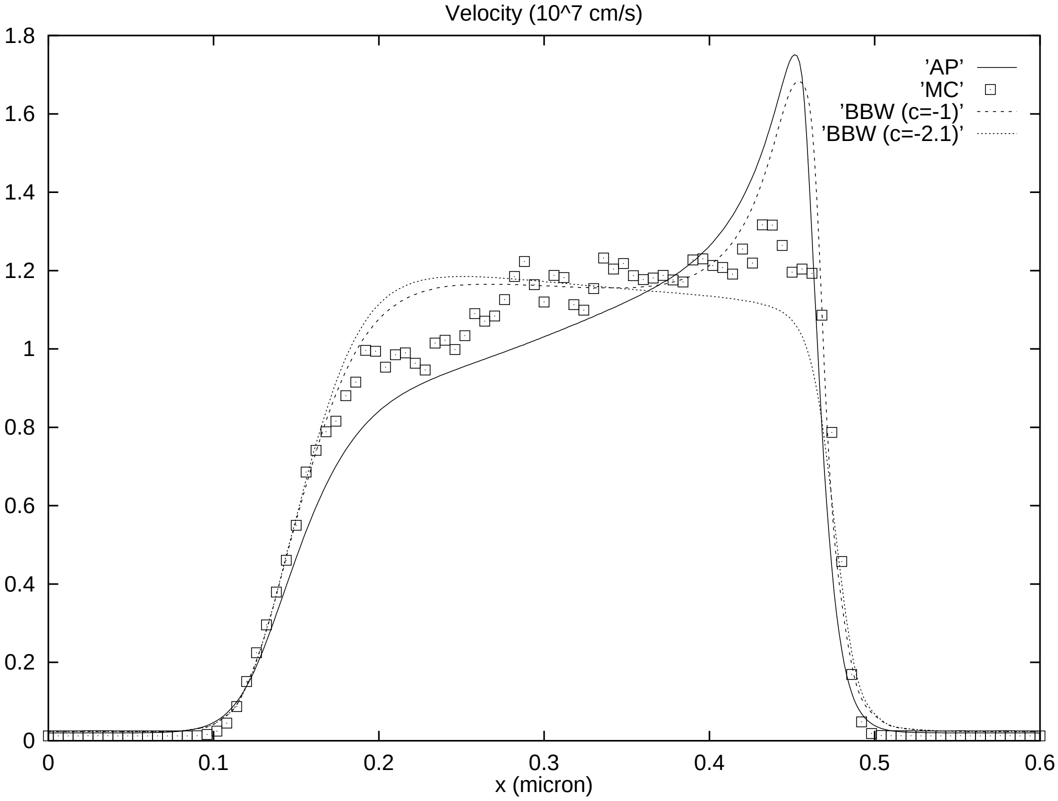

Figure 6: Velocity profile ($\times 10^7$ cm/sec). AP model (continuous line), BBW model with $c = -1.0$ (dashed line), $c = -2.1$ (dotted line) and with Monte Carlo DAMOCLES code (squares). The channel length is $0.4\mu m$, and the applied voltage is 1V

.

Therefore, although AP model gives a better description of the heat flux, it is not yet satisfactory. There is still need for a model without fitting parameters, which gives a more accurate description of carrier dynamics.

Better results are expected by the model obtained with the use of 13 moments of the distribution function, without including Maxwellian iteration. The authors are presently investigating the properties of this model, and the results will be presented in a following article.

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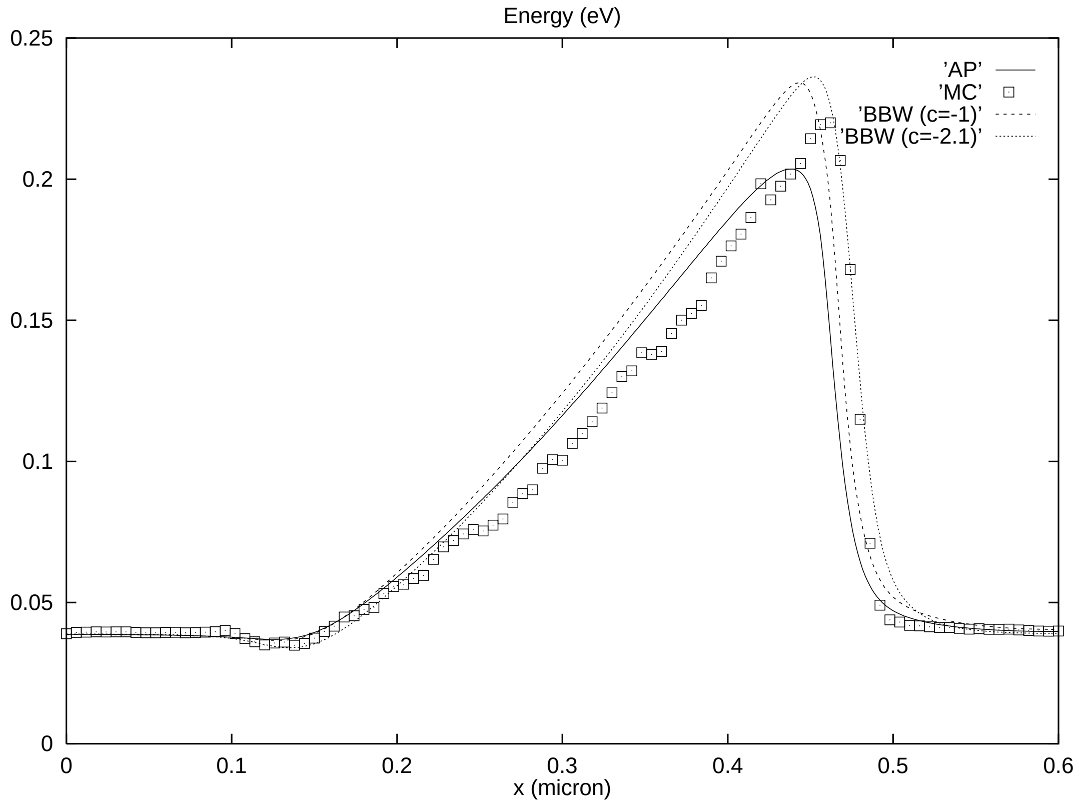

Figure 7: Energy profile (eV). The notation is as in Fig.(6)

cietà", and by CORIMME, a consortium between the University of Catania and SGS-Thomson Microelectronics.

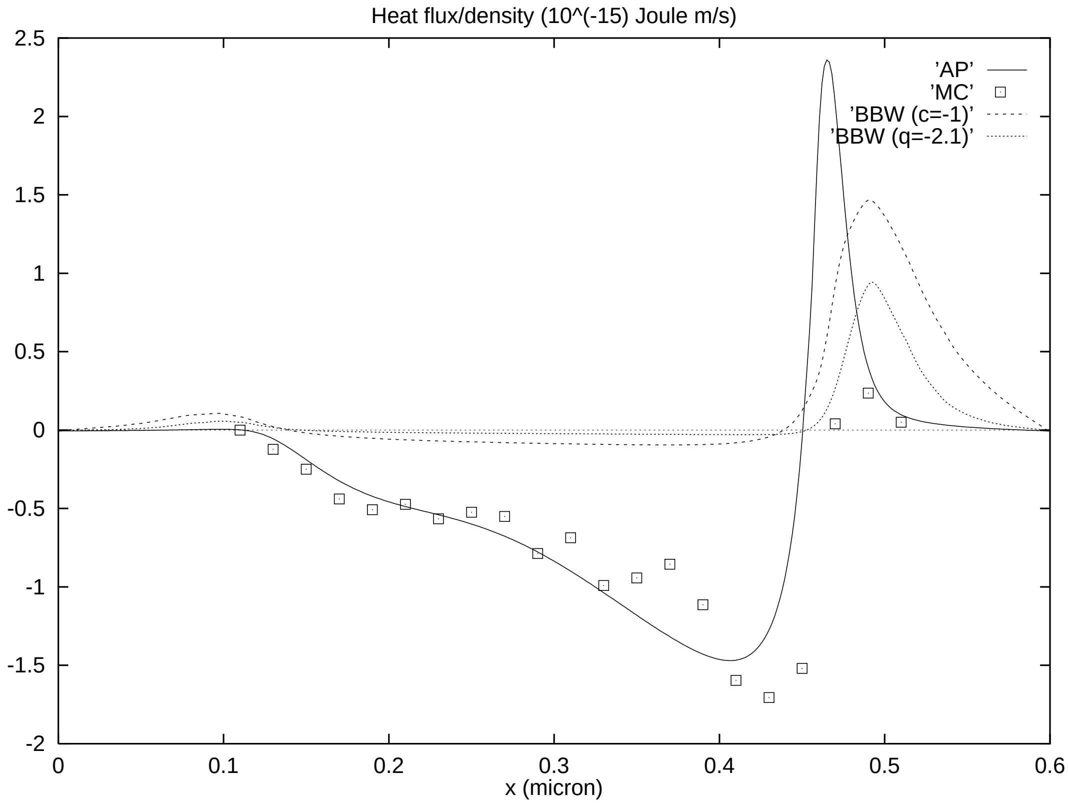

Figure 8: Heat flux/density (J m/sec). The notation is as in Fig.(6)

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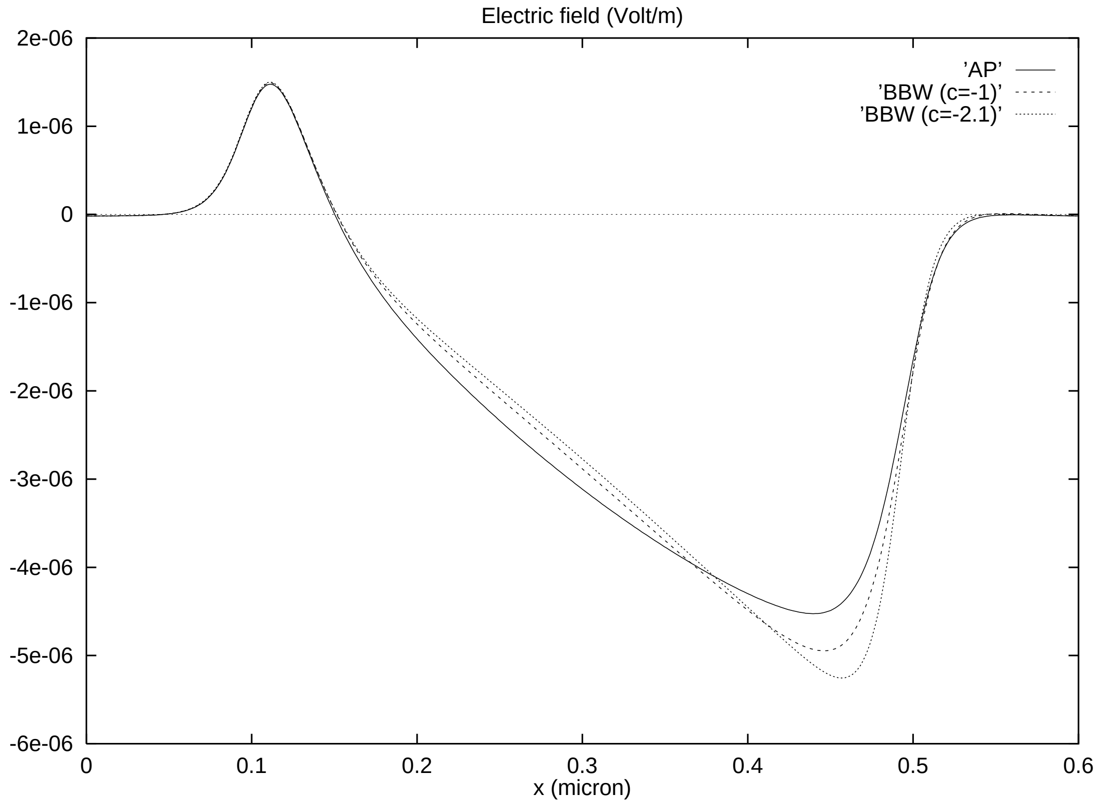

Figure 9: Electric field (Volt/m). The notation is as in Fig.(6)

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