Numerical schemes for semiconductors energy-transport models

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Abstract We introduce some finite volume schemes for unipolar energy-transport models. Using a reformulation in dual entropy variables, we can show the decay of a discrete entropy with control of the discrete entropy dissipation.

Key words: energy-tranport model, finite volumes, entropy method.

MSC (2010)**:** 65M08, 65M12, 35K20.

1 Energy-transport models

Presentation

In this article, we are interested in the discretization of unipolar energy-transport models for semiconductor devices. Such models describe the flow of electrons through a semiconductor crystal, influenced by diffusive, electrical and thermal effects. As they have a drift-diffusion form, they remain simpler than hydrodynamic equations or semiconductor Boltzmann equations. As explained for example in [17] (and the references therein), these energy-transport models can be derived from the Boltzmann equation by the moment method.

The unipolar energy-transport system consists in two continuity equations for the electron density ρ_1 and the internal energy density ρ_2, coupled with a Poisson equation describing the electrical potential V. Following the framework adopted in

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[6], we consider that the electron and energy densities are defined as functions of the entropy variables $u_1 = \mu/T$ and $u_2 = -1/T$ where μ is the chemical potential and T the temperature. We set $u = (u_1, u_2)$.

Let Ω be an open bounded subset of $\mathbb{R}^d$ ($d \geq 1$) describing the geometry of the considered semiconductor device and let $T_{max} > 0$ be a finite time horizon. The energy transport model writes in $\Omega \times (0, T_{max})$

$$\partial_t \rho_1(u) + \text{div} J_1 = 0, \tag{1a}$$
$$\partial_t \rho_2(u) + \text{div} J_2 = \nabla V \cdot J_1 + W(u), \tag{1b}$$
$$-\lambda^2 \Delta V = C(x) - \rho_1(u), \tag{1c}$$

where J_1 and J_2 are respectively the electron and energy current densities, $\nabla V \cdot J_1$ corresponds to a Joule heating term and $W(u)$ is an energy relaxation term. The doping profile $C(x)$ describes the fixed charged background and λ is the rescaled Debye length. The electron and energy current densities are given by:

$$J_1 = -L_{11}(u)(\nabla u_1 + u_2 \nabla V) - L_{12}(u) \nabla u_2, \tag{2a}$$
$$J_2 = -L_{21}(u)(\nabla u_1 + u_2 \nabla V) - L_{22}(u) \nabla u_2, \tag{2b}$$

where $\mathbb{L}(u) = (L_{ij}(u))_{1 \leq i,j \leq 2}$ is a symmetric uniformly positive definite matrix.

The system (1)-(2) is supplemented with an initial condition $u_0 = (u_{1,0}, u_{2,0})$ and with mixed boundary conditions. There are Dirichlet boundary conditions on the ohmic contacts and homogeneous Neumann boundary conditions on insulating segments. More precisely, we assume that Ω is an open bounded polygonal (or polyhedral) subset of $\mathbb{R}^d$, such that its boundary $\partial\Omega$ is split into $\partial\Omega = \Gamma^D \cup \Gamma^N$, with $\Gamma^D \cup \Gamma^N = \emptyset$ and $\text{m}_{d-1}(\Gamma^D) > 0$. We denote by $\mathbf{n}$ the normal to $\partial\Omega$ outward Ω. The boundary conditions write

$$u_1 = u_1^D, \; u_2 = u_2^D, \; V = V^D \text{ on } \Gamma^D \times [0, T_{max}], \tag{3a}$$
$$J_1 \cdot \mathbf{n} = J_2 \cdot \mathbf{n} = \nabla V \cdot \mathbf{n} \quad \text{on } \Gamma^N \times [0, T_{max}]. \tag{3b}$$

We assume that the Dirichlet boundary conditions u_1^D, u_2^D and V^D do not depend on time and are the traces of some functions defined on the whole domain Ω, still denoted by u_1^D, u_2^D and V^D. Moreover, we assume that $u_2^D < 0$ is constant on Γ^D and that the energy relaxation term $W(u)$ verifies, for all $u \in \mathbb{R}^2$ and $u_2^D < 0$,

$$W(u)(u_2 - u_2^D) \leq 0. \tag{4}$$

The main results on the energy-transport model (1)-(2)-(3) are presented in [15]: existence of solutions to the transient system, regularity, uniqueness and existence and uniqueness of steady-states. The main assumptions needed on the function $u \mapsto \rho(u) = (\rho_1(u), \rho_2(u))$ for the existence result are the following:

$$\rho \in W^{1,\infty}(\mathbb{R}^2;\mathbb{R}^2), \tag{5a}$$

$$\exists c_0 > 0 \text{ such that } (\rho(u)-\rho(v))\cdot(u-v) \geq c_0|u-v|^2 \quad \text{for } u,v \in \mathbb{R}^2, \tag{5b}$$

$$\exists \chi \in C^1(\mathbb{R}^2;\mathbb{R}) \text{ strictly convex such that } \rho = \nabla_u \chi. \tag{5c}$$

These hypotheses are rather hard to satisfy in the applications (see Section 4), as well as the hypothesis on uniform positive definiteness of the diffusion matrix $\mathbb{L}$. Existence results for physically more realistic diffusion matrices (only positive semi-definite) are established in [10, 12] for the stationary model and in [4, 5] for the transient system, but only in the case of data close to thermal equilibrium. More recently, existence of solutions has been proved in a simplified degenerate case, namely for a model with a simplified temperature equation in [16] and for vanishing electric fields (avoiding the coupling with Poisson equation) in [20].

The existence result due to Degond, Génieys and Jüngel [6, 15] is based on a reformulation of the system in terms of dual entropy variables. This reformulation symmetrizes the system and allows to apply an entropy method. Since we are going to adapt the results of [6] to the discrete framework, let us now introduce the system reformulated in terms of dual entropy variables and give the outline of the entropy structure.

The system in dual entropy variables

The key point of the analysis of the primal model (1)-(2) is to use another set of variables which symmetrizes the problem, see [6]. Let us define the so-called dual entropy variables $w = (w_1, w_2)$ (w_1 is an electrochemical potential):

$$w_1 = u_1 + u_2 V, \tag{6a}$$

$$w_2 = u_2. \tag{6b}$$

Through this change of variables, the problem (1)-(2) is equivalent to

$$\partial_t b_1(w,V) + \mathrm{div} I_1(w,V) = 0, \tag{7a}$$

$$\partial_t b_2(w,V) + \mathrm{div} I_2(w,V) = \widetilde{W}(w) - \partial_t V b_1(w,V), \tag{7b}$$

$$-\lambda^2 \Delta V = C - b_1(w,V), \tag{7c}$$

where the function $b(w,V) = (b_1(w,V), b_2(w,V))$ is related to ρ and V by

$$b_1(w,V) = \rho_1(u), \quad b_2(w,V) = \rho_2(u) - V\rho_1(u), \tag{8}$$

and the new energy relaxation term is defined by $\widetilde{W}(w) = W(u)$. Moreover, the symmetrized currents are given by $I_1 = J_1$ and $I_2 = J_2 - VJ_1$, which leads to

$$I_1(w,V) = -D_{11}(w,V)\nabla w_1 - D_{12}(w,V)\nabla w_2, \tag{9a}$$

$$I_2(w,V) = -D_{21}(w,V)\nabla w_1 - D_{22}(w,V)\nabla w_2, \tag{9b}$$

where the new diffusion matrix $\mathbb{D}(w,V) = (D_{ij}(w,V))_{1\le i,j\le 2}$ is defined by

$$\mathbb{D}(w,V) = \mathbb{P}(V)^T \mathbb{L}(u)\mathbb{P}(V), \quad \text{with } \mathbb{P}(V) = \begin{pmatrix} 1 & -V \\ 0 & 1 \end{pmatrix}. \tag{10}$$

It is therefore clear that the new diffusion matrix $\mathbb{D}$ is also symmetric and uniformly positive definite.

Entropy structure

We recall in this section the entropy/entropy-dissipation property satisfied by the energy-transport model (1)-(3) established in [6]. The entropy function is defined by

$$S(t) = \int_\Omega \left[\rho(u)\cdot(u-u^D) - (\chi(u)-\chi(u^D))\right] dx - \frac{\lambda^2}{2} u_2^D \int_\Omega |\nabla(V-V^D)|^2 dx. \tag{11}$$

Since $u_2^D < 0$ and χ is a convex function such that $\rho = \nabla_u \chi$, $S(t)$ is nonnegative for all $t \ge 0$.

In addition to the hypotheses already given above, we assume that the Dirichlet boundary conditions are at thermal equilibrium, namely

$$\nabla w_1^D = \nabla w_2^D = 0. \tag{12}$$

Then the entropy function satisfies the following identity:

$$\frac{d}{dt} S(t) = -\int_\Omega (\nabla w)^T \mathbb{D} \nabla w + \int_\Omega W(u)(u_2 - u_2^D) \le 0. \tag{13}$$

The proof of (13) is given in [6], even for more general boundary conditions.

2 Numerical schemes

Different kind of numerical schemes have already been designed for the energy-transport systems, essentially for the stationary systems: finite difference schemes in [11, 19], finite element schemes in [7, 14]. We also refer to [3] for DDFV (Discrete Duality Finite Volume) schemes for the evolutive case. Up to our knowledge, there exists no convergence analysis of these numerical schemes. In this paper, we are interested in the design and the analysis of some finite volume schemes for the system (1)–(3), with two-point flux approximations (TPFA) of the numerical fluxes. We pay attention, while building the scheme, on the possibility of adapting the entropy method to the discrete setting. This will be crucial in order to fulfill the convergence analysis of the scheme.

Mesh and notations

Let $\Delta t > 0$ be the time step and set $t^n = n\Delta t$ for all $n \geq 0$. We now define the mesh of the domain Ω. It is given by a family $\mathcal{T}$ of open polygonal (or polyhedral in 3D) control volumes, a family $\mathcal{E}$ of edges (or faces), and a family $\mathcal{P} = (x_K)_{K\in\mathcal{T}}$ of points. The schemes we will consider are based on two-points flux approximations, so that we assume that the mesh is admissible in the sense of [9, Definition 9.1].

In the set of edges $\mathcal{E}$, we distinguish the interior edges $\sigma = K|L \in \mathcal{E}_{int}$ and the boundary edges $\sigma \in \mathcal{E}_{ext}$. Due to the mixed boundary conditions, we have to distinguish the edges included in Γ^D from the edges included in Γ^N: $\mathcal{E}_{ext} = \mathcal{E}^D \cup \mathcal{E}^N$. For a control volume $K \in \mathcal{T}$, we define $\mathcal{E}_K$ the set of its edges, which is also split into $\mathcal{E}_K = \mathcal{E}_{K,int} \cup \mathcal{E}_K^D \cup \mathcal{E}_K^N$.

In the sequel, we denote by d the distance in $\mathbb{R}^d$ and m the measure in $\mathbb{R}^d$ or $\mathbb{R}^{d-1}$. For all $\sigma \in \mathcal{E}$, we define $\mathrm{d}_\sigma = d(x_K, x_L)$ if $\sigma = K|L \in \mathcal{E}_{int}$ and $\mathrm{d}_\sigma = d(x_K, \sigma)$ if $\sigma \in \mathcal{E}_{ext}$, with $\sigma \in \mathcal{E}_K$. Then the transmissibility coefficient is defined by $\tau_\sigma = \mathrm{m}(\sigma)/\mathrm{d}_\sigma$, for all $\sigma \in \mathcal{E}$.

A finite volume scheme with two-point flux approximation provides, for an unknown v, a vector $\mathbf{v} = (v_K)_{K\in\mathcal{T}} \in \mathbb{R}^\theta$ (with $\theta = \mathrm{Card}(\mathcal{T})$) of approximate values on each cells. We can associate to $\mathbf{v}$ a piecewise constant function, still denoted $\mathbf{v}$. For all $K \in \mathcal{T}$ and all $\sigma \in \mathcal{E}_K$, we define

$$v_{K,\sigma} = \begin{cases} v_L & \text{if } \sigma = K|L \in \mathcal{E}_{int}, \\ v_\sigma^D & \text{if } \sigma \in \mathcal{E}^D, \\ v_K & \text{if } \sigma \in \mathcal{E}^N, \end{cases}$$

and

$$D_{K,\sigma}\mathbf{v} = v_{K,\sigma} - v_K, \qquad D_\sigma \mathbf{v} = |D_{K,\sigma}\mathbf{v}|.$$

Schemes in primal and dual entropy variables

Our aim is to design a scheme for the energy transport model in the primal entropy variables (1)-(3). This scheme must lead to an equivalent scheme for the system written in the dual entropy variables (7)-(9). Indeed, in this case, it will be possible to apply the entropy method at the discrete level. This step is crucial as it brings *a priori* estimates on the sequences of approximate solutions, leading to compactness results. Moreover, it also permits to prove existence of a solution to the scheme.

One main difficulty in writing a TPFA scheme for the energy-transport model (1)-(3) comes from the approximation of the Joule heating term $\nabla V \cdot J_1$. One possibility would be to apply the technique developed in [1], and further used in [18, 8], to discretize de Joule heating term. However, with such discretization, the rewriting of the scheme in dual entropy variables is not straightforward. Therefore, following [2], we propose an approximation of the Joule heating term which is based on its following reformulation:

$$\nabla V \cdot J_1 = \mathrm{div}(VJ_1) - V\mathrm{div}J_1.$$

Let us now turn to the definition of the scheme for the model (1)-(3). Initial and Dirichlet boundary conditions are discretized as usually: $u^0_{i,K}$ is the mean value of $u_{i,0}$ over K for all $K \in \mathscr{T}$ and $i = 1,2$, $u^D_{i,\sigma}$ and V^D_σ are the mean values of u^D_i for $i = 1,2$ and V^D for $\sigma \in \mathscr{E}^D$ and we define:

$$u^n_{1,\sigma} = u^D_{1,\sigma}, \quad u^n_{2,\sigma} = u^D_{2,\sigma}, \quad V^n_\sigma = V^D_\sigma, \quad \forall \sigma \in \mathscr{E}^D, \quad \forall n \geq 0. \tag{14}$$

The scheme is backward Euler in time and finite volume in space with a two-point flux approximation. It writes, for all $n \geq 0$, for all $K \in \mathscr{T}$:

$$\mathrm{m}(K)\frac{\rho^{n+1}_{1,K} - \rho^n_{1,K}}{\Delta t} + \sum_{\sigma\in\mathscr{E}_K} \mathscr{F}^{n+1}_{1,K,\sigma} = 0, \tag{15a}$$

$$\mathrm{m}(K)\frac{\rho^{n+1}_{2,K} - \rho^n_{2,K}}{\Delta t} + \sum_{\sigma\in\mathscr{E}_K} \mathscr{F}^{n+1}_{2,K,\sigma} = \mathrm{m}(K)W^{n+1}_K + \sum_{\sigma\in\mathscr{E}_K} V^{n+1}_\sigma \mathscr{F}^{n+1}_{1,K,\sigma} - V^{n+1}_K \sum_{\sigma\in\mathscr{E}_K} \mathscr{F}^{n+1}_{1,K,\sigma}, \tag{15b}$$

$$-\lambda^2 \sum_{\sigma\in\mathscr{E}_K} \tau_\sigma D_{K,\sigma} V^{n+1} = \mathrm{m}(K)(C_K - \rho^{n+1}_{1,K}), \tag{15c}$$

where

$$\rho^{n+1}_{i,K} = \rho_i(u^{n+1}_K), \quad i = 1,2 \text{ and } W^{n+1}_K = W(u^{n+1}_K) \text{ for all } K \in \mathscr{T}.$$

The numerical fluxes are given by

$$\mathscr{F}^{n+1}_{1,K,\sigma} = -\tau_\sigma \left(L^n_{11,\sigma}(D_{K,\sigma}\mathbf{u}_1{}^{n+1} + u^{n+1}_{2,\sigma} D_{K,\sigma}\mathbf{V}^{n+1}) + L^n_{12,\sigma} D_{K,\sigma}\mathbf{u}_2{}^{n+1} \right), \tag{16a}$$

$$\mathscr{F}^{n+1}_{2,K,\sigma} = -\tau_\sigma \left(L^n_{12,\sigma}(D_{K,\sigma}\mathbf{u}_1{}^{n+1} + u^{n+1}_{2,\sigma} D_{K,\sigma}\mathbf{V}^{n+1}) + L^n_{22,\sigma} D_{K,\sigma}\mathbf{u}_2{}^{n+1} \right), \tag{16b}$$

where the matrix $\mathbb{L}^n_\sigma = (L^n_{ij,\sigma})_{1\leq i,j\leq n}$ is defined as

$$\mathbb{L}^n_\sigma = \mathbb{L}\left(\frac{u^n_K + u^n_{K,\sigma}}{2}\right) \qquad \text{for all } K \in \mathscr{T}, \sigma \in \mathscr{E}_K. \tag{17}$$

At this point, it remains to define V^{n+1}_σ involved in (15b) and $u^{n+1}_{2,\sigma}$ involved in (16) for all $\sigma \in \mathscr{E}$. We will do it later. The choice will be driven by the expected equivalence with a scheme for (7)–(10).

In order to obtain an equivalent scheme for the energy transport system in the dual entropy variables (7)–(10), we apply the change of variables (6), associated with the new functions defined in (8), (9) and (10), to (15)-(16). Let us define for all $K \in \mathscr{T}$, for all $n \geq 0$,

$$w^n_{1,K} = u^n_{1,K} + u^n_{2,K} V^n_K, \qquad w^n_{2,K} = u^n_{2,K}, \tag{18a}$$

$$b^n_{1,K} = \rho^n_{1,K} = b_1(w^n_K, V^n_K), \qquad b^n_{2,K} = \rho^n_{2,K} - \rho^n_{1,K} V^n_K = b_2(w^n_K, V^n_K). \tag{18b}$$

We similarly define $w^D_{1,\sigma}$ and $w^D_{2,\sigma}$ for $\sigma \in \mathscr{E}^D$. From (15a) and (15b), we deduce

$$\mathrm{m}(K)\frac{b^{n+1}_{1,K}-b^n_{1,K}}{\Delta t}+\sum_{\sigma\in\mathscr{E}_K}\mathscr{F}^{n+1}_{1,K,\sigma}=0,$$

$$\mathrm{m}(K)\frac{b^{n+1}_{2,K}-b^n_{2,K}}{\Delta t}+\sum_{\sigma\in\mathscr{E}_K}\left(\mathscr{F}^{n+1}_{2,K,\sigma}-V^{n+1}_\sigma\mathscr{F}^{n+1}_{1,K,\sigma}\right)$$
$$=\mathrm{m}(K)W^{n+1}_K-\mathrm{m}(K)\frac{V^{n+1}_K-V^n_K}{\Delta t}b^n_{1,K}.$$

It leads to the following scheme for the system written in the dual variables (7):

$$\mathrm{m}(K)\frac{b^{n+1}_{1,K}-b^n_{1,K}}{\Delta t}+\sum_{\sigma\in\mathscr{E}_K}\mathscr{G}^{n+1}_{1,K,\sigma}=0, \tag{19a}$$

$$\mathrm{m}(K)\frac{b^{n+1}_{2,K}-b^n_{2,K}}{\Delta t}+\sum_{\sigma\in\mathscr{E}_K}\mathscr{G}^{n+1}_{2,K,\sigma}=\mathrm{m}(K)\tilde{W}^{n+1}_K-\mathrm{m}(K)\frac{V^{n+1}_K-V^n_K}{\Delta t}b^n_{1,K}, \tag{19b}$$

$$-\lambda^2\sum_{\sigma\in\mathscr{E}_K}\tau_\sigma D_{K,\sigma}V^{n+1}=\mathrm{m}(K)(C_K-b^{n+1}_{1,K}), \tag{19c}$$

with

$$\mathscr{G}^{n+1}_{1,K,\sigma}=\mathscr{F}^{n+1}_{1,K,\sigma},\quad \forall K\in\mathscr{T},\forall\sigma\in\mathscr{E}_K, \tag{20a}$$

$$\mathscr{G}^{n+1}_{2,K,\sigma}=\mathscr{F}^{n+1}_{2,K,\sigma}-V^{n+1}_\sigma\mathscr{F}^{n+1}_{1,K,\sigma},\quad \forall K\in\mathscr{T},\forall\sigma\in\mathscr{E}_K, \tag{20b}$$

and $\tilde{W}^{n+1}_K=W^{n+1}_K=\tilde{W}(w^{n+1}_K)$.

The crucial point now is to ensure that the new numerical fluxes $\mathscr{G}^{n+1}_{1,K,\sigma}$, $\mathscr{G}^{n+1}_{2,K,\sigma}$ can be seen as approximations of the currents I_1 and I_2 defined by (9). This means that we want to rewrite the numerical fluxes as

$$\mathscr{G}^{n+1}_{1,K,\sigma}=-\tau_\sigma(\mathrm{D}^*_{11,\sigma}D_{K,\sigma}\mathbf{w}^{n+1}_1+\mathrm{D}^*_{12,\sigma}D_{K,\sigma}\mathbf{w}^{n+1}_2), \tag{21a}$$

$$\mathscr{G}^{n+1}_{2,K,\sigma}=-\tau_\sigma(\mathrm{D}^*_{21,\sigma}D_{K,\sigma}\mathbf{w}^{n+1}_1+\mathrm{D}^*_{22,\sigma}D_{K,\sigma}\mathbf{w}^{n+1}_2), \tag{21b}$$

with the coefficients $(\mathrm{D}^*_{ij,\sigma})_{1\le i,j\le 2}$ defined such that the associate matrix $\mathbb{D}^*_\sigma$ is symmetric and uniformly positive definite. This property will now depend on the definition of V^{n+1}_σ and $u^{n+1}_{2,\sigma}$, respectively involved in (15b) and (16), for each edge $\sigma\in\mathscr{E}$.

Equivalence of the schemes in the primal and dual entropy variables

Proposition 1. *Let us supplement the scheme* (15)-(16) *with the definition of the* $(V^{n+1}_\sigma)_{\sigma\in\mathscr{E},\,n\ge 0}$ *and* $(u^{n+1}_{2,\sigma})_{\sigma\in\mathscr{E},\,n\ge 0}$. *We distinguish two cases:*

- *Case 1: centered scheme. For all* $\sigma\in\mathscr{E}$ *and* $n\ge 0$*, we set:*

$$u_{2,\sigma}^{n+1} = \frac{u_{2,K}^{n+1} + u_{2,K,\sigma}^{n+1}}{2} \quad \textit{and} \quad V_\sigma^{n+1} = \frac{V_K^{n+1} + V_{K,\sigma}^{n+1}}{2}. \tag{22}$$

- *Case 2: upwind scheme. For all* $\sigma \in \mathscr{E}$ *and* $n \geq 0$*, we set:*

$$u_{2,\sigma}^{n+1} = \begin{cases} u_{2,K,\sigma}^{n+1}, & \textit{if } D_{K,\sigma}V^{n+1} > 0, \\ u_{2,K}^{n+1}, & \textit{if } D_{K,\sigma}V^{n+1} \leq 0, \end{cases} \textit{and } V_\sigma^{n+1} = \min(V_K^{n+1}, V_{K,\sigma}^{n+1}). \tag{23}$$

Then, in both cases, the scheme (15)-(16) *written in the primal entropy variables is equivalent with the scheme* (19)-(21) *written in the dual entropy variables, provided that*

$$\mathbb{D}_\sigma^* = (\mathbb{P}_\sigma^{n+1})^T \mathbb{L}^n \mathbb{P}_\sigma^{n+1} \textit{ with } \mathbb{P}_\sigma^{n+1} = \begin{pmatrix} 1 & -V_\sigma^{n+1} \\ 0 & 1 \end{pmatrix}. \tag{24}$$

Proof. Starting from the definition (20) of the numerical fluxes $\mathscr{G}_{1,K,\sigma}^{n+1}$ and $\mathscr{G}_{2,K,\sigma}^{n+1}$, we want to establish (21) with $\mathbb{D}_\sigma^*$ defined by (24).

Let us first notice that, due to the change of variables (18a), we can rewrite $D_{K,\sigma}\mathbf{u}_1{}^{n+1}$ and $D_{K,\sigma}\mathbf{u}_2{}^{n+1}$ for all $K \in \mathscr{T}$ and $\sigma \in \mathscr{E}_K$. It is clear that $D_{K,\sigma}\mathbf{u}_2{}^{n+1} = D_{K,\sigma}\mathbf{w}_2{}^{n+1}$. Moreover, we have

$$\begin{aligned} D_{K,\sigma}\mathbf{u}_1{}^{n+1} &= D_{K,\sigma}\mathbf{w}_1{}^{n+1} - V_K^{n+1} D_{K,\sigma}\mathbf{w}_2{}^{n+1} - w_{2,K,\sigma}^{n+1} D_{K,\sigma}\mathbf{V}^{n+1}, \\ &= D_{K,\sigma}\mathbf{w}_1{}^{n+1} - V_{K,\sigma}^{n+1} D_{K,\sigma}\mathbf{w}_2{}^{n+1} - w_{2,K}^{n+1} D_{K,\sigma}\mathbf{V}^{n+1}. \end{aligned}$$

This yields, for Case 1 as well as for Case 2,

$$D_{K,\sigma}\mathbf{u}_1{}^{n+1} = D_{K,\sigma}\mathbf{w}_1{}^{n+1} - V_\sigma^{n+1} D_{K,\sigma}\mathbf{w}_2{}^{n+1} - w_{2,\sigma}^{n+1} D_{K,\sigma}\mathbf{V}^{n+1},$$

with $w_{2,\sigma}^{n+1} = u_{2,\sigma}^{n+1}$. Therefore, from (16) and (20), we deduce that

$$\begin{aligned} \mathscr{G}_{1,K,\sigma}^{n+1} &= -\tau_\sigma \left(L_{11,\sigma}^n D_{K,\sigma}\mathbf{w}_1{}^{n+1} + (L_{12,\sigma}^n - V_\sigma^{n+1} L_{11,\sigma}^n) D_{K,\sigma}\mathbf{w}_2{}^{n+1} \right), \\ \mathscr{G}_{2,K,\sigma}^{n+1} &= -\tau_\sigma \left((L_{12,\sigma}^n - V_\sigma^{n+1} L_{11,\sigma}^n) D_{K,\sigma}\mathbf{w}_1{}^{n+1} \right) \\ &\qquad + (L_{22,\sigma}^n - 2V_\sigma^{n+1} L_{12,\sigma}^n + (V_\sigma^{n+1})^2 L_{11,\sigma}^n) D_{K,\sigma}\mathbf{w}_2{}^{n+1} \big). \end{aligned}$$

This corresponds to (21) with $\mathbb{D}_\sigma^*$ defined by (24). We have shown that the scheme (15)-(16), supplemented either with (22) or (23), implies (19)-(21)-(24). Starting from (19)-(21)-(24), we similarly get (15)-(16).

3 Discrete entropy inequality

In this Section, we establish the discrete counterpart of the decay of the entropy, with the control of its dissipation, (13). The result is stated in Proposition 2.

Main result

First of all, since the functions u_1^D, u_2^D, V^D are assumed to be defined on the whole domain Ω, we can set

$$(u_{1,K}^D, u_{2,K}^D, V_K^D) = \frac{1}{\mathrm{m}(K)} \int_K (u_1^D(x), u_2^D(x), V^D(x))dx, \quad \forall K \in \mathscr{T}.$$

Moreover, we remember that u_2^D is a constant function, such that

$$u_{K,2}^D = u_2^D < 0, \quad \forall K \in \mathscr{T}. \tag{25}$$

Let $(u_K^n = (u_{1,K}^n, u_{2,K}^n)^T, V_K^n)_{K\in\mathscr{T}, n\geq 0}$ be a solution to the scheme (14)–(17), supplemented with either (22) or (23). For all $n \geq 0$, we define the discrete entropy functional as follows:

$$\begin{aligned} S^n = \sum_{K\in\mathscr{T}} \mathrm{m}(K) \left[\rho_K^n \cdot (u_K^n - u_K^D) - (\chi(u_K^n) - \chi(u_K^D))\right] \\ -\frac{\lambda^2}{2} u_2^D \sum_{\sigma\in\mathscr{E}} \tau_\sigma (D_\sigma(\mathbf{V}^n - \mathbf{V}^D))^2. \end{aligned} \tag{26}$$

We recall that $\rho_K^n = \rho(u_K^n) = (\rho_1(u_K^n), \rho_2(u_K^n))^T$ and that ρ is related to χ by (5c). Therefore, S^n is nonnegative for all $n \geq 0$.

Proposition 2 (Discrete entropy dissipation). *Assume* (4), (5), (25) *and let* $(u_K^n = (u_{1,K}^n, u_{2,K}^n)^T, V_K^n)_{K\in\mathscr{T}, n\geq 0}$ *be a solution to the scheme* (14)–(17)*, supplemented with either* (22) *or* (23)*. The discrete entropy satisfies the following inequality: for all* $n \geq 0$*,*

$$\begin{aligned} \frac{S^{n+1} - S^n}{\Delta t} \leq &- \sum_{\sigma\in\mathscr{E}} \tau_\sigma (D_{K,\sigma}\mathbf{w}^{n+1})^T \mathbb{D}_\sigma^* D_{K,\sigma}\mathbf{w}^{n+1} \\ &+ \sum_{K\in\mathscr{T}} \mathrm{m}(K) W_K^{n+1} (w_{2,K}^{n+1} - w_{2,K}^D) \leq 0, \end{aligned} \tag{27}$$

where $D_{K,\sigma}\mathbf{w}^{n+1} = (D_{K,\sigma}\mathbf{w}_1^{n+1}, D_{K,\sigma}\mathbf{w}_2^{n+1})^T$.

Proof. Using the definition (26) of the discrete entropy, one has

$$S^{n+1} - S^n = A + B, \tag{28}$$

where

$$\begin{aligned} A = \sum_{K\in\mathscr{T}} \mathrm{m}(K) \Big(&\rho_K^{n+1} \cdot (u_K^{n+1} - u_K^D) - (\chi(u_K^{n+1}) - \chi(u_K^D)) \\ &- \rho_K^n \cdot (u_K^n - u_K^D) + (\chi(u_K^n) - \chi(u_K^D))\Big), \end{aligned} \tag{29}$$

$$B = -\frac{\lambda^2}{2} u_2^D \sum_{\sigma\in\mathscr{E}} \tau_\sigma \Big[(D_\sigma(\mathbf{V}^{n+1} - \mathbf{V}^D))^2 - (D_\sigma(\mathbf{V}^n - \mathbf{V}^D))^2\Big]. \tag{30}$$

We first consider the term A. As χ is a convex function such that $\rho = \nabla_u \chi$, leading to $\rho_K^n = \nabla_u \chi(u_K^n)$, we have:

$$\chi(u_K^{n+1}) - \chi(u_K^n) - \rho_K^n \cdot (u_K^{n+1} - u_K^n) \geq 0.$$

This yields

$$A \leq \sum_{K\in\mathcal{T}} m(K)(\rho_K^{n+1} - \rho_K^n)\cdot(u_K^{n+1} - u_K^D). \tag{31}$$

We now address the term B. Since $(a^2-b^2)/2 \leq a(a-b)$, for all $a,b\in\mathbb{R}$, and $u_2^D \leq 0$, we get:

$$B \leq -\lambda^2 u_2^D \sum_{\sigma\in\mathcal{E}} \tau_\sigma D_{K,\sigma}(\mathbf{V}^{n+1} - \mathbf{V}^D)\, D_{K,\sigma}(\mathbf{V}^{n+1} - \mathbf{V}^n).$$

A discrete integration by part leads to

$$B \leq \lambda^2 u_2^D \sum_{K\in\mathcal{T}} (V_K^{n+1} - V_K^D)\left(\sum_{\sigma\in\mathcal{E}_K} \tau_\sigma D_{K,\sigma}(\mathbf{V}^{n+1} - \mathbf{V}^n)\right).$$

Using the scheme for the Poisson equation (15c), we obtain

$$B \leq u_2^D \sum_{K\in\mathcal{T}} \mathrm{m}(K)(V_K^{n+1} - V_K^D)(\rho_{1,K}^{n+1} - \rho_{1,K}^n). \tag{32}$$

From (28), (31) and (32), we deduce:

$$\begin{aligned} S^{n+1} - S^n \leq \sum_{K\in\mathcal{T}} \mathrm{m}(K)(\rho_{1,K}^{n+1} - \rho_{1,K}^n)\big((u_{1,K}^{n+1} - u_{1,K}^D) + u_2^D(V_K^{n+1} - V_K^D)\big) \\ + \sum_{K\in\mathcal{T}} \mathrm{m}(K)(\rho_{2,K}^{n+1} - \rho_{2,K}^n)(u_{2,K}^{n+1} - u_{2,K}^D). \end{aligned} \tag{33}$$

Using the primal scheme (15a), (15b), the inequality (33) becomes

$$\frac{S^{n+1} - S^n}{\Delta t} \leq C + D + \sum_{K\in\mathcal{T}} m(K) W_K^{n+1}(u_{2,K}^{n+1} - u_{2,K}^D), \tag{34}$$

with

$$\begin{aligned} C = -\sum_{K\in\mathcal{T}} \left(\sum_{\sigma\in\mathcal{E}_K} \mathcal{F}_{1,K,\sigma}^{n+1}\right)\Big[(u_{1,K}^{n+1} - u_{1,K}^D) + V_K^{n+1}(u_{2,K}^{n+1} - u_{2,K}^D)\Big] \\ - u_2^D \sum_{K\in\mathcal{T}} \left(\sum_{\sigma\in\mathcal{E}_K} \mathcal{F}_{1,K,\sigma}^{n+1}\right)(V_K^{n+1} - V_K^D), \end{aligned}$$

$$D = -\sum_{K\in\mathcal{T}} \left(\sum_{\sigma\in\mathcal{E}_K} \mathcal{F}_{2,K,\sigma}^{n+1} - V_\sigma^{n+1} F_{1,K,\sigma}^{n+1}\right)(u_{2,K}^{n+1} - u_{2,K}^D).$$

Using the change of variables (18a), the relations (20) on the numerical fluxes written in the primal and dual entropy variables and the hypothesis (25), we get

$$
\begin{aligned}
C &= -\sum_{K\in\mathscr{T}}\left(\sum_{\sigma\in\mathscr{E}_K}\mathscr{G}_{1,K,\sigma}^{n+1}\right)(w_{1,K}^{n+1}-w_{1,K}^{D}),\\
D &= -\sum_{K\in\mathscr{T}}\left(\sum_{\sigma\in\mathscr{E}_K}\mathscr{G}_{2,K,\sigma}^{n+1}\right)(w_{2,K}^{n+1}-w_{2,K}^{D}).
\end{aligned}
\tag{35}
$$

Accounting for the boundary conditions, we conclude by a discrete integration by parts which gives (27):

$$
\begin{aligned}
\frac{S^{n+1}-S^n}{\Delta t} \le \sum_{\sigma\in\mathscr{E}}\mathscr{G}_{1,K,\sigma}^{n+1}D_{K,\sigma}\mathbf{w}_1^{n+1} + \sum_{\sigma\in\mathscr{E}}\mathscr{G}_{2,K,\sigma}^{n+1}D_{K,\sigma}\mathbf{w}_2^{n+1}\\
+\sum_{K\in\mathscr{T}}\mathrm{m}(K)W_K^{n+1}(w_{2,K}^{n+1}-w_{2,K}^{D}).
\end{aligned}
\tag{36}
$$

The formulation (21) of the numerical fluxes $\mathscr{G}_{i,K,\sigma}^{n+1}$ permits to rewrite

$$
\begin{aligned}
\sum_{\sigma\in\mathscr{E}}\mathscr{G}_{1,K,\sigma}^{n+1}D_{K,\sigma}\mathbf{w}_1^{n+1} + \sum_{\sigma\in\mathscr{E}}\mathscr{G}_{2,K,\sigma}^{n+1}D_{K,\sigma}\mathbf{w}_2^{n+1}\\
= -\sum_{\sigma\in\mathscr{E}}\tau_\sigma\begin{pmatrix}D_{K,\sigma}\mathbf{w}_1^{n+1}\\ D_{K,\sigma}\mathbf{w}_2^{n+1}\end{pmatrix}^T\mathbb{D}_\sigma^*\begin{pmatrix}D_{K,\sigma}\mathbf{w}_1^{n+1}\\ D_{K,\sigma}\mathbf{w}_2^{n+1}\end{pmatrix}.
\end{aligned}
\tag{37}
$$

From (36) and (37), we deduce (27). The hypothesis (4) on the energy relaxation term and the positive definiteness of the matrices $\mathbb{D}_\sigma$ ensure the nonpositivity of the right-hand-side in (27) and the decay of the discrete entropy.

Consequences

From Proposition 2, we deduce the uniform bound: $S^n \le S^0$ for all $n \ge 0$. The control of the dissipation writes

$$\sum_{n=0}^{N}\sum_{\sigma\in\mathscr{E}}\tau_\sigma(D_{K,\sigma}\mathbf{w}^{n+1})^T\mathbb{D}_\sigma^* D_{K,\sigma}\mathbf{w}^{n+1} \le S^0.$$

This yields a discrete $L^2(0,T_{max},H^1)$ estimates on w_1 and w_2. But, following the ideas of [6, 17], we may obtain other *a priori* estimates on the solution. They permit first to prove the existence of a solution to the scheme, thanks to a topological degree argument, and second to show the compactness of the sequence of approximate solutions leading to the convergence of the scheme. The existence result and the convergence analysis will be detailed in a forthcoming paper.

4 Numerical experiments

For the numerical experiments, we consider the unipolar energy-transport model under Boltzmann statistics, as in [17, 6]. It is based on the following definitions of the densities $\rho_i(u)$, $i = 1,2$:

$$\begin{cases} \rho_1(u) = \left(-\dfrac{1}{u_2}\right)^{3/2} \exp(u_1), \\ \rho_2(u) = \dfrac{3}{2}\left(-\dfrac{1}{u_2}\right)^{5/2} \exp(u_1). \end{cases} \tag{38}$$

so that $\rho(u) = \nabla_u \chi(u)$ with $\chi(u) = (-u_2)^{-3/2} \exp(u_1)$.

The diffusion matrix $\mathbb{L}(u) = (L_{ij}(u))_{1\le i,j\le 2}$ actually depends on u under the following form [17]:

$$\mathbb{L} = c_o \rho_1(u) T^{1/2-\beta} \begin{pmatrix} 1 & (2-\beta)T \\ (2-\beta)T & (3-\beta)(2-\beta)T^2 \end{pmatrix}, \tag{39}$$

where $c_0 > 0$ is a constant (and we recall that $T = -1/u_2$). The usual values of β are $1/2$, corresponding to the Chen model, and 0, corresponding to the Lyumkis model [17]. The matrix $\mathbb{L}(u)$ is symmetric positive definite.

Presentation of the test case

We consider a test case of a 2-D n^+nn^+ silicon diode, uniform in one space direction, already introduced in [7, 13, 3]. It is a simple model for the channel of a MOS transistor. The adopted model is the Chen model ($\beta = 1/2$ in (39)). Additional test cases will be given in a forthcoming paper.

The domain is $\Omega = (0,l_x)\times(0,l_y)$ with $l_x = 0.6\,\mu m$ and $l_y = 0.2\,\mu m$. The channel length is $0.4\,\mu m$, see Fig. 1.

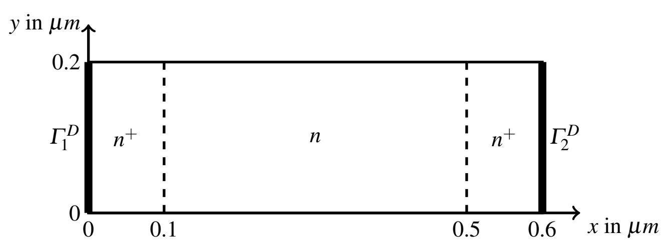

Fig. 1 Geometry of the n^+nn^+ ballistic diode.

The numerical values of the physical parameters for a silicon diode are given in Table 1. The doping profile is

Table 1 Physical parameters.

Parameter	Physical meaning	Numerical value
q	elementary charge	10^{-19} As
ε	permittivity constant	$10^{-12}\mathrm{AsV}^{-1}\mathrm{cm}^{-1}$
μ_0	low field mobility	$1.5\times 10^{3}\mathrm{cm}^{2}\mathrm{V}^{-1}\mathrm{s}^{-1}$
U_T	thermal voltage at $T_0 = 300$K	0.0259 V
τ_0	energy relaxation time	0.4×10^{-12} s

$$C = C_m = 5\times 10^{17} cm^{-3} \quad \text{in the } n^+ \text{ region,}$$
$$C = C_m = 2\times 10^{15} cm^{-3} \quad \text{in the } n \text{ region.}$$

The boundary conditions are

$$V = 1.5\text{V on } \Gamma_1^D \text{ and } V = 0 \text{ on } \Gamma_2^D,$$
$$u_2 = -1/T_0, \text{ with } T_0 = 300K, \text{ on } \Gamma_1^D \cup \Gamma_2^D,$$
$$\rho_1(u) = C_m \text{ on } \Gamma_1^D \cup \Gamma_2^D,$$

the latest giving the boundary condition for u_1 according to (38). The initial conditions for u_1 and u_2 are constant and equal to the boundary conditions.

The function W reads

$$W(u) = c_1\rho_1(u) - c_2\rho_2(u),$$

with

$$c_1 = \frac{3}{2}\frac{l_x^2}{\tau_0\mu_0 U_T}, \quad c_2 = \frac{l_x^2}{\tau_0\mu_0 U_T},$$

and the scaling ensures that the Debye length is

$$\lambda^2 = \frac{\varepsilon U_T}{q l_x^2 C_m}.$$

Numerical results

We use an admissible mesh made of 896 triangles. Figure 2 presents the results obtained by the scheme (15)-(16) in the centered case (22). The results are plotted for the final time $T_{\text{final}} = 1$s, as the equilibrium state is reached. Although the discretization is fully implicit, it is necessary to use an adaptative time step during the first iterations, in order to allow the convergence of the Newton's method. As expected, the computed quantities are almost uniform in one space direction. Moreover one observes the expected hot electron effect in the channel, which compares with the results given in [7, 13, 3].

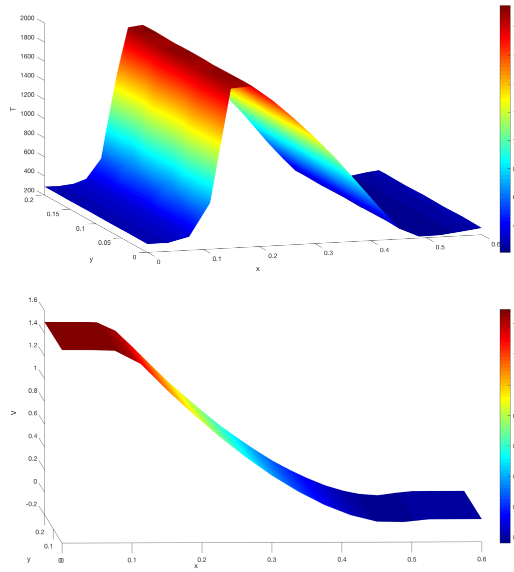

Fig. 2 2-D n^+nn^+ diode: temperature (above) and electrostatic potential (below).

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