Asymptotic preserving schemes in the quasi-neutral limit for the drift-diffusion system

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Abstract We are interested in the drift-diffusion system near quasi-neutrality. This system, constituted of coupled elliptic and parabolic equations, arises in semiconductor modeling. For this system, classical explicit schemes are decoupled but, they are subject to severe numerical constraints in the quasi-neutral regime. By constrast, the implicit discretizations are unconditionally stable. But, they are non linearly coupled. Then, an iterative method must be used yielding a large numerical cost. Here, we propose a new decoupled asymptotic preserving scheme. We perform one and two dimensional numerical experiments which show its good behavior.

1 Presentation of the problem

Let $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) be an open bounded domain describing the geometry of a semiconductor device. The unknowns of the linear drift-diffusion system are the density of electrons and holes, N and P, and the electrostatic potential Ψ. It writes:

$$\partial_t N + \mathrm{div}(-\nabla N + N\nabla\Psi) = 0 \text{ on } \Omega \times [0,T], \tag{1a}$$

$$\partial_t P + \mathrm{div}(-\nabla P - P\nabla\Psi) = 0 \text{ on } \Omega \times [0,T], \tag{1b}$$

$$-\lambda^2 \Delta\Psi = P - N + C \text{ on } \Omega \times [0,T], \tag{1c}$$

where C is the given doping profile non depending on t. The parameter λ comes from the scaling of the physical model. It is called the rescaled Debye length and is

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given by the ratio of the Debye length to the size of the domain. The Debye length measures the typical scale of electric interactions in the semiconductor.

The system (1) is supplemented with initial conditions N_0, P_0 and with mixed boundary conditions: Dirichlet boundary conditions on Γ^D (N^D, P^D and Ψ^D) and homogeneous Neumann boundary conditions on Γ^N (with $\partial\Omega = \Gamma^D \cup \Gamma^N$).

We are interested in the so-called quasi-neutral regime. This regime occurs when the parameter λ tends to zero. There has been an intense literature on the rigorous quasi-neutral limit of the drift-diffusion model; we can refer for instance to [9] for a zero doping profile C and to [10] for a regular doping profile.

Many different numerical methods have been already developed for the approximation of (1); see for instance [1] and [12, 13] in the non linear case. The convergence of some finite volume schemes has been proved in [2, 3]. But, up to our knowledge, all the schemes are studied in the case $\lambda = 1$. In this paper, we focus on the behavior of schemes in the quasi-neutral limit, that means when λ tends to zero. In this regime, the local electric charge vanishes everywhere. However, simultaneously, very high frequency oscillations, of order $1/\lambda^2$, are triggered. When a standard explicit scheme is used, the scale of these very high frequency oscillations must be resolved by the time step. Hence, the time step must be smaller than λ^2 otherwise a numerical instability appears. The satisfaction of this constraint requires huge computational resources which makes the explicit methods unusable.

Here, the purpose is to define numerical schemes free of such constraints. For a given time step, we look for schemes which may be used as well as for values of λ of order 1 and for values of λ as small as possible. Furthermore, these schemes must preserve the behavior of the continuous problem in the quasi-neutral limit ($\lambda \to 0$). Such schemes are called asymptotic preserving schemes, this name has been introduced in [11] for relaxation limits of kinetic systems. Asymptotic preserving schemes in the quasi-neutral limit have been developed in [5] for the Euler-Poisson problem and in [6, 7] for the Vlasov-Poisson system. For the drift-diffusion model, implicit strategies have been proposed in [15].

This paper is organized as follows. In Section 2, we present the formal quasi-neutral limit of the drift-diffusion system. Then, in Section 3, we recall two classical schemes and discuss their stability. Section 4 is devoted to the presentation of a new scheme for the drift-diffusion model. Finally, in Section 5, we conclude with numerical simulations.

2 The formal quasi-neutral limit

Formally, passing to the limit $\lambda \to 0$ in system (1) gives the quasi-neutral drift-diffusion system. It is constituted of the mass equations (1a), (1b) and of the quasi-neutrality constraint $P - N + C = 0$. The Poisson equation is lost, and the electrostatic potential becomes the Lagrange multiplier of this constraint. In order to obtain an explicit equation for the potential we subtract the mass equations (1a), (1b) and

we remark that thanks to the quasi-neutrality constraint $P-N=-C$. This yields an elliptic equation for the potential: $-\mathrm{div}((P+N)\nabla\Psi)=-\Delta C$.

Let us perform the same transformations on the original drift-diffusion system. We begin by subtracting the mass equations. Then, remarking that, thanks to Poisson equation, $\partial_t(P-N)=\partial_t(P-N+C)=\partial_t(-\lambda^2\Delta\Psi)$,we obtain

$$-\lambda^2\,\partial_t\Delta\Psi-\mathrm{div}((P+N)\nabla\Psi)=\Delta(P-N). \tag{2}$$

Following [5], we call this equation the reformulated Poisson equation. If P and N are constant, this equation is an order one differential equation on the quantity $-\Delta\Psi$. And, we can note that solutions oscillate in time at the period λ^2.

Thus, an explicit discretization of the electric force terms in (1) will give an explicit discretization of equation (2) and so a stability non uniform in λ. By contrast, an implicit discretization of these terms will give an implicit discretization of (2) and so a stability uniform in λ. This remark will be used in Section 4 for the construction of our decoupled asymptotic preserving scheme.

3 "Classical" schemes

In this section, we present the classical schemes used for the discretization of the drift-diffusion system. The mesh is given by $\mathscr{T}$, a family of control volumes, $\mathscr{E}$, a family of edges and $\mathscr{P}=(x_K)_{K\in\mathscr{T}}$ a family of points. We assume that the mesh is admissible in the sense of [8]. The set of edges will be split into $\mathscr{E}=\mathscr{E}_{int}\cup\mathscr{E}_{ext}$ and for the exterior edges, we distinguish the edges included in Γ^D from the edges included in Γ^N: $\mathscr{E}_{ext}=\mathscr{E}_{ext}^D\cup\mathscr{E}_{ext}^N$. For a given control volume $K\in\mathscr{T}$, we define $\mathscr{E}_K$ the set of its edges, which is also split into $\mathscr{E}_K=\mathscr{E}_{K,int}\cup\mathscr{E}_{K,ext}^D\cup\mathscr{E}_{K,ext}^N$.

For all edge $\sigma\in\mathscr{E}$, we define $\mathrm{d}_\sigma=\mathrm{d}(x_K,x_L)$ if $\sigma=K|L\in\mathscr{E}_{int}$ and $\mathrm{d}_\sigma=\mathrm{d}(x_K,\sigma)$ if $\sigma\in\mathscr{E}_{K,int}$. Then, the transmissibility coefficient is defined by $\tau_\sigma=\mathrm{m}(\sigma)/\mathrm{d}_\sigma$, for all $\sigma\in\mathscr{E}$.

Let Δt be the time step. A finite volume scheme for (1) writes:

$$\begin{aligned}
&\mathrm{m(K)}\frac{\mathrm{N_K^{n+1}}-\mathrm{N_K^n}}{\Delta\mathrm{t}}+\sum_{\sigma\in\mathscr{E}_\mathrm{K}}\mathscr{F}_{\mathrm{K},\sigma}^{\mathrm{n+1}}=0,\forall\mathrm{K}\in\mathscr{T},\forall\mathrm{n}\geq 0,\\
&\mathrm{m(K)}\frac{\mathrm{P_K^{n+1}}-\mathrm{P_K^n}}{\Delta\mathrm{t}}+\sum_{\sigma\in\mathscr{E}_\mathrm{K}}\mathscr{G}_{\mathrm{K},\sigma}^{\mathrm{n+1}}=0,\forall\mathrm{K}\in\mathscr{T},\forall\mathrm{n}\geq 0,\\
&-\lambda^2\sum_{\sigma\in\mathscr{E}_K}\tau_\sigma D\Psi_{K,\sigma}^n=\mathrm{m(K)}(\mathrm{P_K^n}-\mathrm{N_K^n}+\mathrm{C_K}),\forall\mathrm{K}\in\mathscr{T},\forall\mathrm{n}\geq 0.
\end{aligned}$$

It remains to define the numerical fluxes $D\Psi_{K,\sigma}^n$, $\mathscr{F}_{K,\sigma}^{n+1}$ and $\mathscr{G}_{K,\sigma}^{n+1}$. As usually, we set $D\Psi_{K,\sigma}^n=\Psi_L^n-\Psi_K^n$ if $\sigma=K|L$, $D\Psi_{K,\sigma}^n=\Psi_\sigma^D-\Psi_K^n$ if $\sigma\in\mathscr{E}_{K,ext}^D$ and $D\Psi_{K,\sigma}^n=0$ elsewhere. The numerical approximations of the convection-diffusion fluxes in (1a) and (1b), $\mathscr{F}_{K,\sigma}^{n+1}$ and $\mathscr{G}_{K,\sigma}^{n+1}$, are written with the following compact form:

$$\mathscr{F}_{K,\sigma}^{n+1} = \tau_\sigma \left(B(-D\Psi_{K,\sigma}^m) N_K^{n+1} - B(D\Psi_{K,\sigma}^m) N_L^{n+1} \right), \ \forall \sigma \in \mathscr{E}_{int}, \sigma = K|L \qquad (3a)$$

$$\mathscr{G}_{K,\sigma}^{n+1} = \tau_\sigma \left(B(D\Psi_{K,\sigma}^m) P_K^{n+1} - B(-D\Psi_{K,\sigma}^m) P_L^{n+1} \right), \ \forall \sigma \in \mathscr{E}_{int}, \sigma = K|L. \qquad (3b)$$

If $\sigma \in \mathscr{E}_{K,ext}^D$, we replace N_L^{n+1} by N_σ^D in (3a) and P_L^{n+1} by P_σ^D in (3b). If $\sigma \in \mathscr{E}_{K,ext}^N$, we set $\mathscr{F}_{K,\sigma}^{n+1} = \mathscr{G}_{K,\sigma}^{n+1} = 0$.

The case $m = n$ corresponds to a semi-implicit and decoupled scheme: at each time step $(N_K^{n+1})_{K\in\mathscr{T}}$, $(P_K^{n+1})_{K\in\mathscr{T}}$, and $(\Psi_K^{n+1})_{K\in\mathscr{T}}$, are obtained by solving three linear systems. With $m = n+1$, we write a fully implicit scheme. For the function B, we may choose either $B(x) = 1 - \min(x,0)$ or $B(x) = x/(\exp(x)-1)$ with $B(0) = 1$. The first choice corresponds to a classical two-points discretization of the diffusion with an upwinding for the convection. With the Bernoulli function, we get the Scharfetter-Gummel scheme. One main advantage of this last choice, well-known in semiconductor device simulation, is that the scheme is order 2 in space (see [14]). Moreover, as shown in [4], the Scharfetter-Gummel scheme satisfies some crucial properties like energy and energy dissipation decrease.

The decoupled scheme ($m = n$) has been studied in [2] for $B(x) = 1 - \min(x,0)$ and the convergence has been established (for the nonlinear drift-diffusion system). The proof can be extended to the Scharfetter-Gummel scheme (in the linear case). However, in [2], the convergence proof has been done for $\lambda^2 = 1$ and in fact all the a priori estimates (leading to stability, compactness and convergence) depend on λ^2. More precisely, when there is no doping profile or when the doping profile is constant in space, there exists uniform in time L^∞ estimates on the densities N and P (see [10]). In this case, the L^∞ estimates holds at the discrete level, but only under a condition of the form: $\Delta t \leq D\lambda^2$ with $D \in \mathbb{R}$. It means that such a scheme might not be used for small values of λ.

Let us now consider the fully implicit scheme ($m = n+1$). In this case, existence of a solution to the scheme can be proved via a fixed point theorem. Moreover, when the doping profile is constant in space, we can prove that the scheme is unconditionally stable. However, the implementation of the scheme needs the resolution of a nonlinear system of equations at each iteration. This might be done using a Newton's method. It has a numerical cost and the solution is computed up to a precision criterion.

In the next section, we propose a new scheme with the same numerical cost as the decoupled scheme, but remaining stable and consistent when λ tends to 0.

4 Construction of an asymptotic preserving scheme

Following the remark given in Section 2, let us first consider the following semi-discretization of (1) in which the electric force terms are discretized implicitly.

$$\frac{N^{n+1} - N^n}{\Delta t} + \operatorname{div}(-\nabla N^n + N^n \nabla \Psi^{n+1}) = 0 \text{ on } \Omega \times [0,T], \qquad (4a)$$

$$\frac{P^{n+1}-P^n}{\Delta t}+\operatorname{div}(-\nabla P^n - P^n\nabla\Psi^{n+1})=0 \text{ on } \Omega\times[0,T], \tag{4b}$$

$$-\lambda^2\Delta\Psi^{n+1}=P^{n+1}-N^{n+1}+C \text{ on } \Omega\times[0,T]. \tag{4c}$$

We eliminate P^{n+1} and N^{n+1} in (4c) using their expression respectively given in (4b) and (4a). It yields:

$$-\lambda^2\Delta\Psi^{n+1}-\Delta t\operatorname{div}((P^n+N^n)\nabla\Psi^{n+1})=P^n-N^n+C+\Delta t\Delta(P^n-N^n). \tag{5}$$

The semi-discretization given by (4a), (4b) and (5) is uniformally stable in λ but not unconditionaly stable. Then, in order to construct an unconditionally stable semi-discretization we just have to change the discretizations (4a), (4b) into the implicit semi-discretizations of the mass equations.

This corresponds to the following fully discrete scheme:

$$\mathrm{m(K)}\frac{\mathrm{N_K^{n+1}-N_K^n}}{\Delta\mathrm{t}}+\sum_{\sigma\in\mathscr{E}_\mathrm{K}}\mathscr{F}_{\mathrm{K},\sigma}^{\mathrm{n+1}}=0,\forall\mathrm{K}\in\mathscr{T},\forall\mathrm{n}\geq 0, \tag{6a}$$

$$\mathrm{m(K)}\frac{\mathrm{P_K^{n+1}-P_K^n}}{\Delta\mathrm{t}}+\sum_{\sigma\in\mathscr{E}_\mathrm{K}}\mathscr{G}_{\mathrm{K},\sigma}^{\mathrm{n+1}}=0,\forall\mathrm{K}\in\mathscr{T},\forall\mathrm{n}\geq 0, \tag{6b}$$

$$\begin{aligned}-\sum_{\sigma\in\mathscr{E}_K}\tau_\sigma(\lambda^2+\Delta t(P_\sigma^n+N_\sigma^n))D\Psi_{K,\sigma}^{n+1}&=\mathrm{m(K)(P_K^n-N_K^n+C_K)}\\&\quad+\Delta t\sum_{\sigma\in\mathscr{E}_K}\tau_\sigma(DP_{K,\sigma}^n-DN_{K,\sigma}^n)\,\forall K\in\mathscr{T},\forall n\geq 0,\end{aligned} \tag{6c}$$

with the values (3a), (3b) and $m=n+1$ for the numerical fluxes $\mathscr{F}_{K,\sigma}^{n+1}$, $\mathscr{G}_{K,\sigma}^{n+1}$. The interface values, P_σ^n and N_σ^n are defined by taking the mean value between the values of N^n and P^n at two neighboring control volumes. Let us also note that we keep an implicit discretization on N and P in (6a) and (6b) in order to avoid any CFL condition on the time step.

We stress that our scheme is decoupled. It means that, at each time step, if the values $(N_K^n)_{K\in\mathscr{T}}$, $(P_K^n)_{K\in\mathscr{T}}$ are known,

- we first compute $(\Psi_K^{n+1})_{K\in\mathscr{T}}$ by solving the linear system (6c), whose matrix and right-hand-side depend on N^n and P^n,
- then we compute $(N_K^{n+1})_{K\in\mathscr{T}}$ and $(P_K^{n+1})_{K\in\mathscr{T}}$ solutions of the linear systems (6a) and (6b), whose matrices depend on Ψ^{n+1}.

The matrices from (6a) and (6b) are identical to that obtained in the classical decoupled scheme. They are M-matrices, which ensure the positivity at N^n and P^n for all n (starting with positive initial and boundary conditions). However, the numerical analysis of the scheme (6) is not straightforward and is in progress. In the next section, we present the results of numerical simulations in which we compare our new decoupled scheme to the fully implicit scheme. We will focus on the behavior when the rescaled Debye length tends to 0.

5 Numerical experiments

Test case 1. The first test case is a one-dimensional test case ($\Omega =]0,1[$). The doping profile is a continuous function satisfying $C(x) = -1$ for $0 \leq x \leq 0.4$, $C(x) = +1$ for $0.6 \leq x \leq 1$ and $C(x)$ affine on $[0.4, 0.6]$. The initial and the boundary conditions satisfy the quasi-neutrality condition $P + C - N = 0$, in order to avoid any boundary or initial time layers:

$$N^D = 0, P^D = 1, \Psi^D = 0 \text{ in } x = 0, \quad N^D = 1,\ P^D = 0, \Psi^D = 4 \text{ in } x = 1, \tag{7a}$$

$$N_0(x) = \max(C(x), 0) \quad P_0(x) = -\min(C(x), 0). \tag{7b}$$

With a time step $\Delta t = 10^{-3}$, we run computations with the fully implicit scheme and with the new one for different values of λ^2 on a mesh made of 100 cells. The solution is computed at the final time $T = 1$. For the Newton's method used in the fully implicit scheme the precision criterion is set to 10^{-10} and the maximal number of iterations to 60. In Table 1, we present the CPU times needed by both schemes and also the relative error between the two solutions in a discrete L^2-norm.

We note that the CPU time needed by the new scheme is almost independent of λ. For the fully implicit scheme, we see that for $\lambda^2 \leq 10^{-6}$ the CPU time has a ratio 3 with those of the new scheme. For smaller values of λ^2, it appears some default of convergence of the Newton's method with the given time step for the fully implicit scheme. However, the new scheme still works and we show on Figure 1(a) the density profiles obtained for $\lambda^2 = 10^{-14}$.

Table 1 Comparison of the fully implicit scheme with the new scheme for the Test Case 1.

λ^2	CPU time fully implicit	CPU time new scheme	ratio	relative error on N	relative error on P	relative error on Ψ
1	1.92	0.64	3.00	1.32e-08	1.32e-08	5.94e-09
1e-2	1.82	0.59	3.08	5.73e-06	5.73e-06	2.98e-06
1e-4	2.07	0.59	3.51	2.77e-04	2.77e-04	1.99e-04
1e-6	1.67	0.60	2.78	5.15e-04	5.15e-04	5.70e-04
1e-8	51.46	0.60	85.77	5.24e-04	5.24e-04	5.88e-04

Test Case 2. We change the doping profile for a discontinuous doping profile: $C(x) = -1$ for $x \leq 0.5$ and $C(x) = +1$ for $x \geq 0.5$. We keep (7) as initial and boundary conditions. The numerical results, presented in Table 2, are similar to those of Test Case 1. We just observe that the relative errors are bigger. This is due to the discontinuity appearing in the density profiles (due to the discontinuity in C): the two schemes do not capture the discontinuity similarly. However, we still note that the new scheme has the same efficiency up to very small values of λ. On Figure 1(b), we present the density profiles obtained for $\lambda^2 = 10^{-14}$.

Test Case 3. We consider now the simulation of a two-dimensional forward PN diode. The device is made of two different regions : a P-region with a doping profile

(a) Test case 1 (b) Test case 2

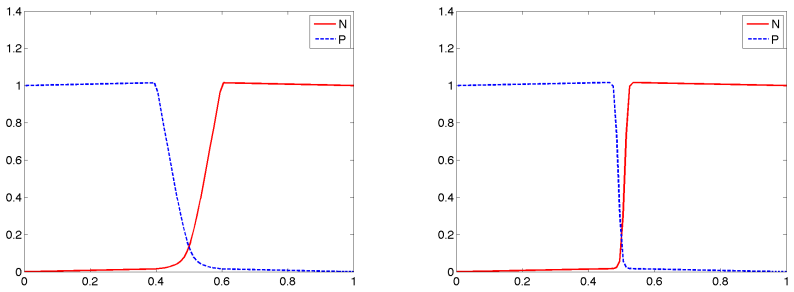

Fig. 1 Density profiles computed by the new scheme for $\lambda^2 = 10^{-14}$ on a mesh made of 100 cells, with $\Delta t = 10^{-3}$.

Table 2 Comparison of the fully implicit scheme with the new scheme for the Test Case 2.

λ^2	CPU time fully implicit	CPU time new scheme	ratio	relative error on N	relative error on P	relative error on Ψ
1	2.09	0.67	3.12	1.31e-08	1.31e-08	5.89e-09
1e-2	1.88	0.60	3.13	7.50e-06	7.50e-06	4.22e-06
1e-4	2.15	0.61	3.52	1.36e-02	1.36e-02	9.51e-03
1e-6	1.73	0.61	2.84	1.03e-01	1.03e-01	6.07e-02
1e-8	51.51	0.60	85.85	1.08e-01	1.08e-01	6.23e-02

equal to -1 and an N-region with a doping profile equal to 1 (see [3]). We use a triangular mesh made of 896 triangles and we set the time step $\Delta t = 5 \cdot 10^{-4}$.

Table 3 shows the efficiency of the new scheme. It really runs faster than the fully implicit scheme. Moreover, the fully implicit scheme did not give results for values of λ^2 less that 10^{-3}, while the new scheme still works. We show on Figure 2, the density profiles obtained with the new scheme for $\lambda^2 = 10^{-10}$.

Table 3 Comparison of the fully implicit scheme with the new scheme for the Test Case 3.

λ^2	CPU time fully implicit	CPU time new scheme	ratio	relative error on N	relative error on P	relative error on Ψ
1	203.28	14.68	13.85	1.13e-01	2.78e-01	2.54e-03
1e-1	219.85	14.52	15.14	8.54e-02	2.19e-01	3.01e-02
1e-2	310.72	14.52	21.40	3.21e-02	1.00e-01	4.50e-02
1e-3	718.09	14.68	48.92	4.84e-02	8.30e-02	7.49e-02

As a conclusion, we recall that we have proposed in this paper a new scheme for the drift-diffusion system, whose efficiency is independent of the value of the rescaled Debye length. This scheme can be used at the quasi-neutral limit. Numerical analysis of the scheme is in progress.

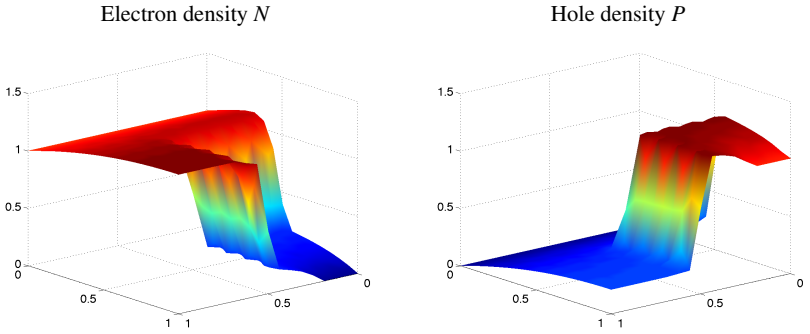

Fig. 2 Test case 3. Density profiles computed by the new scheme for $\lambda^2 = 10^{-10}$ on a mesh made of 896 triangles, with $\Delta t = 5 \cdot 10^{-4}$.

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