Entropy Method and Asymptotic Behaviours of Finite Volume Schemes

Claire Chainais-Hillairet

Abstract When deriving a numerical scheme for a system of PDEs coming for instance from physics or engineering, it is crucial to propose a scheme which preserves the asymptotic behaviour of the continuous system, with respect to time as with respect to some parameters. In this paper, we want to show how the entropy method can be applied to some finite volume schemes and permits to show that some schemes are asymptotic preserving. We focus on two problems: the nonlinear diffusion equation (long time behaviour) and the drift-diffusion system (long time behaviour and quasi-neutral limit). Some results have been obtained in collaboration with Jüngel and Schuchnigg [10] and the others with Bessemoulin-Chatard and Vignal [4].

1 Introduction

1.1 Entropy Method and Long Time Behaviour

The entropy method is initially devoted to the study of the convergence to equilibrium of systems composed of a large number of particules. Roughly speaking, the trend to equilibrium is governed by a thermodynamical principle: a given functional, called physical entropy, increases when the time increases and the equilibrium is defined as the maximum of the entropy. The entropy method has been widely studied and applied since the beginning of the 90s: see [1] and all the references therein. As

C. Chainais-Hillairet (✉)
Laboratoire P. Painlevé, UMR CNRS 8524, Université Lille 1,
59655 Villeneuve d'Ascq Cedex, France
e-mail: Claire.Chainais@math.univ-lille1.fr

Team MEPHYSTO, INRIA Lille Nord Europe, 40 av. Halley,
59650 Villeneuve d'Ascq Cedex, France

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written in this paper, it appears that "entropy methods have proved over the last years to be an efficient tool for the understanding of the qualitative properties of physically sound models, for accurate numerics and for a more mathematical understanding of nonlinear PDEs".

In order to explain the principles of the entropy method, let us consider a system of partial differential equations written basically under the form:

$$\begin{aligned} &\partial_t f + Af = 0, \quad t \geq 0, \\ &f(0) = f_0, \end{aligned}$$

where A is a partial differential operator containing also the boundary conditions. A stationary state is defined by $Af_\infty = 0$. The question worthy of interest concerns the convergence of $f(t)$ towards f_∞ when t tends to $+\infty$. The strategy consists in proving the convergence in relative entropy: considering an entropy (a convex nonnegative Lyapunov functional), the idea is to prove that $E(f) \to E(f_\infty)$ or equivalently $E(f|f_\infty) = E(f) - E(f_\infty) \to 0$ when $t \to +\infty$. The result is based on the relation

$$\frac{d}{dt}(E(f(t)|f_\infty) + D(f(t))) = 0, \text{ with } D(f) = \langle Af, E'(f)\rangle.$$

The term $D(f)$ is the entropy dissipation. It must be nonnegative so that the entropy is nonincreasing (the mathematical entropy is the opposite of the physical entropy). Moreover, if the dissipation is related to the entropy thanks to some relation like $D(f) \geq \lambda E(f|f_\infty)$ (respectively $D(f) \geq KE(f|f_\infty)^{1+\gamma}$), an exponential (respectively polynomial) convergence of the relative entropy towards the equilibrium can be obtained.

This technique has been widely used for many systems of PDEs coming from the physics in many different areas of applications. We can refer to the survey paper [1] and the references therein. The entropy method has been applied for instance for electro-reaction-diffusion systems [22], thin-film type equations [5], reaction-diffusion equations [13], coagulation-fragmentation models [6].

In the sequel of the paper, we will consider two different problems: the nonlinear diffusion equation (porous medium/fast diffusion equation) and the drift-diffusion system coming from the modelling of semiconductor devices.

The Nonlinear Diffusion Equation

Let Ω be an open bounded domain of $\mathbb{R}^d$ such that $\mathrm{m}(\Omega) = 1$ and $\beta > 0$. We consider the following nonlinear diffusion equation supplemented with initial and homogeneous Neumann boundary conditions:

$$\partial_t u - \Delta(u^\beta) = 0, \text{ in } \Omega, t > 0 \text{ with } u(\cdot, 0) = u_0, \text{ in } \Omega, \tag{1a}$$

$$\nabla(u^\beta)\cdot\nu = 0, \text{ on } \partial\Omega, t>0. \tag{1b}$$

When $\beta > 1$, it is called the porous-medium equation, describing the flow of an isentropic gas through a porous medium. When $\beta < 1$, it is referred as the fast-diffusion equation. In [9], the entropy-entropy dissipation method was applied to (1a) in the whole space to prove the decay of the solutions to the asymptotic self-similar profile. The convergence towards the constant steady-state on the one-dimensional torus was proved in [7].

We note that the solution to (1a), (1b) satisfies $\int_\Omega u(x,t)dx = \int_\Omega u_0(x)dx$ for all $t \geq 0$. Therefore, the stationary state is constant and equal to $u_\infty = \int_\Omega u_0(x)dx$. In order to study the convergence towards the stationary state, we introduce the following family of zeroth-order relative entropies:

$$E_\alpha(u) = \frac{1}{\alpha+1}\left(\int_\Omega u^{\alpha+1}dx - \left(\int_\Omega u dx\right)^{\alpha+1}\right), \quad \alpha > 0. \tag{2}$$

In [10], we study, among other things, the algebraic and the exponential decay of these entropies. The functional inequalities relating entropy and dissipation are obtained from generalized Beckner inequalities.

The Drift-Diffusion System

The drift-diffusion-Poisson system has been introduced by van Roosbroeck [27] for the modelling of semiconductor devices. Let Ω be an open bounded set of $\mathbb{R}^d$ describing the geometry of the semiconductor device, the system writes:

$$\partial_t N + \operatorname{div}(\mu_N(-\nabla N + N\nabla\Psi)) = -R(N,P), \text{ in } \Omega,\ t>0, \tag{3a}$$

$$\partial_t P + \operatorname{div}(\mu_P(-\nabla P - P\nabla\Psi)) = -R(N,P), \text{ in } \Omega,\ t>0, \tag{3b}$$

$$-\lambda^2\Delta\Psi = P - N + C, \text{ in } \Omega,\ t>0. \tag{3c}$$

where the given function $C(x)$ is the doping profile and $R(N,P)$ the recombination-generation rate. The dimensionless physical parameters μ_N, μ_P and λ are the rescaled mobilities of electrons and holes and the rescaled Debye length. This system is generally supplemented with Dirichlet-Neumann boundary conditions ($\partial\Omega = \Gamma^D \cup \Gamma^N$):

$$N = N^D,\ P = P^D,\ \Psi = \Psi^D \text{ on } \Gamma^D \times (0,T), \tag{4a}$$

$$\nabla N\cdot\nu = 0,\ \nabla P\cdot\nu = 0,\ \nabla\Psi\cdot\nu = 0, \text{ on } \Gamma^N \times (0,T), \tag{4b}$$

and with initial conditions N_0, P_0.

The stationary state for the drift-diffusion model is referred as the thermal equilibrium (N^*, P^*, Ψ^*). It is defined under some compatibility assumptions on the boundary data. The convergence of the solution to (3a)–(4b) towards the thermal equilibrium has been established by Jüngel in [24] (including the case of nonlinear diffusion) and Gajewski and Gärtner in [16] (for the linear system with magnetic field). Both proofs are based on an entropy method. In this case, the relative entropy is defined by:

$$\mathbb{E}(t) = \int_\Omega \Big(H(N) - H(N^*) - \log(N^*)(N - N^*) \\ + H(P) - H(P^*) - \log(P^*)(P - P^*) + \frac{\lambda^2}{2}|\nabla\Psi - \nabla\Psi^*|^2 \Big) dx,$$

with $H(x) = x\log x - x + 1$.

1.2 Entropy Method and Quasi-Neutral Limit

In the drift-diffusion model (3a)–(4b), the quasi-neutral limit consists in letting the scaled Debye length λ tend to 0. From a physical point of view, this means that only the large scale structures with respect to the Debye length are taken into account. For the sake of simplicity, we will now assume that $\mu_N = \mu_P = 1$, $R(N, P) = 0$ and that the doping profile vanishes. Under these hypotheses, the system (3a)–(4b) will be denoted $(\mathscr{P}_\lambda)$. The quasi-neutral limit is formally obtained by setting $\lambda = 0$ in $(\mathscr{P}_\lambda)$. It implies that the Poisson equation reduces to an algebraic equation on N and P. The system $(\mathscr{P}_0)$ rewrites:

$$\partial_t N - \Delta N = 0, \tag{5a}$$

$$\operatorname{div}(N\nabla\Psi) = 0, \tag{5b}$$

$$P = N. \tag{5c}$$

Jüngel and Peng [25] performed rigorously the quasi-neutral limit for the drift-diffusion system with a zero doping profile and mixed Dirichlet and homogeneous Neumann boundary conditions. Under quasi-neutrality assumptions on the initial and boundary conditions ($N_0 - P_0 = 0$ and $N^D - P^D = 0$), they prove that a weak solution to $(\mathscr{P}_\lambda)$, denoted by $(N^\lambda, P^\lambda, \Psi^\lambda)$, converges, when $\lambda \to 0$, to (N^0, P^0, Ψ^0) solution to $(\mathscr{P}_0)$ in the following sense:

$$N^\lambda \to N^0,\ P^\lambda \to P^0 \text{ in } L^p(\Omega \times (0, T)) \text{ strongly, for all } p \in [1, +\infty),$$
$$N^\lambda \rightharpoonup N^0,\ P^\lambda \rightharpoonup P^0,\ \Psi^\lambda \rightharpoonup \Psi^0 \text{ in } L^2(0, T, H^1(\Omega)) \text{ weakly.}$$

The same kind of result is established for the drift-diffusion system with homogeneous Neumann boundary conditions by Gasser in [17] for a zero doping profile and by Gasser et al. in [18] for a regular doping profile. In all these papers, the rigorous proof of the quasi-neutral limit is based on an entropy method.

In the case of Dirichlet-Neumann boundary conditions, we will consider that the boundary data N^D, P^D, Ψ^D are defined on the whole domain Ω and verify $N^D, P^D \in L^\infty \cap H^1(\Omega)$, $\Psi^D \in H^1(\Omega)$. Then, the entropy functional, which has the physical meaning of a free energy, is defined (see [25]) by

$$\mathbb{E}(t) = \int_\Omega \Big(H(N) - H(N^D) - \log(N^D)(N - N^D) \\ + H(P) - H(P^D) - \log(P^D)(P - P^D) + \frac{\lambda^2}{2} |\nabla\Psi - \nabla\Psi^D|^2 \Big) dx$$

and the entropy dissipation functional is defined by

$$\mathbb{D}(t) = \int_\Omega \Big(N\, |\nabla(\log N - \Psi)|^2 + P\, |\nabla(\log P + \Psi)|^2 \Big)\, dxdt.$$

The entropy and the entropy dissipation satisfy the following relation:

$$\frac{d\mathbb{E}}{dt}(t) + \frac{1}{2}\mathbb{D}(t) \le K_D \quad \forall t \ge 0, \tag{6}$$

where K_D is a constant depending only on data. This inequality is crucial in order to perform rigorously the quasi-neutral limit. Indeed, if $\mathbb{E}(0)$ is uniformly bounded in λ, (6) provides a uniform bound on $\int_0^T \mathbb{D}(s)ds$. It implies a priori uniform bounds on $(N^\lambda, P^\lambda, \Psi^\lambda)$ solution to $(\mathscr{P}_\lambda)$ and therefore compactness of a sequence of solutions.

1.3 Aim of the Paper

The preservation of the structure of the equations (or system of equations) is a very important property of a numerical scheme. Positivity, maximum principle, appropriate a priori estimates are the bases for the proof of convergence of finite volume schemes for instance. The properties of entropy consistency or entropy dissipation by numerical schemes are also crucial and have been investigated in different frameworks, see for instance [8, 14, 19–21, 23].

In this paper, we want to present some recent results obtained with Jüngel and Schuchnigg for the nonlinear diffusion equation [10] and with Bessemoulin-Chatard and Vignal for the drift-diffusion system [4]. In both cases, we study the asymptotic behaviour of some finite volume schemes using a discrete entropy method.

Section 2 is devoted to the presentation of the notations. In Sect. 3, we are interested in the long time behaviour of some numerical schemes. We first present results obtained in [10] for the nonlinear diffusion equation. In this case, thanks to discrete functional inequalities, we can establish polynomial or exponential decay of a family of discrete relative entropies. We will also mention some known results for the numerical approximation of the drift-diffusion system.

In Sect. 4, we consider a Euler implicit in time and finite volume in space scheme for the drift-diffusion system. With the choice of Scharfetter-Gummel approximation for the convection-diffusion fluxes [26], we can derive a discrete counterpart of (6). We then prove that the scheme is asymptotic preserving at the quasi-neutral limit : it converges for all $\lambda \geq 0$ and the corresponding limit (N, P, Ψ) is a solution to $(\mathscr{P}_\lambda)$, for $\lambda > 0$ as for $\lambda = 0$.

2 Notations

In order to define the numerical schemes under consideration in this paper, we need to introduce the discretization settings and some notations. We restrict the presentation to a two-dimensional case but generalization to higher dimension is straightforward. We consider that Ω is an open bounded polygonal subset of $\mathbb{R}^2$.

The mesh $\mathscr{M} = (\mathscr{T}, \mathscr{E}, \mathscr{P})$ is given by $\mathscr{T}$, a family of open polygonal control volumes, $\mathscr{E}$, a family of edges and $\mathscr{P} = (x_K)_{K\in\mathscr{T}}$ a family of points. As it is classical in the finite volume discretization of elliptic or parabolic equations with a two-points flux approximations, we assume that the mesh is admissible in the sense of [15] (Definition 9.1).

We distinguish in $\mathscr{E}$ the interior edges, $\sigma = K|L$, from the exterior edges, $\sigma \subset \partial\Omega$. Therefore $\mathscr{E}$ is split into $\mathscr{E} = \mathscr{E}_{int} \cup \mathscr{E}_{ext}$. Within the exterior edges, we distinguish (if necessary) 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 each edge $\sigma \in \mathscr{E}$, there exists at least one cell $K \in \mathscr{T}$ such that $\sigma \in \mathscr{E}_K$. Then, we can denote this cell K_σ. In the case where σ is an interior edge ($\sigma = K|L$), K_σ can be either equal to K or to L.

For all edges $\sigma \in \mathscr{E}$, 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 $\sigma \in \mathscr{E}_{ext}$ with $\sigma \in \mathscr{E}_K$. Then, the transmissibility coefficient is defined by $\tau_\sigma = \mathrm{m}(\sigma)/\mathrm{d}_\sigma$, for all $\sigma \in \mathscr{E}$. We assume that the mesh satisfies the following regularity constraint:

$$\exists \xi > 0 \text{ such that } \mathrm{d}(x_K, \sigma) \geq \xi\, \mathrm{d}_\sigma, \quad \forall K \in \mathscr{T}, \forall \sigma \in \mathscr{E}_K. \tag{7}$$

Let $T > 0$, we consider a subdivision of the interval $[0, T]$ defined by $(t^n = n\Delta t)_{0\leq n\leq N_T}$, where Δt is the time step and $N_T \Delta t = T$. A classical finite volume approximation provides an approximate solution which is constant on each cell of the mesh and on each time interval. Let $X(\mathscr{T})$ be the linear space of functions $\Omega \to \mathbb{R}$ which are constant on each cell $K \in \mathscr{T}$. To a discrete set $(u_K)_{K\in\mathscr{T}}$, we associate

$u_{\mathcal{T}} = \sum_{K\in\mathcal{T}} u_K \mathbf{1}_K \in X(\mathcal{T})$. The L^p-norm of $u_{\mathcal{T}}$ is

$$\|u_{\mathcal{T}}\|_{0,p} = \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K)|u_K|^p\right)^{1/p}.$$

When there are Dirichlet boundary conditions on a part of the boundary, we need to define approximate values for u at the corresponding boundary edges: $u_{\mathcal{E}^D} = (u_\sigma)_{\sigma\in\mathcal{E}^D_{ext}} \in \mathbb{R}^{\theta^D}$ (with $\theta^D = \mathrm{Card}(\mathcal{E}^D_{ext})$). Therefore, the vector containing the approximate values in the control volumes and the approximate values at the boundary edges is denoted by $u_{\mathcal{M}} = (u_{\mathcal{T}}, u_{\mathcal{E}^D})$. For any vector $u_{\mathcal{M}} = (u_{\mathcal{T}}, u_{\mathcal{E}^D})$, we define, for all $K \in \mathcal{T}$, for all $\sigma \in \mathcal{E}_K$,

$$u_{K,\sigma} = \begin{cases} u_L, & \text{if } \sigma = K|L \in \mathcal{E}_{K,int}, \\ u_\sigma, & \text{if } \sigma \in \mathcal{E}^D_{K,ext}, \\ u_K, & \text{if } \sigma \in \mathcal{E}^N_{K,ext}, \end{cases} \tag{8a}$$

$$Du_{K,\sigma} = u_{K,\sigma} - u_K \quad \text{and} \quad D_\sigma u = \left|Du_{K,\sigma}\right|. \tag{8b}$$

It permits to define the discrete H^1-semi-norm $|\cdot|_{1,2,\mathcal{M}}$:

$$|u_{\mathcal{M}}|^2_{1,2,\mathcal{M}} = \sum_{\sigma\in\mathcal{E}} \tau_\sigma \; (D_\sigma u)^2, \quad \forall u_{\mathcal{M}} = (u_{\mathcal{T}}, u_{\mathcal{E}^D}).$$

If $\mathcal{E}^D = \emptyset$, we have $u_{\mathcal{M}} = u_{\mathcal{T}}$ and we will write $|u_{\mathcal{T}}|_{1,2,\mathcal{T}} = |u_{\mathcal{M}}|_{1,2,\mathcal{M}}$.

3 Long Time Behaviour of Some Finite Volume Schemes

3.1 First Example: Nonlinear Diffusion Equations

In this section, we consider a classical Euler implicit in time and finite volume in space discretization of the nonlinear diffusion Eq. (1a), (1b).

Theoretical Results

We assume that $u_0 \in L^\infty(\Omega)$, with $m \leq u_0 \leq M$ a.e. on Ω, with $m \geq 0$. For the sake of simplicity, we also assume that $\mathrm{m}(\Omega) = 1$. The scheme writes:

$$\mathrm{m}(K)\frac{u_K^{n+1}-u_K^n}{\Delta t}+\sum_{\substack{\sigma\in\mathcal{E}_{K,int},\\ \sigma=K|L}}\tau_\sigma\left((u_K^{n+1})^\beta-(u_L^{n+1})^\beta\right)=0, \tag{9a}$$

$$u_K^0=\frac{1}{\mathrm{m}(K)}\int_K u_0(x)dx. \tag{9b}$$

Existence and uniqueness of a discrete solution to (9a), (9b) is a well-known result (see [15]). Moreover, it is clear that $m\le u_K^n\le M$ for all $K\in\mathcal{T}$ and for all $0\le n\le N_T$. Due to the Neumann boundary conditions, we also have:

$$\sum_{K\in\mathcal{T}}\mathrm{m}(K)u_K^n=\|u_0\|_{L^1(\Omega)}.$$

At each time step, we can reconstruct the approximate solution $u_{\mathcal{T}}^n\in X(\mathcal{T})$. Our aim is to study the convergence of $(u_{\mathcal{T}}^n)_{n\ge 0}$ when n tends to $+\infty$ towards the constant function equal to $\|u_0\|_{L^1(\Omega)}$. Therefore, we can use the relative entropies E_α defined in (2) for $\alpha>0$. Let us note that

$$E_\alpha[u_{\mathcal{T}}^n]=\frac{1}{\alpha+1}\left(\sum_{K\in\mathcal{T}}\mathrm{m}(K)(u_K^n)^{\alpha+1}-\left(\sum_{K\in\mathcal{T}}\mathrm{m}(K)u_K^n\right)^{\alpha+1}\right),$$

Using the convexity of the function $x\mapsto x^{\alpha+1}$ and the scheme (9a), (9b), we easily get:

$$E_\alpha[u_{\mathcal{T}}^{n+1}]-E_\alpha[u_{\mathcal{T}}^n]\le-\Delta t\sum_{\substack{\sigma\in\mathcal{E}_{int},\\ \sigma=K|L}}\tau_\sigma\left((u_K^{n+1})^\alpha-(u_L^{n+1})^\alpha\right)\left((u_K^{n+1})^\beta-(u_L^{n+1})^\beta\right).$$

Then, using the following inequality:

$$(y^\alpha-x^\alpha)(y^\beta-x^\beta)\ge\frac{4\alpha\beta}{(\alpha+\beta)^2}(y^{(\alpha+\beta)/2}-x^{(\alpha+\beta)/2})^2,\quad\forall x,y\ge 0,$$

we get that

$$E_\alpha[u_{\mathcal{T}}^{n+1}]-E_\alpha[u_{\mathcal{T}}^n]\le-\frac{4\alpha\beta\Delta t}{(\alpha+\beta)^2}\left|(u_{\mathcal{T}}^{n+1})^{(\alpha+\beta)/2}\right|_{1,2,\mathcal{T}}^2. \tag{10}$$

With another choice of inequality:

$$(y^\beta-x^\beta)(y^\alpha-x^\alpha)\ge\frac{4\alpha\beta}{(\alpha+1)^2}\min(x^{\beta-1},y^{\beta-1})(y^{(\alpha+1)/2}-x^{(\alpha+1)/2})^2,\ \forall x,y\ge 0,$$

we get:

$$E_\alpha[u_{\mathcal{T}}^{n+1}] - E_\alpha[u_{\mathcal{T}}^n] \le -\frac{4\alpha\beta\Delta t}{(\alpha+1)^2} \inf_{K\in\mathcal{T}} (u_K^{n+1})^{\beta-1} \left|(u_{\mathcal{T}}^{n+1})^{(\alpha+1)/2}\right|_{1,2,\mathcal{T}}^2. \quad (11)$$

In both cases, the dissipation of the entropy of the approximate solution is stated in terms of the discrete H^1-semi-norm of some discrete function. In order to relate the dissipation to the entropy, we need some functional inequalities. The relation between either $|(u_{\mathcal{T}}^{n+1})^{(\alpha+\beta)/2}|_{1,2,\mathcal{T}}^2$ or $|(u_{\mathcal{T}}^{n+1})^{(\alpha+1)/2}|_{1,2,\mathcal{T}}^2$, to $E_\alpha[u_{\mathcal{T}}^{n+1}]$ will be done through discrete generalized Beckner inequalities, established in [10].

Lemma 1

- *Let $0 < q < 2$, $pq > 1$ or $q = 2$ and $0 < p \le 1$, and $f_{\mathcal{T}} \in X(\mathcal{T})$. Then*

$$\int_\Omega |f_{\mathcal{T}}|^q dx - \left(\int_\Omega |f_{\mathcal{T}}|^{1/p} dx\right)^{pq} \le \frac{C_b(p,q)}{\xi^{q/2}} |f_{\mathcal{T}}|_{1,2,\mathcal{T}}^q \quad (12)$$

  holds, where $C_b(p,q)$ only depends on p, q, Ω and with ξ defined in (7).
- *Let $0 < q < 2$, $pq \ge 1$, and $f_{\mathcal{T}} \in X(\mathcal{T})$. Then*

$$\|f_{\mathcal{T}}\|_{0,q,\mathcal{T}}^{2-q} \left(\int_\Omega |f_{\mathcal{T}}|^q dx - \left(\int_\Omega |f_{\mathcal{T}}|^{1/p} dx\right)^{pq}\right) \le \frac{C_b'(p,q)}{\xi} |f_{\mathcal{T}}|_{1,2,\mathcal{T}}^2 \quad (13)$$

  holds, where $C_b'(p,q)$ only depends on p, q, Ω and with ξ defined in (7).

Applying (12) with $p = (\alpha+\beta)/2$, $q = 2(\alpha+1)/(\alpha+\beta)$ and $f_{\mathcal{T}} = (u_{\mathcal{T}}^{n+1})^{(\alpha+\beta)/2}$, we deduce from (10):

$$E_\alpha[u_{\mathcal{T}}^{n+1}] - E_\alpha[u_{\mathcal{T}}^n] \le -K\Delta t\, E_\alpha[u_{\mathcal{T}}^{n+1}]^{(\alpha+\beta)/(\alpha+1)},$$

with K depending on α, β, Ω and ξ. Then, a discrete nonlinear Gronwall lemma (see [10]) leads to the polynomial decay of the discrete entropy.

Theorem 1 (Polynomial decay) *Let $\alpha > 0$ and $\beta > 1$. Let $(u_{\mathcal{T}}^n)_{n\ge0}$ be the solution to the finite-volume scheme (9a), (9b) with $\inf_{K\in\mathcal{T}} u_K^0 \ge 0$. Then*

$$E_\alpha[u_{\mathcal{T}}^n] \le \frac{1}{(c_1 t^n + c_2)^{(\alpha+1)/(\beta-1)}}, \quad \forall n \ge 0,$$

where c_1 depends on α, β, Ω, ξ and Δt (but stays bounded when Δt tends to 0) and $c_2 = E_\alpha[u_{\mathcal{T}}^0]^{-(\beta-1)/(\alpha+1)}$.

Applying (13) with $p = (\alpha+1)/2$, $q = 2$ and $f_{\mathcal{T}} = (u_{\mathcal{T}}^{n+1})^{(\alpha+1)/2}$, we deduce from (11):

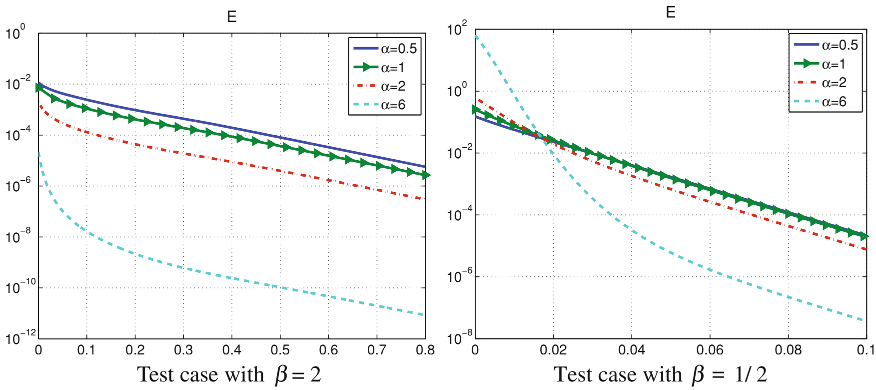

Fig. 1 Evolution of the discrete entropies with respect to time for different values of α

$$E_\alpha[u_{\mathscr{T}}^{n+1}] - E_\alpha[u_{\mathscr{T}}^n] \leq -K' \Delta t \inf_{K \in \mathscr{T}} (u_K^0)^{\beta-1} E_\alpha[u_{\mathscr{T}}^{n+1}],$$

with K' depending on α, β, Ω and ξ. Then, we can conclude to the exponential decay of the discrete entropy.

Theorem 2 (Exponential decay) *Let* $0 < \alpha \leq 1$ *and* $\beta > 0$. *Let* $(u_{\mathscr{T}}^n)_{n \geq 0}$ *be the solution to the finite-volume scheme* (9a), (9b) *with* $\inf_{K \in \mathscr{T}} u_K^0 \geq 0$. *Then*

$$E_\alpha[u_{\mathscr{T}}^n] \leq E_\alpha[u_{\mathscr{T}}^0] e^{-\lambda t^n}, \quad \forall n \geq 0,$$

with λ *depending on* α, β, Ω, ξ *and* $\inf_{K \in \mathscr{T}} (u_K^0)^{\beta-1}$.

Numerical Experiments

We illustrate on Fig. 1 the time decay of the solutions to the discretized porous-medium equation ($\beta = 2$) and to the fast-diffusion equation ($\beta = 1/2$). Both test cases are two-dimensional, with $\Omega = (0, 1) \times (0, 1)$. When $\beta = 2$, we choose a Barenblatt profile as initial condition. We observe that the decay of the discrete entropies seems to be exponential for large times, even for values of α not covered by Theorem 2. When $\beta = 1/2$, we choose $u_0(x) = C((R^2 - |x - x_0|^2)^+)^2$ with $x_0 = (0.5, 0.5)$, $R = 0.2$, $C = 3000$ as initial condition. We observe similarly an exponential decay of the discrete entropies for large times.

3.2 Second Example: Drift-Diffusion System

As recalled in the introduction, the drift-diffusion system (3a), (3b), (3c) is made of two convection-diffusion-reaction equations on the densities coupled with a Poisson equation on the electric potential. Writing a two-points finite volume scheme for this system is not difficult. However, the choice of the time discretization and of the numerical approximation of the convection-diffusion fluxes will be crucial for the preservation of the asymptotic behaviours.

When writing the scheme, we have to define for instance $\mathscr{F}_{K,\sigma}$ the numerical approximation of $\int_\sigma (-\nabla N + N\nabla\Psi) \cdot \nu_{K,\sigma}$. Scharfetter and Gummel [26] have proposed to discretize simultaneously the convection and diffusion terms. It leads to the following numerical fluxes:

$$\mathscr{F}_{K,\sigma} = \tau_\sigma \left(B(-D\Psi_{K,\sigma})N_K - B(D\Psi_{K,\sigma})N_{K,\sigma} \right)$$

where B is the Bernoulli function defined by:

$$B(0) = 1 \text{ and } B(x) = \frac{x}{\exp(x) - 1} \ \forall x \neq 0. \tag{14}$$

Gajewski and Gärtner [16] have shown that the Euler implicit in time and finite volume in space scheme, with a Scharfetter-Gummel approximation of the convection-diffusion fluxes, is entropy dissipative (the scheme is detailed in the next section). Later, Chatard [12] has also obtained a discrete counterpart of the entropy method for this scheme (with a different way of proof). The numerical experiments in [12] show the exponential decay in time of the discrete entropy for the Scharfetter-Gummel scheme. They also show that this property is no more satisfied by the scheme proposed in [11], where the diffusion terms are discretized classically and the convection terms are discretized with upwind fluxes.

4 Finite Volume Scheme at the Quasi-Neutral Limit

In this Section, we study a numerical scheme for the simplified drift-diffusion system $(\mathscr{P}_\lambda)$, similar to the schemes studied in [16] or in [12]. We will use the entropy method in order to show that the scheme is asymptotic preserving at the quasi-neutral limit $\lambda \to 0$. More precisely, we will establish that the a priori estimates needed for the proof of convergence hold for all $\lambda \geq 0$.

We make the following assumptions on the data:

$$N_0, P_0 \in L^\infty(\Omega), \tag{15a}$$

$$N^D, P^D \in L^\infty \cap H^1(\Omega), \ \Psi^D \in H^1(\Omega), \tag{15b}$$

$$\exists m > 0, M > 0 \text{ such that } m \leq N_0, P_0, N^D, P^D \leq M \text{ a.e. on } \Omega. \tag{15c}$$

4.1 Presentation of the Scheme

For $u = N, P, \Psi$, the approximate solution is defined by $u^n_{\mathcal{T}}$ and the approximate values at the boundary are $u^n_{\mathcal{E}^D} = (u^n_\sigma)_{\sigma\in\mathcal{E}^D_{ext}}$, at each time step, $0 \le n \le N_T$. Let us first discretize the initial and the boundary conditions. We set:

$$u^0_K = \frac{1}{\mathrm{m}(K)}\int_K u_0(x)\,dx, \quad \forall K \in \mathcal{T}, \text{ for } u = N, P, \tag{16}$$

$$u^D_\sigma = \frac{1}{\mathrm{m}(\sigma)}\int_\sigma u(\gamma)d\gamma, \quad \forall \sigma \in \mathcal{E}^D_{ext}, \text{ for } u = N, P, \Psi.$$

Moreover, we define

$$u^n_\sigma = u^D_\sigma, \quad \forall\sigma \in \mathcal{E}^D_{ext}, \forall n \ge 0, \text{ for } u = N, P, \Psi. \tag{17}$$

We consider a Euler implicit in time and finite volume in space discretization. The scheme writes:

$$\mathrm{m}(K)\frac{N^{n+1}_K - N^n_K}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} \mathcal{F}^{n+1}_{K,\sigma} = 0, \quad \forall K \in \mathcal{T}, \forall n \ge 0, \tag{18a}$$

$$\mathrm{m}(K)\frac{P^{n+1}_K - P^n_K}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} \mathcal{G}^{n+1}_{K,\sigma} = 0, \quad \forall K \in \mathcal{T}, \forall n \ge 0, \tag{18b}$$

$$-\lambda^2 \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma D\Psi^n_{K,\sigma} = \mathrm{m}(K)(P^n_K - N^n_K), \quad \forall K \in \mathcal{T}, \forall n \ge 0. \tag{18c}$$

We choose a Scharfetter-Gummel approximation for the convection-diffusion fluxes:

$$\mathcal{F}^{n+1}_{K,\sigma} = \tau_\sigma\left(B(-D\Psi^{n+1}_{K,\sigma})N^{n+1}_K - B(D\Psi^{n+1}_{K,\sigma})N^{n+1}_{K,\sigma}\right), \quad \forall K \in \mathcal{T}, \forall\sigma \in \mathcal{E}_K, \tag{19a}$$

$$\mathcal{G}^{n+1}_{K,\sigma} = \tau_\sigma\left(B(D\Psi^{n+1}_{K,\sigma})P^{n+1}_K - B(-D\Psi^{n+1}_{K,\sigma})P^{n+1}_{K,\sigma}\right), \quad \forall K \in \mathcal{T}, \forall\sigma \in \mathcal{E}_K, \tag{19b}$$

where B is the Bernoulli function defined by (14).

In the sequel, we denote by $(\mathcal{S}_\lambda)$ the scheme (16)–(19b). It is a fully implicit in time scheme: the numerical solution $(N^{n+1}_K, P^{n+1}_K, \Psi^{n+1}_K)_{K\in\mathcal{T}}$ at each time step is defined as a solution of the nonlinear system of Eqs. (18a)–(19b). When choosing $D\Psi^n_{K,\sigma}$ instead of $D\Psi^{n+1}_{K,\sigma}$ in the definition of the fluxes (19a), (19b), we would get a decoupled scheme whose solution is obtained by solving successively three linear systems of equations for N, P and Ψ. However, this other choice of time discretization induces a stability condition of the form $\Delta t \leq C\lambda^2$ (see for instance [2]). Therefore, it cannot be used in practice for small values of λ and it does not preserve the quasi-neutral limit.

Setting $\lambda = 0$ in the scheme $(\mathscr{S}_\lambda)$ leads to the scheme $(\mathscr{S}_0)$ defined hereafter. The scheme for the Poisson Eq. (18c) becomes $P_K^n - N_K^n = 0$ for all $K \in \mathscr{T}, n \in \mathbb{N}$. In order to avoid any incompatibility condition at $n = 0$ (which would correspond to an initial layer), we assume that the initial conditions N_0 and P_0 satisfy the quasi-neutrality assumption:

$$P_0 - N_0 = 0. \tag{20}$$

Adding and subtracting (18a) and (18b), and using $P_K^n = N_K^n$ for all $K \in \mathscr{T}$ and $n \in \mathbb{N}$, we get

$$\mathrm{m}(K)\frac{N_K^{n+1} - N_K^n}{\Delta t} + \frac{1}{2}\sum_{\sigma\in\mathscr{E}_K}\left(\mathscr{F}_{K,\sigma}^{n+1} + \mathscr{G}_{K,\sigma}^{n+1}\right) = 0, \forall K \in \mathscr{T}, \forall n \geq 0,$$

$$\text{and} \quad \sum_{\sigma\in\mathscr{E}_K}\left(\mathscr{F}_{K,\sigma}^{n+1} - \mathscr{G}_{K,\sigma}^{n+1}\right) = 0, \forall K \in \mathscr{T}, \forall n \geq 0.$$

But, using the following property of the Bernoulli function $B(x) - B(-x) = -x$, $\forall x \in \mathbb{R}$, we have, $\forall K \in \mathscr{T}, \forall \sigma \in \mathscr{E}_{K,int} \cup \mathscr{E}_{K,ext}^N$:

$$\mathscr{F}_{K,\sigma}^{n+1} - \mathscr{G}_{K,\sigma}^{n+1} = \tau_\sigma D\Psi_{K,\sigma}^{n+1}(N_K^{n+1} + N_{K,\sigma}^{n+1}),$$

$$\text{and} \quad \mathscr{F}_{K,\sigma}^{n+1} + \mathscr{G}_{K,\sigma}^{n+1} = -\tau_\sigma\left(B(D\Psi_{K,\sigma}^{n+1}) + B(-D\Psi_{K,\sigma}^{n+1})\right)DN_{K,\sigma}^{n+1}.$$

Let us note that these equalities still hold for each Dirichlet boundary edge $\sigma \in \mathscr{E}_{K,ext}^D$ if $N_\sigma^D = P_\sigma^D$. In the sequel, when studying the scheme at the quasi-neutral limit $(\mathscr{S}_0)$, we assume the quasi-neutrality of the initial conditions (20) and of the boundary conditions:

$$P^D - N^D = 0. \tag{21}$$

Finally, the scheme $(\mathscr{S}_0)$ can be rewritten: $\forall K \in \mathscr{T}, \forall n \geq 0$,

$$\mathrm{m}(K)\frac{N_K^{n+1} - N_K^n}{\Delta t} - \sum_{\sigma\in\mathscr{E}_K}\tau_\sigma\frac{B(D\Psi_{K,\sigma}^{n+1}) + B(-D\Psi_{K,\sigma}^{n+1})}{2}DN_{K,\sigma}^{n+1} = 0, \tag{22a}$$

$$-\sum_{\sigma\in\mathscr{E}_K}\tau_\sigma D\Psi_{K,\sigma}^{n+1}(N_K^{n+1} + N_{K,\sigma}^{n+1}) = 0, \tag{22b}$$

$$P_K^n - N_K^n = 0, \tag{22c}$$

with the initial conditions (15a), (15b), (15c) and the boundary conditions (17).

Existence of a solution to the scheme $(\mathscr{S}_\lambda)$ is proved in [4] without any condition on Δt and for all $\lambda \geq 0$. Moreover, under the hypotheses (15a), (15b), (15c), we have:

$$m \leq N_K^n, P_K^n \leq M, \forall n \in \mathbb{N}.$$

It means in particular that all the densities are positive.

4.2 Entropy-Dissipation Estimate

In this Section, we establish the discrete counterpart of the entropy-dissipation inequality (6). As N^D, P^D and Ψ^D are defined on the whole domain, we can set:

$$u_K^D = \frac{1}{\mathrm{m}(K)} \int_K u(x)dx, \ \forall K \in \mathscr{T}, \text{ for } u = N, P, \Psi.$$

Then, for all $n \in \mathbb{N}$, the discrete entropy is defined by:

$$\begin{aligned}\mathbb{E}^n = &\sum_{K \in \mathscr{T}} \mathrm{m}\,(K) \Big(H(N_K^n) - H(N_K^D) - \log(N_K^D) \left(N_K^n - N_K^D \right) \Big) \\ &+ \sum_{K \in \mathscr{T}} \mathrm{m}\,(K) \Big(H(P_K^n) - H(P_K^D) - \log(P_K^D)(P_K^n - P_K^D) \Big) \\ &+ \frac{\lambda^2}{2} \left| \Psi_{\mathscr{M}}^n - \Psi_{\mathscr{M}}^D \right|_{1,2,\mathscr{M}}^2,\end{aligned}$$

and the discrete entropy dissipation by:

$$\begin{aligned}\mathbb{D}^n = &\sum_{\substack{\sigma \in \mathscr{E}, \\ (K = K_\sigma)}} \tau_\sigma \Bigg[\min\left(N_K^n, N_{K,\sigma}^n\right) \Big(D_\sigma \left(\log N^n - \Psi^n \right) \Big)^2 \\ &+ \min\left(P_K^n, P_{K,\sigma}^n\right) \Big(D_\sigma \left(\log P^n + \Psi^n \right) \Big)^2 \Bigg],\end{aligned}$$

where the notation $\sum_{\substack{\sigma \in \mathscr{E}, \\ (K = K_\sigma)}}$ means a sum over all the edges $\sigma \in \mathscr{E}$, with $K = K_\sigma$ (and therefore σ is an edge of the cell K) in the term inside the sum.

Theorem 3 (Discrete entropy-dissipation inequality) *Let assume* (15a), (15b), (15c) *and let $\mathscr{T}$ be an admissible mesh of Ω satisfying* (7) *and $\Delta t > 0$. Then, there exists K_E, not depending on λ, Δt and* size$(\mathscr{T})$*, such that, for all $\lambda \geq 0$, a solution to the scheme $(\mathscr{S}_\lambda)$, $(N_{\mathscr{T}}^n, P_{\mathscr{T}}^n, \Psi_{\mathscr{T}}^n)_{0 \leq n \leq N_T}$, satisfies the following inequality:*

$$\frac{\mathbb{E}^{n+1} - \mathbb{E}^n}{\Delta t} + \frac{1}{2}\,\mathbb{D}^{n+1} \leq K_E, \quad \forall n \geq 0. \tag{23a}$$

Furthermore, if N^0 and P^0 satisfy the quasi-neutrality assumption (20)*, we have*

$$\sum_{n=0}^{N_T-1} \Delta t\,\mathbb{D}^{n+1} \leq K_E(1+\lambda^2). \tag{23b}$$

Sketch of the proof We mimic the proof at the continuous level. The scheme on N (18a) is multiplied by $\Delta t(\log(N_K^{n+1} - \log(N_K^D))$ and a sum over the control volumes $K \in \mathscr{T}$ is achieved. A similar procedure is applied to the scheme on P (18b). Both terms are summed up and the sums are rearranged in order to use the scheme on Ψ (18c). In order to let the discrete entropy dissipation appear $\mathbb{D}^{n+1}$, we crucially use the discretization by the Scharfetter-Gummel fluxes. In practice, the result is based on the following properties satisfied by the Scharfetter-Gummel fluxes:

$$\begin{aligned}
\mathscr{F}_{K,\sigma}^{n+1}\, D(\log N - \Psi)_{K,\sigma}^{n+1} &\leq -\,\tau_\sigma \min(N_K^{n+1}, N_{K,\sigma}^{n+1}) \left(D_\sigma(\log N - \Psi)^{n+1}\right)^2,\\
\mathscr{G}_{K,\sigma}^{n+1}\, D(\log P + \Psi)_{K,\sigma}^{n+1} &\leq -\,\tau_\sigma \min(P_K^{n+1}, P_{K,\sigma}^{n+1}) \left(D_\sigma(\log P + \Psi)^{n+1}\right)^2.
\end{aligned}$$

Moreover, if $\min(N_K^{n+1}, N_{K,\sigma}^{n+1}) \geq 0$ and $\min(P_K^{n+1}, P_{K,\sigma}^{n+1}) \geq 0$, we also have

$$\begin{aligned}
\left|\mathscr{F}_{K,\sigma}^{n+1}\right| &\leq \tau_\sigma \max(N_K^{n+1}, N_{K,\sigma}^{n+1}) \left|D_\sigma\,(\log N - \Psi)^{n+1}\right|,\\
\left|\mathscr{G}_{K,\sigma}^{n+1}\right| &\leq \tau_\sigma \max(P_K^{n+1}, P_{K,\sigma}^{n+1}) \left|D_\sigma\,(\log P + \Psi)^{n+1}\right|.
\end{aligned}$$

4.3 New a Priori Estimates in Order to Get the Compactness

As it is classical in the finite volume framework and especially for elliptic and parabolic equations, we want to prove some a priori estimates satisfied by the discrete solution. In our case, it is crucial to establish a priori estimates which remain satisfied when $\lambda \to 0$. They will be deduced from the bound on the entropy dissipation (23b).

Theorem 4 (A priori estimates satisfied by the approximate solution) *Let assume* (15a)*,* (15b)*,* (15c) *and let $\mathscr{T}$ be an admissible mesh of Ω satisfying* (7) *and $\Delta t > 0$. We also assume that the initial and boundary conditions satisfy the quasi-neutrality relations* (20) *and* (21)*. Then, there exists a constant K_F not depending on λ, Δt and* $\text{size}(\mathscr{T})$*, such that, for all $\lambda \geq 0$, a solution to the scheme ($\mathscr{S}_\lambda$), $(N_{\mathscr{T}}^n, P_{\mathscr{T}}^n, \Psi_{\mathscr{T}}^n)_{0\leq n\leq N_T}$, satisfies the following inequalities:*

$$\sum_{n=0}^{N_T-1} \Delta t \sum_{\sigma\in\mathscr{E}} \tau_\sigma D_\sigma \Psi^{n+1}\Big((D_\sigma P^{n+1})^2 + (D_\sigma N^{n+1})^2\Big) \le K_F(1+\lambda^2), \tag{24a}$$

$$\sum_{n=0}^{N_T-1} \Delta t \sum_{\sigma\in\mathscr{E}} \tau_\sigma (D_\sigma N^{n+1})^2 + \sum_{n=0}^{N_T-1} \Delta t \sum_{\sigma\in\mathscr{E}} \tau_\sigma (D_\sigma P^{n+1})^2 \le K_F(1+\lambda^2), \tag{24b}$$

$$\sum_{n=0}^{N_T-1} \Delta t \sum_{\sigma\in\mathscr{E}} \tau_\sigma (D_\sigma \Psi^{n+1})^2 \le K_F(1+\lambda^2). \tag{24c}$$

We refer to [4] for the proof of this Theorem. The estimates are obtained successively: first, we establish the weak-BV inequality on N and P (24a); then, we deduce the $L^2(0, T, H^1)$ estimate on N and P and finally we conclude with the $L^2(0, T, H^1)$ estimate on Ψ.

The $L^2(0, T, H^1(\Omega))$-estimates on N, P (24b) and Ψ (24c) lead to compactness in space of the sequences of approximate solutions. The compactness in time is deduced from estimates on the time translates obtained by reusing the scheme. To prove the convergence of the numerical method, it remains to pass to the limit in the scheme and by this way prove that the limit of the sequence of approximate solutions is a weak solution to $(\mathscr{P}_\lambda)$. It can be done as in [11], but dealing with the Scharfetter-Gummel fluxes as in [3].

4.4 Some Numerical Experiments

We illustrate now the stability of the fully implicit Scharfetter-Gummel scheme for all nonnegative values of the rescaled Debye length λ. Therefore, we consider a one dimensional test case on $\Omega = (0, 1)$. Initial data are constant $N_0(x) = P_0(x) = 0.5$, $\forall x \in (0, 1)$. We consider quasi-neutral Dirichlet boundary conditions $N^D(0) = P^D(0) = 0.1$, $\Psi^D(0) = 0$ and $N^D(1) = P^D(1) = 0.9$, $\Psi^D(1) = 4$.

Since the exact solution to the problem $(\mathscr{P}_\lambda)$ is not available, we compute a reference solution on a uniform mesh made of $10240 = 20 \times 2^9$ cells, with time step $\Delta t = 10^{-6}$, for different values of λ^2 in [0, 1]. This reference solution is then used to compute the L^1 error for the variables N, P and Ψ. In order to prove the asymptotic preserving behaviour of the scheme, we compute L^1 errors at time $T = 0.1$ for different numbers of cells $\theta = 20 \times 2^i$, $i \in \{0, ..., 8\}$, with different time steps Δt in $[10^{-5}, 10^{-2}]$ and various rescaled Debye length λ^2 in [0, 1]. Figure 2 presents the L^1 error on the electron density and on the electrostatic potential as functions of Δt for different values of λ^2. It clearly shows the uniform behaviour in the limit $\lambda \to 0$ since the convergence rate is of order 1 for all variables even for small values of λ^2, including zero.

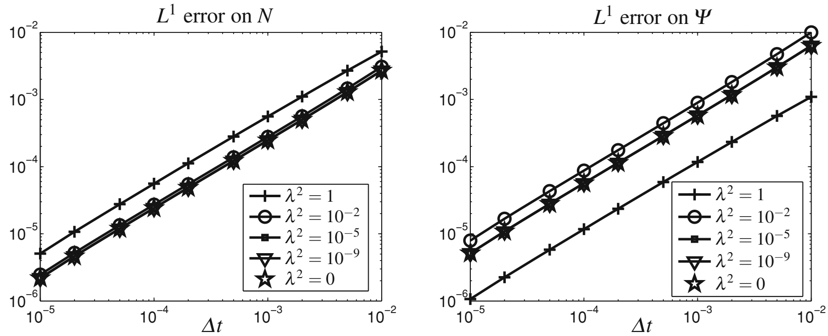

Fig. 2 Errors in L^1 norm as functions of Δt, for different values of λ^2

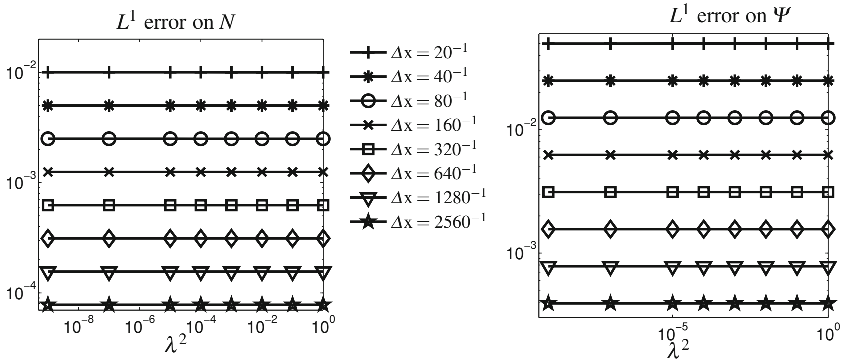

Fig. 3 Errors in L^1 norm as functions of λ^2, for different values of Δx

On Fig. 3, we plot the L^1 errors as functions of λ^2 for different values of the space step. We still observe the asymptotic preserving property of the scheme in the limit $\lambda \to 0$. Moreover, the errors are independent of λ^2.

Further numerical experiments (in 2D, with a non-vanishing doping profile,...) can be found in [4].

5 Conclusion

In this paper, we have first presented some results obtained with Jüngel and Schuchnigg on the long time behaviour of a classical scheme for nonlinear diffusion equations. We have obtained the exponential/polynomial decay of discrete zeroth-order relative entropies. The proof is based on an entropy method and on discrete functional inequalities. We refer to [10] for further results on first-order entropies (like the Fisher information).

On the drift-diffusion system, we have explained how the discrete counterpart of the entropy method can take part in the proof of convergence of a particular (but widely used) finite volume scheme. Particularly, it permits to establish that the considered scheme is asymptotic preserving at the quasi-neutral limit. We refer to the joint work with Bessemoulin-Chatard and Vignal [4] for the details of the proofs.

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