Exponential time decay of a finite volume scheme for drift-diffusion systems

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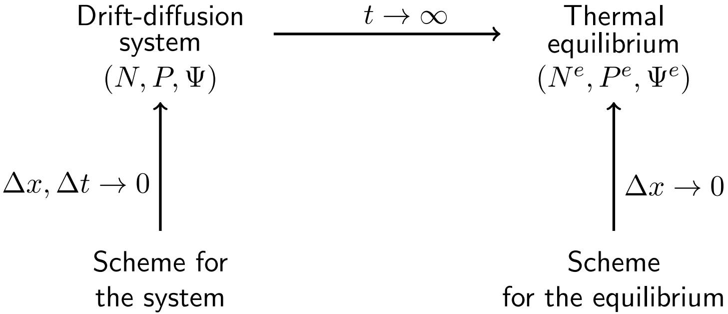
Joint work with M. Bessemoulin-Chatard (Nantes)

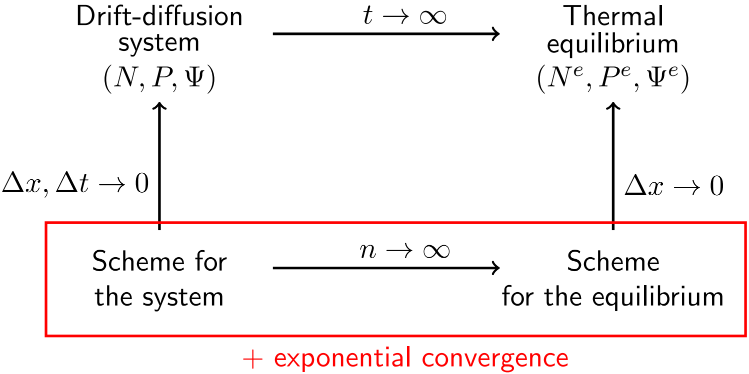
Overview

Drift-diffusion system (N, P, Ψ) $\xrightarrow{t \to \infty}$ Thermal equilibrium (N^e, P^e, Ψ^e)

Overview


Drift-diffusion system
(N, P, Ψ)
$t \to \infty$
Thermal equilibrium
(N^e, P^e, Ψ^e)
$\Delta x, \Delta t \to 0$
$\Delta x \to 0$
Scheme for the system
Scheme for the equilibrium

Overview


Drift-diffusion system (N, P, Ψ)
$t \to \infty$
Thermal equilibrium (N^e, P^e, Ψ^e)
$\Delta x, \Delta t \to 0$
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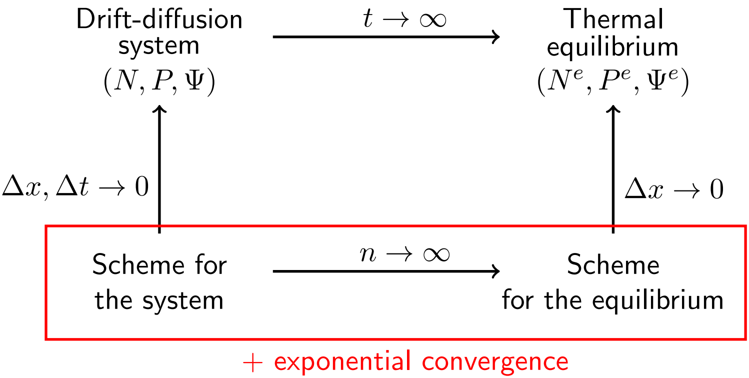
Scheme for the system
$n \to \infty$
Scheme for the equilibrium
$+$ exponential convergence

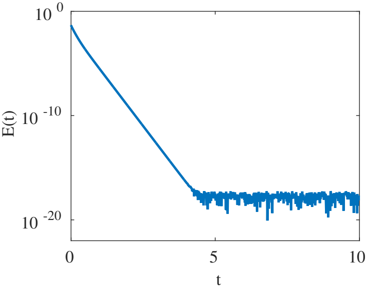
Overview



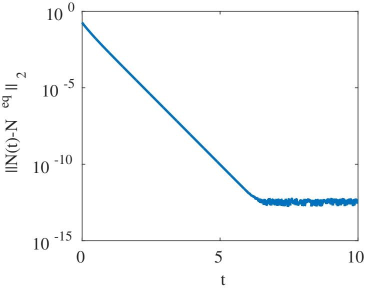
- Model : Linear or non-linear drift-diffusion systems
- Scheme : Backward Euler in time + Finite volume in space

  + (extended) Scharfetter-Gummel numerical fluxes

Illustration



relative entropy

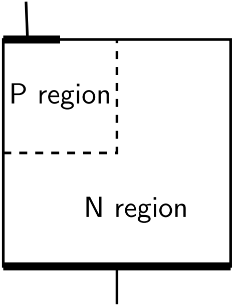


L^2 error

Outline of the talk

1. About the drift-diffusion systems
2. Numerical scheme for the drift-diffusion systems
3. Exponential decay to the thermal equilibrium

Drift-diffusion systems



Unknowns

- N, P : densities of charge carriers
- Ψ : electrical potential

Data

- Doping profile : C
- Initial and boundary conditions

The equations

$$\begin{cases} \partial_t N + \operatorname{div}(J_N) = -R(N,P), \quad J_N = -\nabla r(N) + N\nabla\Psi, \\ \partial_t P + \operatorname{div}(J_P) = -R(N,P), \quad J_P = -\nabla r(P) - P\nabla\Psi, \\ -\lambda^2 \Delta\Psi = P - N + C. \end{cases}$$

λ : Debye length

Linear/non-linear diffusion

$$\begin{cases} \partial_t N + \mathrm{div}(J_N) = -R(N,P), & J_N = -\nabla r(N) + N\nabla\Psi, \\ \partial_t P + \mathrm{div}(J_P) = -R(N,P), & J_P = -\nabla r(P) - P\nabla\Psi, \\ -\lambda^2 \Delta\Psi = P - N + C. \end{cases}$$

Van Roosbroeck model (1950)

- Boltzmann statistics

  $\longrightarrow r(s) = s$

- different choices for the recombination-generation terms R :

$$R(N,P) = R_0(N,P)(1 - NP).$$

Non-linear diffusion

- other statistics than Boltzmann (Fermi-Dirac for instance)

  $\longrightarrow r(s) = s^\gamma$, avec $\gamma > 1$ ($\gamma = 5/3$)

- recombination-generation ?

Known results

Assumptions

- $N_0, P_0 \in L^\infty(\Omega)$, $C \in L^\infty(\Omega)$,
- $N^D, P^D \in L^\infty \cap H^1(\Omega)$, $\Psi^D \in H^1(\Omega)$,
- $\exists m \geq 0, M > 0$ such that

$$m \leq N_0, P_0, N^D, P^D \leq M \text{ a.e. in } \Omega.$$

- $r(s) = s$ and $R(N, P) = R_0(NP - 1)$

  or $r(s) = s^\gamma$ and $R = 0$.

Existence of a weak solution

- Gajewski, 1985
- Gajewski, Gröger, 1986
- Jüngel, 1994

The thermal equilibrium

Definition

$$\begin{cases} -\nabla r(N) + N\nabla\Psi = 0 = -N\ \nabla(h(N) - \Psi) \\ -\nabla r(P) - P\nabla\Psi = 0 = -P\ \nabla(h(P) + \Psi) \\ -\lambda^2\Delta\Psi = P - N + C \end{cases} \qquad (h'(s) = \frac{r'(s)}{s})$$

$+$ Dirichlet/Neumann boundary conditions

Existence and uniqueness (under conditions)

- Markowich, Unterreiter, 1993
- Unterreiter, 1994

g : generalized inverse of h,

$$\begin{cases} N^e = g(\alpha_N + \Psi^e),\ P^e = g(\alpha_P - \Psi^e) \\ \lambda^2\Delta\Psi^e = g(\alpha_N + \Psi^e) - g(\alpha_P - \Psi^e) - C \quad + \text{b. c.} \\ \alpha_N = h(N^D) - \Psi^D,\ \alpha_P = h(P^D) + \Psi^D \end{cases}$$

Convergence in large time to the thermal equilibrium

- Gajewski, Gröger, 1986, 1990
- Gajewski, Gärtner, 1996
- Jüngel, 1995

Relative energy and energy dissipation

$$H(u) = \int_1^u h(s)ds, \text{ convex}$$

$$\begin{aligned}\mathbb{E}(t) &= \int_\Omega \Big(H(N) - H(N^e) - h(N^e)(N - N^e) + \dots \\ &\qquad + \frac{\lambda^2}{2} |\nabla(\Psi - \Psi^e)|^2 \Big) \quad \geq 0 \\ \mathbb{I}(t) &= \int_\Omega \Big(N|\nabla(h(N) - \Psi)|^2 + P|\nabla(h(P) + \Psi)|^2 \Big) \quad \geq 0\end{aligned}$$

Keypoint : an energy/energy dissipation equality

$$\frac{d\mathbb{E}}{dt}(t) + \mathbb{I}(t) = 0$$

Outline of the talk

Schemes for the evolutive drift-diffusion equation

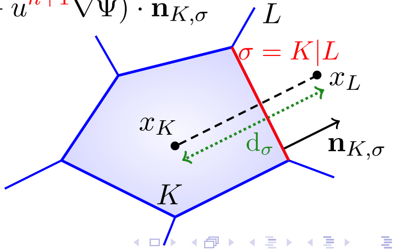
From the equation...

$$\begin{cases} \partial_t u + \mathrm{div}\mathbf{J} = 0, \quad \mathbf{J} = -\nabla u + u\nabla\Psi, \text{ in } \Omega \\ u(\cdot,0) = u_0 \geq 0 \ + \text{Neumann boundary conditions} \end{cases}$$

... to the scheme

$$\begin{cases} \mathrm{m}(K)\dfrac{u_K^{n+1} - u_K^n}{\Delta t} + \displaystyle\sum_{\sigma\in\mathcal{E}_K^{int}} \mathcal{F}_{K,\sigma}^{n+1} = 0 \\ \mathcal{F}_{K,\sigma}^{n+1} \approx \displaystyle\int_\sigma (-\nabla u^{n+1} + u^{n+1}\nabla\Psi)\cdot \mathbf{n}_{K,\sigma} \end{cases}$$

- $\mathcal{T}$: control volumes, $K \in \mathcal{T}$
- $\mathcal{E}$: edges, $\sigma \in \mathcal{E}$
- Δt : time step



Scharfetter-Gummel fluxes

❏ Scharfetter, Gummel, 1969

Definition

$$\mathcal{F}_{K,\sigma} = \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma}\Big(B\big(-\Psi_L + \Psi_K\big)u_K - B\big(\Psi_L - \Psi_K\big)u_L\Big)$$

where B is the Bernoulli function : $B(x) = \dfrac{x}{e^x - 1} \quad (B(0) = 1)$.

Properties

- Existence, uniqueness of the solution to the scheme
- Preservation of positivity, conservation of mass
- Preservation of the thermal equilibrium :

$$u_K = \exp(\Psi_K) \Longrightarrow \mathcal{F}_{K,\sigma} = 0.$$

Generalization to nonlinear diffusion

$$\mathbf{J} = -\nabla r(u) + u\nabla\Psi = -r'(u)\nabla u + u\nabla\Psi = -u\nabla(h(u) - \Psi).$$

Extended SG fluxes

$$D\Psi_{K,\sigma} = \Psi_L - \Psi_K \qquad \text{(and } D_\sigma\Psi = |\Psi_L - \Psi_L|\text{)}$$

$$\mathcal{F}_{K,\sigma} = \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma} dr(u_K, u_L) \Big(B\big(\frac{-D\Psi_{K,\sigma}}{dr(u_K, u_L)}\big)u_K - B\big(\frac{D\Psi_{K,\sigma}}{dr(u_K, u_L)}\big)u_L \Big)$$

Definition of dr $\quad \Psi_K = h(u_K) \Longrightarrow \mathcal{F}_{K,\sigma} = 0$

$$dr(a,b) = \begin{cases} \dfrac{h(b) - h(a)}{\log(b) - \log(a)} & \text{if } a, b > 0,\ a \neq b \\ r'\big(\dfrac{a+b}{2}\big) & \text{elsewhere} \end{cases}$$

Overview of the schemes for the drift-diffusion system

Scheme for the drift-diffusion system

$$
\begin{cases}
\mathrm{m}(K)\dfrac{N_K^{n+1}-N_K^n}{\Delta t}+\displaystyle\sum_{\sigma\in\mathcal{E}_K}\mathcal{F}_{K,\sigma}^{n+1}=0,\\[2ex]
\mathrm{m}(K)\dfrac{P_K^{n+1}-P_K^n}{\Delta t}+\displaystyle\sum_{\sigma\in\mathcal{E}_K}\mathcal{G}_{K,\sigma}^{n+1}=0,\\[2ex]
-\lambda^2\displaystyle\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma D\Psi_{K,\sigma}^{n+1}=\mathrm{m}(K)(P_K^{n+1}-N_K^{n+1}+C_K).
\end{cases}
$$

Scheme for the thermal equilibrium

$$
\begin{cases}
-\lambda^2\displaystyle\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma D\Psi_{K,\sigma}^{e}=\mathrm{m}(K)\Big(g(\alpha_P-\Psi_K^e)-g(\alpha_N+\Psi_K^e)+C_K\Big),\\[2ex]
\qquad N_K^e=g(\alpha_N+\Psi_K^e),\quad P_K^e=g(\alpha_P-\Psi_K^e).
\end{cases}
$$

Crucial property of the SG fluxes

At the continuous level

$$\mathbf{J} = -u\nabla(h(u) - \Psi)$$

$$\mathbb{I} = \int_\Omega -\mathbf{J} \cdot \nabla(h(u) - \Psi) = \int_\Omega u|\nabla(h(u) - \Psi)|^2$$

At the discrete level

$$-\mathcal{F}_{K,\sigma} D(h(u) - \Psi)_{K,\sigma} \geq \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma} \min(u_K, u_L)\big(D_\sigma(h(u) - \Psi)\big)^2$$

Definition of the discrete dissipation

$$\mathbb{I}^n = \sum_{\sigma \in \mathcal{E}} \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma} \Bigg(\min(N_K^n, N_L^n)\Big(D_\sigma\big(h(N^n) - \Psi^n\big)\Big)^2 + \min(P_K^n, P_L^n)\Big(D_\sigma\big(h(P^n) + \Psi^n\big)\Big)^2 \Bigg)$$

Discrete energy/dissipation inequality

Definition of the discrete energy

$$\mathbb{E}^n = \sum_{K\in\mathcal{T}} \mathrm{m}(K)\big(H(N_K^n) - H(N_K^e) - h(N_K^e)(N_K^n - N_K^e) + \ldots$$

$$+ \frac{\lambda^2}{2}\sum_{\sigma\in\mathcal{E}} \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma}\Big(D_\sigma(\Psi^n - \Psi^e)\Big)^2.$$

Proposition

If the scheme has a solution which satisfies

$$0 \le N_K^n, P_K^n \le M, \quad \forall K \in \mathcal{T}, \forall n \ge 0,$$

then,

$$0 \le \mathbb{E}^{n+1} + \Delta t \mathbb{I}^{n+1} \le \mathbb{E}^n, \quad \forall n \ge 0.$$

Outline of the talk

How to get the exponential decay ?

$$0 \le \mathbb{E}^{n+1} + \Delta t \mathbb{I}^{n+1} \le \mathbb{E}^n, \quad \forall n \ge 0.$$

If we prove

$$\mathbb{E}^n \le C_{EI} \mathbb{I}^n$$

then

$$\mathbb{E}^{n+1} - \mathbb{E}^n \le -\frac{\Delta t}{C_{EI}} \mathbb{E}^{n+1},$$

and

➔ $\mathbb{E}^n \le (1 - \frac{\Delta t}{C_{EI}})^n \mathbb{E}^0 \quad \forall n \ge 0,$

➔ $\mathbb{E}^n \le e^{-\alpha n \Delta t} \, \mathbb{E}^0 \quad \forall n \ge 0,$ with $\alpha = \dfrac{e^{-\Delta t_{max}}}{C_{EI}}.$

Relation between energy and dissipation

Proposition

Let assume some hypotheses on the data, including :

- boundary conditions at thermal equilibrium.

If moreover the scheme has a solution which satisfies

$$0 < m \leq N_K^n, P_K^n \leq M, \quad \forall K \in \mathcal{T}, \forall n \geq 0.$$

Then,

$$\mathbb{E}^n \leq C_{EF} \mathbb{F}^n \leq C_{EI} \mathbb{I}^n,$$

where,

$$\mathbb{F}^n = \|N_{\mathcal{T}}^n - N_{\mathcal{T}}^e\|_0^2 + \|P_{\mathcal{T}}^n - P_{\mathcal{T}}^e\|_0^2 + \frac{\lambda^2}{2} |\Psi_{\mathcal{T}}^n - \Psi_{\mathcal{T}}^e|_{1,\mathcal{T}}^2.$$

➔ exponential decay of $\mathbb{F}^n$ as a by-product.

About the existence and the uniform bounds

- The scheme leads to a nonlinear system of equations at each time step.
- Existence is obtained *via* a fixed point theorem :
  - ➔ linearization of the scheme :

    $$T^n_\mu : (N_\mathcal{T}, P_\mathcal{T}) \to (\Psi_\mathcal{T} \to)\ (\hat{N}_\mathcal{T}, \hat{P}_\mathcal{T}),$$

    T^n_μ based on the resolution of 3 linear systems of eq.
  - ➔ proof of L^∞-estimates :

    T^n_μ preserves the set $\mathcal{C}^{n+1} = \left\{ m^{n+1} \leq N_K, P_K \leq M^{n+1} \right\},$
  - ➔ application of Brouwer's fixed point theorem.

Existence and L^∞-estimates

Proposition

Under some hypotheses on the data, including :

- $0 < m \leq N_0, P_0, N^D, P^D \leq M$.

If the time step verifies

$$\Delta t \leq \frac{\lambda^2}{\|C\|_\infty}$$

Then, the scheme has a solution, which satisfies the following L^∞-estimates on the approximate densities :

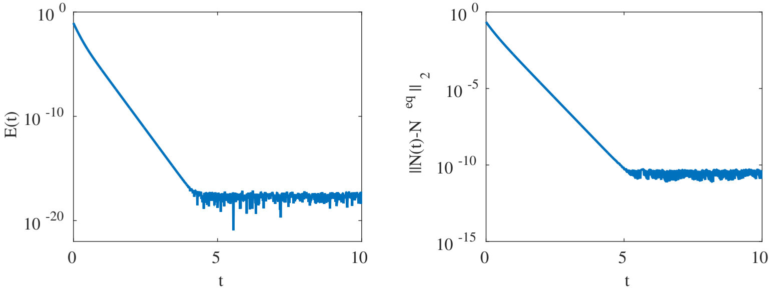
$$m^n \leq N_K^n, P_K^n \leq M^n,$$

where

$$m^n = m(1 + \frac{\Delta t}{\lambda^2}\|C\|_\infty)^{-n}, \quad M^n = M(1 - \frac{\Delta t}{\lambda^2}\|C\|_\infty)^{-n}$$

Comments

- If the doping profile vanishes $(C = 0)$
  - ➔ uniform L^∞ estimates on the discrete densities,
  - ➔ without any assumption on the time step,
  - ➔ exponential decay is established.
- What happens when the doping profile does not vanish ?



Conclusion and perspectives

For the drift-diffusion systems

- At the discrete level,the exponential decay towards the thermal equilibrium is established,...
- ...provided that uniform bounds on the densities are satisfied.
- OK when $C = 0$.

Uniform estimates when $C \neq 0$

❒ Gajewski, Gröger, 1986

- Moser iterations process...
- ... to be adapted at the discrete level
- Ongoing work with M. Bessemoulin-Chatard and A. Jüngel

Finite Volumes for Complex Applications

FVCA 8

Lille - France
June 12-16, 2017

Invited speakers

- A. R. Brodtkorb
- A. Chertock
- I. Faille
- E. Fernandez-Nieto
- T. Gallouët
- B. Haasdonk
- S. Mishra
- C. W. Shu

➘ Peer-reviewed proceedings (submission before 2017/1/6)
➘ Special benchmark session on incompressible flows

https://indico.math.cnrs.fr/event/1299/overview