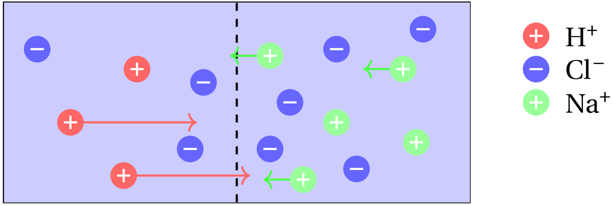
Finite volumes for a generalized Poisson–Nernst–Planck system with cross-diffusion

Clément Cancès, Maxime Herda, **Annamaria Massimini**

CANUM 2026 – Méthodes numériques pour les plasmas

Introduction to the model

Aim: to describe the evolution of I ion species, immersed in a solvent like water, through long and narrow channels:



Applications: batteries, human cells, …

The continuous model

Then, over $\Omega \times [0, +\infty)$:

$$\begin{cases} \partial_t u_i + \nabla \cdot F_i = 0, & i = 1, \dots, I, \\ -\lambda^2 \Delta\phi = \sum_{i=1}^{I} z_i u_i, & (\lambda > 0, z_i \in \mathbb{R}) \end{cases}$$

with the flux of the species i being given by

$(D_i > 0)$

$$F_i = -D_i \Big(u_0 \nabla u_i - u_i \nabla u_0 + u_0 u_i z_i \nabla\phi \Big).$$

where the *solvent concentration* satisfies

(size exclusion)

$$u_0 = 1 - \sum_{i=1}^{I} u_i$$

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where the *solvent concentration* satisfies

(size exclusion)
$$u_0 = 1 - \sum_{i=1}^{I} u_i$$

and leads to cross-diffusion.

Initial and boundary conditions

- We consider boundary conditions of mixed type for the electric potential:

$$\nabla\phi\cdot n=0 \quad \text{on } \Gamma^N \qquad \text{and} \qquad \phi=\phi^D \text{ on } \Gamma^D.$$

- We assume for simplicity that the system is isolated, in the sense that

$$F_i\cdot n=0 \quad \text{on } \partial\Omega, \qquad i=1,\dots,I.$$

- The system is finally complemented with initial conditions $u_i(t=0)=u_i^0$ with

$$u_i^0\geq 0 \quad \text{and} \quad \int_\Omega u_i^0>0 \quad \text{for} \quad i=0,\dots,I \quad \text{and} \quad \sum_{i=0}^{I} u_i^0=1.$$

Entropy structure of the model

The system posses a free energy

$$\mathscr{H} = \int_\Omega \left(u_0 \log(u_0) + \sum_{i=1}^{I} u_i \log(u_i) \right) + \frac{\lambda^2}{2} \int_\Omega |\nabla \phi|^2 - \lambda^2 \int_{\Gamma^D} \phi^D \nabla \phi \cdot n.$$

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Indeed, by rewriting the fluxes via the Slotboom variables $w_i = \frac{u_i}{u_0} e^{z_i \phi}$,

$$F_i = -D_i u_0^2 e^{-z_i \phi} \nabla w_i, \qquad i = 1, \ldots, I,$$

we deduce that

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathscr{H} + \underbrace{4 \int_\Omega \sum_{i=1}^{I} D_i u_0^2 e^{-z_i \phi} |\nabla \sqrt{w_i}|^2}_{\mathscr{D} \text{ dissipation}} = 0.$$

The boundedness-by-entropy method

- By solving $\mu_i = \log(u_i/u_0) + z_i\Phi$, the ion profiles obey the Fermi–Dirac statistics[0]

$$u_i = \frac{\exp(\mu_i - z_i\Phi)}{1 + \sum_{j=1}^{n} \exp(\mu_j - z_j\Phi)} \in [0,1] \qquad i = 1, \dots, I.$$

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[0] Gerstenmayer and Jüngel 2018

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- Since $\mathscr{H}$ is bounded, then the dissipation $\mathscr{D}$ also is

$$\iint_{\mathbb{R}_+ \times \Omega} \sum_{i=1}^{I} D_i u_0^2 e^{-z_i\phi} |\nabla \sqrt{w_i}|^2 \leq C$$

  and so all the terms in the following expression of the fluxes

$$F_i = -D_i \left(\nabla(u_0 u_i) - 4u_i \sqrt{u_0} \nabla \sqrt{u_0} + u_i u_0 z_i \nabla \phi \right) \qquad 1 \leq i \leq I,$$

  have a clear mathematical sense.

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A steady state (u^∞, ϕ^∞)

- It should correspond to constant-in-space $\boldsymbol{\mu}^\infty = \left(\mu_i^\infty\right)_{1\le i\le I}$[1], calculated to guarantee the conservation-of-total-mass

$$\int_\Omega u_i^\infty = \int_\Omega u_i^0.$$

- Then the densities $U^\infty = \left(u_i^\infty\right)_{1\le i\le I}$ satisfy

$$u_i^\infty(x) = \frac{e^{\mu_i^\infty - z_i\phi^\infty(x)}}{1+\sum_{j=1}^I e^{\mu_j^\infty - z_j\phi^\infty(x)}}, \qquad i = 1,\dots,I,\ x\in\Omega,$$

  and $u_0^\infty(x) = 1-\sum_{j=1}^I u_j^\infty(x)$.
- Plugging these expressions in the Poisson equation provides

$$-\lambda^2\Delta\phi^\infty = f + \sum_{i=1}^I z_i \frac{e^{\mu_i^\infty - z_i\phi^\infty(x)}}{1+\sum_{j=1}^I e^{\mu_j^\infty - z_j\phi^\infty(x)}} \quad \text{in } \Omega.$$

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[1] Burger, Schlake, and Wolfram 2012

Equilibrium

The solution $(\phi^\infty, \boldsymbol{\mu}^\infty)$ is the unique minimizer of the convex functional $\Psi : (\phi^D + V) \times \mathbb{R}^I \to \mathbb{R}$ defined by

$$\Psi(y, \boldsymbol{\xi}) = \int_\Omega \left[\frac{\lambda^2}{2} |\nabla y|^2 + \log\left(1 + \sum_{i=1}^{I} e^{\xi_i - z_i y}\right) - fy - \sum_{i=1}^{I} \xi_i u_i^0 \right].$$

Two numerical schemes for the modified PNP model

Motivations: To propose and to analyze a scheme for the model which shares the best with the approaches proposed so far [a] [b] [c]:

- positivity of the volume fractions
- decay of free energy,
- unconditional convergence,
- second order accuracy in space,
- well behaviour (even for small λ^2),
- preserve the form of the steady states.

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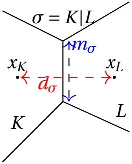
[a] Bailo, Carrillo, and Hu 2023
[b] Cancès, C. Chainais-Hillairet, et al. 2019
[c] Gerstenmayer and Jüngel 2019

The space-time discretisation

- We introduce a partition $\mathscr{T}$ of Ω in polytopes (*control volumes*), and a time discretisation $\left(t^n\right)_{n\geq 0}$ of $[0,+\infty)$.



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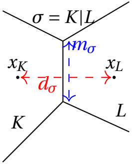

- The discretization of the Poisson equation relies on a classical two-point flux approximation:

$$-\lambda^2 \int_K \Delta\phi = \sum_{i=1}^{I} z_i \int_K u_i \qquad K \in \mathcal{T}, n \geq 1.$$

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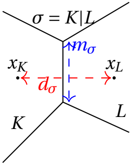

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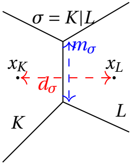

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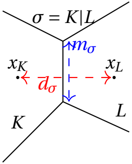

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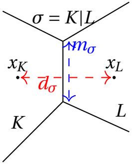

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- The conservation laws are discretized using a backward Euler method in time and finite volumes in space:

$$\frac{u_{i,K}^n - u_{i,K}^{n-1}}{\tau^n} m_K + \sum_{\sigma\in\mathcal{E}_K} F_{i,K\sigma}^n = 0, \qquad i=1,\ldots,I,\ K\in\mathcal{T},\ n\geq 1.$$

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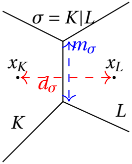

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$$\sum_{\sigma\in\mathcal{E}_K} m_\sigma \frac{(\phi_K^n - \phi_{K\sigma}^n)}{d_\sigma} = \frac{1}{\lambda^2} m_K \sum_{i=1}^{I} z_i u_{i,K}^n \qquad K\in\mathcal{T}, n\geq 1.$$

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The SQRA scheme

The continuous model was originally derived thanks to a hopping process[a], suggesting the choice

$$F_{i,K\sigma}^{n} = a_\sigma D_i \left(u_{i,K}^{n} u_{0,L}^{n} e^{\frac{1}{2} z_i (\phi_K^n - \phi_L^n)} - u_{i,L}^{n} u_{0,K}^{n} e^{\frac{1}{2} z_i (\phi_L^n - \phi_K^n)} \right),$$

leading to the *square-root approximation scheme*[b].

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[a] Burger, Schlake, and Wolfram 2012

[b] Cancès and Venel 2023

The SQRA scheme

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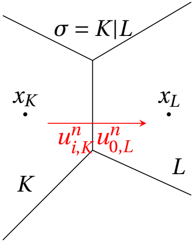


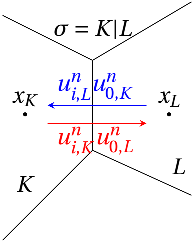
The probability that a $i-$particle jumps from K to L is proportional to:

$u_{i,K}^n$ = #{candidates in K for a jump}

$u_{0,L}^n$ = #{available sites to host the $i-$ particle in the cell L}

The SQRA scheme

$$F^n_{i,K\sigma} = a_\sigma D_i \left(u^n_{i,K} u^n_{0,L} e^{\frac{1}{2} z_i (\phi^n_K - \phi^n_L)} - u^n_{i,L} u^n_{0,K} e^{\frac{1}{2} z_i (\phi^n_L - \phi^n_K)} \right),$$



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$u^n_{i,L}$ = #{candidates in L for a jump}

$u^n_{0,K}$ = #{available sites to host the $i-$ particle in the cell K}

A generalisation of the Scharfetter-Gummel scheme

Hence the scheme can be re-written using the function

$$\mathfrak{B}(y) = e^{-y/2}$$

as

$$F^n_{i,K\sigma} \quad = \quad a_\sigma D_i \left(u^n_{i,K} u^n_{0,L} \mathfrak{B}\left(z_i(\phi^n_L - \phi^n_K)\right) - u^n_{i,L} u^n_{0,K} \mathfrak{B}\left(z_i(\phi^n_K - \phi^n_L)\right)\right)$$[2][3][4]

where

- $\mathfrak{B} \in C^1(\mathbb{R}, \mathbb{R})$;
- $\mathfrak{B}(0) = 1$, $\mathfrak{B}(y) > 0$;
- in general, $\mathfrak{B}(y) - \mathfrak{B}(-y) \neq -y$, but $\mathfrak{B}(-y) - \mathfrak{B}(y) = y + \mathcal{O}(y^2)$.

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[2] Lie, Fackeldey, and Weber 2013

[3] Heida 2018

[4] Claire Chainais-Hillairet and Droniou 2011

Behaviour for small λ^2

However, when λ^2 become small,

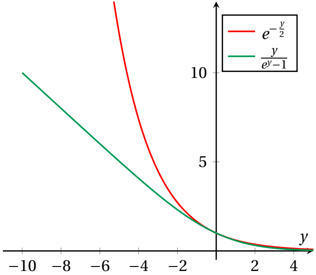
$$\sum_{\sigma \in \mathcal{E}_K} \frac{m_\sigma}{d_\sigma} (\phi_K^n - \phi_{K\sigma}^n) = \frac{1}{\lambda^2} m_K \sum_{i=1}^{I} z_i u_{i,K}^n,$$

the drift

$$e^{\frac{1}{2} z_i (\phi_K^n - \phi_L^n)}$$

becomes too large to evaluate its exponential.

The SG scheme



Instead of using the function

(SQRA) $$\mathfrak{B}(y) = e^{-y/2},$$

another natural choice for the drift term is the function

(SG) $$\mathfrak{B}(y) = \frac{y}{e^y - 1},$$

leading to the *Scharfetter-Gummel scheme*, with fluxes:

$$F^n_{i,K\sigma} = a_\sigma D_i \left(u^n_{i,K} u^n_{0,L} \frac{z_i(\phi^n_L - \phi^n_K)}{e^{z_i(\phi^n_L - \phi^n_K)} - 1} - u^n_{i,L} u^n_{0,K} \frac{z_i(\phi^n_K - \phi^n_L)}{e^{z_i(\phi^n_K - \phi^n_L)} - 1} \right).$$

Consistency of the fluxes

By taking advantages of the entropy structure of the model the fluxes re-write as

$$F_i = -D_i\Big(u_0 \nabla u_i - u_i \nabla u_0 + u_0 u_i z_i \nabla\phi\Big) = -D_i u_0^2 e^{-z_i\phi} \nabla w_i$$

where $w_i := \frac{u_i}{u_0} e^{z_i\phi}$ are the *Slotboom variables.*

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[5] Heida, Kantner, and Stephan 2021

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where $w_i := \frac{u_i}{u_0} e^{z_i\phi}$ are the *Slotboom variables*. Hence

$$F^n_{i,K\sigma} = a_\sigma\, D_i\, u^n_{0,K}\, u^n_{0,L} \mathfrak{M}(e^{-z_i\phi^n_K}, e^{-z_i\phi^n_L}) \Big(w^n_{i,K} - w^n_{i,L}\Big)$$

where $\mathfrak{M}$ is a Stolarsky mean[5]:

$$\mathfrak{B}(y) = \mathfrak{M}(1, e^{-y}).$$

We used:

$(a, b > 0 \text{ with } a \neq b)$ $\quad \mathfrak{M}^{\mathrm{SQRA}}(a,b) := \sqrt{ab}, \quad \mathfrak{M}^{\mathrm{SG}}(a,b) := \dfrac{\log(1/a) - \log(1/b)}{1/a - 1/b}$

---

[5] Heida, Kantner, and Stephan 2021

Theorem (Existence - C. Cancès, M. Herda, A. M)

There exists (at least) one solution to the scheme which satisfies

$$0 < u_{i,K}^n < 1 \qquad \forall i = 0, \dots, I,\ K \in \mathcal{T},\ n \geq 1.$$

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Moreover, the discrete free energy $\mathcal{H}_{\mathcal{T}}^n$ *is decaying along the time iterations*

$$\mathcal{H}_{\mathcal{T}}^n + \tau^n \mathcal{D}_{\mathcal{T}}^n \leq \mathcal{H}_{\mathcal{T}}^{n-1}, \qquad n \geq 1,$$

where $\mu_{i,K}^n = \log\left(\frac{u_{i,K}^n}{u_{0,K}^n}\right) + z_i \phi_K^n$ *is the discrete electrochemical potentials of species i, and*

$$\mathcal{D}_{\mathcal{T}}^n = \sum_{i=1}^{I} \sum_{\sigma \in \mathcal{E}_{int}} F_{i,K\sigma}^n (\mu_{i,K}^n - \mu_{i,L}^n) \geq 0.$$

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The dissipation $\mathcal{D}_{\mathcal{T}}^n$ *vanishes iff* $\left(\left(U_K^n\right)_{K \in \mathcal{T}}, \left(\phi_K^n\right)_{K \in \mathcal{T}}\right)$ *is the stationary solution.*

Theorem (Convergence of the scheme - C. Cancès, M. Herda, A. M)

There exists a weak solution (U,ϕ) *such that, up to the extraction of a subsequence,*

$$\phi_{\mathcal{T}_\ell,\tau_\ell} \underset{\ell\to+\infty}{\longrightarrow} \phi \quad \textit{and} \quad u_{0,\mathcal{T}_\ell,\tau_\ell} \underset{\ell\to+\infty}{\longrightarrow} u_0 \quad \textit{in}\ L^p_{loc}(\mathbb{R}_+;L^p(\Omega)) \quad \forall p\in[1,+\infty),$$

$$\textit{and} \quad U_{\mathcal{T}_\ell,\tau_\ell} \underset{\ell\to+\infty}{\longrightarrow} U \quad \textit{in the}\ L^\infty(\mathbb{R}_+\times\Omega)^I\ \textit{weak-}\star\ \textit{sense.}$$

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We proceed by compactness and then we identify the limit.

Let $\varphi\in C_c^\infty(\mathbb{R}_+\times\overline{\Omega})$ and $\varphi_K^n := \varphi(x_K,t^n)$. We multiply the scheme by $\tau^n\varphi_K^n$ and sum over $K\in\mathcal{T}$ and $n\geq 1$:

$$\sum_{n\geq1}\sum_{K\in\mathcal{T}} m_K\left(u_{i,K}^n - u_{i,K}^{n-1}\right)\varphi_K^n + \sum_{n\geq1}\tau^n\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} F_{i,K\sigma}^n\varphi_K^n = 0.$$

Reformulation of the discrete fluxes

In particular, the proof is based on the reformulation of the fluxes

$$F_i = -D_i \left(\nabla(u_0 u_i) - 4 u_i \sqrt{u_0} \nabla \sqrt{u_0} + u_i u_0 z_i \nabla \phi \right).$$

One splits the flux into:

$$F_{i,K\sigma}^n = F_{i,K\sigma}^{\text{conv},n} + F_{i,K\sigma}^{\text{diff},n},$$

with

$$F_{i,K\sigma}^{\text{conv},n} = a_\sigma D_i \frac{u_{i,K}^n u_{0,L}^n + u_{i,L}^n u_{0,K}^n}{2} \left[\mathfrak{B}\left(z_i(\phi_L^n - \phi_K^n)\right) - \mathfrak{B}\left(z_i(\phi_K^n - \phi_L^n)\right) \right]$$

$$F_{i,K\sigma}^{\text{diff},n} = a_\sigma D_i \frac{u_{i,K}^n u_{0,L}^n - u_{i,L}^n u_{0,K}^n}{2} \left[\mathfrak{B}\left(z_i(\phi_L^n - \phi_K^n)\right) + \mathfrak{B}\left(z_i(\phi_K^n - \phi_L^n)\right) \right]$$

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$$\begin{aligned} F_{i,K\sigma}^{\text{conv},n} &= a_\sigma D_i \frac{u_{i,K}^n u_{0,L}^n + u_{i,L}^n u_{0,K}^n}{2} \left[\mathfrak{B}\left(z_i(\phi_L^n - \phi_K^n) \right) - \mathfrak{B}\left(z_i(\phi_K^n - \phi_L^n) \right) \right] \\ &= a_\sigma D_i \frac{u_{i,K}^n u_{0,L}^n + u_{i,L}^n u_{0,K}^n}{2} z_i(\phi_K^n - \phi_L^n) + \mathcal{O}\left(a_\sigma (\phi_K^n - \phi_L^n)^2 \right), \end{aligned}$$

$$\begin{aligned} F_{i,K\sigma}^{\text{diff},n} &= a_\sigma D_i \frac{u_{i,K}^n u_{0,L}^n - u_{i,L}^n u_{0,K}^n}{2} \left[\mathfrak{B}\left(z_i(\phi_L^n - \phi_K^n) \right) + \mathfrak{B}\left(z_i(\phi_K^n - \phi_L^n) \right) \right] \\ &= a_\sigma D_i \left(u_{i,K}^n u_{0,L}^n - u_{i,L}^n u_{0,K}^n \right) \left(1 + \mathcal{O}\left((\phi_K^n - \phi_L^n)^2 \right) \right) \end{aligned}$$

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$$F_{i,K\sigma}^{\mathrm{conv},n} = a_\sigma D_i \frac{u_{i,K}^n u_{0,L}^n + u_{i,L}^n u_{0,K}^n}{2} z_i(\phi_K^n - \phi_L^n) + \mathcal{O}\left(a_\sigma(\phi_K^n - \phi_L^n)^2\right),$$

$$\begin{aligned}
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&= a_\sigma D_i\left(u_{i,K}^n u_{0,L}^n - u_{i,L}^n u_{0,K}^n\right)\left(1 + \mathcal{O}\left((\phi_K^n - \phi_L^n)^2\right)\right) \\
&= a_\sigma D_i (u_{i,K}^n u_{0,K}^n - u_{i,L}^n u_{0,L}^n)\left(1 + \mathcal{O}\left((\phi_K^n - \phi_L^n)^2\right)\right) \\
&\quad + a_\sigma D_i (u_{i,K}^n + u_{i,L}^n)(u_{0,L}^n - u_{0,K}^n)\left(1 + \mathcal{O}\left((\phi_K^n - \phi_L^n)^2\right)\right)
\end{aligned}$$

Reformulation of the discrete fluxes

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$$F_i = -D_i\left(\nabla(u_0 u_i) - 4u_i\sqrt{u_0}\,\nabla\sqrt{u_0} + u_i u_0 z_i \nabla\phi\right).$$

$$F_{i,K\sigma}^{\mathrm{conv},n} = a_\sigma D_i \frac{u_{i,K}^n u_{0,L}^n + u_{i,L}^n u_{0,K}^n}{2} z_i(\phi_K^n - \phi_L^n) + \mathcal{O}\left(a_\sigma(\phi_K^n - \phi_L^n)^2\right),$$

$$\begin{aligned} F_{i,K\sigma}^{\mathrm{diff},n} = a_\sigma D_i \Big[& (u_{i,K}^n u_{0,K}^n - u_{i,L}^n u_{0,L}^n) \\ & + (u_{i,K}^n + u_{i,L}^n)(\sqrt{u_{0,L}^n} - \sqrt{u_{0,K}^n})(\sqrt{u_{0,L}^n} + \sqrt{u_{0,K}^n}) \Big] \\ & \times \left(1 + \mathcal{O}\left((\phi_K^n - \phi_L^n)^2\right)\right) \end{aligned}$$

A simulations with $\lambda^2 = 10^{-2}$ (1D)

- $\Omega = (0,1)$
- $z_1 = 2$, $z_2 = 1$, and $D_1 = D_2 = 1$
- $\phi^D(t,0) = 10$ and $\phi^D(t,1) = 0$.
- Initial configurations: $u_1^0(x) = 0.2 + 0.1(x-1)$ and $u_2^0 \equiv 0.4$

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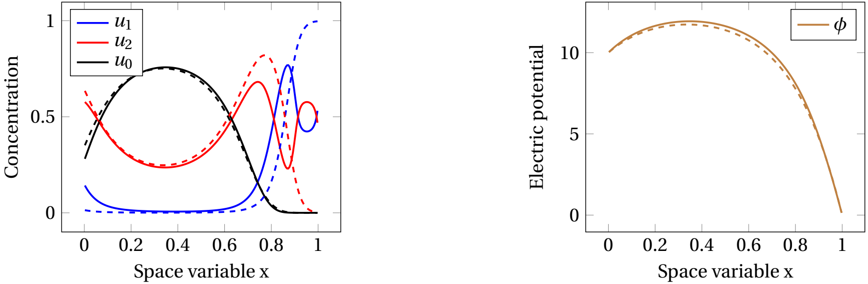
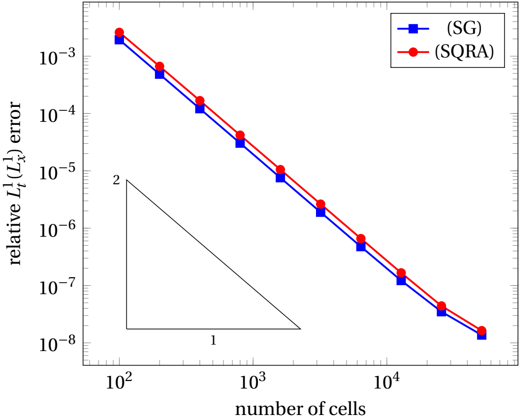


Figure 1: Solid lines: Solutions at time $T = 1$. Dashed lines: Long-time limit.

Second order convergence of the schemes



A reference solution is computed on a grid made of 1638400 cells and with a constant time step $\tau = 10^{-3}$, to which are compared solutions computed on successively refined grids but with the same constant time step.

The steady state of the scheme

We are interested in steady states $(U_{\mathcal{T}}^{\infty}, \phi_{\mathcal{T}}^{\infty})$ of the scheme, i.e. solutions to

$$\lambda^2 \sum_{\sigma\in\mathcal{E}_K} a_\sigma (\phi_K^\infty - \phi_{K\sigma}^\infty) = m_K \left(f_K + \sum_{i=1}^{I} z_i u_{i,K}^\infty \right), \qquad K \in \mathcal{T},$$

$$\sum_{\sigma\in\mathcal{E}_K} F_{i,K\sigma}^\infty = 0, \qquad i = 1,\ldots,I,\ K \in \mathcal{T},$$

with $F_{i,K\sigma}^\infty = 0$ if $\sigma \in \mathcal{E}_{\text{ext}}$ and

$$F_{i,K\sigma}^\infty = a_\sigma D_i \left(u_{i,K}^\infty u_{0,L}^\infty \mathfrak{B}\left(z_i(\phi_L^\infty - \phi_K^\infty)\right) - u_{i,L}^\infty u_{0,K}^\infty \mathfrak{B}\left(z_i(\phi_K^\infty - \phi_L^\infty)\right)\right)$$

for $\sigma = K|L \in \mathcal{E}_{\text{int}}$, where we have set

$$u_{0,K}^\infty = 1 - \sum_{i=1}^{I} u_{i,K}^\infty, \qquad K \in \mathcal{T},$$

complemented with

$$\sum_{K\in\mathcal{T}} m_K u_{i,K}^\infty = \int_\Omega u_i^0, \qquad i = 1,\ldots,I.$$

Proposition (Existence of the (discrete) steady state)

There exists a solution to the steady scheme, with constant in space potentials in the sense that there exists $\boldsymbol{\mu}_{\mathcal{T}}^{\infty} = \left(\mu_{i,\mathcal{T}}^{\infty}\right)_{1\le i\le I} \in \mathbb{R}^I$ *such that*

$$\log \frac{u_{i,K}^{\infty}}{u_{0,K}^{\infty}} + z_i \phi_K^{\infty} = \mu_{i,\mathcal{T}}^{\infty}, \qquad K \in \mathcal{T},\ 1 \le i \le I,$$

such that,

$$(U_{\mathcal{T}}^{n}, \phi_{\mathcal{T}}^{n}) \underset{n\to+\infty}{\longrightarrow} (U_{\mathcal{T}}^{\infty}, \phi_{\mathcal{T}}^{\infty}).$$

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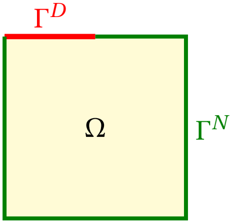
Proposition (Uniqueness)

The solution $(\phi_{\mathcal{T}}^{\infty}, \boldsymbol{\mu}_{\mathcal{T}}^{\infty})$ *minimizes the strictly convex functional* $\Psi_{\mathcal{T}} : \mathbb{R}^{\mathcal{T}} \times \mathbb{R}^I \to \mathbb{R}$ *defined by*

$$\Psi_{\mathcal{T}}(y_{\mathcal{T}}, \boldsymbol{\xi}) = \frac{\lambda^2}{2} \sum_{\sigma\in\mathcal{E}} a_\sigma (y_K - y_{K\sigma})^2 + \sum_{K\in\mathcal{T}} m_K \log\left(1 + \sum_{i=1}^{I} e^{\xi_i - z_i y_K}\right) - \sum_{K\in\mathcal{T}} m_K \left[f_K y_K + \sum_{i=1}^{I} \xi_i u_{i,K}^0 \right].$$

Long-time behavior of the scheme (2D)



- $\Omega = (0,1)^2$, with $\partial\Omega = \Gamma^D \cup \Gamma^N$
- $\phi^D = 0$

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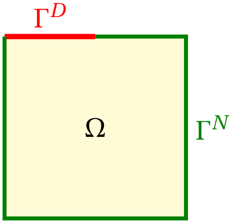

- $\Omega = (0,1)^2$, with $\partial\Omega = \Gamma^D \cup \Gamma^N$
- $\phi^D = 0$
- $z_1 = 2$, $z_2 = 1$, $z_3 = -1$
- $D_1 = 1$, $D_2 = 2$,$D_3 = 2$

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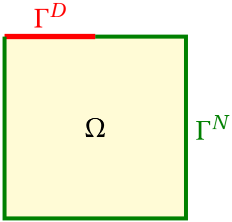

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- $D_1 = 1$, $D_2 = 2$, $D_3 = 2$

Two initial globally neutral profiles:

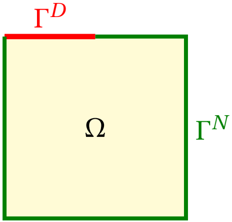
(1)

$$\begin{cases} u_1^{0,(1)}(x) = 0.3 \times 1_{(0,1/2)^2}(x), \\ u_2^{0,(1)}(x) = 0.3 \times 1_{(1/2,1)\times(0,1/2)}(x), \\ u_3^{0,(1)}(x) = 0.9 \times 1_{(1/2,1)^2}(x). \end{cases}$$

(2)

$$\begin{cases} u_1^{0,(2)}(x) = 0.1 \times u_1^{0,(1)}(x), \\ u_2^{0,(2)}(x) = 0.1 \times u_2^{0,(1)}(x) + 0.9 \times 1_{(0,1)\times(1/2,1)}(x), \\ u_3^{0,(2)}(x) = 0.1 \times u_3^{0,(1)}(x) + 0.9 \times 1_{(0,1)\times(0,1/2)}(x). \end{cases}$$

Long-time behavior of the scheme (2D)



- $\Omega = (0,1)^2$, with $\partial\Omega = \Gamma^D \cup \Gamma^N$
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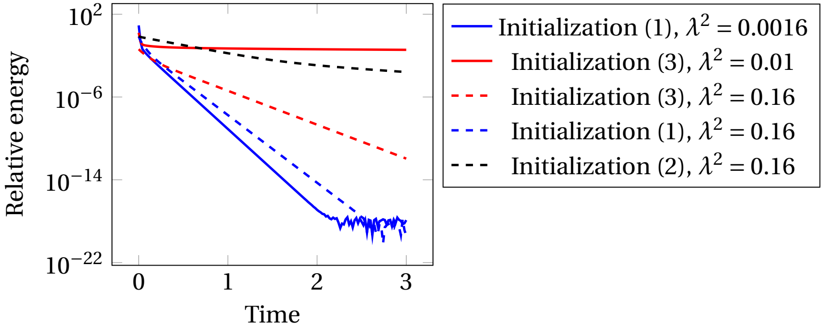
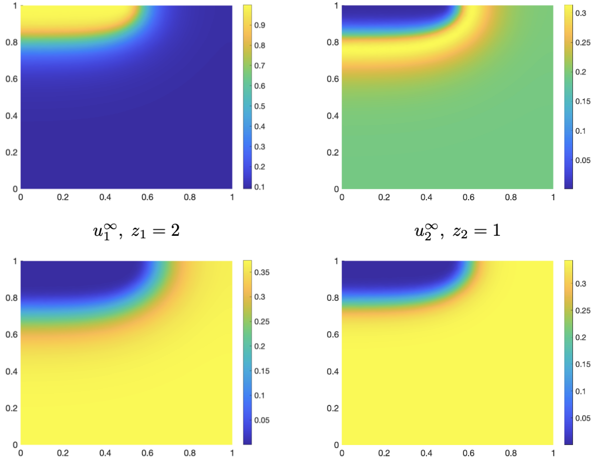
A third initial globally charged and constant in space:

(3) $\quad u_1^{0,(3)}(x) = 0.2, \quad u_2^{0,(3)}(x) = 0.2, \quad u_3^{0,(3)}(x) = 0.3.$

Convergence towards the steady long-time behavior ($\mathcal{H}_{\mathcal{T}}^{n} - \mathcal{H}_{\mathcal{T}}^{\infty}$)



We run our scheme with a constant time step $\tau = 10^{-4}$ and for two different Debye length until a final time $T = 3$, and look for the evolution of the relative energy $\mathcal{H}_{\mathcal{T}}^{n} - \mathcal{H}_{\mathcal{T}}^{\infty}$ along time. The relative energy is decaying for all the curves, but the velocity at which the decay occurs varies strongly depending on the Debye length and on the initial profile.



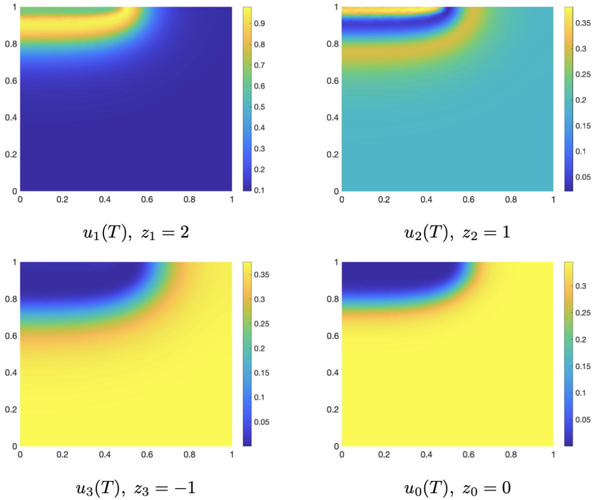
$u_1^\infty,\ z_1 = 2$

$u_2^\infty,\ z_2 = 1$

$u_3^\infty,\ z_3 = -1$

$u_0^\infty,\ z_0 = 0$

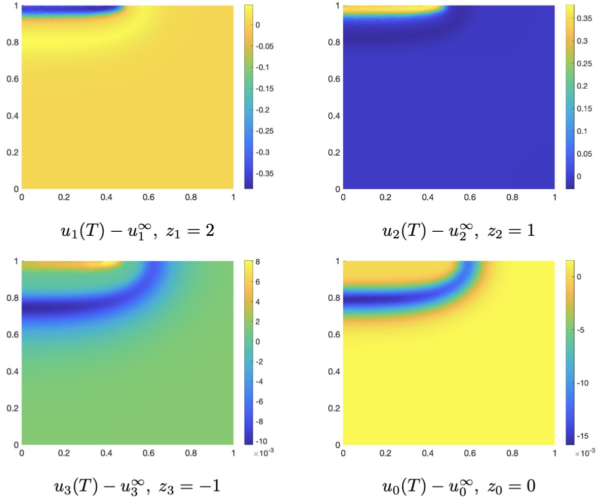
Figure 2: Stationary concentration profiles with initial configuration (3), $\lambda^2 = 0.01$.



$u_1(T),\ z_1 = 2$ $u_2(T),\ z_2 = 1$

$u_3(T),\ z_3 = -1$ $u_0(T),\ z_0 = 0$

Figure 3: Concentration profiles at final time $T = 3$, with initial configuration (3), $\lambda^2 = 0.01$.



$u_1(T) - u_1^{\infty},\ z_1 = 2$

$u_2(T) - u_2^{\infty},\ z_2 = 1$

$u_3(T) - u_3^{\infty},\ z_3 = -1$

$u_0(T) - u_0^{\infty},\ z_0 = 0$

Figure 4: Difference between the final concentration profiles, with initial configuration (3), $\lambda^2 = 0.01$.