A convergent finite volume scheme for a cross-diffusion model for ion transport

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The Cross-Diffusion Model[1]

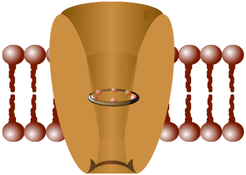

Figure: schematic picture of an ion channel

2 major effects for modelling flow through an ion channel:

- electrostatic interaction
- size exclusion

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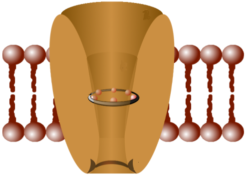

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2 major effects for modelling flow through an ion channel:

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Evolution of the ion concentrations u_i, $i = 1, \ldots, n$

$$\partial_t u_i = \operatorname{div}\Big(\underbrace{D_i \left(u_0 \nabla u_i - u_i \nabla u_0 \right)}_{\text{Diffusion}} + \underbrace{D_i \mu z_i u_i u_0 \nabla \Phi}_{\text{Drift}} \Big)$$

Volume filling: solvent concentration $u_0 = 1 - \sum_{i=1}^{n} u_i$

Electric potential: $-\Delta \Phi = \sum_{i=1}^{n} z_i u_i + f$

$D_i > 0$	... diffusion coefficient	$\mu > 0$	... mobility constant
$z_i \in \mathbb{R}$	... ion charge	$f \in L^\infty$	... permanent charge density

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Mathematical Difficulties

Equation for u_i can be rewritten as system

$$\partial_t u = \operatorname{div}\left(A(u)\nabla u + F(u, \Phi)\right)$$

with diffusion matrix $A(u)$ given by

$$A_{ii}(u) = D_i u_i, \quad A_{ij}(u) = D_i(u_0 + u_i), \quad j \neq i$$

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- A is nonsymmetric and not positive semidefinite
- no maximum principle for cross-diffusion systems
- degenerate structure of the equations

Boundedness-by-entropy Method[1]

System possesses **entropy functional** $\mathcal{H}[u] = \int_\Omega h(u)dx$ with

$$h(u) = \sum_{i=0}^{n} u_i(\log u_i - 1) + \sum_{i=1}^{n} \mu z_i u_i \Phi$$

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- transform system to **entropy variables**

$$w_i = \partial h(u)/\partial u_i = \log(u_i/u_0) + \mu z_i \Phi$$

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- gradient estimates for $u_0^{1/2}$ and $u_0^{1/2} u_i$ from **entropy inequality**

$$\frac{d\mathcal{H}[u]}{dt} + \mathcal{I}[u] \leq 0, \quad \text{with } \mathcal{I}[u] = \frac{1}{2}\int_\Omega \sum_{i=1}^{n} D_i u_0 u_i |\nabla w_i|^2 dx$$

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$\Rightarrow$ weak formulation by rewriting $u_0 \nabla u_i - u_i \nabla u_0 = u_0^{1/2}\left(\nabla(u_0^{1/2} u_i) - 3 u_i \nabla u_0^{1/2}\right)$

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Analytic Results

- Stationary equations: existence of bounded weak solutions and uniqueness in special cases [Burger, Schlake, Wolfram, 2012][1]
- $\Phi \equiv 0$: global existence of bounded weak solutions and uniqueness for $D_i = D$ [Zamponi, Jüngel, 2017][2]
- Global existence for full problem with potential and mixed B.C. and uniqueness for $D_i = D$ [G., Jüngel][3]

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Our Aim

Find a finite volume scheme that preserves the entropy inequality and gradient estimates (and ideally converges)

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Simplified Problem

Simplified Equations

$$
\begin{aligned}
\partial_t u_i = D\,\mathrm{div}(u_0 \nabla u_i - u_i \nabla u_0) \quad & \text{in } \Omega \times (0,T), \text{ for } i = 1,\dots,n, \\
\nabla u_i \cdot \nu = 0 \quad & \text{on } \partial\Omega \times (0,T), \\
u(0) = u^0 \quad & \text{in } \Omega.
\end{aligned}
$$

Assumptions:

- vanishing potential $\Phi \equiv 0$
- equal diffusion coefficients $D_i = D > 0$
- homogeneous Neumann B.C.
- $u^0 \in L^\infty(\Omega)$ with $0 \leq u^0 \leq 1$
- $\Omega \subset \mathbb{R}^2$ polygonal domain

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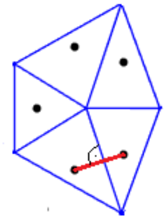
Finite Volume Methods

Admissible mesh $\mathcal{M} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$:

$\mathcal{T}$ ... family of open polygonal cells
$\mathcal{E}$ ... family of edges
$\mathcal{P} = (x_K)_{K \in \mathcal{T}}$ ... family of cell centers



FVM provides functions $u_{\mathcal{T}} = \sum_{K \in \mathcal{T}} \mathbb{I}_K u_K$ .. constant on each cell

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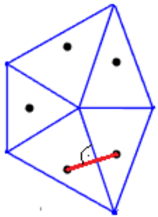

FVM provides functions $u_{\mathcal{T}} = \sum_{K\in\mathcal{T}} \mathbb{I}_K u_K$ .. constant on each cell

For example:

$$-\int_K \mathrm{div}(u_i \nabla u_0) dx = \sum_{\sigma\in\mathcal{E}_K} \int_\sigma u_i \nabla u_0 \cdot \nu ds \approx -\sum_{\sigma\in\mathcal{E}_K} \underbrace{\frac{\mathrm{m}(\sigma)}{d_\sigma}}_{=:\tau_\sigma} u_{i,\sigma}(u_{0,K} - u_{0,L})$$

The Scheme

Find $u^k_{i,\mathcal{T}}$ and $\Phi^k_{\mathcal{T}}$ such that for $K \in \mathcal{T}$, $k \geq 1$ and $1 \leq i \leq n$

$$\mathrm{m}(K)\frac{u^k_{i,K} - u^{k-1}_{i,K}}{\Delta t} + \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}^k_{i,K,\sigma} = 0\,,$$

The Scheme

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$$\mathrm{m}(K) \frac{u_{i,K}^k - u_{i,K}^{k-1}}{\Delta t} + \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{i,K,\sigma}^k = 0 \,,$$

... implicit Euler in time & finite volume discretization in space with fluxes

$$\mathcal{F}_{i,K,\sigma}^k = \tau_\sigma D \left(u_{0,\sigma}^k (u_{i,K}^k - u_{i,L}^k) - u_{i,\sigma}^k (u_{0,K}^k - u_{0,L}^k) \right) ,$$

with

$$u_{0,\sigma}^k = \max\{u_{0,K}^k, u_{0,L}^k\},$$

$$u_{i,\sigma}^k = \begin{cases} u_{i,K}^k & \text{if } u_{0,K}^k - u_{0,L}^k \leq 0 \\ u_{i,L}^k & \text{if } u_{0,K}^k - u_{0,L}^k > 0 \end{cases} \quad \text{for } i \geq 1.$$

Well-posedness of the Scheme

Proposition 1

There exists a unique solution (u, Φ) to the scheme that satisfies $0 \leq u_{i,K}^k \leq 1$ for all $k \geq 1$, $i = 0, \ldots, n$ and $K \in \mathcal{T}$.

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2. Existence with topological degree method
3. Uniqueness for u_0
4. Uniqueness for u_i: with discrete version of Gajewski's method, show that

$$d(u^k, v^k) = \int_\Omega \sum_{i=1}^n \left(H(u_i^k) + H(v_i^k) - 2H\left(\frac{u_i^k + v_i^k}{2}\right)\right)$$

is non-increasing along two solutions u and v, with $H(u) = u(\log u - 1) + 1$.

Discrete Entropy Inequality and Gradient Estimates

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The solution to the scheme satisfies the discrete entropy-production inequality

$$\frac{\mathcal{H}^k - \mathcal{H}^{k-1}}{\Delta t} + \mathcal{I}^k \leq 0,$$

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with the discrete entropy

$$\mathcal{H}^k = \sum_{K \in \mathcal{T}} \mathrm{m}(K) \sum_{i=0}^{n} \left(u_{i,K}^k (\log u_{i,K}^k - 1) + 1 \right),$$

and the discrete entropy production

$$\mathcal{I}^k = D \sum_{\sigma \in \mathcal{E}} \tau_\sigma \left(4 \sum_{i \geq 1} u_{0,\sigma}^k \left(\sqrt{u_{i,K}^k} - \sqrt{u_{i,L}^k} \right)^2 + 4 \left(\sqrt{u_{0,K}^k} - \sqrt{u_{0,L}^k} \right)^2 + (u_{0,K}^k - u_{0,L}^k)^2 \right).$$

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$\Rightarrow$ discrete gradient estimates for $u_0^{1/2}$ and $u_0^{1/2} u_i$

Important: $\sum_{i=0}^n u_{i,\sigma}^k \ge 1$!

Convergence

Theorem

Let $\mathcal{T}_m$ and Δt_m be a sequence of regular admissible meshes and time steps such that $h(\mathcal{T}_m)$, $\Delta t_m \to 0$, and set $u_m = u_{\mathcal{T}_m,\Delta t_m}$ the solution of the scheme. Then there exist functions $u_0, \ldots, u_n \in L^\infty(0, T; L^\infty(\Omega))$ such that

$$u_0^{1/2},\ u_0^{1/2} u_i \in L^2(0, T; H^1(\Omega)),$$
$$u_{0,m}^{1/2} \to u_0^{1/2},\ u_{0,m}^{1/2} u_{i,m} \to u_0^{1/2} u_i \quad \text{in } L^2(\Omega \times (0, T)),$$

and $u = (u_1, \ldots, u_n)$ is a weak solution to the ion transport model.

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Main Difficulty: compactness of the sequence $(u_{0,m}^{1/2}u_{i,m})_m$

Solution: prove discrete version of a degenerate Aubin-Lions lemma

Generalisations of the Results

Scheme with Φ

$$\mathcal{F}_{i,K,\sigma}^k = -\tau_\sigma D\Big(u_{0,\sigma}^k(u_{i,K}^k - u_{i,L}^k) - u_{i,\sigma}^k\Big(\underbrace{(u_{0,K}^k - u_{0,L}^k) - \hat{u}_{0,\sigma_i}^k \mu z_i(\Phi_K^k - \Phi_L^k)}_{=:\mathcal{V}_{i,K,\sigma}^k}\Big)\Big),$$

where now

$$\hat{u}_{0,\sigma_i}^k = \begin{cases} u_{0,K}^k & \text{if } z_i(\Phi_K^k - \Phi_L^k) \leq 0 \\ u_{0,L}^k & \text{if } z_i(\Phi_K^k - \Phi_L^k) > 0 \end{cases} \quad \text{for } i \geq 1,$$

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Existence and L^∞-**bounds** still hold, **entropy inequality** only if $\sum_{i=0}^n u_{i,\sigma}^k \geq \delta > 0$!

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Existence and L^∞**-bounds** still hold, **entropy inequality** only if $\sum_{i=0}^{n} u_{i,\sigma}^{k} \ge \delta > 0$!

Bad news: until now not able to prove anything when D_i not constant..
Good news: simulations still look fine

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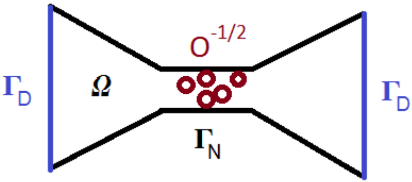
Test Case: Calcium Channel

3 types of ions

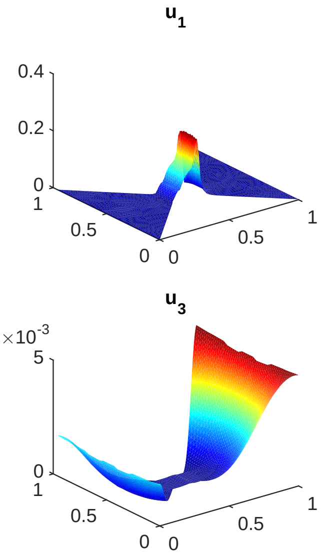
- u_1 ... Calcium Ca^{2+}
- u_2 ... Sodium Na^{+}
- u_3 ... Chloride Cl^{-}



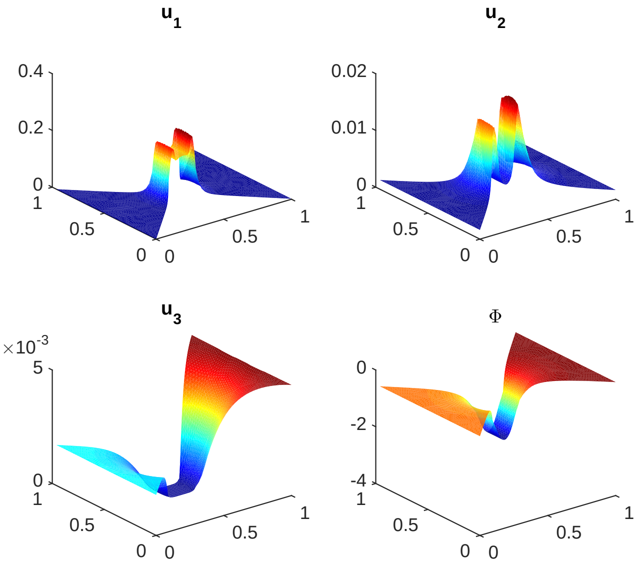
Confined Oxygen $O^{-1/2}$ ions inside the channel contribute to

- permanent charge density $f = -u_O/2$
- sum of concentrations $u_0 = 1 - u_1 - u_2 - u_3 - u_O$

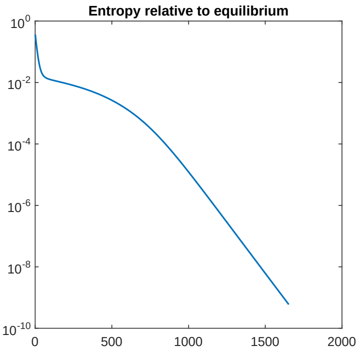
Solution after few time steps

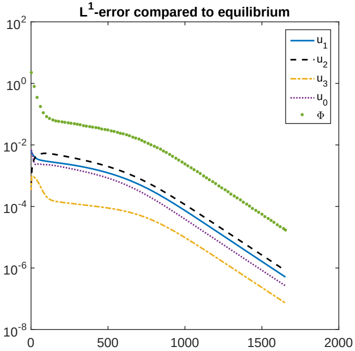


Solution close to equilibrium



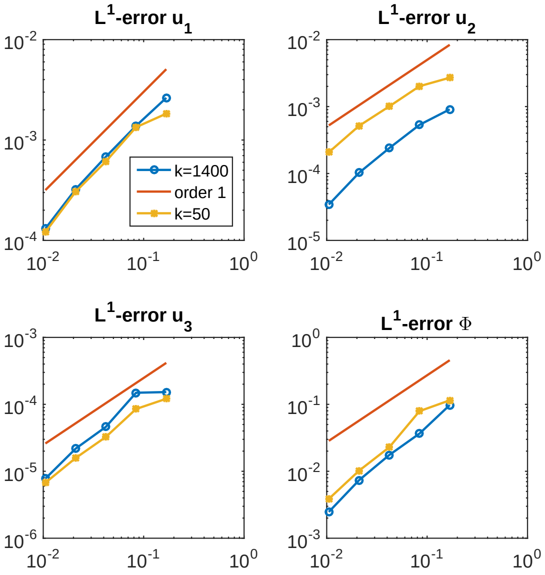
Long-time Behaviour





Observation: Exponential decay of the relative entropy and exponential convergence of solution to equilibrium

Convergence in Space



Thank you for your attention!