Cross-diffusion systems coupled by a moving interface

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Outline of the talk

Motivations

Multispecies and multiphasic diffusion models with moving interfaces to model:

- thin-film vapor deposition (solar cells)

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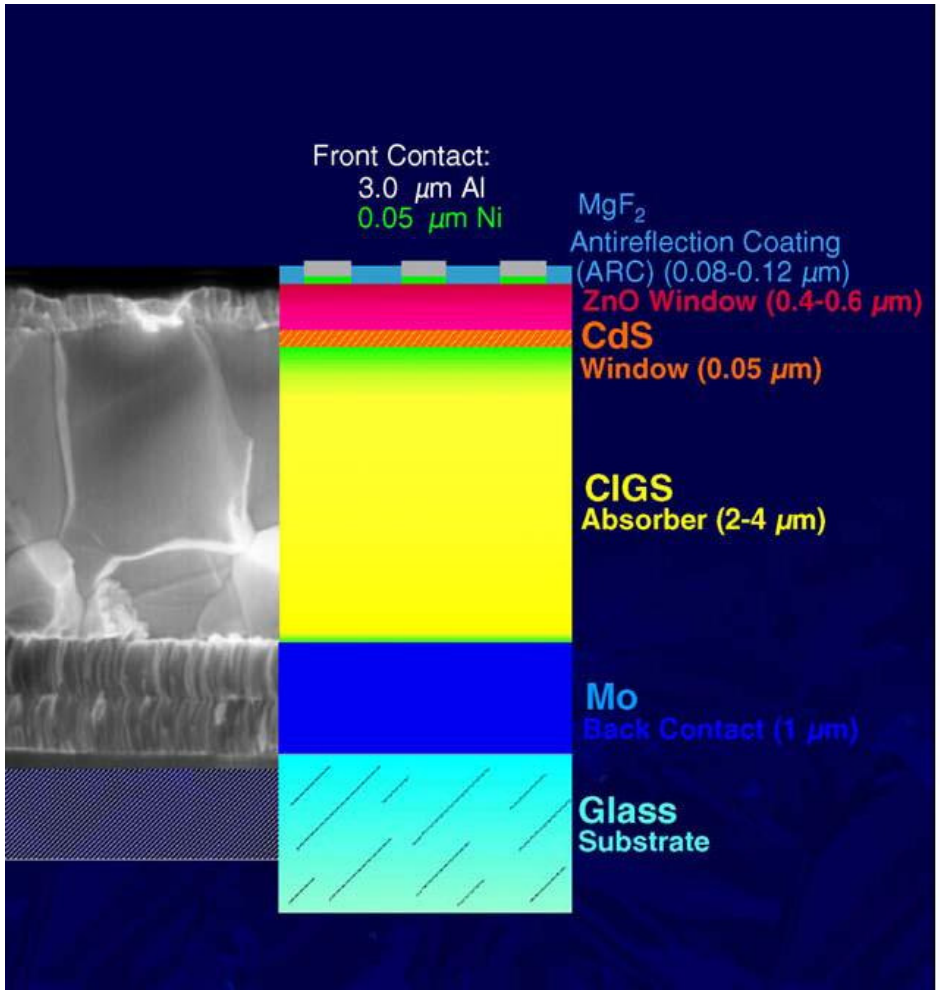
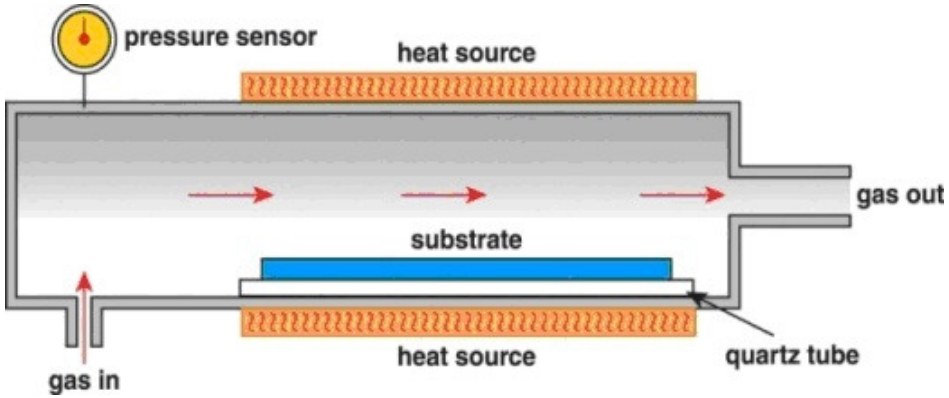
- thin-film vapor deposition (solar cells)
- corrosion (nuclear waste storing)

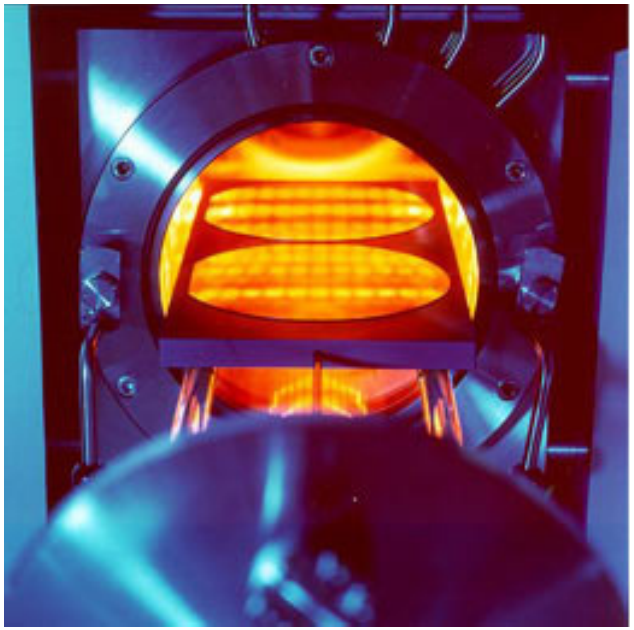
- concrete carbonation (structure engineering)...

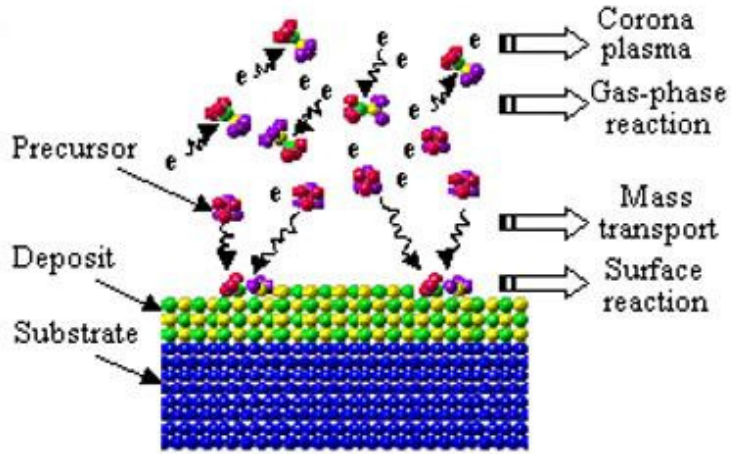
Thin film solar cell



Production process: Physical Vapor Decomposition (PVD)







Modelisation

One has to take into account:

- the cross-diffusion phenomena occuring inside the solid phase and inside the gaseous phase between the different chemical species;
- the evolution of the boundary between the two phases.

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General form of a diffusion system:

$$\partial_t u_i - \operatorname{div}(J_i) = 0, \quad u_i(t=0,\cdot) = u_i^0, \quad 1 \leqslant i \leqslant n$$

with no-flux boundary conditions on $\partial\Omega$, and $J_i(t,x) \in \mathbb{R}^d$ the flux of the i^{th} species at point x and time $t > 0$. $\Rightarrow$ **mass preservation for each chemical species**

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Fick's law is not always valid and in general J_i may depend on $\nabla u_1, \cdots, \nabla u_n$ in multicomponent systems.

Cross-diffusion systems

In general,

$$\forall 1 \leqslant i \leqslant n, \quad J_i = \sum_{j=1}^{n} A_{ij}(u) \nabla u_j, \tag{1}$$

where $A_{ij} : \mathbb{R}^n \to \mathbb{R}$ is a smooth function for all $1 \leqslant i, j \leqslant n$.

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Equations (1) can be rewritten in a more condensed form using the notation

$$u = (u_1, \cdots, u_n), \quad J = (J_1, \cdots, J_n)$$

as

$$J = A(u) \nabla u$$

where for all $u \in \mathbb{R}^n$, $A(u) = \left(A_{ij}(u)\right)_{1 \leqslant i,j \leqslant n} \in \mathbb{R}^{n \times n}$ is called the diffusion matrix of the system.

General form of a cross-diffusion system:

$$\partial_t u - \operatorname{div}\left(A(u) \nabla u\right) = 0, \quad u(t = 0, \cdot) = u^0 = (u_1^0, \cdots, u_n^0)$$

Cross-diffusion systems as hydrodynamic limits

Hydrodynamic limits of microscopic and mesoscopic models lead to cross-diffusion systems with non-diagonal diffusion matrices:

- Markov chains on discrete state space: Quastel 1991; Erignoux 2018; ...
- Continuous stochastic differential equations: Chen, Daus, Jüngel 2019; ...
- Kinetic equations: Boudin, Grec, Salvarini, 2015; Boudin, Grec, Pavant, 2017; Bondesant, Briant, 2019; ...

Cross-diffusion systems with entropic structure

$$\partial_t u - \operatorname{div}\left(A(u)\nabla u\right) = 0$$

We focus in the talk on a particular type of cross-diffusion systems which satisfy specific properties

- **Volumic constraints:** $\forall 1 \leqslant i \leqslant n, \quad u_i(t,x) \geqslant 0 \quad$ and $\quad \sum_{i=1}^n u_i(t,x) = 1$

  i.e. $u(t,x) \in \mathcal{A} := \left\{u \in {\mathbb{R}_+}^n : \sum_{i=1}^n u_i = 1\right\}$.

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- **Entropic structure**

More precisely, we consider here cross-diffusion systems such that there exists an entropy functional which is a Lyapunov function for the system (key ingredient in order to establish the existence of solutions).

In general, such an entropy functional reads as $\mathcal{H}(u) = \int_\Omega h(u)$ for some convex function $h : \mathcal{A} \to \mathbb{R}$ such that $D^2h(u)A(u)$ is a positive semi-definite matrix

$$\begin{aligned}\frac{d}{dt}\mathcal{H}(u) = \frac{d}{dt}\int_\Omega h(u) = \int_\Omega Dh(u)\cdot\partial_t u = -\int_\Omega \nabla Dh(u)\cdot A(u)\nabla u \\ = -\int_\Omega \nabla u \cdot D^2h(u)A(u)\nabla u \leqslant 0.\end{aligned}$$

Cross-diffusion systems with entropic structure

Denoting by $M(u) := A(u)(D^2h(u))^{-1}$ the mobility matrix, then the cross-diffusion system formally reads as

$$\partial_t u - \operatorname{div}(M(u)\nabla Dh(u)) = 0$$

and it formally holds that

$$\begin{aligned}\frac{d}{dt}\mathcal{H}(u) = \frac{d}{dt}\int_\Omega h(u) = \int_\Omega Dh(u)\cdot\partial_t u &= -\int_\Omega \nabla Dh(u)\cdot A(u)\nabla u \\ &= -\int_\Omega \nabla u\cdot D^2h(u)A(u)\nabla u \\ &= -\int_\Omega \nabla Dh(u)\cdot M(u)\nabla Dh(u) \leqslant 0.\end{aligned}$$

Global existence results obtained using the so-called boundedness by entropy principle, first introduced in [Burger, Di Francesco, Pietschmann, Schlake (2010)], and then further developped in [Jüngel (2015)].

Example 1: model for the solid phase

Model for solid phase: Cross-diffusion equations formally derived from a stochastic hopping model on a network: for $1 \leqslant i \leqslant n$,

$$\partial_t u_i - \operatorname{div}\left(\sum_{j=1}^{n} c_{ij}^s \left(u_j \nabla u_i - u_i \nabla u_j\right)\right) = 0$$

for some coefficients $c_{ij}^s = c_{ji}^s > 0$.

$$J_i = \sum_{j=1}^{n} c_{ij}^s \left(u_j \nabla u_i - u_i \nabla u_j\right) \qquad \text{i.e.} \qquad J = A_s(u)\nabla u$$

Gradient flow structure: $h(u) = \sum_{i=1}^n u_i \log u_i$

Important remarks:

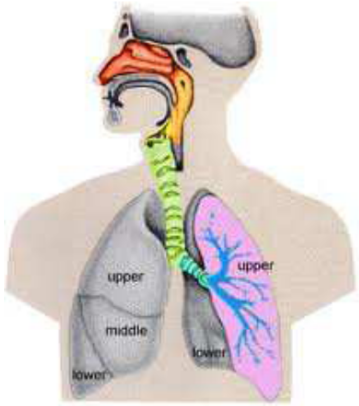
- When $c_{ij}^s = c$ for all $1 \leqslant i \neq j \leqslant n$, the system boils down to a system of decoupled heat equations:

$$\partial_t u_i - c\Delta u_i = 0$$

- $\sum_{i=1}^n J_i = 0$

Example 2: the Stefan-Maxwell system

- Proposed by Maxwell 1866/Stefan 1871.
- Models the evolution of a gas mixture in non dilute regime
- Duncan-Toor 1962: Comparison between the Stefan-Maxwell model and experimental measurements for a system composed of hydrogen, nitrogen and carbon dioxide.
- Boudin, Grec, Salvarini, 2015: derivation from the Boltzmann equation for simple mixtures.
- Application: Patients with airways obstruction inhale Heliox to speed up diffusion



The Stefan-Maxwell system

The Stefan-Maxwell system reads, together with appropriate initial and no-flux boundary conditions,

$$\begin{cases} \partial_t u_i - \operatorname{div}(J_i) = 0, \\ \nabla u_i + \sum_{j=1}^n B_{ij}(u) J_j = 0, \\ \sum_{i=1}^n J_i = 0 \end{cases}$$

where

$$\forall 1 \leqslant i \neq j \leqslant n, \quad B_{ij}(u) = -c_{ij}^g u_i, \quad B_{ii}(u) = \sum_{1 \leqslant j \neq i \leqslant n} c_{ij}^g u_j$$

with

$$c_{ij}^g = c_{ji}^g > 0.$$

Notation: $\langle u, v \rangle := \sum_{i=1}^n u_i v_i$ for all $u := (u_i)_{1 \leqslant i \leqslant n}, v := (v_i)_{1 \leqslant i \leqslant n} \in \mathbb{R}^n$.

Condensed form:

$$\begin{cases} \partial_t u - \operatorname{div}(J) = 0, \\ \nabla u + B(u) J = 0, \\ \langle 1, J \rangle = 0 \end{cases} \tag{2}$$

where $1 = (1, \cdots, 1)$.

Properties of the matrix $B(u)$

Giovangigli, 1999; Bothe, 2011; Boudin, Grec, Salvarani, 2012; Jüngel, Steltzer, 2013...

$$\mathcal{A} := \left\{ u := (u_i)_{1 \leqslant i \leqslant n} \in \mathbb{R}_+^n, \quad \sum_{i=1}^n u_i = \langle 1, u \rangle = 1 \right\}$$

$$\mathcal{V} := \left\{ v := (v_i)_{1 \leqslant i \leqslant n} \in \mathbb{R}^n, \quad \sum_{i=1}^n v_i = \langle 1, v \rangle = 0 \right\}$$

Lemma (Jüngel, Steltzer, 2013)

Let $u \in (\mathbb{R}_+^*)^n \cap \mathcal{A}$. Then, it holds that

$$\textit{Span } B(u) = \mathcal{V} \quad \textit{and} \quad \textit{Ker } B(u) = \textit{Span}\{u\}.$$

Properties of the matrix $B(u)$

Consequence: Thus, for any $u \in (\mathbb{R}_+^*)^n \cap \mathcal{A}$, for any vector $z \in \mathcal{V}$ and any vector $y \in \mathbb{R}^n$ such that $\langle y, u \rangle \neq 0$, there exists a unique solution $x \in \mathbb{R}^n$ solution to

$$B(u)x = z \quad \text{and } \langle y, x \rangle = 0.$$

Assume now that there exists a solution (u, J) to (2) such that $u(t,x) \in (\mathbb{R}_+^*)^n \cap \mathcal{A}$ for almost all $t > 0$ and $x \in \Omega$. Then, $\nabla u(t,x) \in \mathcal{V}^d$ since

$$\sum_{i=1}^n u_i = 1 \text{ a.e. implies that } \sum_{i=1}^n \nabla u_i = 0 \text{ a.e.}$$

Besides, $\langle 1, u \rangle = 1 \neq 0$ a.e. Then, a.e., there exists a unique solution $J(t,x) \in \mathbb{R}^{n \times d}$ such that, a.e.

$$\begin{cases} B(u)J + \nabla u = 0, \\ \langle 1, J \rangle = 0, \end{cases}$$

and there exists a matrix field $A_g : (\mathbb{R}_+^*)^n \cap \mathcal{A} \to \mathbb{R}^{n \times n}$ such that

$$J = A_g(u)\nabla u.$$

Gradient flow structure: $h(u) = \sum_{i=1}^n u_i \log u_i$

Weak solution for the solid/Stefan-Maxwell system

Let $T > 0$ be some final time and $Q_T := (0, T) \times \Omega$.

Definition (Weak solution)

A weak solution (u, J) to the the solid/Stefan-Maxwell system, corresponding to the initial profile $u^0 \in L^\infty(\Omega; \mathcal{A})$, with no-flux boundary conditions, is a pair (u, J) such that $u \in L^\infty(Q_T; \mathcal{A}) \cap L^2((0, T); H^1(\Omega)^n)$, $\nabla\sqrt{u} \in L^2(Q_T)^{n\times d}$, $J \in L^2(Q_T; \mathcal{V}^d)$ satisfies

$$J = A_s(u)\nabla u \quad \text{or} \quad B(u)J + \nabla u = 0 \text{ a.e. in } Q_T$$

and such that for all $\phi := (\phi_i)_{1\leqslant i\leqslant n} \in \mathcal{C}_c^\infty([0, T) \times \overline{\Omega})^n$,

$$-\int\int_{Q_T} \langle u, \partial_t\phi\rangle + \int_\Omega \langle u^0, \phi(0, \cdot)\rangle + \int\int_{Q_T} \sum_{i=1}^n J_i \cdot \nabla\phi_i = 0.$$

Theorem (Jüngel, Steltzer, 2013, Jüngel, 2015)

There exists at least one weak solution to (2) in the sense of the previous definition.

Entropy dissipation for the solid/Stefan-Maxwell system

For both systems,

$$h(u) = \sum_{i=1}^{n} u_i \log u_i$$

Let $c^* := \min_{1 \leqslant i \neq j \leqslant n} c_{ij} > 0$, $\overline{c}_{ij} = c_{ij} - c^* \geqslant 0$ and $\overline{c} := \max_{1 \leqslant i \neq j \leqslant n} \overline{c}_{ij}$.

Then, the following inequality holds for all u solution to the solid/Stefan-Maxell system

$$\frac{d}{dt}\mathcal{H}(u) \leqslant -\frac{1}{2}\alpha \sum_{i=1}^{n} \int_\Omega |\nabla \sqrt{u_i}|^2 - \frac{1}{2} c^* \int_\Omega |J|^2 \leqslant 0, \tag{3}$$

with

$$\alpha = \alpha(c^*, \overline{c}) > 0.$$

This inequality enables to obtain bounds on

$$\int\int_{Q_T} |\nabla \sqrt{u_i}|^2 \quad \text{and} \quad \int\int_{Q_T} |J|^2$$

Numerical scheme for the solid/Stefan-Maxwell system: wishlist

- the non-negativity of the volumic fractions;
- the conservation of mass

$$\int_\Omega u_i(t) = \int_\Omega u_i^0 = m_i^0, \quad \forall 1 \leqslant i \leqslant n.$$

- the preservation of the volume-filling constraint

$$u_i \geqslant 0 \quad \text{and} \quad \sum_{i=1}^{n} u_i = 1 \text{ a.e.}$$

- the entropy dissipation relation (3) (or a discrete version of it).

Numerical schemes for the solid/Stefan-Maxwell system: literature

Burger, Cancès, Carillo, Chainais-Hillaret, Daus, Filbet, Guichard, Jüngel, Perugia, Pietschamnn, Schmidtchen...

In the particular case of the Stefan-Maxell system,

- Boudin, Grec, Salvarani, 2012: ternary system, dimension 1
- Jüngel, Leingang, 2019: finite element approximation

Here, we use finite volume schemes based on two-point flux approximation:

- solid phase [Cancès, Gaudeul, 2020]
- Stefan-Maxwell [Cancès, Ehrlacher, Monasse, 2024]

Focus on the Stefan-Maxwell case: fundamental remark for the scheme

For all $u \in \mathbb{R}^n_+$, it holds that

$$B(u) = c^* \langle 1, u \rangle I + c^* C(u) + \overline{B}(u)$$

where, for all $1 \leqslant i, j \leqslant n$,

$$c_{ij}(u) = u_i, \quad \overline{B}_{ii}(u) = \sum_{1 \leqslant i \neq j \leqslant n} \overline{c}_{ij} u_j, \quad \overline{B}_{ij}(u) = -\overline{c}_{ij} u_i \ i \neq j$$

The matrix $\overline{B}$ has the same expression as B except that the coefficients c_{ij} are replaced by $\overline{c}_{ij}$.

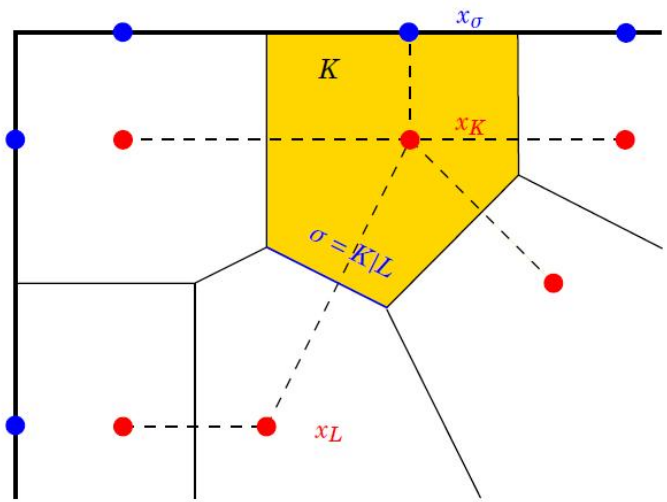
In particular, if $u \in \mathcal{A}$, $B(u) = c^* I + c^* C(u) + \overline{B}(u)$. Moreover, for all $J \in \mathcal{V}$, $C(u)J = 0$. Thus,

$$\boxed{B(u)J = c^* J + \overline{B}(u)J}$$

Admissible mesh with orthogonality property

$\mathcal{T}$: set of cells $\mathcal{E}$: set of faces (or edges) $(x_K)_{K\in\mathcal{T}}$: set of cell centers

Assumption: orthogonality property



Time discretization

Let $\Delta t > 0$, $t_p = p\Delta t$ for all $p \in \mathbb{N}$ and $P_T \in \mathbb{N}^*$ such that $t_{P_T} = P_T \Delta = T$.

The numerical method is an iterative scheme, where for all $p \in \mathbb{N}^*$, a discrete solution

$$\boldsymbol{u}^p := (\boldsymbol{u}_i^p)_{1 \leqslant i \leqslant n} \in \left(\mathbb{R}^{\mathcal{T}}\right)^n,$$

so that $\boldsymbol{u}_i^p = \left(u_{i,K}^p\right)_{K \in \mathcal{T}} \in \mathbb{R}^{\mathcal{T}}$ with

$$u_{i,K}^p \text{ an approximation of the function } u_i \text{ at time } t_p \text{ in the cell } K,$$

will be computed given the value of the discrete solution at the previous time step $\boldsymbol{u}^{p-1}$.

Let $\boldsymbol{u}^0 = (\boldsymbol{u}_i^0)_{1 \leqslant i \leqslant n} \in \left(\mathbb{R}^{\mathcal{T}}\right)^n$ be a discretized initial condition.

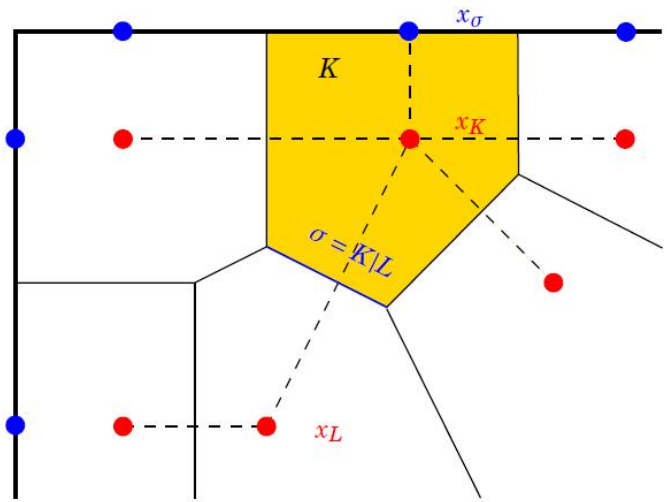
Notation

- For all $K \in \mathcal{T}$, $m_K = |K|$ the Lebesgue measure of the cell K;
- For all $\sigma \in \mathcal{E}$, $m_\sigma = \mathcal{H}^{d-1}(\sigma)$ the $d-1$-dimensional Hausdorff measure of the face σ,

$$d_\sigma := \begin{cases} |x_K - x_L| & \text{if } \sigma = K|L \text{ is an interior face;} \\ d(x_K, \sigma) & \text{if } \sigma \in \mathcal{E}_K \text{ is an exterior face,} \end{cases}$$

and

$$\tau_\sigma = \frac{m_\sigma}{d_\sigma}$$



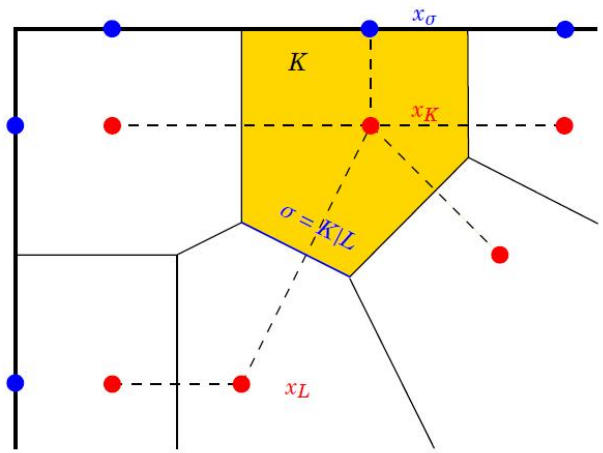
Notation

For all $\boldsymbol{v} = (v_K)_{K\in\mathcal{T}} \in \mathbb{R}^{\mathcal{T}}$, for all $K \in \mathcal{T}$ and all $\sigma \in \mathcal{E}_K$, we denote by $v_{K\sigma}$ the mirror value of v_K across σ, i.e.

$$v_{K\sigma} = \begin{cases} v_L & \text{if } \sigma = K|L \text{ for some } L \in \mathcal{T}, \\ v_K & \text{if } \sigma \text{ is an exterior face,} \end{cases}$$

The oriented jump of $\boldsymbol{v}$ across σ is defined by

$$D_{K\sigma}\boldsymbol{v} := v_{K\sigma} - v_K$$



Finally, $v_{\sigma,\log}$ denotes the logarithmic mean between v_K and $v_{K\sigma}$, i.e.

$$v_{\sigma,\log} := \begin{cases} 0 & \text{if } \min(v_K, v_{K\sigma}) \leqslant 0, \\ v_K & \text{if } v_K = v_{K\sigma} \geqslant 0, \\ \frac{v_K - v_{K\sigma}}{\log(v_K) - \log(v_{K\sigma})} & \text{otherwise.} \end{cases}$$

Numerical scheme

For all $K \in \mathcal{T}$ and all $1 \leqslant i \leqslant n$,

$$m_K \frac{u_{i,K}^p - u_{i,K}^{p-1}}{\Delta t} + \sum_{\sigma \in \mathcal{E}_K} m_\sigma J_{i,K\sigma}^p = 0, \tag{4}$$

where for all $\sigma \in \mathcal{E}_K$, $J_{K\sigma}^p = \left(J_{i,K\sigma}^p\right)_{1 \leqslant i \leqslant n} \in \mathbb{R}^n$ is computed as follows:

- if $\sigma = K|L$ is an interior face,

$$\frac{1}{d_\sigma} D_{K\sigma} \boldsymbol{u}_i^p + c^* J_{i,K\sigma}^p + \sum_{1 \leqslant j \leqslant n} \overline{B}_{ij}(u_{\sigma,\log}^p) J_{j,K\sigma}^p = 0, \quad \forall 1 \leqslant i \leqslant n, \tag{5}$$

  where $u_{\sigma,\log}^p = \left(u_{i,\sigma,\log}^p\right)_{1 \leqslant i \leqslant n}$, and

$$J_{L\sigma} = -J_{K\sigma} \tag{6}$$

- if σ is an exterior face,

$$J_{K\sigma}^p = 0. \tag{7}$$

Properties of the scheme

Solid phase: [Cancès, Gaudeul, 2020]

Theorem (Cancès, VE, Monasse, 2024)

Let $(\mathcal{T}, \mathcal{E}, (x_K)_{K\in\mathcal{T}})$ be an admissible mesh of Ω and let $\boldsymbol{u}^0$ be an initial condition such that $\boldsymbol{u}^0 \in \mathcal{A}^{\mathcal{T}}$. Then, for all $p \in \mathbb{N}^*$, the nonlinear system of equations (4)-(5)-(6)-(7) has at least a (strictly) positive solution $\boldsymbol{u}^p \in \mathcal{A}^{\mathcal{T}}$. This solution satisfies

$$\sum_{K\in\mathcal{T}} u_{i,K}^p = \sum_{K\in\mathcal{T}} u_{i,K}^0.$$

In addition, the corresponding fluxes $\boldsymbol{J}^p = \left(J_{K\sigma}^p\right)_{\sigma\in\mathcal{E}}$ are uniquely determined by (5)-(6)-(7) and belong to $\mathcal{V}^{\mathcal{E}}$, i.e.

$$\forall K \in \mathcal{T},\ \forall \sigma \in \mathcal{E}_K, \quad \sum_{i=1}^n J_{i,K\sigma}^p = 0.$$

Moreover, the following discrete entropy dissipation estimate holds

$$E_{\mathcal{T}}(\boldsymbol{u}^p) + \Delta t \sum_{\sigma=K|L\in\mathcal{E}_{int}} \left(\frac{c^*}{2} m_\sigma d_\sigma |J_{K\sigma}^p|^2 + \frac{\alpha}{2}\tau_\sigma |D_{K\sigma}\sqrt{\boldsymbol{u}^p}|^2 \right) \leqslant E_{\mathcal{T}}(\boldsymbol{u}^{p-1})$$

where the discrete entropy functional is defined as

$$E_{\mathcal{T}}(\boldsymbol{u}) = \sum_{K\in\mathcal{T}} \sum_{i=1}^n m_K u_{i,K} \log(u_{i,K}), \quad \forall \boldsymbol{u} = (\boldsymbol{u}_i)_{1\leqslant i\leqslant n} \in \mathcal{A}^{\mathcal{T}}.$$

Convergence of the scheme

Let $\left(\mathcal{T}_m, \mathcal{E}_m, (x_K^m)_{K\in\mathcal{T}_m}\right)_{m\in\mathbb{N}}$ be a sequence of admissible meshes such that

$$h_{\mathcal{T}_m} := \max_{K\in\mathcal{T}_m} \operatorname{diam}(K) \underset{m\to+\infty}{\longrightarrow} 0$$

and

$$\zeta_{\mathcal{T}_m} := \min_{K\in\mathcal{T}_m} \min_{\sigma\in\mathcal{E}_K} \frac{d(x_K,\sigma)}{d_\sigma} \geqslant \eta, \quad \forall m \in \mathbb{N},$$

for some $\eta > 0$ independent of m.

Let $(\Delta t_m)_{m\in\mathbb{N}}$ be a sequence of positive time steps such that $\Delta t_m \underset{m\to+\infty}{\longrightarrow} 0$.

Solid phase: [Cancès, Gaudeul, 2020]

Theorem (Cancès, VE, Monasse, 2024)

There exist $u \in L^\infty(Q_T;\mathcal{A}) \cap L^2((0,T);H^1(\Omega)^n)$ with $\sqrt{u} \in L^2((0,T);H^1(\Omega)^n)$ and $J \in L^2(Q_T,\mathcal{V}^d)$ such that, up to the extraction of a subsequence,

$$u_{\mathcal{T}_m,\Delta t_m} = (u_{i,\mathcal{T}_m,\Delta t_m})_{1\leqslant i\leqslant n} \underset{m\to+\infty}{\longrightarrow} u \text{ a.e. in } Q_T,$$

$$J_{\mathcal{E}_m,\Delta t_m} = \left(J_{i,\mathcal{E}_m,\Delta t_m}\right)_{1\leqslant i\leqslant n} \underset{m\to+\infty}{\longrightarrow} J \text{ weakly in } L^2(Q_T)^{n\times d}.$$

Besides, (u,J) is a weak solution of the Stefan-Maxwell problem.

See also [Jüngel, Zurek, 2022]

Outline of the talk

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- $\alpha = s, g$ index refering to the solid (s) or gaseous (g) phase
- for $1 \leqslant i \leqslant n$, $u_i(t,x) = u_i^s(t,x)$: local volumic fraction of the chemical species i at time t and point $0 < x < X(t)$ in the solid phase;
- for $1 \leqslant i \leqslant n$, $u_i(t,x) = u_i^g(t,x)$: local volumic fraction of the chemical species i at time t and point $X(t) < x < 1$ in the gaseous phase;

A toy model

For any function $f : \Omega \to \mathbb{R}^n$ regular enough on $(0, X(t))$ and $(X(t), 1)$:

$$f^s := f(X(t)^-),\ f^g(t) = f(X(t)^+),\ [\![f]\!] = f^s - f^g$$

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Coupled cross-diffusion system:

$$\begin{aligned} \partial_t u - \partial_x J = 0, \quad & x \in \Omega, \\ J = A_s(u)\partial_x u, \ & x \in (0, X(t)), \\ J = A_g(u)\partial_x u, \ & x \in (X(t), 1). \end{aligned}$$

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Zero-flux conditions on the fixed boundary $\boldsymbol{J}(t,0) = \boldsymbol{J}(t,1) = 0$ and at the interface, if $X(t) \in (0,1)$,

$$J^s(t) + X'(t)u^s(t) = J^g(t) + X'(t)u^g(t) = F(t).$$

F accounts for the flux of chemical species from one phase to the other. We assume it to be of Butler-Volmer type: for $i \in \{1, \dots, n\}$, $\mu_i^{*,s}, \mu_i^{*,g} \in \mathbb{R}$,

$$F_i = u_i^s \exp(\frac{1}{2}[\![\mu_i^*]\!]) - u_i^g \exp(-\frac{1}{2}[\![\mu_i^*]\!]).$$

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Interface evolution: $X'(t) = -\sum_{i=1}^n F_i(t)$.

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- Total mass conservation for each species because at the interface $[\![J(t)]\!] + X'(t)[\![u(t)]\!] = 0$.

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$$\mathcal{H}(u, X) = \int_0^X h_s(u) + \int_X^1 h_g(u),$$

with, for $\alpha \in \{s, g\}$,

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- Dissipation equality:

$$\frac{d}{dt}\mathcal{H}(u(t), X(t)) + \int_0^{X(t)} \partial_x \log(u(t))^T \boldsymbol{M}_s(u(t))\partial_x \log(u(t)) + \int_{X(t)}^1 \partial_x \log(u(t))^T \boldsymbol{M}_g(u(t))\partial_x \log(u(t)) - F(t)^T[\![\mu(t)]\!] = 0.$$

M_s, M_g are positive semi-definite mobility matrices.

Properties of the model II

Reformulation of the Butler-Volmer fluxes: for $i \in \{1, \dots, n\}$,

$$F_i = u_i^s \exp(\frac{1}{2}[\![\mu_i^*]\!]) - u_i^g \exp(-\frac{1}{2}[\![\mu_i^*]\!]) = 2\sqrt{u_i^s u_i^g} \sinh\left(-\frac{1}{2}[\![\mu_i(t)]\!]\right),$$

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Stationary solutions $(\overline{u}, \overline{X})$ must be constant in each connected part of $\overline{\Omega} := (0, \overline{X}) \cup (\overline{X}, 1)$.

Proposition (Stationary states)

In addition to the trivial pure phase solutions, there exists a non-trivial stationary solution $(\overline{u}^s, \overline{u}^g, \overline{X}) \in \mathcal{A} \times \mathcal{A} \times (0,1)$ *if and only if*

$$\min\left(\sum_{i=1}^n m_i^0 \exp\left([\![\mu_i^*]\!]\right), \sum_{i=1}^n m_i^0 \exp\left(-[\![\mu_i^*]\!]\right)\right) > 1.$$

Moreover, under the latter assumption, this stationary state is unique.

Discretization

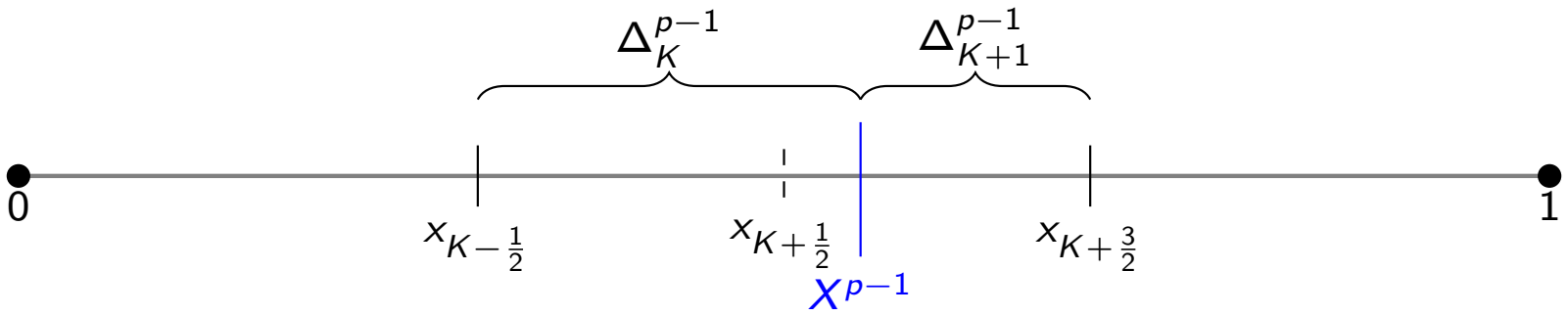

Figure: Mesh deformation at time $t^{p-1} = (p-1)\Delta t$ where $K := K^{p-1}$ is the interface cell.

- Background mesh: $N \in \mathbb{N}^*$ reference cells of uniform size $\Delta x = \frac{1}{N}$. $N+1$ edge vertices $0 = x_{\frac{1}{2}} \leqslant x_{\frac{3}{2}} \leqslant \cdots \leqslant x_{N+\frac{1}{2}} = 1$, $x_{K+\frac{1}{2}} = K\Delta x$ for all $K \in \{0, \ldots, N\}$. Time horizon $T > 0$ and a time discretization with mesh parameter Δt defined such that $N_T \Delta t = T$ with $N_T \in \mathbb{N}^*$.

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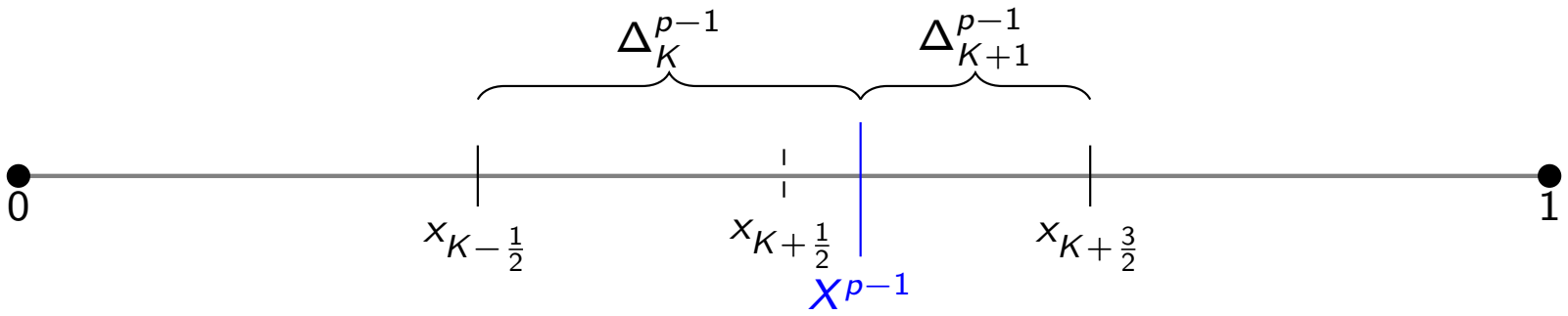

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- Discrete concentrations $\boldsymbol{u}_{\Delta x}^p = (u_{i,K}^p)_{i\in\{1,\ldots,n\},\ K\in\{1,\ldots,N\}}$ for $p \in \{0, \ldots, N_T\}$. Time-discrete interface X^p for $p \in \{0, \ldots, N_T\}$. $K^p \in \{0, \ldots, N\}$ the index of the left interface cell.

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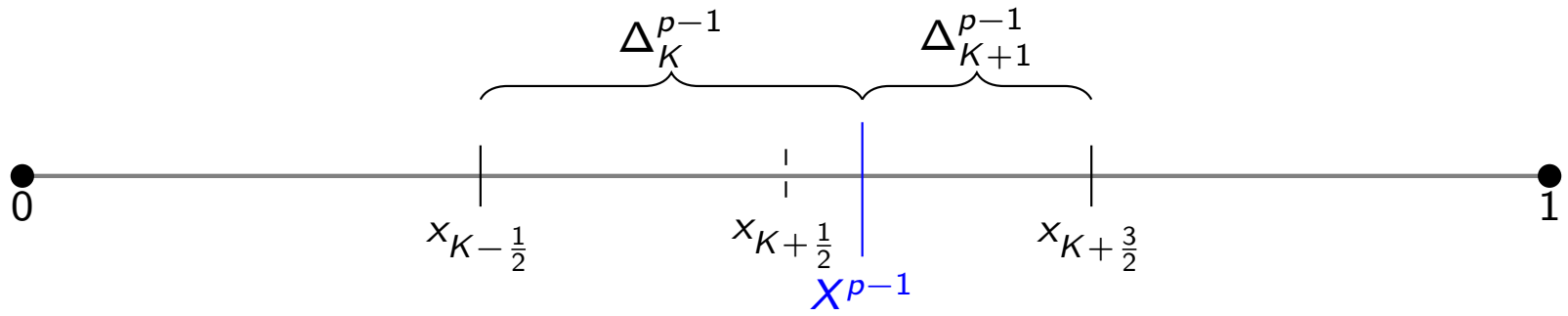

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- The mesh is locally modified around X^{p-1}: for all $K \in \{1, \ldots, N\}$, the size of the K^{th} cell is

$$\Delta_K^{p-1} = \begin{cases} (X^{p-1} - x_{K^{p-1}-\frac{1}{2}}) & \text{if } K = K^{p-1}, \\ (x_{K^{p-1}+\frac{3}{2}} - X^{p-1}) & \text{if } K = K^{p-1}+1, \\ \Delta x & \text{otherwise.} \end{cases}$$

First step: solving the conservation laws

- $(\boldsymbol{u}_{\Delta x}^{p-1}, X^{p-1}) \to (\boldsymbol{u}_{\Delta x}^{p,\star}, X^{p})$: solving the conservation laws and updating the interface.
  Implicit discretization: $K \in \{1, \dots, N\}$, $i \in \{1, \dots, n\}$,

$$\frac{1}{\Delta t}(\Delta_K^{p,\star} u_{i,K}^{p,\star} - \Delta_K^{p-1} u_{i,K}^{p-1}) + J_{i,K+\frac{1}{2}}^{p,\star} - J_{i,K-\frac{1}{2}}^{p,\star} = 0,$$

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- Interface evolution discretized as

$$X^p = X^{p-1} - \Delta t \sum_{i=1}^{n} F_i^{p,\star}.$$

Second step: moving the mesh and post-processing

- When X^p crosses the center of a cell, one needs to update the mesh (change the interface cell from K^{p-1} to K^p) and to post-process the concentrations into the final values $\boldsymbol{u}^p_{\Delta x}$ accordingly.

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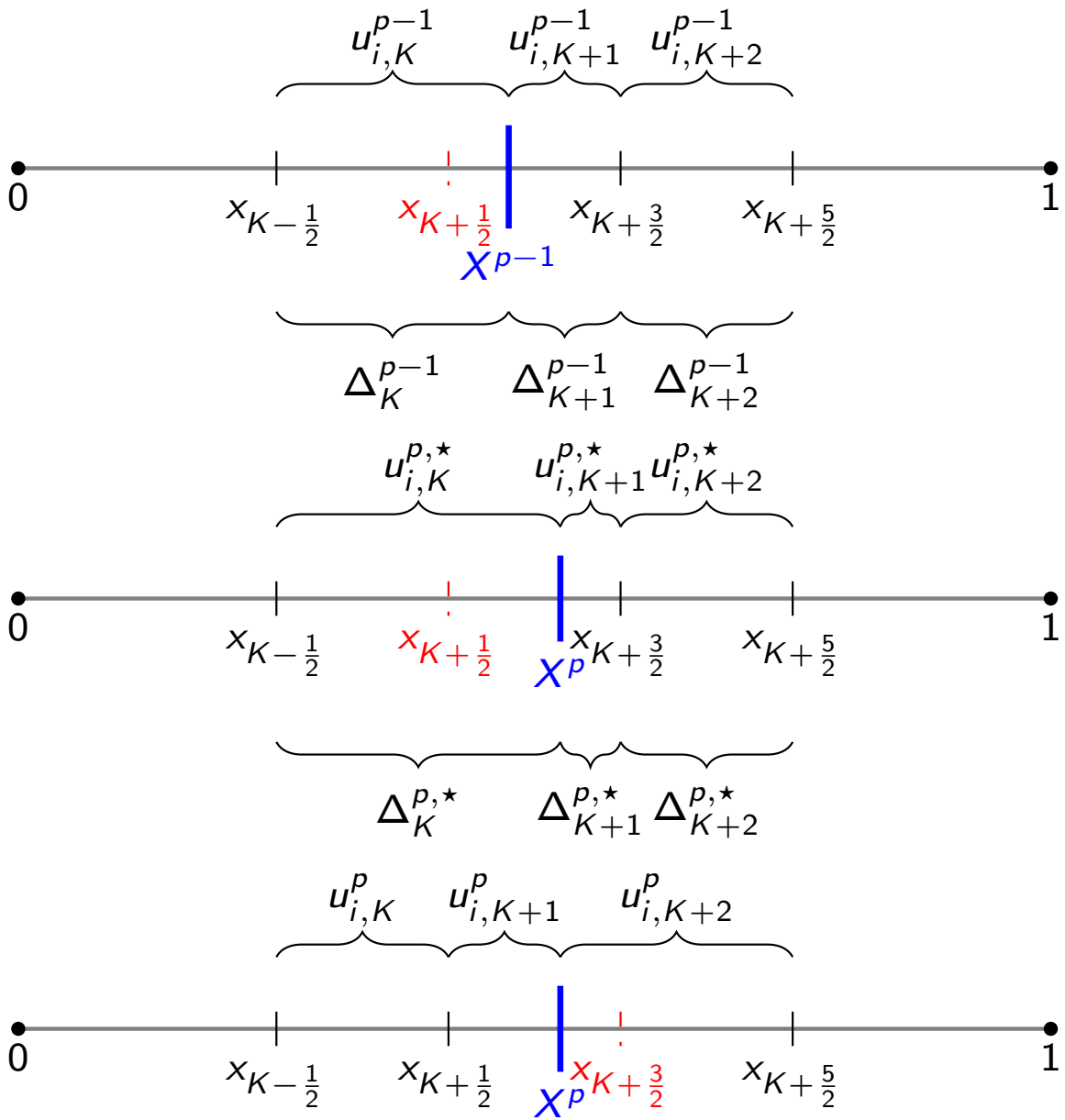
- Otherwise, we project and average the values of $\boldsymbol{u}_{\Delta x}^{p,\star}$ onto the new mesh (dictated by mass conservation). By convexity of the energy functional, these operations decrease the total free energy.

Illustration of the two steps of the scheme



Discrete free energy functional

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Proposition (Structure preservation)

Let $(\boldsymbol{u}^{p-1}_{\Delta x}, X^{p-1})$ *be such that* $\boldsymbol{u}^{p-1}_{\Delta x} \geqslant 0$ *and* $\sum_{i=1}^n u^{p-1}_{i,K} = 1$ *for any* $K \in \{1, \dots, N\}$. *There exists a solution* $(\boldsymbol{u}^p_{\Delta x}, X^p)$ *to the scheme such that it holds*

$$u^p_{i,K} > 0, \ \forall i \in \{1, \dots, n\}, \ \forall K \in \{1, \dots, N\},$$

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$$u^p_{i,K} > 0, \ \forall i \in \{1, \dots, n\}, \ \forall K \in \{1, \dots, N\},$$

$$\sum_{i=1}^{n} u^p_{i,K} = 1, \ \forall K \in \{1, \dots, N\},$$

$$\sum_{K=1}^{N} \Delta^p_K u^p_{i,K} = \sum_{K=1}^{N} \Delta^{p-1}_K u^{p-1}_{i,K}, \ \forall i \in \{1, \dots, n\},$$

$$\mathcal{H}^p(\boldsymbol{u}^p_{\Delta x}, X^p) \leqslant \mathcal{H}^{p-1}(\boldsymbol{u}^{p-1}_{\Delta x}, X^{p-1}).$$

Proof: topological degree argument on a modified scheme (truncations, scalings) to satisfy all the a priori estimates.

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  - **Long-time asymptotics:** relative free energy $\mathcal{H}^p(\boldsymbol{u}_{\Delta x}^p, X^p) - \mathcal{H}^\infty(\boldsymbol{u}^\infty, X^\infty)$ and relative interface $|X^\infty - X^p|$ over time.

Long-time asymptotics

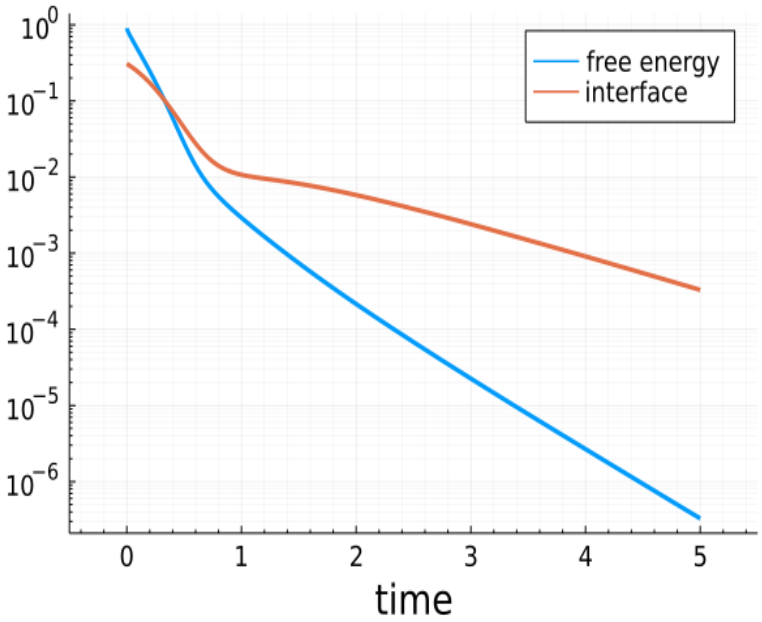

Figure: Equilibrium case.

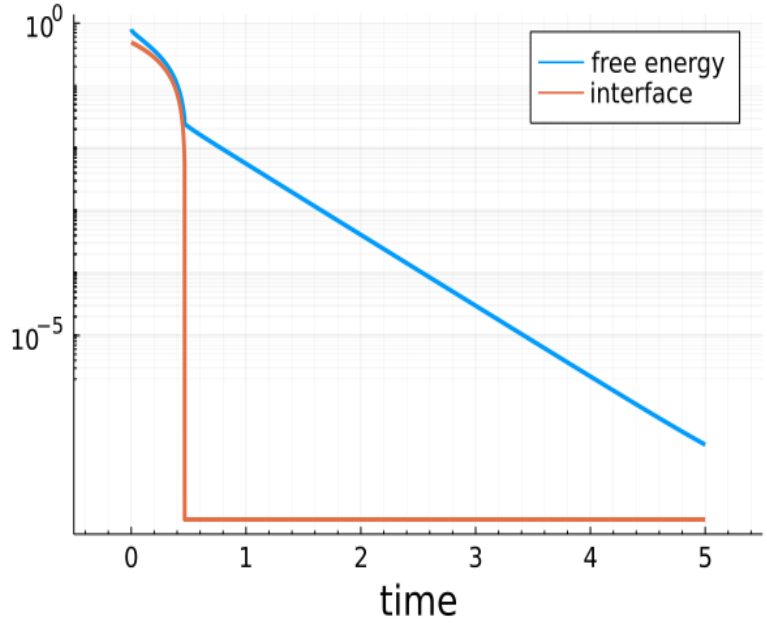

Figure: Non-equilibrium case: convergence to a one-phase stationary state.

Convergence of the scheme

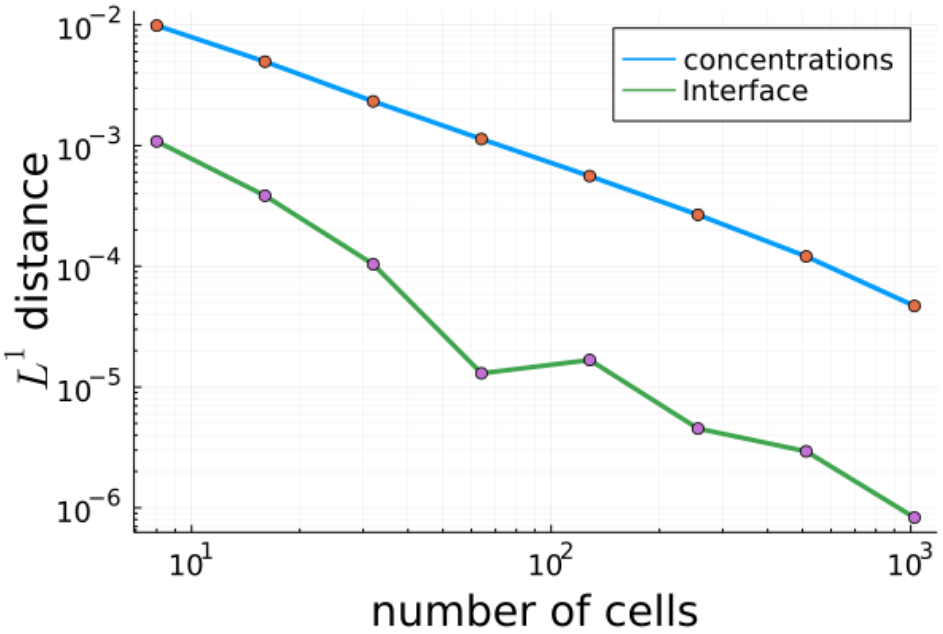

Figure: Convergence analysis of the solution under space grid refinement

Loss of order: first-order accurate on the concentrations in the case of a moving interface, second-order in fixed domains.

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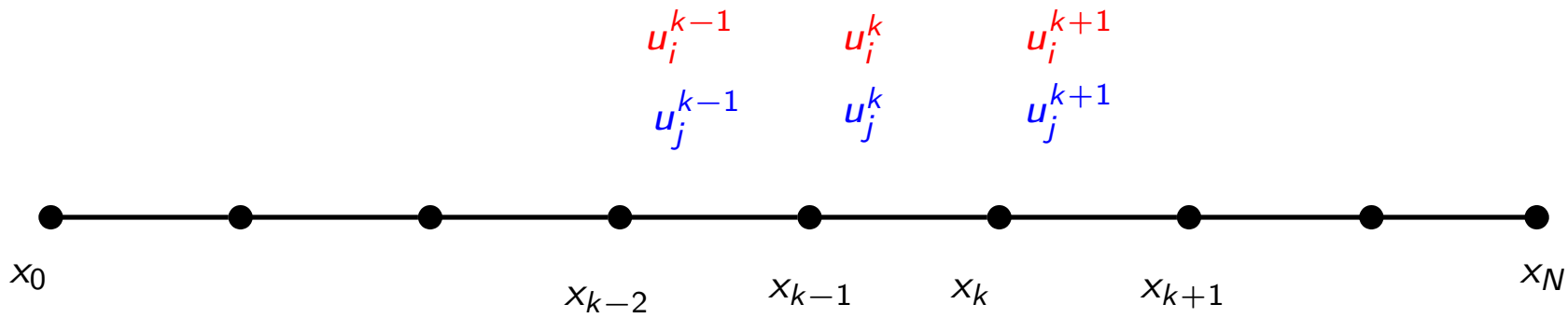
- Generalizations to higher dimension, including geometric effects such as surface diffusion.
- Hybrid finite volume schemes for cross-diffusion ? (remove the orthogonality assumption on the mesh)

Thank you for your attention

Formal (1d) derivation of the model for the cross-diffusion equations inside the solid



Let $\Delta t > 0$. Let $p_{ij} = p_{ji}$ represent the probability that an atom of type i exchange its position in the solid with an atom of type j.

Assume for the moment that $d = 1$, $\Omega = (0, e_0)$ with $e_0 > 0$ and let us introduce a uniform discretization grid $(x_k)_{0 \leqslant k \leqslant N}$ of $(0, e_0)$ defined by $x_k = k\Delta x$ with $\Delta x = \frac{e_0}{N}$ for $N \in \mathbb{N}^*$.

Let us denote by $u_i^k(t)$ the local concentration of atom i in the k^{th} cell (x_{k-1}, x_k).

$$
\begin{aligned}
& u_i^k(t + \Delta t) - u_i^k(t) \\
\approx & \sum_{0 \leqslant j \leqslant n,\ j \neq i} p_{ij}[u_j^k(t)u_i^{k+1}(t) + u_j^k(t)u_i^{k-1}(t) - u_j^{k-1}(t)u_i^k(t) + u_j^{k+1}(t)u_i^k(t)] \\
\approx & \sum_{0 \leqslant j \leqslant n,\ j \neq i} p_{ij}[u_j^k(t)(u_i^{k+1}(t) + u_i^{k-1}(t) - 2u_i^k(t)) - u_i^k(t)(u_j^{k-1} + u_j^{k+1}(t) - 2u_j^k(t))]
\end{aligned}
$$

Formal derivation of the model for the diffusion equations inside the solid

Taking now (for instance) the scaling $\Delta t = 2Q\Delta x^2$ for some constant $Q > 0$ and denoting by $c_{ij}^s := \frac{p_{ij}}{Q}$, we obtain the limit equation

$$\begin{aligned}\partial_t u_i &= \sum_{0\leqslant j\leqslant n,\ j\neq i} c_{ij}^s (u_j \partial_{xx} u_i - u_i \partial_{xx} u_j) \\ &= \partial_x \left[\sum_{0\leqslant j\leqslant n,\ j\neq i} c_{ij}^s \left(u_j \partial_x u_i - u_i \partial_x u_j\right) \right].\end{aligned}$$

Remark: Rigorous hydrodynamic limit of multi-species symmetric exclusion systems [Quastel, 91], [Erignoux, 2018], [Dabaghi, VE, Strössner, 2018]