Structure-preserving reduced basis method for cross-diffusion systems

JAD DABAGHI, Virginie Ehrlacher

École des Ponts ParisTech (CERMICS) & INRIA Paris (MATHERIALS)

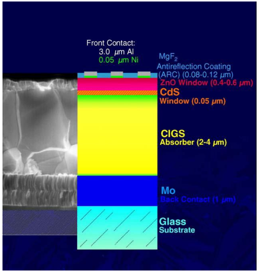
SIAM UQ-22 Conference 12$^{\text{nd}}$ April 2022

Outline

Motivation

Numerical simulation of the PVD process for the fabrication of CIGS (Copper-Indium-Galium-Selenium) solar panels

1. The chemical species are injected under gazeous form in a hot chamber.
2. A cross-diffusion process occurs and the local volumic fraction of the species evolve with respect to time
3. **goal :** optimize the injected flux to obtain high performance solar cells



The numerical simulation of the cross-diffusion system is highly expensive

Need to construct robust schemes to reduce the computational time

Outline

Model Problem

$\Omega \subset \mathbb{R}^2$: polygonal domain, $T > 0$: final simulation time, N_s : number of chemical species.

Cross-diffusion model

$$\partial_t u_i - \nabla \cdot \left(\sum_{j=1}^{N_s} a_{i,j} \left(u_j \nabla u_i - u_i \nabla u_j \right) \right) = 0 \quad \text{in} \quad \Omega \times [0, T], \text{ for } i \in [1, N_s],$$

$$\left(\sum_{j=1}^{N_s} a_{i,j} \left(u_j \nabla u_i - u_i \nabla u_j \right) \right) \cdot \boldsymbol{n} = 0 \quad \text{on} \quad \partial\Omega \times [0, T], \text{ for } i \in [1, N_s],$$

$$u_i(\boldsymbol{x}, 0) = u_i^0(\boldsymbol{x}) \quad \text{in} \quad \Omega, \text{ for } i \in [1, N_s].$$

- Assume $\mathbb{A} \in \mathbb{R}^{N_s,N_s}$, $\mathbb{A} = (a_{i,j})_{1 \le i,j \le N_s}$ is symmetric with nonnegative coefficients and that its diagonal terms vanish.

Gradient flow structure

Entropy functional:

$$E(\boldsymbol{u}) := \int_\Omega \sum_{i=1}^{N_s} u_i(x)\ln(u_i(x))\,\mathrm{d}x \qquad \boldsymbol{u} = (u_i)_{i\in[\![1,N_s]\!]}$$

The cross-diffusion system has a gradient flow structure and can be rewritten as

$$\partial_t \boldsymbol{u} - \boldsymbol{\nabla}\cdot(\mathbb{C}(\boldsymbol{u})\boldsymbol{\nabla} dE(\boldsymbol{u}))$$
$$(\mathbb{C}(\boldsymbol{u})\boldsymbol{\nabla} dE(\boldsymbol{u}))\cdot \boldsymbol{n} = 0$$
$$\boldsymbol{u}(\boldsymbol{x},0) = \boldsymbol{u}^0(\boldsymbol{x}) \quad \text{in} \quad \Omega.$$

- $\mathbb{C}(\boldsymbol{u}) \in \mathbb{R}^{N_s,N_s}$: mobility matrix
- dE: Entropy differential defined by

$$(dE(\boldsymbol{u}))_i := \frac{\partial E(\boldsymbol{u})}{\partial u_i} = 1 + \ln(u_i).$$

Theorem

There exists a weak solution $\mathbf{u}$ satisfying

$$\mathbf{u} \in \left[L^2_{\text{loc}}(\mathbb{R}^+, H^1(\Omega, \mathbb{R}^{N_s}))\right]^{N_s} \quad \text{and} \quad \partial_t \mathbf{u} \in \left[L^2_{\text{loc}}(\mathbb{R}^+, \left[H^1(\Omega, \mathbb{R}^{N_s})\right]')\right]^{N_s}.$$

Theorem

There exists a weak solution $\boldsymbol{u}$ *satisfying*

$$\boldsymbol{u} \in \left[L^2_{\mathrm{loc}}(\mathbb{R}^+, H^1(\Omega, \mathbb{R}^{N_s}))\right]^{N_s} \quad \textit{and} \quad \partial_t \boldsymbol{u} \in \left[L^2_{\mathrm{loc}}(\mathbb{R}^+, \left[H^1(\Omega, \mathbb{R}^{N_s})\right]')\right]^{N_s}.$$

Structural properties of the solution: Consider $\boldsymbol{u}^0 \in L^\infty(\Omega, \mathcal{A})$. Then

Theorem

There exists a weak solution $\boldsymbol{u}$ satisfying

$$\boldsymbol{u} \in \left[L^2_{\text{loc}}(\mathbb{R}^+, H^1(\Omega, \mathbb{R}^{N_s}))\right]^{N_s} \quad \textit{and} \quad \partial_t \boldsymbol{u} \in \left[L^2_{\text{loc}}(\mathbb{R}^+, \left[H^1(\Omega, \mathbb{R}^{N_s})\right]')\right]^{N_s}.$$

Structural properties of the solution: Consider $\boldsymbol{u}^0 \in L^\infty(\Omega, \mathcal{A})$. Then

1. mass conservation: $\int_\Omega u_i(x,t)\,\mathrm{dx} = \int_\Omega {u_i}^0(x)\,\mathrm{dx} \;\; \forall t \in [0, T], \;\; \forall i \in [1, N_s]$.

Theorem

There exists a weak solution $\boldsymbol{u}$ *satisfying*

$$\boldsymbol{u} \in \left[L^2_{\mathrm{loc}}(\mathbb{R}^+, H^1(\Omega, \mathbb{R}^{N_s}))\right]^{N_s} \quad \text{and} \quad \partial_t \boldsymbol{u} \in \left[L^2_{\mathrm{loc}}(\mathbb{R}^+, \left[H^1(\Omega, \mathbb{R}^{N_s})\right]')\right]^{N_s}.$$

Structural properties of the solution: Consider $\boldsymbol{u}^0 \in L^\infty(\Omega, \mathcal{A})$. Then

1. mass conservation: $\int_\Omega u_i(x,t)\,\mathrm{dx} = \int_\Omega {u_i}^0(x)\,\mathrm{dx} \;\; \forall t \in [0,T], \;\; \forall i \in [1, N_s]$.
2. positivity: $u_i(x,t) \geq 0 \quad \forall x \in \Omega, \quad \forall t \in [0,T], \quad \forall i \in [1, N_s]$.

Theorem

There exists a weak solution $\boldsymbol{u}$ satisfying

$$\boldsymbol{u} \in \left[L^2_{\mathrm{loc}}(\mathbb{R}^+, H^1(\Omega, \mathbb{R}^{N_s}))\right]^{N_s} \quad \textit{and} \quad \partial_t \boldsymbol{u} \in \left[L^2_{\mathrm{loc}}(\mathbb{R}^+, \left[H^1(\Omega, \mathbb{R}^{N_s})\right]')\right]^{N_s}.$$

Structural properties of the solution: Consider $\boldsymbol{u}^0 \in L^\infty(\Omega, \mathcal{A})$. Then

1. mass conservation: $\int_\Omega u_i(x,t)\,\mathrm{dx} = \int_\Omega {u_i}^0(x)\,\mathrm{dx} \;\; \forall t \in [0,T], \;\; \forall i \in [1, N_s]$.
2. positivity: $u_i(x,t) \geq 0 \quad \forall x \in \Omega, \quad \forall t \in [0,T], \quad \forall i \in [1, N_s]$.
3. preservation of the volume filling constraint: $\boldsymbol{u} \in \mathbb{R}^{N_s}_+$ such that $\sum_{i=1}^{N_s} = 1$.

Theorem

There exists a weak solution $\boldsymbol{u}$ satisfying

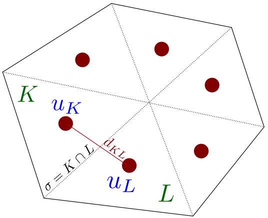
$$\boldsymbol{u} \in \left[L^2_{\mathrm{loc}}(\mathbb{R}^+, H^1(\Omega, \mathbb{R}^{N_s}))\right]^{N_s} \quad \textit{and} \quad \partial_t \boldsymbol{u} \in \left[L^2_{\mathrm{loc}}(\mathbb{R}^+, \left[H^1(\Omega, \mathbb{R}^{N_s})\right]')\right]^{N_s}.$$

Structural properties of the solution: Consider $\boldsymbol{u}^0 \in L^\infty(\Omega, \mathcal{A})$. Then

1. mass conservation: $\displaystyle\int_\Omega u_i(x,t)\,\mathrm{d}x = \int_\Omega {u_i}^0(x)\,\mathrm{d}x \;\; \forall t \in [0,T], \;\forall i \in [1, N_s]$.
2. positivity: $u_i(x,t) \geq 0 \quad \forall x \in \Omega, \quad \forall t \in [0,T], \quad \forall i \in [1, N_s]$.
3. preservation of the volume filling constraint: $\boldsymbol{u} \in \mathbb{R}^{N_s}_+$ such that $\sum_{i=1}^{N_s} = 1$.
4. entropy-entropy dissipation relation

$$\frac{d}{dt}E(\boldsymbol{u}) + \int_\Omega \sum_{1 \leq i < j \leq N} a_{i,j} u_i(x) u_j(x) |\nabla \ln(u_i(x)) - \nabla \ln(u_j(x))|^2 \,\mathrm{d}x = 0.$$

The cell-centered finite Volume method



$D_{K\sigma}\mathbf{u}_i^n = u_{i,L}^n - u_{i,K}^n$

- N_s unknowns per cell $\boldsymbol{U}^n := (u_{i,K}^n)_{K\in\mathcal{T}_h, i\in[\![1,N_s]\!]} \in \mathbb{R}^{N_e\times N_s}$
- $\boldsymbol{U}^0 \in \mathbb{R}^{N_s\times N_e}$ where $u_{i,K}^0 = \dfrac{1}{|K|}\displaystyle\int_K u_i{}^0(x)\,\mathrm{d}x$
- FV scheme : find $\boldsymbol{U}^n \in \mathbb{R}^{N_e\times N_s}$ satisfying

$$|K|\frac{u_{i,K}^n - u_{i,K}^{n-1}}{\Delta t_n} + \sum_{\sigma\in\mathcal{E}_K} \mathcal{F}_{i,K\sigma}^n(\boldsymbol{U}^n) = 0$$

Flux: $$\mathcal{F}_{i,K\sigma}^n(\boldsymbol{U}^n) := -a^\star \tau_\sigma D_{K\sigma}\boldsymbol{u}_i^n - \tau_\sigma\left(\sum_{j=1}^{N}(a_{i,j}-a^\star)\left(u_{j,\sigma}^n D_{K\sigma}\boldsymbol{u}_i^n - u_{i,\sigma}^n D_{K\sigma}\boldsymbol{u}_j^n\right)\right).$$

edge unknown $$u_{i,\sigma}^n := \begin{cases} 0 & \text{if} \quad \min(u_{i,K}^n, u_{i,K\sigma}^n) < 0, \\ u_{i,K}^n & \text{if} \quad u_{i,K}^n = u_{i,K\sigma}^n \geq 0, \\ \dfrac{u_{i,K}^n - u_{i,K\sigma}^n}{\ln(u_{i,K}^n) - \ln(u_{i,K\sigma}^n)} & \text{if} \quad u_{i,K}^n \neq u_{i,K\sigma}^n \geq 0. \end{cases}$$

Remark

- *The main idea of the introduction of the parameter* $a^\star > 0$ *is to avoid unphysical solutions* *Cancès, Gaudeul 2020*.
- *The numerical flux is conservative in the sense that for* $\sigma \in \mathcal{E}_h^{\mathrm{int}}$, $\sigma = K|L$, $F_{i,L\sigma}^n = -F_{i,K\sigma}^n$.

Remark

- *The main idea of the introduction of the parameter $a^\star > 0$ is to avoid unphysical solutions Cancès, Gaudeul 2020.*
- *The numerical flux is conservative in the sense that for $\sigma \in \mathcal{E}_h^{\text{int}}$, $\sigma = K|L$, $F^n_{i,L\sigma} = -F^n_{i,K\sigma}$.*

Structural properties of the discrete solution:

Remark

- *The main idea of the introduction of the parameter $a^\star > 0$ is to avoid unphysical solutions Cancès, Gaudeul 2020.*
- *The numerical flux is conservative in the sense that for $\sigma \in \mathcal{E}_h^{\text{int}}$, $\sigma = K|L$, $F^n_{i,L\sigma} = -F^n_{i,K\sigma}$.*

Structural properties of the discrete solution:

Theorem (Cancès, Gaudeul 2020)

1. *mass conservation* $\sum_{K\in\mathcal{T}_h} |K| u^n_{i,K} = \int_\Omega u_i{}^0(x)\,\mathrm{d}x \quad \forall i \in [1, N_s], \quad \forall n \in [0, N_t]$.
2. *positivity* $u^n_{i,K} > 0 \quad \forall K \in \mathcal{T}_h, \quad \forall i \in [1, N_s], \quad \forall n \in [0, N_t]$.
3. *Volume filling constraints:* $\sum_{i=1}^{N_s} u^n_{i,K} = 1 \quad \forall K \in \mathcal{T}_h, \quad \forall n \in [0, N_t]$.
4. *Decays of the discrete entropy* $E_{\mathcal{T}_h}(\boldsymbol{U}^n) \le E_{\mathcal{T}_h}(\boldsymbol{U}^{n-1}) \quad \forall n \in [1, N_t]$ *where* $E_{\mathcal{T}_h}(\boldsymbol{U}) := \sum_{K\in\mathcal{T}_h} \sum_{i=1}^{N_s} |K| u_{i,K} \ln(u_{i,K})$.

Newton linearization

The finite volume procedure defines a nonlinear system of algebraic equations

$$G^n(\boldsymbol{U}^n) = 0 \quad \text{where} \quad G^n : \mathbb{R}^{N_e \times N_s} \to \mathbb{R}^{N_e \times N_s}.$$

Newton linearization

The finite volume procedure defines a nonlinear system of algebraic equations

$$G^n(\boldsymbol{U}^n) = 0 \quad \text{where} \quad G^n : \mathbb{R}^{N_e \times N_s} \to \mathbb{R}^{N_e \times N_s}.$$

Initialization of Newton solver: Let $n \in [\![1, N_{\mathrm{t}}]\!]$ and $\boldsymbol{U}^{n,0} \in \mathbb{R}^{N_e \times N_s}$ be fixed (typically $\boldsymbol{U}^{n,0} = \boldsymbol{U}^{n-1}$).

Linear system : the Newton algorithm generates a sequence $(\boldsymbol{U}^{n,k})_{k \geq 1}$, with $\boldsymbol{U}^{n,k} \in \mathbb{R}^{N_e \times N_s}$ solution of

$$\mathbb{A}^{n,k-1} \boldsymbol{U}^{n,k} = \boldsymbol{B}^{n,k-1}.$$

Newton linearization

The finite volume procedure defines a nonlinear system of algebraic equations

$$G^n(\boldsymbol{U}^n) = 0 \quad \text{where} \quad G^n : \mathbb{R}^{N_e \times N_s} \to \mathbb{R}^{N_e \times N_s}.$$

Initialization of Newton solver: Let $n \in [\![1, N_{\mathrm{t}}]\!]$ and $\boldsymbol{U}^{n,0} \in \mathbb{R}^{N_e \times N_s}$ be fixed (typically $\boldsymbol{U}^{n,0} = \boldsymbol{U}^{n-1}$).

Linear system : the Newton algorithm generates a sequence $(\boldsymbol{U}^{n,k})_{k \geq 1}$, with $\boldsymbol{U}^{n,k} \in \mathbb{R}^{N_e \times N_s}$ solution of

$$\mathbb{A}^{n,k-1} \boldsymbol{U}^{n,k} = \boldsymbol{B}^{n,k-1}.$$

The jacobian matrix $\mathbb{A}^{n,k-1} \in \mathbb{R}^{N_e \times N_s, N_e \times N_s}$ and the right-hand side vector $\boldsymbol{B}^{n,k-1} \in \mathbb{R}^{N_e \times N_s}$ are defined by

$$\mathbb{A}^{n,k-1} := \mathbb{J}_{G^n}(\boldsymbol{U}^{n,k-1}) \quad \text{and} \quad \boldsymbol{B}^{n,k-1} := \mathbb{J}_{G^n}(\boldsymbol{U}^{n,k-1})\boldsymbol{U}^{n,k-1} - G^n(\boldsymbol{U}^{n,k-1})$$

Summary

1. We proposed the cell-centered finite volume method to solve the cross-diffusion system.
2. This discrete system preserves the structural properties of the solution.

We want to solve the cross-diffusion problem for a wide variety of cross-diffusion matrices $\mathbb{A}$. It involves high computational cost.

We construct a reduced model to save computational time that preserves the structural properties of the solution.

Outline

The offline stage

Some notation: To each cross-diffusion matrix $\mathbb{A} = (a_{i,j})$ is associated a parameter $\mu \in \mathcal{P}$.

$$\forall \mu \in \mathcal{P} \longleftrightarrow \text{ a solution } \boldsymbol{U}_\mu^n \in \mathbb{R}^{N_s \times N_e}.$$

The offline stage:

1. We compute snapshots of solution $\boldsymbol{U}_\mu^n \in \mathbb{R}^{N_s \times N_e}$ for $\mu \in \mathcal{P}^{\text{off}} \subset \mathcal{P}$ (a certain number of so-called high-fidelity trajectories). Next, compute the corresponding snapshots matrix

$$\mathbb{M} = \begin{bmatrix} \mathbb{M}_{\mu_1} & \mathbb{M}_{\mu_2} & \cdots & \mathbb{M}_{\mu_{p^\star}} \end{bmatrix} \in \mathbb{R}^{N_s \times N_e, N_t \times p^\star}.$$

2. SVD decomposition : $\mathbb{M} = \underbrace{\mathbb{V}}_{\in \mathbb{R}^{N_s \times N_e, N_s \times N_e}} \times \underbrace{\mathbb{S}}_{\in \mathbb{R}^{N_s \times N_e, N_t \times p^\star}} \times \underbrace{\mathbb{W}^T}_{\in \mathbb{R}^{N_t \times p^\star, N_t \times p^\star}}.$

   Here, $\mathbb{S}_{ii} = \sqrt{\sigma_i}$ for $1 \leq i \leq \min(N_s \times N_e, N_t \times p^\star)$ and σ_i are the eigenvalues of $\mathbb{M}\mathbb{M}^T$.

3. Select r columns from the matrice $\mathbb{V}$ as follows : $\sum_{k \geq r+1} \sigma_k^2 \leq \varepsilon$ for $\varepsilon \geq 0$ a fixed tolerance. $\Rightarrow$ We obtain a reduced basis $\mathbb{V}^r = (\boldsymbol{V}_1, \cdots, \boldsymbol{V}_r)$.

The online stage

For each $\mu \in \mathcal{P}$, at each time step $n = 1 \cdots N_t$, the solution of the reduced model denoted by $\widetilde{\boldsymbol{U}}^n_\mu \in \mathbb{R}^{N_s \times N_e}$ is expressed in the basis $(\boldsymbol{V}^1, \cdots, \boldsymbol{V}^r)$ as

$$\widetilde{\boldsymbol{U}}^n_\mu := \sum_{k=1}^{r} c^{k,n}_\mu \boldsymbol{V}^k, \quad \widetilde{\boldsymbol{U}}^0_\mu := \Pi_{\mathrm{span}(\boldsymbol{V}^1,\cdots,\boldsymbol{V}^r)} \boldsymbol{U}^0.$$

How to derive the expression of the coefficients $c^{k,n}_\mu$?

We define the function $H : \mathbb{R}^r \to \mathbb{R}^r$ by $H_l(\boldsymbol{c}^n_\mu) := \langle \boldsymbol{V}^l, G^n(\widetilde{\boldsymbol{U}}^n_\mu) \rangle \quad \forall 1 \leq l \leq r$.
The vector $\boldsymbol{c}^n_\mu \in \mathbb{R}^r$ is solution to the nonlinear problem

$$H(\boldsymbol{c}^n_\mu) = 0.$$

Remark

This reduced model does not necessarily preserve the structural properties of the numerical solution.

Outline

The offline stage

1. Compute snapshots of solutions.
2. Compute the matrix $\overline{\mathbb{M}} \in \mathbb{R}^{N_s \times N_e, N_t \times p^\star}$ defined by

$$\overline{\mathbb{M}} = \left[\overline{\mathbb{M}}_{\mu_1} \quad \overline{\mathbb{M}}_{\mu_2} \quad \cdots \quad \overline{\mathbb{M}}_{\mu_{p^\star}}\right] \in \mathbb{R}^{N_s \times N_e, N_t \times p^\star}.$$

   where each matrix $\overline{\mathbb{M}}_{\mu_\alpha} \in \mathbb{R}^{N_s \times N_e, N_t}$ are defined by $\left[\overline{\mathbb{M}}_{\mu_\alpha}\right]_{i,K} = z^n_{\mu_\alpha,i,K} = \ln(u^n_{\mu_\alpha,i,K})$.
3. SVD decomposition

$$\overline{\mathbb{M}} = \underbrace{\overline{\mathbb{V}}}_{\in \mathbb{R}^{N_s \times N_e, N_s \times N_e}} \times \underbrace{\overline{\mathbb{S}}}_{\in \mathbb{R}^{N_s \times N_e, N_t \times p^\star}} \times \underbrace{\overline{\mathbb{W}}^T}_{\in \mathbb{R}^{N_t \times p^\star, N_t \times p^\star}}.$$

4. Select r basis functions. Add to the matrix $\overline{\mathbb{V}}^r$ N_s identity bloc matrices as follows

Example: $N_s = 3$

$$
\overline{\mathbb{V}}^{r^\star} = \begin{bmatrix}
\overline{v}^1_{1,K1} & \overline{v}^2_{1,K1} & \cdots & \overline{v}^r_{1,K1} & 1 & 0 & 0 \\
\overline{v}^1_{1,K2} & \overline{v}^2_{1,K2} & \cdots & \overline{v}^r_{1,K2} & 1 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\overline{v}^1_{1,K_{N_e}} & \overline{v}^2_{1,K_{N_e}} & \cdots & \overline{v}^r_{1,K_{N_e}} & 1 & 0 & 0 \\
\overline{v}^1_{2,K1} & \overline{v}^2_{2,K1} & \cdots & \overline{v}^r_{2,K1} & 0 & 1 & 0 \\
\overline{v}^1_{2,K2} & \overline{v}^2_{2,K2} & \cdots & \overline{v}^r_{2,K2} & 0 & 1 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\overline{v}^1_{2,K_{N_e}} & \overline{v}^2_{2,K_{N_e}} & \cdots & \overline{v}^r_{2,K_{N_e}} & 0 & 1 & 0 \\
\overline{v}^1_{3,K1} & \overline{v}^2_{3,K1} & \cdots & \overline{v}^r_{3,K1} & 0 & 0 & 1 \\
\overline{v}^1_{3,K2} & \overline{v}^2_{3,K2} & \cdots & \overline{v}^r_{3,K2} & 0 & 0 & 1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\overline{v}^1_{3,K_{N_e}} & \overline{v}^2_{3,K_{N_e}} & \cdots & \overline{v}^r_{3,K_{N_e}} & 0 & 0 & 1
\end{bmatrix}
$$

Remark

The matrix $\overline{\mathbb{V}}^{r^\star}$ is not orthogonal. We employ a QR factorization on the matrix $\overline{\mathbb{V}}^{r^\star}$ so that $\overline{\mathbb{V}}^{r^\star} = \mathbb{Q} \times \widetilde{\mathbb{R}}$ where $\mathbb{Q} \in \mathbb{R}^{N_s \times N_e, r^\star}$ is orthogonal, and $\widetilde{\mathbb{R}} \in \mathbb{R}^{r^\star, r^\star}$ is upper triangular.

Remark

The matrix $\overline{\mathbb{V}}^{r^\star}$ is not orthogonal. We employ a QR factorization on the matrix $\overline{\mathbb{V}}^{r^\star}$ so that $\overline{\mathbb{V}}^{r^\star} = \mathbb{Q} \times \widetilde{\mathbb{R}}$ where $\mathbb{Q} \in \mathbb{R}^{N_s \times N_e, r^\star}$ is orthogonal, and $\widetilde{\mathbb{R}} \in \mathbb{R}^{r^\star, r^\star}$ is upper triangular.

For each $\mu \in \mathcal{P}$, at each time step $n = 1 \cdots N_{\mathrm{t}}$, we define a “temporary reduced solution” denoted by $\overline{\boldsymbol{Z}}_\mu^n \in \mathbb{R}^{N_s \times N_e}$. It is expressed in the basis $(\boldsymbol{Q}^1, \cdots, \boldsymbol{Q}^{r^\star})$ as

$$\overline{\boldsymbol{Z}}_\mu^n := \sum_{k=1}^{r^\star} \overline{c}_\mu^{k,n} \boldsymbol{Q}^k \quad \text{and} \quad \overline{\boldsymbol{Z}}_\mu^0 := \Pi_{\mathrm{Span}(\boldsymbol{Q}^1, \cdots, \boldsymbol{Q}^{r^\star})} \boldsymbol{Z}_\mu^0 \quad \text{where} \quad z_{\mu,i,K}^0 := \ln(u_{\mu,i,K}^0).$$

Remark

The matrix $\overline{\mathbb{V}}^{r^\star}$ is not orthogonal. We employ a QR factorization on the matrix $\overline{\mathbb{V}}^{r^\star}$ so that $\overline{\mathbb{V}}^{r^\star} = \mathbb{Q} \times \widetilde{\mathbb{R}}$ where $\mathbb{Q} \in \mathbb{R}^{N_s \times N_e, r^\star}$ is orthogonal, and $\widetilde{\mathbb{R}} \in \mathbb{R}^{r^\star, r^\star}$ is upper triangular.

For each $\mu \in \mathcal{P}$, at each time step $n = 1 \cdots N_t$, we define a “temporary reduced solution” denoted by $\overline{\boldsymbol{Z}}_\mu^n \in \mathbb{R}^{N_s \times N_e}$. It is expressed in the basis $(\boldsymbol{Q}^1, \cdots, \boldsymbol{Q}^{r^\star})$ as

$$\overline{\boldsymbol{Z}}_\mu^n := \sum_{k=1}^{r^\star} \overline{c}_\mu^{k,n} \boldsymbol{Q}^k \quad \text{and} \quad \overline{\boldsymbol{Z}}_\mu^0 := \boldsymbol{\Pi}_{\mathrm{Span}(\boldsymbol{Q}^1, \cdots, \boldsymbol{Q}^{r^\star})} \boldsymbol{Z}_\mu^0 \quad \text{where} \quad z_{\mu,i,K}^0 := \ln(u_{\mu,i,K}^0).$$

Definition of the coefficient $\overline{\boldsymbol{c}}_\mu^{k,n}$

Solve the nonlinear problem $\overline{H}_l(\overline{\boldsymbol{c}}_\mu^n) = 0$ with $\overline{H}_l(\overline{\boldsymbol{c}}_\mu^n) := \left\langle \boldsymbol{Q}^l, G^n(\overline{\boldsymbol{U}}_\mu^n) \right\rangle \quad \forall 1 \leq l \leq r^\star.$

How can we construct a structure preserving reduced model ?

Safe reduced solution

$$\overline{\boldsymbol{U}}^n_{\mu} := (\overline{u}^n_{\mu,i,K})_{i\in[1,N_s],K\in\mathcal{T}_h} \quad \text{with} \quad \overline{u}^n_{\mu,i,K} := \exp(\overline{z}^n_{\mu,i,K}) \Big/ \sum_{j=1}^{N_s} \exp(\overline{z}^n_{\mu,j,K}).$$

Structural properties of the reduced solution

1. Positivity $\quad \overline{u}^n_{\mu,i,K} > 0 \quad \forall \mu \in \mathcal{P} \quad \forall K \in \mathcal{T}_h \quad \forall i \in [1, N_s] \quad \forall n \in [0, N_t]$.
2. Volume filling constraint: $\sum_{i=1}^{N_s} \overline{u}^n_{\mu,i,K} = 1 \quad \forall \mu \in \mathcal{P} \quad \forall K \in \mathcal{T}_h, \quad \forall n \in [1, N_t]$.
3. mass conservation

$$\sum_{K\in\mathcal{T}_h} |K| \overline{u}^n_{\mu,i,K} = \sum_{K\in\mathcal{T}_h} |K| \overline{u}^{n-1}_{\mu,i,K} = \int_\Omega \overline{u}^0_i(x)\,\mathrm{d}x \quad \forall i \in [1, N_s] \quad \forall n \in [1, N_t]\,.$$

4. The discrete counterpart of the entropy decays along time

$$E_{\mathcal{T}_h}(\overline{\boldsymbol{U}}^n_{\mu}) - E_{\mathcal{T}_h}(\overline{\boldsymbol{U}}^{n-1}_{\mu}) + \Delta t_n \min_{i,j} a_{i,j} \sum_{\sigma\in\mathcal{E}_h^{\mathrm{int}}} \sum_{i=1}^{N_s} \tau_\sigma \overline{u}^n_{\mu,i\sigma} \left(D_{K\sigma}(\ln(\overline{\boldsymbol{u}}^n_{\boldsymbol{\mu},\boldsymbol{i}}))\right)^2 \le 0 \quad \forall n \in [1, N_t]\,.$$

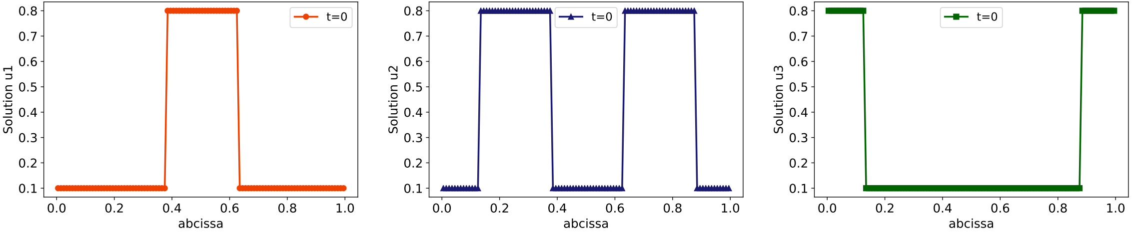
Outline

First test case

- We consider 3 species.
- Ω is a one dimensional domain consisting in a segment of length $L = 1m$.
- $\Delta x = 10^{-2}$.
- Final simulation time $T = 0.5$s and $\Delta t = 5 \times 10^{-4}$ s.
- Compute $\mu = 20$ snapshots of solutions.

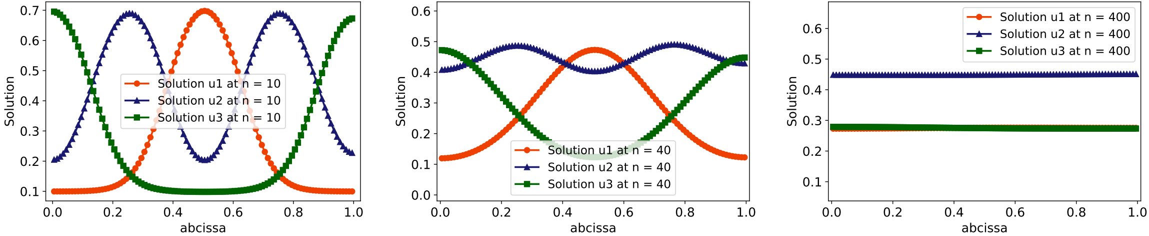
Initial condition

- discontinuous solution



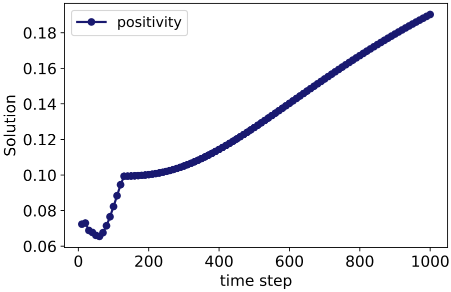
Shape of the solution

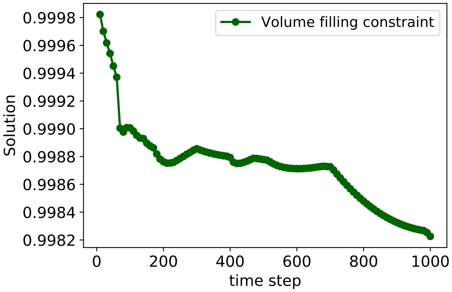
$$\mathbb{A}_\mu := \begin{pmatrix} 0 & 0.75 & 0.73 \\ 0.75 & 0 & 0.84 \\ 0.73 & 0.84 & 0 \end{pmatrix}$$



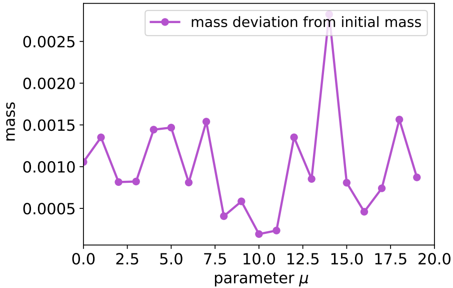
Typical behavior of a cross-diffusion system

Structural properties of the solution





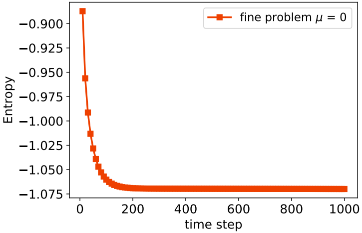
$$\mathcal{P}_U(t_n) := \inf_{\color{red}{\mu}\in\mathcal{P}^{\text{off}}} \inf_{K\in\mathcal{T}_h} U^n_{\color{red}{\mu},K} \qquad \mathcal{S}_U(t_n) := \inf_{\color{red}{\mu}\in\mathcal{P}^{\text{off}}} \inf_{K\in\mathcal{T}_h} \sum_{i=1}^{N_s} U^n_{\color{red}{\mu},i,K}$$

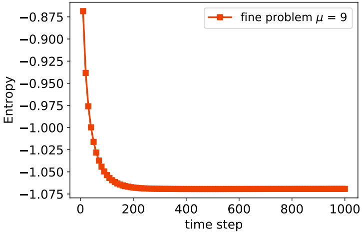


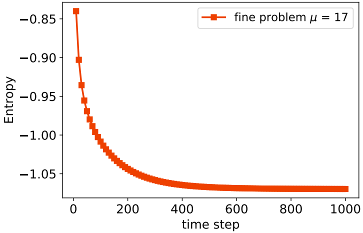
$$\mathcal{E}_U(\mu) := \max_{i \in [\![1,N_s]\!]} \max_{n \in [\![1,N_t]\!]} \left| \sum_{K \in \mathcal{T}_h} |K| U^n_{\mu,i,K} - \int_\Omega {u_i}^0(x)\, \mathrm{dx} \right|$$

Structural properties of the Solution

$$\mathbb{A}_{\mu_0} := \begin{pmatrix} 0 & 0.75 & 0.73 \\ 0.75 & 0 & 0.84 \\ 0.73 & 0.84 & 0 \end{pmatrix} \mathbb{A}_{\mu_9} = \begin{pmatrix} 0 & 0.93 & 0.71 \\ 0.93 & 0 & 0.44 \\ 0.71 & 0.44 & 0 \end{pmatrix} \quad \mathbb{A}_{\mu_{17}} = \begin{pmatrix} 0 & 0.37 & 0.004 \\ 0.37 & 0 & 0.72 \\ 0.004 & 0.72 & 0 \end{pmatrix}$$

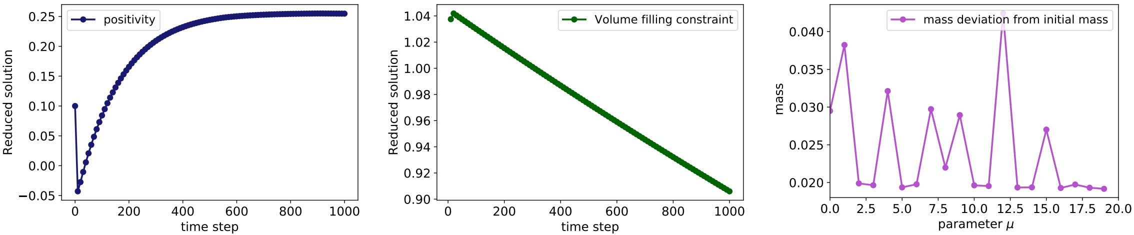






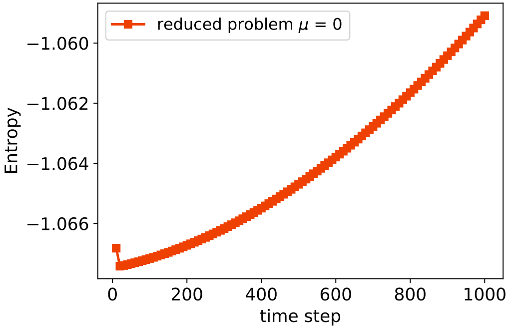
First POD reduced model

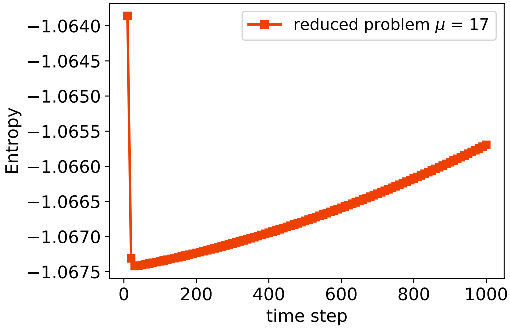
Violation of the structural properties of the solution



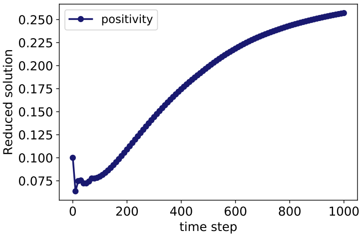
$r = 2$ $\qquad r = 1$ $\qquad r = 1$

$$\mathbb{A}_0 = \begin{pmatrix} 0 & 0.93 & 0.71 \\ 0.93 & 0 & 0.44 \\ 0.71 & 0.44 & 0 \end{pmatrix} \qquad \mathbb{A}_{17} = \begin{pmatrix} 0 & 0.37 & 0.004 \\ 0.37 & 0 & 0.72 \\ 0.004 & 0.72 & 0 \end{pmatrix}$$

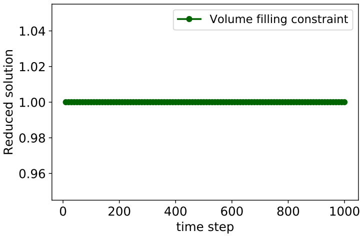




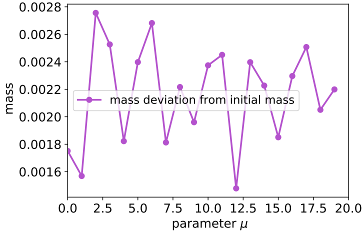
Second POD reduced model



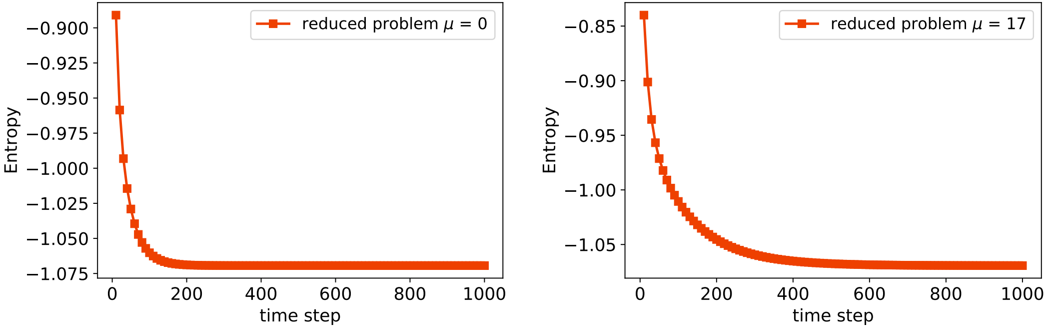
$r = 2$



$r = 1$



$r = 1$



The entropy decreases with respect to time.

Second test case

- We consider the PVD process : 4 species.
- Ω is a one dimensional domain consisting in a segment of length $L = 1m$.
- $\Delta x = 10^{-2}$.
- Final simulation time $T = 0.5$ s and $\Delta t = 2.5 \times 10^{-4}$ s.
- Compute $\mu = 20$ snapshots of solutions.

Initial guess

We take

$$w_1^0(x) = e^{-25(x-0.5)^2}, \quad w_2^0(x) = x^2 + \varepsilon, \quad w_3(x) = 1 - e^{-25(x-0.5)^2}, \quad w_4(x) = |\sin(\pi x)|$$

where $\varepsilon = 10^{-6}$.

To satisfy the volume filling constraint property we use a renormalization

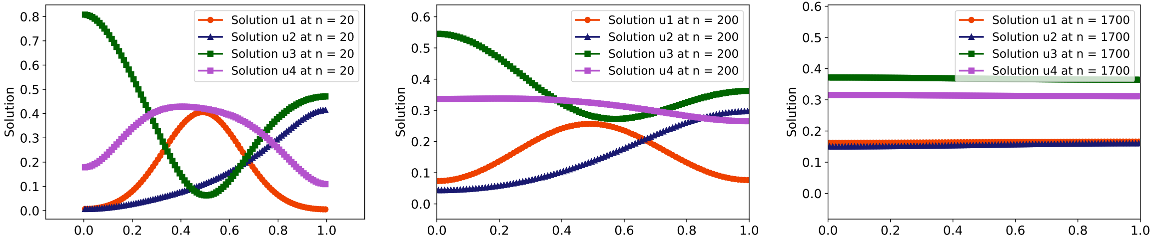
$$u_i{}^0(x_j) = \frac{w_i^0(x_j)}{\sum_{l=1}^{N_s} w_l^0(x_j)}$$

where x_j, $j \in [1, N_e]$ are the cell centers of the mesh.

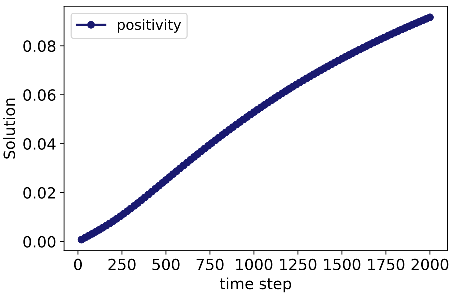
Fine solution

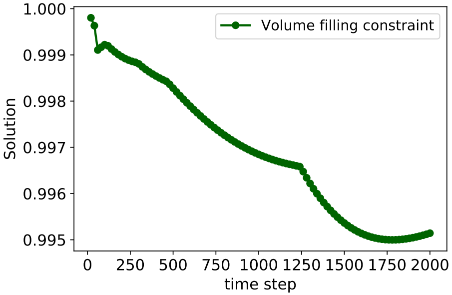
Cross-diffusion matrix

$$\mathbb{A}_{17} = \begin{pmatrix} 0 & 0.64 & 0.31 & 0.53 \\ 0.64 & 0 & 0.99 & 0.84 \\ 0.32 & 0.99 & 0 & 0.99 \\ 0.53 & 0.84 & 0.99 & 0 \end{pmatrix}$$



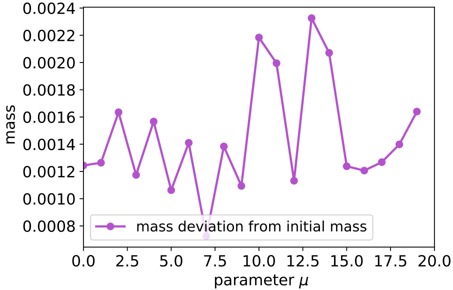
Properties of the solution





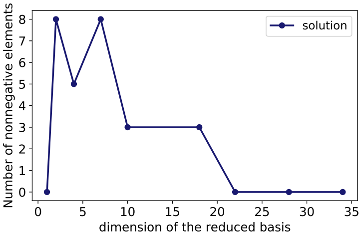
$$\mathcal{P}_{\overline{U}}(t_n) := \inf_{\color{red}{\mu}\in\mathcal{P}^{\mathrm{off}}} \inf_{K\in\mathcal{T}_h} \overline{U}^n_{\color{red}{\mu},K}$$

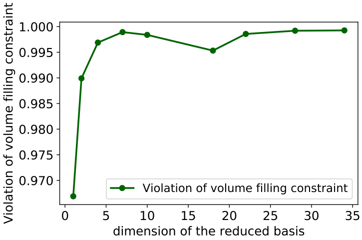
$$\mathcal{S}_{\overline{U}}(t_n) := \inf_{\color{red}{\mu}\in\mathcal{P}^{\mathrm{off}}} \inf_{K\in\mathcal{T}_h} \sum_{i=1}^{N_s} \overline{U}^n_{\color{red}{\mu},i,K}$$

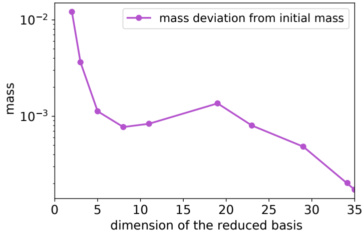


$$\mathcal{E}_{\overline{U}}(\mu) := \max_{i \in [\![1, N_s]\!]} \max_{n \in [\![1, N_t]\!]} \left| \sum_{K \in \mathcal{T}_h} |K| \overline{U}^n_{\mu,i,K} - \int_\Omega \overline{u}^0_i(x)\, \mathrm{d}x \right|$$

First POD reduced model



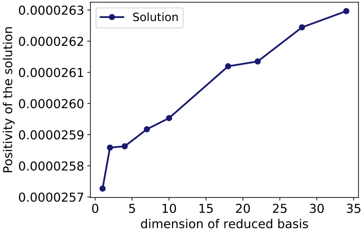


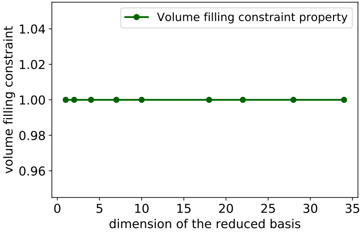


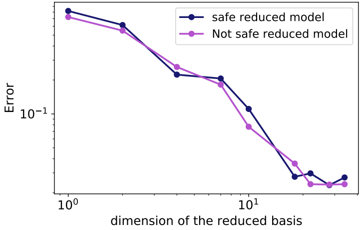
$$\inf_{n\in[\![1,N_t]\!]} \inf_{\mu\in\mathcal{P}^{\text{off}}} \inf_{K\in\mathcal{T}_h} \sum_{i=1}^{N_s} \widetilde{U}^n_{\mu,i,K} \qquad \max_{\mu\in\mathcal{P}^{\text{off}}} \max_{i\in[\![1,N_s]\!]} \max_{n\in[\![1,N_t]\!]} \left| \sum_{K\in\mathcal{T}_h} |K| \overline{U}^n_{\mu,i,K} - \int_\Omega \overline{u}^0_i(x)\,\mathrm{d}x \right|$$

Violation of the physical properties.

Safe POD reduced model







$$\inf_{n\in[\![1,N_t]\!]}\ \inf_{\mu\in\mathcal{P}^{\text{off}}}\ \inf_{K\in\mathcal{T}_h} \overline{U}^{n}_{\mu,K} \qquad \inf_{n\in[\![1,N_t]\!]}\ \inf_{\mu\in\mathcal{P}^{\text{off}}}\ \inf_{K\in\mathcal{T}_h} \sum_{i=1}^{N_s} \overline{U}^{n}_{\mu,i,K}$$

$$\max_{i\in[\![1,N_s]\!]} \left\| u^{i}_{\mu} - u^{i,\text{red}}_{\mu} \right\|_{L^\infty(\mathcal{P}^{\text{off}},L^2(\Omega),L^\infty([0,T]))} := \max_{\mu\in\mathcal{P}^{\text{off}}}\ \max_{n\in[\![1,N_t]\!]} \left(\sum_{K\in\mathcal{T}_h} \left| U^{n}_{\mu,i,K} - U^{n,\text{red}}_{\mu,i,K} \right|^2 \right)^{\frac{1}{2}}$$

Outline

Conclusion and perspectives

Conclusion

- We constructed an efficient reduced model preserving the physical properties of the cross-diffusion system.

Perspectives

- Construct a reduced basis method with a posteriori estimators for high accuracy.
- EIM algorithm to reduce the computational time.