

# Structure-preserving reduced basis method for cross-diffusion systems

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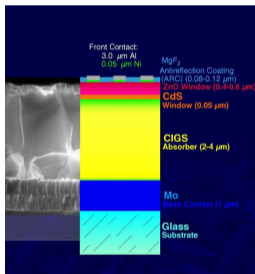
# Outline

- 1 Introduction
- 2 Model problem and discretization
- 3 A first POD reduced model
- 4 A structure preserving POD reduced model
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# 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 gaseous 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.**

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# Model Problem

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

## Cross-diffusion model

$$\begin{aligned} \partial_t u_i - \nabla \cdot \left( \sum_{j=1}^{N_s} a_{i,j} (u_j \nabla u_i - u_i \nabla u_j) \right) &= 0 \quad \text{in } \Omega \times [0, T], \text{ for } i \in [1, N_s], \\ \left( \sum_{j=1}^{N_s} a_{i,j} (u_j \nabla u_i - u_i \nabla u_j) \right) \cdot \mathbf{n} &= 0 \quad \text{on } \partial\Omega \times [0, T], \text{ for } i \in [1, N_s], \\ u_i(\mathbf{x}, 0) &= u_i^0(\mathbf{x}) \quad \text{in } \Omega, \text{ for } i \in [1, N_s]. \end{aligned}$$

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

## Gradient flow structure

### Entropy functional:

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

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

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

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

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

# Theorem

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

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

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**Structural properties of the solution:** Consider  $\mathbf{u}^0 = (u_1^0, \dots, u_{N_s}^0) \in \mathbb{R}_+^{N_s}$  such that  $\sum_{i=1}^{N_s} u_i^0 = 1$  and  $\|\mathbf{u}^0\|_{L^\infty(\Omega)} < +\infty$ . Then,



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



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- 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:  $\mathbf{u} \in \mathbb{R}_+^{N_s}$  such that  $\sum_{i=1}^{N_s} u_i = 1$ .

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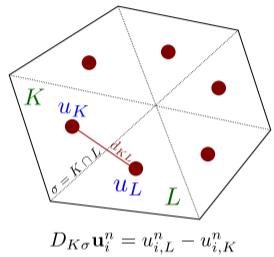
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- 4 entropy-entropy dissipation relation

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

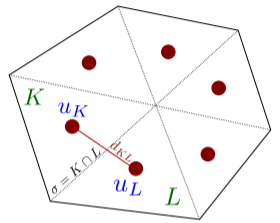
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- $N_s$  unknowns per cell  $\mathbf{U}^n := (u_{i,K}^n)_{K \in \mathcal{T}_h, i \in [1, N_s]} \in \mathbb{R}^{N_e \times N_s}$
- $\mathbf{U}^0 \in \mathbb{R}^{N_s \times N_e}$  where  $u_{i,K}^0 = \frac{1}{|K|} \int_K u_i^0(x) dx$
- FV scheme : find  $\mathbf{U}^n \in \mathbb{R}^{N_e \times N_s}$  satisfying
 
$$|K| \frac{u_{i,K}^n - u_{i,K}^{n-1}}{\Delta t_n} + \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{i,K\sigma}^n(\mathbf{U}^n) = 0$$

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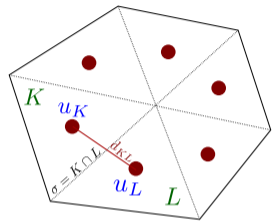
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**Flux:**  $\mathcal{F}_{i,K\sigma}^n(\mathbf{U}^n) := -a^* \tau_\sigma D_{K\sigma} \mathbf{u}_i^n - \tau_\sigma \left( \sum_{j=1}^N (a_{i,j} - a^*) (u_{j,\sigma}^n D_{K\sigma} \mathbf{u}_i^n - u_{i,\sigma}^n D_{K\sigma} \mathbf{u}_j^n) \right).$

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





## Remark

- The main idea of the introduction of the parameter  $a^* > 0$  is to avoid unphysical solutions Cancès, Gaudoul 2020.
- The numerical flux is conservative in the sense that for  $\sigma \in \mathcal{E}_h^{\text{int}}, \sigma = K|L$ ,  
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### Structural properties of the discrete solution:

#### Theorem (*Cancès, Gaudeul 2020*)

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- 2 positivity  $u_{i,K}^n > 0 \quad \forall K \in \mathcal{T}_h, \quad \forall i \in [1, N_s], \quad \forall n \in [0, N_t].$
- 3 Volume filling constraints:  $\sum_{i=1}^{N_s} u_{i,K}^n = 1 \quad \forall K \in \mathcal{T}_h, \quad \forall n \in [0, N_t].$
- 4 Decays of the discrete entropy  $E_{\mathcal{T}_h}(\mathbf{U}^n) \leq E_{\mathcal{T}_h}(\mathbf{U}^{n-1}) \quad \forall n \in [1, N_t]$  where  

$$E_{\mathcal{T}_h}(\mathbf{U}) := \sum_{K \in \mathcal{T}_h} \sum_{i=1}^{N_s} |K| u_{i,K} \ln(u_{i,K}).$$



# Newton linearization

The finite volume procedure defines a nonlinear system of algebraic equations

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

**Initialization of Newton solver:** Let  $n \in \llbracket 1, N_t \rrbracket$  and  $\mathbf{U}^{n,0} \in \mathbb{R}^{N_e \times N_s}$  be fixed (typically  $\mathbf{U}^{n,0} = \mathbf{U}^{n-1}$ ).

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

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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  $\mathbf{B}^{n,k-1} \in \mathbb{R}^{N_e \times N_s}$  are defined by

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

# 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.**

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# The offline stage

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

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

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- 1 We compute snapshots of solution  $\mathbf{U}_{\mu}^n \in \mathbb{R}^{N_s \times N_e}$  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

$$\mathbf{M} = [\mathbf{M}_{\mu_1} \quad \mathbf{M}_{\mu_2} \quad \dots \quad \mathbf{M}_{\mu_{p^*}}] \in \mathbb{R}^{N_s \times N_e, N_t \times p^*}.$$

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

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- 3 Select  $r$  columns from the matrix  $\mathbb{V}$  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  $\mathbb{V}^r = (\mathbf{V}_1, \dots, \mathbf{V}_r)$ .

## The online stage

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

$$\tilde{\mathbf{U}}_\mu^n := \sum_{k=1}^r c_\mu^{k,n} \mathbf{V}^k, \quad \tilde{\mathbf{U}}_\mu^0 := \Pi_{\text{span}(\mathbf{V}^1, \dots, \mathbf{V}^r)} \mathbf{U}^0.$$

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

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

$$H(\mathbf{c}_\mu^n) = 0.$$

#### Remark

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

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where each matrix  $\bar{\mathbf{M}}_{\mu_\alpha} \in \mathbb{R}^{N_s \times N_e, N_t}$  are defined by  $[\bar{\mathbf{M}}_{\mu_\alpha}]_{i,K} = z_{\mu_\alpha, i, K}^n = \ln(u_{\mu_\alpha, i, K}^n)$ .

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- 3 SVD decomposition

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

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

**Example:  $N_s = 3$**

$$\bar{V}^{r*} = \begin{bmatrix} \bar{V}_{1,K1}^1 & \bar{V}_{1,K1}^2 & \cdots & \bar{V}_{1,K1}^r & 1 & 0 & 0 \\ \bar{V}_{1,K2}^1 & \bar{V}_{1,K2}^2 & \cdots & \bar{V}_{1,K2}^r & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \bar{V}_{1,K_{N_e}}^1 & \bar{V}_{1,K_{N_e}}^2 & \cdots & \bar{V}_{1,K_{N_e}}^r & 1 & 0 & 0 \\ \bar{V}_{2,K1}^1 & \bar{V}_{2,K1}^2 & \cdots & \bar{V}_{2,K1}^r & 0 & 1 & 0 \\ \bar{V}_{2,K2}^1 & \bar{V}_{2,K2}^2 & \cdots & \bar{V}_{2,K2}^r & 0 & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \bar{V}_{2,K_{N_e}}^1 & \bar{V}_{2,K_{N_e}}^2 & \cdots & \bar{V}_{2,K_{N_e}}^r & 0 & 1 & 0 \\ \bar{V}_{3,K1}^1 & \bar{V}_{3,K1}^2 & \cdots & \bar{V}_{3,K1}^r & 0 & 0 & 1 \\ \bar{V}_{3,K2}^1 & \bar{V}_{3,K2}^2 & \cdots & \bar{V}_{3,K2}^r & 0 & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \bar{V}_{3,K_{N_e}}^1 & \bar{V}_{3,K_{N_e}}^2 & \cdots & \bar{V}_{3,K_{N_e}}^r & 0 & 0 & 1 \end{bmatrix}$$

## Remark

The matrix  $\bar{\mathbf{V}}^{r^*}$  is not orthogonal. We employ a QR factorization on the matrix  $\bar{\mathbf{V}}^{r^*}$  so that  $\bar{\mathbf{V}}^{r^*} = \mathbf{Q} \times \tilde{\mathbf{R}}$  where  $\mathbf{Q} \in \mathbb{R}^{N_s \times N_{e,r^*}}$  is orthogonal, and  $\tilde{\mathbf{R}} \in \mathbb{R}^{r^*, r^*}$  is upper triangular.

## Remark

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

$$\bar{\mathbf{z}}_{\mu}^n := \sum_{k=1}^{r^*} \bar{c}_{\mu}^{k,n} \mathbf{Q}^k \quad \text{and} \quad \bar{\mathbf{z}}_{\mu}^0 := \Pi_{\text{Span}(\mathbf{Q}^1, \dots, \mathbf{Q}^{r^*})} \mathbf{z}_{\mu}^0 \quad \text{where} \quad z_{\mu,i,K}^0 := \ln(u_{\mu,i,K}^0).$$



**Remark**

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

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**Definition of the coefficient  $\bar{c}_\mu^{k,n}$**

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

**How can we construct a structure preserving reduced model ?**



## Safe reduced solution

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

## Structural properties of the reduced solution

## Safe reduced solution

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

## Structural properties of the reduced solution

- ① Positivity  $\bar{u}_{\mu,i,K}^n > 0 \quad \forall \mu \in \mathcal{P} \quad \forall K \in \mathcal{T}_h \quad \forall i \in [1, N_s] \quad \forall n \in [0, N_t].$

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

### Structural properties of the reduced solution

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

## Safe reduced solution

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

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- 3 mass conservation

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

## Safe reduced solution

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

### Structural properties of the reduced solution

- ① Positivity  $\bar{u}_{\mu,i,K}^n > 0 \quad \forall \mu \in \mathcal{P} \quad \forall K \in \mathcal{T}_h \quad \forall i \in [1, N_s] \quad \forall n \in [0, N_t].$
- ② Volume filling constraint:  $\sum_{i=1}^{N_s} \bar{u}_{\mu,i,K}^n = 1 \quad \forall \mu \in \mathcal{P} \quad \forall K \in \mathcal{T}_h, \quad \forall n \in [1, N_t].$
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$$\sum_{K \in \mathcal{T}_h} |K| \bar{u}_{\mu,i,K}^n = \sum_{K \in \mathcal{T}_h} |K| \bar{u}_{\mu,i,K}^{n-1} = \int_{\Omega} \bar{u}_i^0(x) dx \quad \forall i \in [1, N_s] \quad \forall n \in [1, N_t].$$

- ④ The discrete counterpart of the entropy decays along time

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



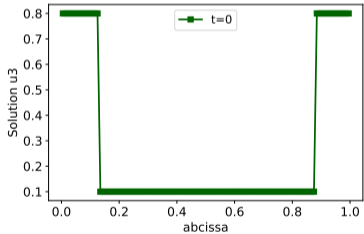
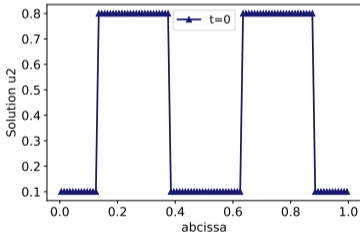
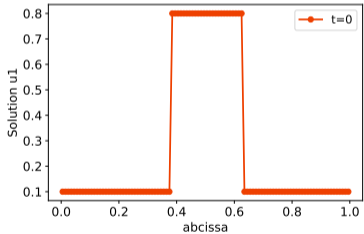


# First test case

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

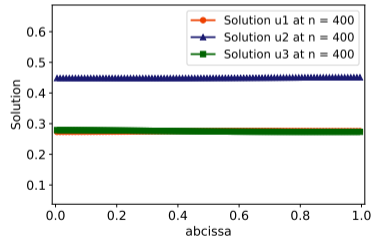
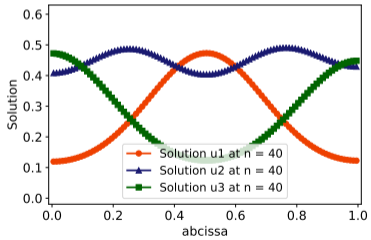
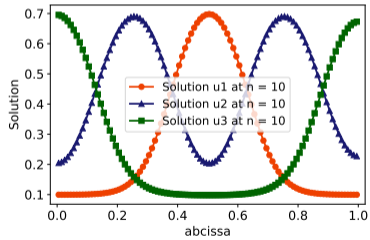
# Initial condition

- discontinuous solution



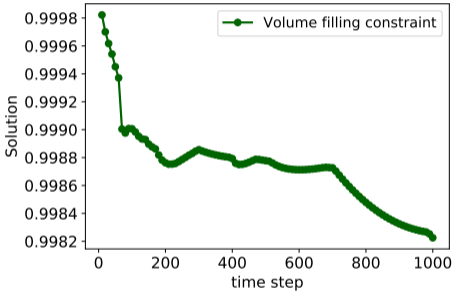
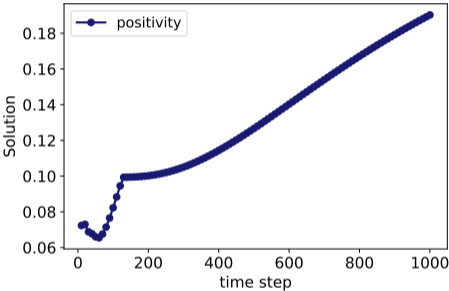
# Shape of the solution

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



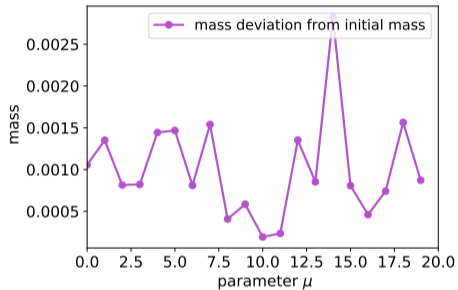
Typical behavior of a cross-diffusion system

# Structural properties of the solution



$$\mathcal{P}_U(t_n) := \inf_{\mu \in \mathcal{P}^{\text{off}}} \inf_{K \in \mathcal{T}_h} U_{\mu, K}^n$$

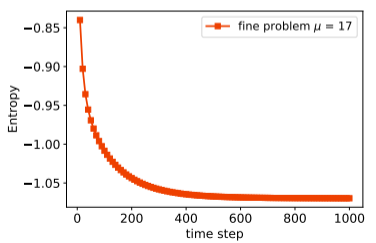
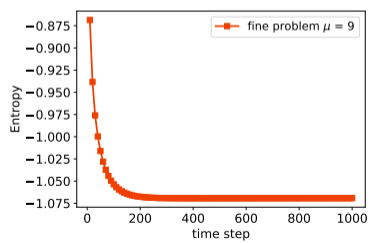
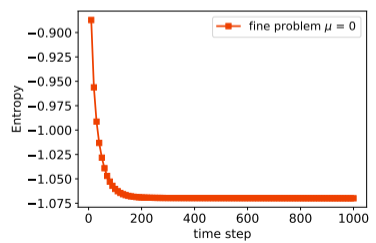
$$\mathcal{S}_U(t_n) := \inf_{\mu \in \mathcal{P}^{\text{off}}} \inf_{K \in \mathcal{T}_h} \sum_{i=1}^{N_s} U_{\mu, i, K}^n$$



$$\mathcal{E}_U(\mu) := \max_{i \in \llbracket 1, N_s \rrbracket} \max_{n \in \llbracket 1, N_t \rrbracket} \left| \sum_{K \in \mathcal{T}_h} |K| U_{\mu, i, K}^n - \int_{\Omega} u_i^0(x) dx \right|$$

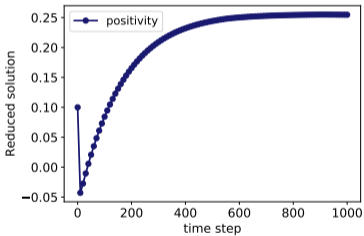
# Structural properties of the Solution

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

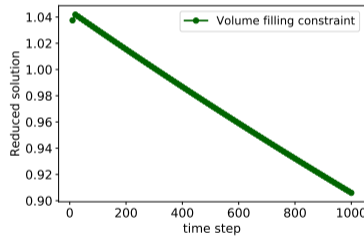


# First POD reduced model

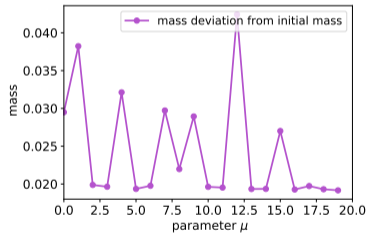
## Violation of the structural properties of the solution



$r = 2$



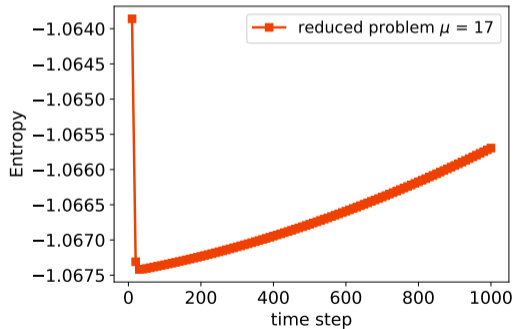
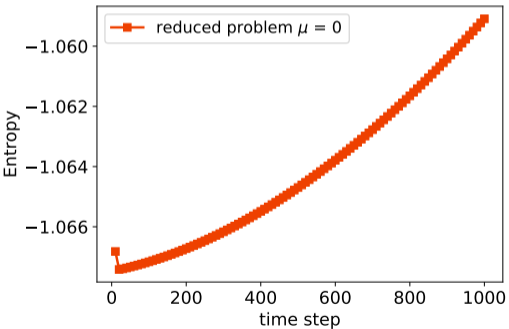
$r = 1$



$r = 1$

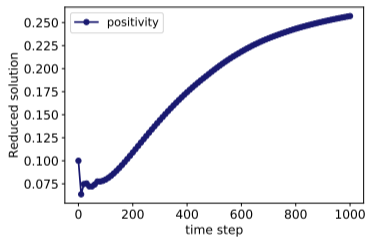
$$\mathbb{A}_0 = \begin{pmatrix} 0 & 0.93 & 0.71 \\ 0.93 & 0 & 0.44 \\ 0.71 & 0.44 & 0 \end{pmatrix}$$

$$\mathbb{A}_{17} = \begin{pmatrix} 0 & 0.37 & 0.004 \\ 0.37 & 0 & 0.72 \\ 0.004 & 0.72 & 0 \end{pmatrix}$$

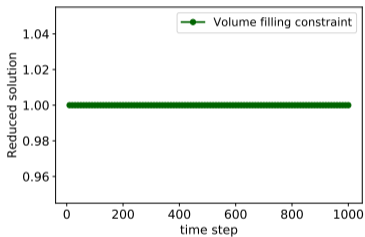




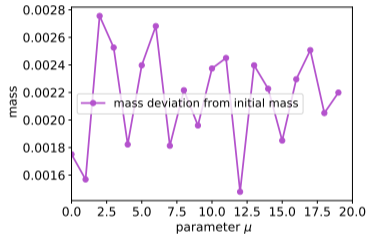
# Second POD reduced model



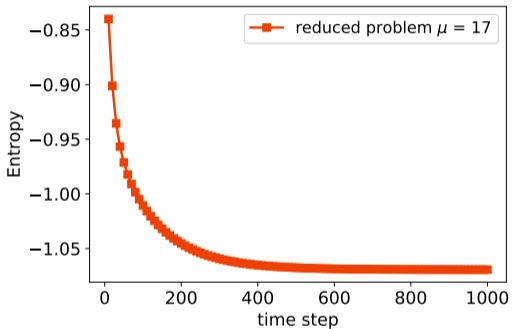
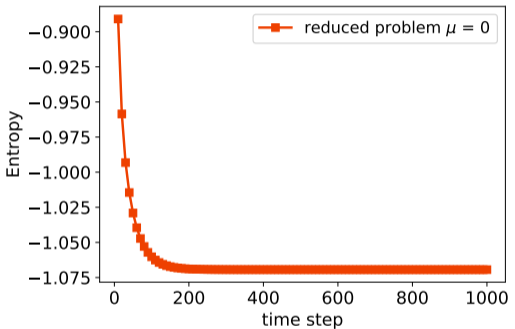
$r = 2$



$r = 1$



$r = 1$



The entropy decreases with respect to time.

## Second test case

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

# Initial condition

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

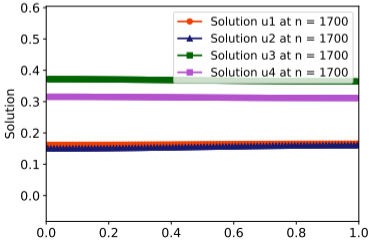
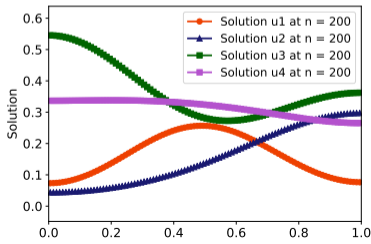
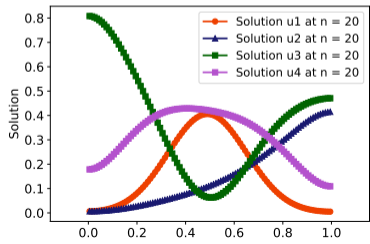
$$u_i^0(x_j) = \frac{w_i^0(x_j)}{\sum_{l=1}^{N_s} w_l^0(x_j)}$$

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

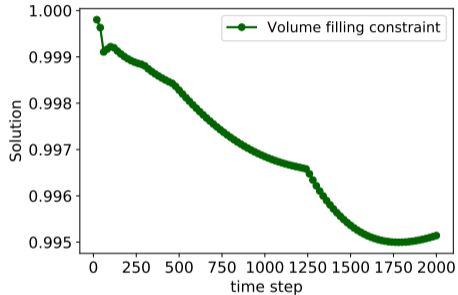
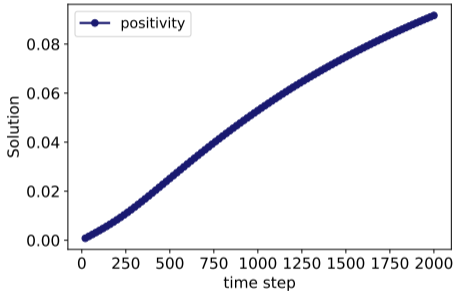
# Fine solution

## Cross-diffusion matrix

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

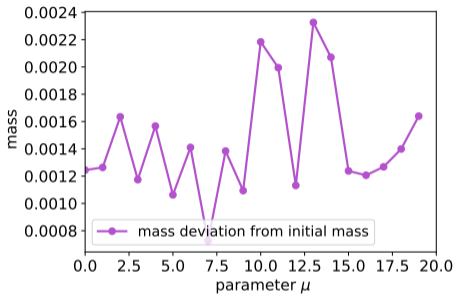


# Properties of the solution



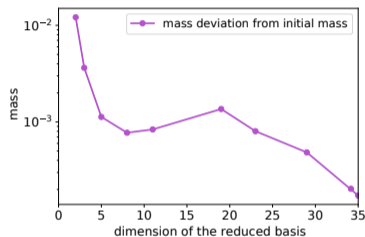
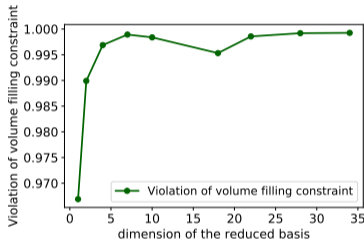
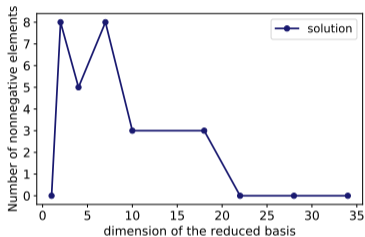
$$\mathcal{P}_{\bar{U}}(t_n) := \inf_{\mu \in \mathcal{P}^{\text{off}}} \inf_{K \in \mathcal{T}_h} \bar{U}_{\mu, K}^n$$

$$\mathcal{S}_{\bar{U}}(t_n) := \inf_{\mu \in \mathcal{P}^{\text{off}}} \inf_{K \in \mathcal{T}_h} \sum_{i=1}^{N_s} \bar{U}_{\mu, i, K}^n$$



$$\mathcal{E}_{\bar{U}}(\mu) := \max_{i \in \llbracket 1, N_s \rrbracket} \max_{n \in \llbracket 1, N_t \rrbracket} \left| \sum_{K \in \mathcal{T}_h} |K| \bar{U}_{\mu, i, K}^n - \int_{\Omega} \bar{u}_i^0(x) dx \right|$$

# First POD reduced model

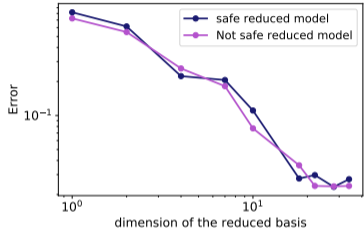
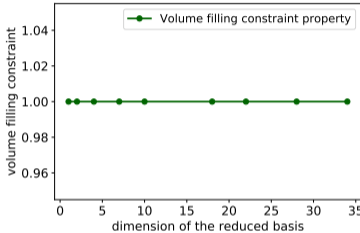
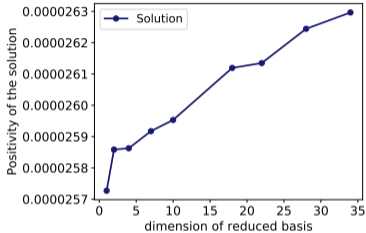


$$\inf_{n \in [1, N_t]} \inf_{\mu \in \mathcal{P}^{\text{off}}} \inf_{K \in \mathcal{T}_h} \sum_{i=1}^{N_s} \tilde{U}_{\mu, i, K}^n \quad \max_{\mu \in \mathcal{P}^{\text{off}}} \max_{i \in [1, N_s]} \max_{n \in [1, N_t]} \left| \sum_{K \in \mathcal{T}_h} |K| \bar{U}_{\mu, i, K}^n - \int_{\Omega} \bar{u}_i^0(x) dx \right|$$

**Violation of the physical properties.**



# Safe POD reduced model



$$\inf_{n \in \llbracket 1, N_t \rrbracket} \inf_{\mu \in \mathcal{P}^{\text{off}}} \inf_{K \in \mathcal{T}_h} \bar{U}_{\mu, K}^n \quad \inf_{n \in \llbracket 1, N_t \rrbracket} \inf_{\mu \in \mathcal{P}^{\text{off}}} \inf_{K \in \mathcal{T}_h} \sum_{i=1}^{N_s} \bar{U}_{\mu, i, K}^n$$

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



