Structure preserving reduced-order model for parametric cross-diffusion systems

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Outline

Motivation

Cross-diffusion systems arise in various application fields:

- *N. Shigesada, K. Kawasaki, E. Teramoto (1979)* population dynamics
- *T. L. Jackson and H. M. Byrne (2002)* growth of vascular tumors in medical biology
- *A. Bakhta and V. Ehrlacher (2018)* evolution of densities of chemical species composing a mixture

$$\partial_t u_i - \nabla \cdot (\sum_{j=0}^{N_s} G_{ij}(u_0, \cdots, u_{N_s}) \nabla u_j) = g_i(u_0, \cdots, u_n) \quad \text{in } \Omega \times [0, T]$$

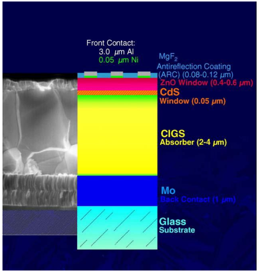
$$u(0, \cdot) = u^0 \quad \text{in} \quad \Omega$$

$$u_i(t, x) \geq 0, \quad \sum_{i=1}^{Ns} u_i(t, x) = 1 \quad \text{in} \quad \Omega \times [0, T]$$

Particular example of cross-diffusion system

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.

Theoretical analysis

Devise existence and uniqueness of solutions satisfying the constraints for n species with arbitrary cross-diffusion matrices is an open problem.

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The analysis framework is based on the so-called boundedness by entropy method. The main idea is to write the system of equations as a formal gradient flow and derive estimates on the solutions using the decay of some entropy functional.

Gradient flow structure

Entropy functional:

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

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*

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

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

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4. entropy-entropy dissipation relation

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

The cell-centered finite Volume method

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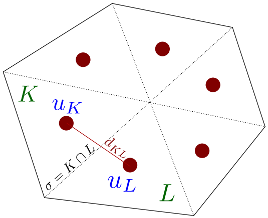

$D_{K\sigma}\mathbf{u}_i^n = u_{i,L}^n - u_{i,K}^n$

- 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 $u_{i,K}^0 = \frac{1}{|K|}\int_K u_i{}^0(x)\,\mathrm{dx}$
- FV scheme : find $\boldsymbol{U}^n \in \mathbb{R}^{N_e\times N_s}$ satisfying

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

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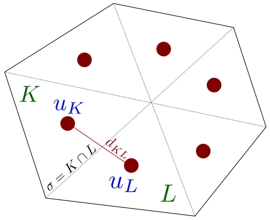

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Flux: $\mathcal{F}_{i,K\sigma}^n(\boldsymbol{U}^n) := -a^\star \tau_\sigma D_{K\sigma}\boldsymbol{u}_i^n - \tau_\sigma \left(\sum_{j=1}^N (a_{i,j} - a^\star)\left(u_{j,\sigma}^n D_{K\sigma}\boldsymbol{u}_i^n - u_{i,\sigma}^n D_{K\sigma}\boldsymbol{u}_j^n\right)\right).$

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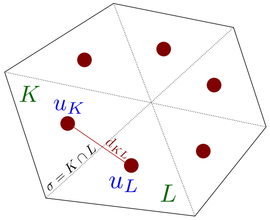

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$$\text{edge unknown } u_{i,\sigma}^n := \begin{cases} 0 & \text{if} \quad \min(u_{i,K}^n, u_{i,K\sigma}^n) < 0, \\ u_{i,K}^n & \text{if} \quad u_{i,K}^n = u_{i,K\sigma}^n \geq 0, \\ \dfrac{u_{i,K}^n - u_{i,K\sigma}^n}{\ln(u_{i,K}^n) - \ln(u_{i,K\sigma}^n)}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

Remark

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

Example:

Consider 2 *species and two elements* K *and* L *such that*

$$u^0_K = (0,1) \quad u^0_L = (1,0).$$

Here,

$$u^0_{1,K|L} = 0 \quad u^0_{2,K|L} = 0$$

Then,

$$\mathcal{F}^n_{i,K\sigma}(\boldsymbol{U}^n) = 0 \Rightarrow \textit{stationnary solution}$$

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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* $E_{\mathcal{T}_h}(\boldsymbol{U}^n) \leq E_{\mathcal{T}_h}(\boldsymbol{U}^{n-1}) \quad \forall n \in [1, N_t]$ *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

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

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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

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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 $\boldsymbol{B}^{n,k-1} \in \mathbb{R}^{N_e \times N_s}$ 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

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

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

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

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

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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 $\mathbb{M}\mathbb{M}^T$.

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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

The online stage

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

$$\widetilde{\boldsymbol{U}}_{\mu}^{n} := \sum_{k=1}^{r} c_{\mu}^{k,n} \boldsymbol{V}^k, \quad \widetilde{\boldsymbol{U}}_{\mu}^{0} := \boldsymbol{U}^0.$$

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

The online stage

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

6. We define the function $H : \mathbb{R}^r \to \mathbb{R}^r$ by $H_l(\boldsymbol{c}_\mu^n) := \langle \boldsymbol{V}^l, G^n(\widetilde{\boldsymbol{U}}_\mu^n) \rangle \quad \forall 1 \leq l \leq r$.

The online stage

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7. The vector $\boldsymbol{c}_{\mu}^{n} \in \mathbb{R}^r$ is solution to the nonlinear problem

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

Remark

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

We want to construct a reduced-order model preserving the structural properties of the solution

1. Positivity of the solution
2. mass conservation
3. Volume filling constraint
4. Decay of entropy

Outline

The offline stage

The offline stage

1. Compute snapshots of solutions.

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 $\overline{\mathbb{M}} = \left[\overline{\mathbb{M}}_{\mu_1} \quad \overline{\mathbb{M}}_{\mu_2} \quad \cdots \quad \overline{\mathbb{M}}_{\mu_{p^\star}} \right]$ where

$$\left[\overline{\mathbb{M}}_{\mu_\alpha}\right]_{i,K} = z^n_{\mu_\alpha,i,K} = \ln(u^n_{\mu_\alpha,i,K}) - \ln(u^n_{\mu_\alpha,N_s,K}) \quad \forall i \in [\![1, N_s - 1]\!] \quad \forall K \in \mathcal{T}_h$$

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3. We then denote by $\boldsymbol{V}^1, \cdots, \boldsymbol{V}^r \in \mathbb{R}^{N_h \times (N_s - 1)}$ the r first POD modes of the family $\left(\boldsymbol{Z}^n_\mu\right)_{\mu \in \mathcal{P}^{\text{off}}, 1 \leq n \leq N_t}$. In addition, for all $1 \leq i \leq N_s - 1$, we define
$$\boldsymbol{V}^{r+i} := \boldsymbol{I}^i,$$
where $\boldsymbol{I}^i \in \mathbb{R}^{(N_s - 1) \times N_h}$ is defined by
$$\boldsymbol{I}^i := (I^i_{j,K})_{K \in \mathcal{T}, 1 \leq j \leq N_s - 1} \quad \text{with} \quad I^i_{j,K} = \delta^i_j$$

Denote by $r^\star := r + N_s - 1$.

Example: $N_s = 3$

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

4. 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.

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5. The SP-ROM method construct a ROM approximation $\overline{\boldsymbol{Z}}_\mu^n$ of $\boldsymbol{Z}_\mu^n$ that reads

$$\overline{\boldsymbol{Z}}_\mu^n := \sum_{k=1}^{r^\star} c_\mu^{k,n} \boldsymbol{V}^k \qquad \text{where} \quad \boldsymbol{c}_\mu^n := \left(c_\mu^{k,n}\right)_{1 \le k \le r^\star} \in \mathbb{R}^{r^\star}$$

Here, the vector $\boldsymbol{c}_\mu^n$ is solution to the nonlinear system

$$\overline{H}_\mu^{n,l}(\boldsymbol{c}) := \left\langle \boldsymbol{W}^l, \overline{G}_\mu^n(\boldsymbol{c}) \right\rangle = 0 \quad \forall 1 \le l \le r^\star$$

6. Assuming that $\overline{\boldsymbol{Z}}_\mu^n$ is computed, a structure preserving ROM approximation $\overline{\boldsymbol{U}}_\mu^n = \left(\overline{u}_{\mu,i,K}^n\right)_{K\in\mathcal{T},1\leq i\leq N_s-1}$ of $\boldsymbol{U}_\mu^n$ is then computed as follows:

$$\overline{u}_{\mu,i,K}^n := \frac{e^{\overline{z}_{\mu,i,K}^n}}{1+\sum_{j=1}^{N_s-1} e^{\overline{z}_{\mu,j,K}^n}} \quad \forall K\in\mathcal{T}_h \quad \forall 1\leq i\leq N_s-1$$

$$\overline{u}_{\mu,N_s,K}^n = \frac{1}{1+\sum_{j=1}^{N_s-1} e^{\overline{z}_{\mu,j,K}^n}} \quad \forall K\in\mathcal{T}_h$$

Structural properties of the solution

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Structural properties of the solution

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

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2. Volume filling constraint: $\sum_{i=1}^{N_s} \overline{u}^n_{\mu,i,K} = 1 \quad \forall \mu \in \mathcal{P} \quad \forall K \in \mathcal{T}_h, \quad \forall n \in [1, N_\mathrm{t}]$.

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3. mass conservation

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

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4. The discrete counterpart of the entropy decays along time

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

Outline

First test case

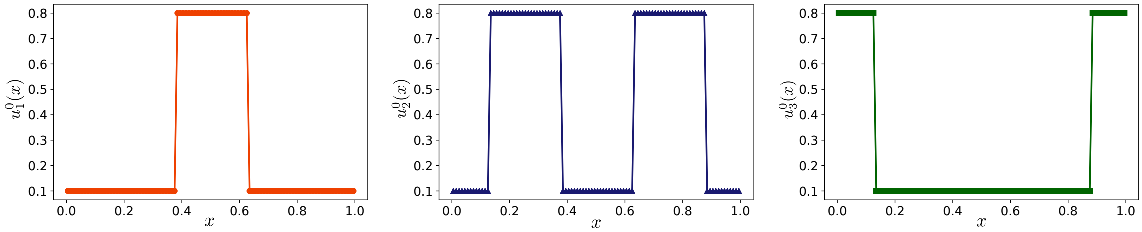
- number of species : $N_s = 3$
- Ω : 1D domain
- number of cells : 70
- $\Delta t = \Delta t_n := 1,6 \times 10^{-4}$ and the final simulation time is $T := 0.5$.
- Compute $\mu = 20$ snapshots of solutions.

Initial condition

$$u_1^0(x) := \begin{cases} 1-2\delta & \text{if } x \in \left[\frac{3}{8}, \frac{5}{8}\right] \\ \delta & \text{else,} \end{cases} \quad u_2^0(x) := \begin{cases} 1-2\delta & \text{if } x \in \left[\frac{1}{8}, \frac{3}{8}\right] \cap \left[\frac{5}{8}, \frac{7}{8}\right] \\ \delta & \text{else} \end{cases}$$

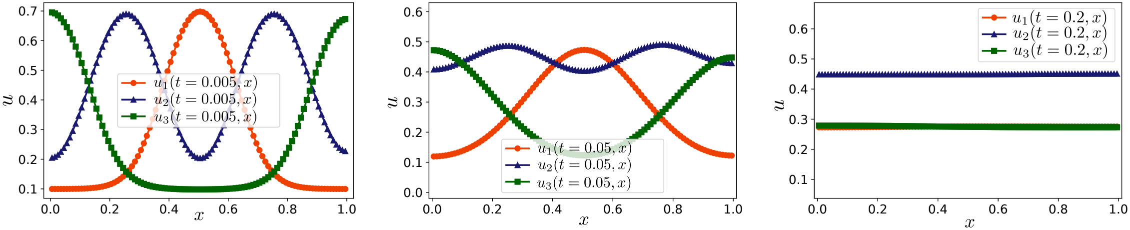
and

$$u_3^0(x) := \begin{cases} 1-2\delta & \text{if } x \in \left[0, \frac{1}{8}\right] \cap \left[\frac{7}{8}, 1\right] \\ \delta & \text{else.} \end{cases}$$



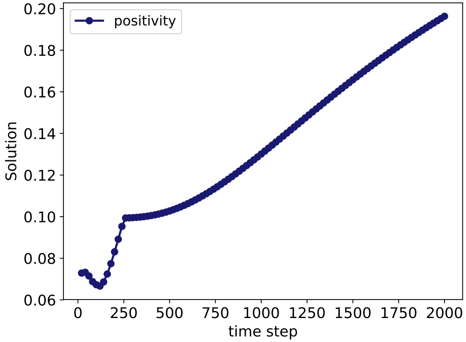
The high-fidelity problem

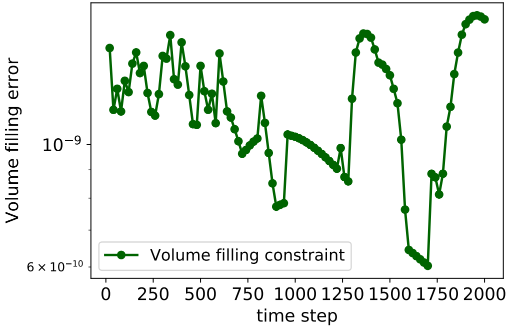
$$\mathbb{A}_{\mu} := \begin{pmatrix} 0 & 0.75 & 0.73 \\ 0.75 & 0 & 0.84 \\ 0.73 & 0.84 & 0 \end{pmatrix}$$



Typical behavior of a cross-diffusion system

Structural properties of the solution

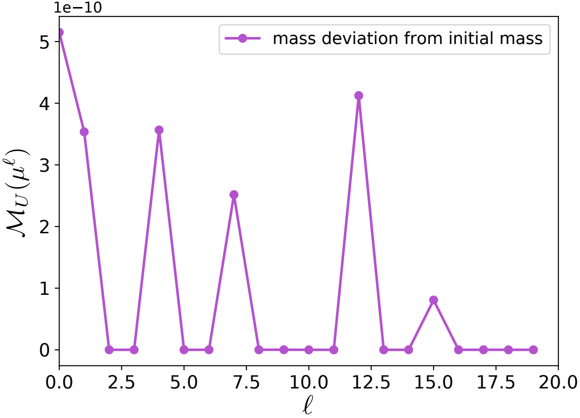




$$\mathcal{P}_U(t_n) := \inf_{\mu \in \mathcal{P}^{\text{off}}} \inf_{K \in \mathcal{T}_h} U^n_{\mu,K}$$

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

Positive and volume-filling constraint satisfied

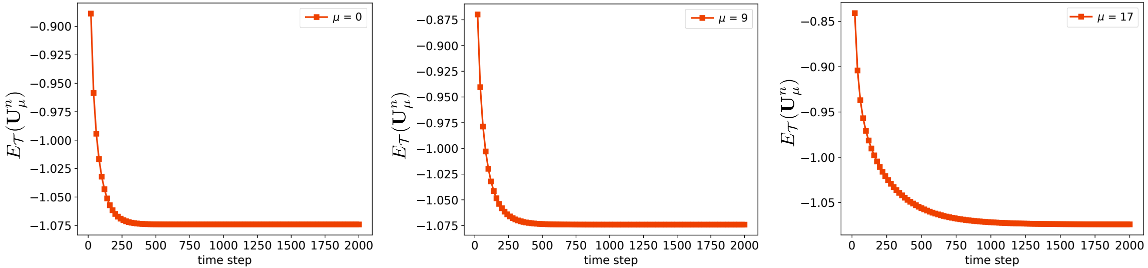


$$\mathcal{M}_U(\mu) := \max_{i\in[\![1,N_s]\!]} \max_{n\in[\![1,N_t]\!]} \left| \sum_{K\in\mathcal{T}_h} |K| U^n_{\mu,i,K} - \int_\Omega u_i{}^0(x)\,\mathrm{d}x \right|$$

Mass conservation property satisfied

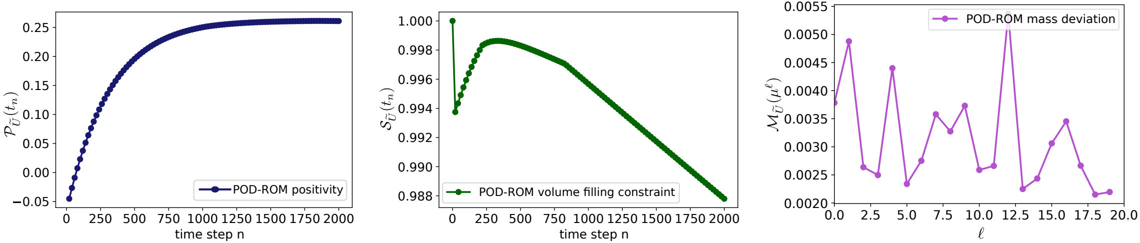
Structural properties of the Solution

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

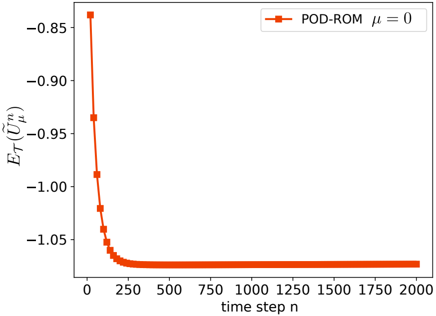


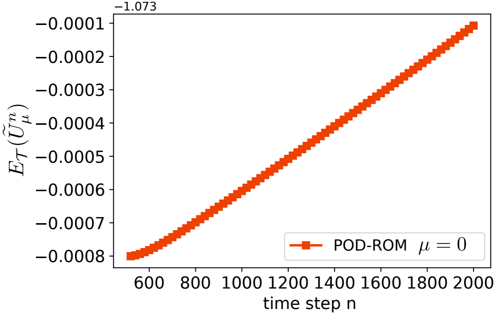
POD reduced model

Violation of the structural properties of the solution



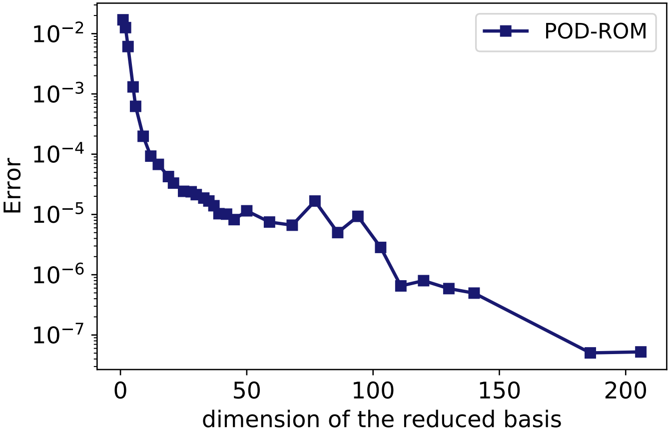
$$\mathbb{A}_0 = \begin{pmatrix} 0 & 0.93 & 0.71 \\ 0.93 & 0 & 0.44 \\ 0.71 & 0.44 & 0 \end{pmatrix}$$





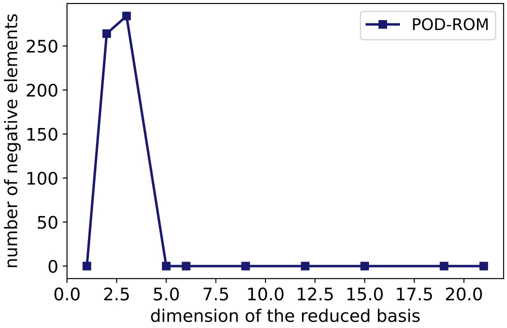
Violation of the decay of entropy

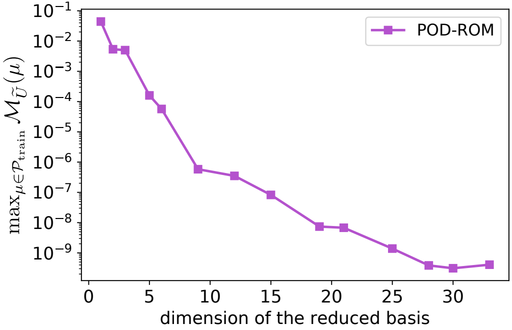
$$\max_{i\in[\![1,N_s]\!]} \left\| u_\mu^i - \tilde{u}_\mu^i \right\|_{L^\infty(\mathcal{P}^{\text{off}},L^2(\Omega),L^2([0,T]))} := \max_{i\in[\![1,N_s]\!]} \max_{\mu\in\mathcal{P}^{\text{off}}} \left(\int_0^T \left\| u_\mu^i - \tilde{u}_\mu^i \right\|^2_{L^2(\Omega)} (t)\, \mathrm{dt} \right)^{\frac{1}{2}}$$



POD-ROM error $\rightarrow 0$.

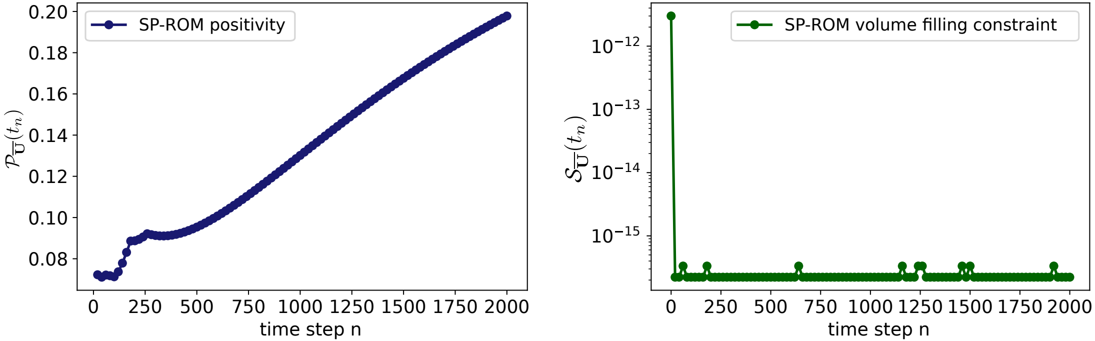
Complements



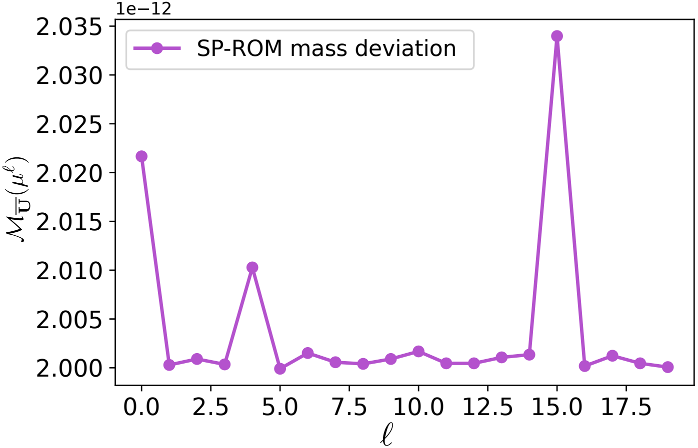


A surprising result occurs for $r = 1$...

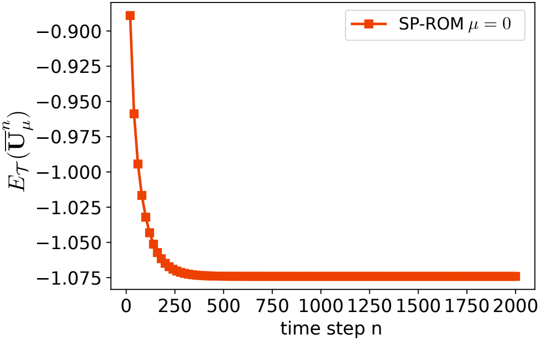
SP-ROM

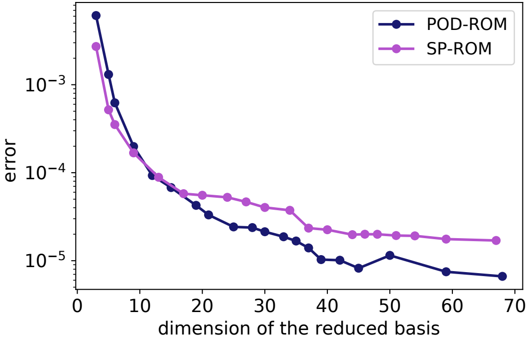


- **The solution is always positive**
- **The volume-filling constraint is satisfied**



The mass conservation property is satisfied





- **The entropy decreases with respect to time.**
- **The POD-ROM and SP-ROM error decrease with respect to the dimension of the reduced basis.**

Second test case : PVD process

- 4 species are injected under gaseous form in a hot chamber : copper, indium, gallium and selenium.
- Ω is a one dimensional domain consisting in a segment of length $L = 1m$.
- Final simulation time $T = 0.5$ s and $\Delta t = 2.5 \times 10^{-4}$ s.
- Compute $\mu = 20$ snapshots of solutions.

Initial condition

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

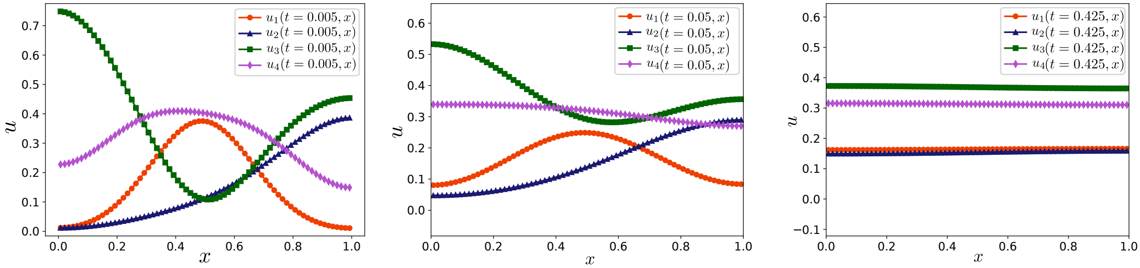
where $\varepsilon = 10^{-6}$, and employ a normalization

$$u_i^0(x) = \frac{w_i^0(x)}{\sum_{l=1}^{N_s} w_l^0(x)} \quad \forall i \in [\![1, 4]\!]$$

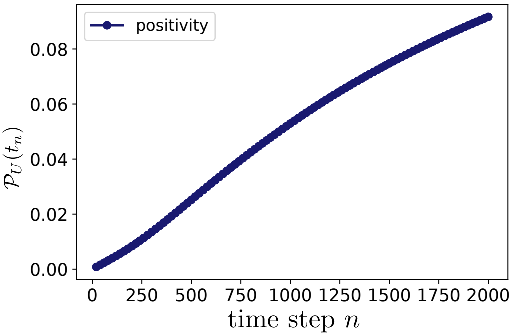
High-fidelity resolution

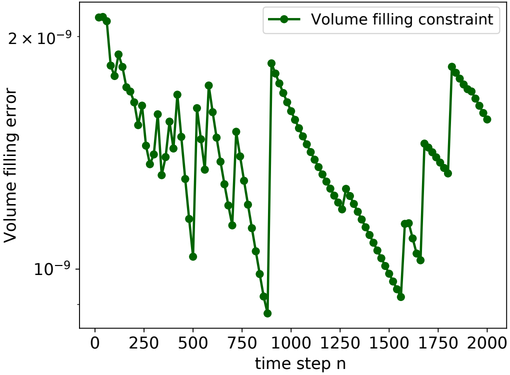
Cross-diffusion matrix

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

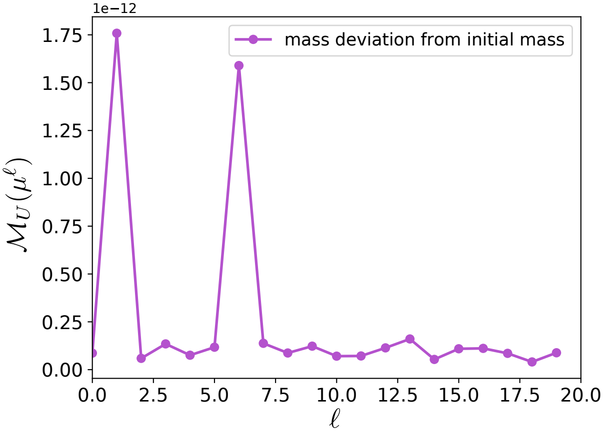


Properties of the solution



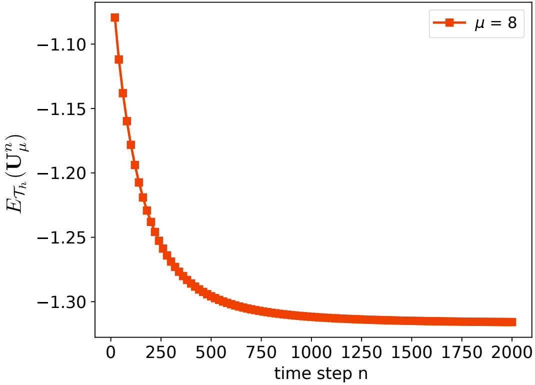


- **The solution is always positive**
- **The volume filling property is satisfied.**



The mass conservation property is satisfied

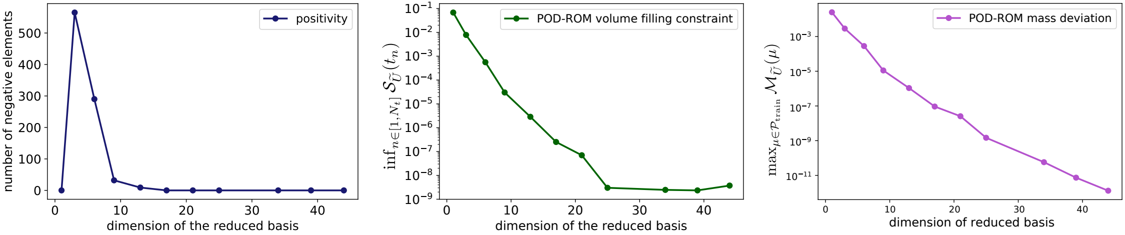
$$\mathbb{A}_8 = \begin{pmatrix} 0 & 0.36 & 0.19 & 0.64 \\ 0.36 & 0 & 0.07 & 0.61 \\ 0.19 & 0.07 & 0 & 0.51 \\ 0.64 & 0.61 & 0.51 & 0 \end{pmatrix}$$

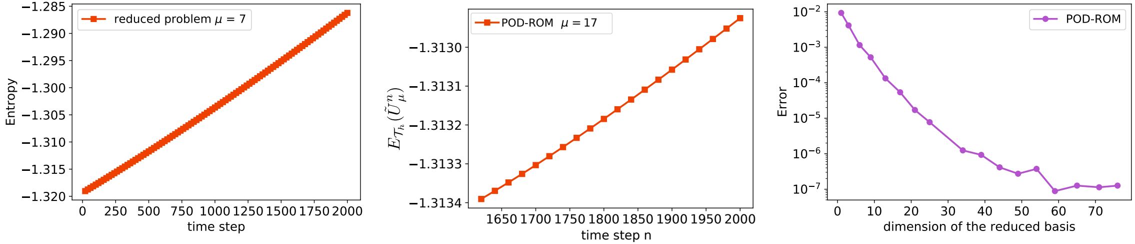


The entropy decreases with respect to time

POD-ROM

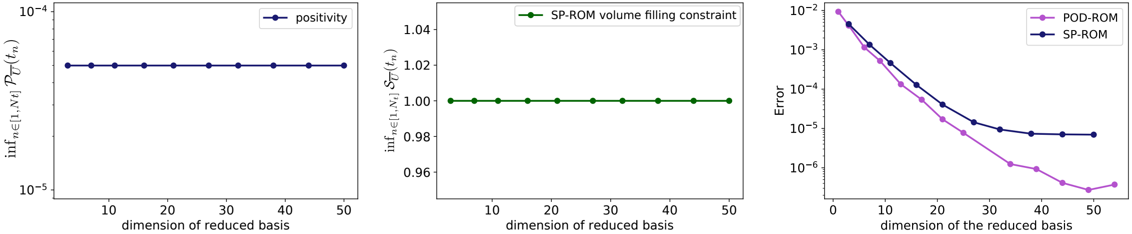
Violation of the physicial properties of the solution





- The entropy increases with respect to time
- The POD-ROM error decreases with respect to the dimension of the reduced basis

SP-ROM

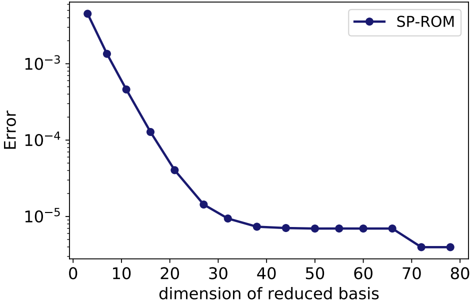


Left Figure : $\inf_{n\in[\![1,N_t]\!]} \inf_{\mu\in\mathcal{P}^{\mathrm{off}}} \inf_{K\in\mathcal{T}} \inf_{i\in[\![1,N_s]\!]} \overline{u}^n_{\mu,i,K}$

Middle figure : $\inf_{n\in[\![1,N_t]\!]} \inf_{\mu\in\mathcal{P}^{\mathrm{off}}} \inf_{K\in\mathcal{T}} \inf_{i\in[\![1,N_s]\!]} \overline{u}^n_{\mu,i,K}$

Validation stage

- We check the validity of the various reduced-order models for cross-diffusion coefficients which do not belong to the training set $\mathcal{P}^{\mathrm{off}}$.
- We select values of parameters μ in a subset $\mathcal{P}_{\mathrm{valid}}$ of $\mathcal{P}$, which is different from $\mathcal{P}^{\mathrm{off}}$
- Compare the error between the high-fidelity model and the ROMs. Here, $\mathrm{Card}(\mathcal{P}_{\mathrm{valid}}) = 20$



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.