A cross-diffusion Cahn-Hilliard system: existence and numerics

Jean Cauvin-Vila, joint work with V.Ehrlacher, G.Marino and J.-F. Pietschmann.

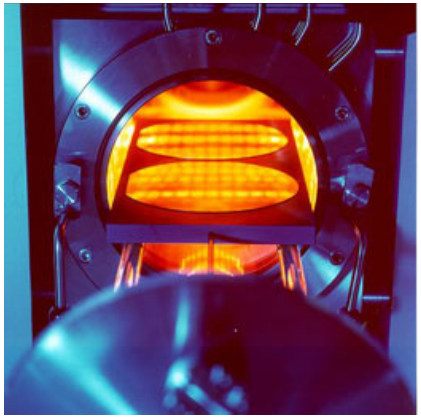
CERMICS, Ecole des Ponts and Inria Paris

NEEA workshop, Chemnitz, Sep 6-9, 2022

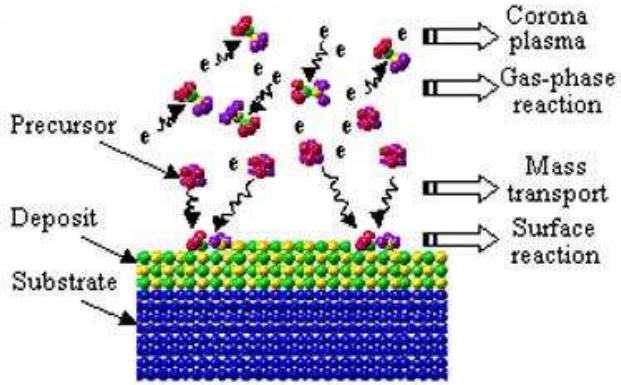
Outline of the talk

Outline of the talk

Motivation: fabrication of thin-film crystalline solar cells



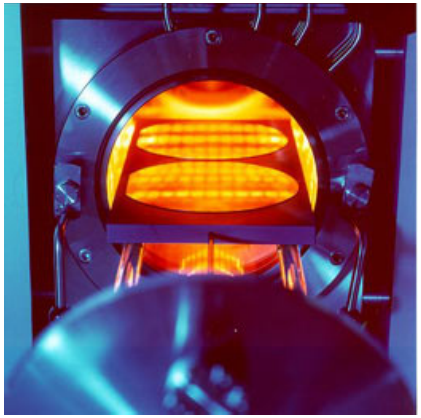
(a) Wafers in hot chamber



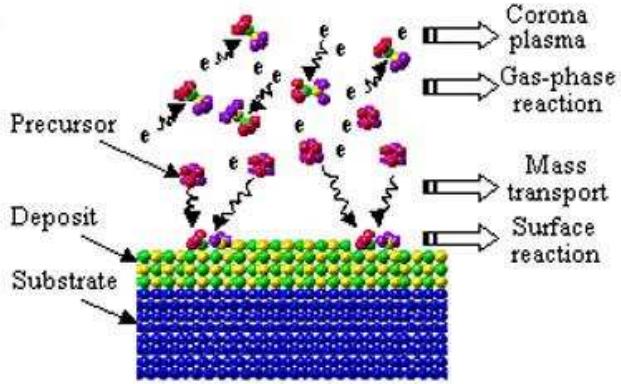
(b) Physical Vapor Deposition

Figure: CIGS cells fabrication

Motivation: fabrication of thin-film crystalline solar cells



(a) Wafers in hot chamber



(b) Physical Vapor Deposition

Figure: CIGS cells fabrication

Two main phenomena:

- Evolution of the surface of the film.
- Diffusion of the various species in the bulk due to the high temperature.

Cross-diffusion with size exclusion: PVD system[1]

- $n+1$ chemical species with volumic fractions $u_0(t,x), \dots, u_n(t,x)$, and volume-filling constraints:

$$\forall\ 0 \leqslant i \leqslant n,\ \ u_i(t,x) \geqslant 0 \text{ and } \sum_{j=0}^{n} u_j(t,x) = 1.$$

[1] Bakhta and V. Ehrlacher 2018.

Cross-diffusion with size exclusion: PVD system[1]

- $n+1$ chemical species with volumic fractions $u_0(t,x), \dots, u_n(t,x)$, and volume-filling constraints:

$$\forall\ 0 \leqslant i \leqslant n,\ \ u_i(t,x) \geqslant 0 \text{ and } \sum_{j=0}^{n} u_j(t,x) = 1.$$

- Cross-diffusion equations formally derived from a stochastic hopping model on a network: for $0 \leqslant i \leqslant n$,

$$\partial_t u_i - \operatorname{div}_x \left(\sum_{j=0}^{n} K_{ij} \left(u_j \nabla_x u_i - u_i \nabla_x u_j \right) \right) = 0,$$

for some coefficients $K_{ij} = K_{ji} > 0$ (non-degeneracy assumption).

[1] Bakhta and V. Ehrlacher 2018.

Cross-diffusion with size exclusion: PVD system[1]

- $n+1$ chemical species with volumic fractions $u_0(t,x), \dots, u_n(t,x)$, and volume-filling constraints:

$$\forall\ 0 \leqslant i \leqslant n,\ \ u_i(t,x) \geqslant 0 \text{ and } \sum_{j=0}^{n} u_j(t,x) = 1.$$

- Cross-diffusion equations formally derived from a stochastic hopping model on a network: for $0 \leqslant i \leqslant n$,

$$\partial_t u_i - \operatorname{div}_x \left(\sum_{j=0}^{n} K_{ij} \left(u_j \nabla_x u_i - u_i \nabla_x u_j \right) \right) = 0,$$

  for some coefficients $K_{ij} = K_{ji} > 0$ (non-degeneracy assumption).

- The unknown vector $u := (u_0, \dots, u_n)^T$ solves the system:

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

  with the (non-symmetric) diffusion matrix

$$\begin{cases} A_{ii}(u) = \displaystyle\sum_{0 \leqslant k \neq i \leqslant n} K_{ik} u_k, \\ A_{ij}(u) = -K_{ij} u_i. \end{cases}$$

[1] Bakhta and V. Ehrlacher 2018.

Entropic structure and analysis of the PVD system[4]

- The system is shown to admit an entropy structure[2], with respect to the Boltzmann entropy:

$$E(u) := \int_\Omega \sum_{i=0}^{n} u_i \log(u_i) - u_i + 1,$$

[2] Jüngel 2015.
[3] Otto 2001.
[4] Bakhta and V. Ehrlacher 2018.

Entropic structure and analysis of the PVD system[4]

- The system is shown to admit an entropy structure[2], with respect to the Boltzmann entropy:

$$E(u) := \int_\Omega \sum_{i=0}^{n} u_i \log(u_i) - u_i + 1,$$

that is, it rewrites formally as a Otto gradient flow[3]

$$\partial_t u - \mathrm{div}_x \left(M(u) \nabla_x \frac{\delta E}{\delta u} \right) = 0,$$

[2] Jüngel 2015.
[3] Otto 2001.
[4] Bakhta and V. Ehrlacher 2018.

Entropic structure and analysis of the PVD system[4]

- The system is shown to admit an entropy structure[2], with respect to the Boltzmann entropy:

$$E(u) := \int_\Omega \sum_{i=0}^{n} u_i \log(u_i) - u_i + 1,$$

that is, it rewrites formally as a Otto gradient flow[3]

$$\partial_t u - \mathrm{div}_x \left(M(u) \nabla_x \frac{\delta E}{\delta u} \right) = 0,$$

with the nonlinear, degenerate, positive semi-definite mobility matrix $M(u)$ given by

$$\begin{cases} M_{ii}(u) = \displaystyle\sum_{0 \leqslant j \neq i \leqslant n} K_{ij} u_i u_j, \\ M_{ij}(u) = -K_{ij} u_i u_j. \end{cases}$$

[2] Jüngel 2015.
[3] Otto 2001.
[4] Bakhta and V. Ehrlacher 2018.

Entropic structure and analysis of the PVD system[4]

- The system is shown to admit an entropy structure[2], with respect to the Boltzmann entropy:

$$E(u) := \int_\Omega \sum_{i=0}^{n} u_i \log(u_i) - u_i + 1,$$

that is, it rewrites formally as a Otto gradient flow[3]

$$\partial_t u - \operatorname{div}_x \left(M(u) \nabla_x \frac{\delta E}{\delta u} \right) = 0,$$

with the nonlinear, degenerate, positive semi-definite mobility matrix $M(u)$ given by

$$\begin{cases} M_{ii}(u) = \displaystyle\sum_{0 \leqslant j \neq i \leqslant n} K_{ij} u_i u_j, \\ M_{ij}(u) = -K_{ij} u_i u_j. \end{cases}$$

- Existence of weak solutions to this system in a fixed domain follows from the *Boundedness by entropy method*. It was extended to a moving one-dimensional domain by Bakhta and Ehrlacher.

[2] Jüngel 2015.
[3] Otto 2001.
[4] Bakhta and V. Ehrlacher 2018.

Adding a Cahn-Hilliard contribution[5]

- Motivation: to understand the evolution of the moving interface → diffuse interface approach.

[5] Ehrlacher, Marino, and Pietschmann 2021.

Adding a Cahn-Hilliard contribution[5]

- Motivation: to understand the evolution of the moving interface → diffuse interface approach.
- Now modify the free energy into

$$E_{\epsilon,\beta}(u) := \int_\Omega \sum_{i=0}^{n} (u_i \log(u_i) - u_i + 1) + \frac{\epsilon}{2}|\nabla u_0|^2 + \beta u_0(1-u_0),$$

for some positive constants $\epsilon, \beta > 0$, and consider the new system:

$$\partial_t u - \mathrm{div}_x \left(M(u) \nabla_x \frac{\delta E_{\epsilon,\beta}}{\delta u} \right) = 0.$$

[5] Ehrlacher, Marino, and Pietschmann 2021.

Adding a Cahn-Hilliard contribution[5]

- Motivation: to understand the evolution of the moving interface → diffuse interface approach.
- Now modify the free energy into

$$E_{\epsilon,\beta}(u) := \int_\Omega \sum_{i=0}^{n} (u_i \log(u_i) - u_i + 1) + \frac{\epsilon}{2}|\nabla u_0|^2 + \beta u_0(1-u_0),$$

for some positive constants $\epsilon, \beta > 0$, and consider the new system:

$$\partial_t u - \mathrm{div}_x \left(M(u) \nabla_x \frac{\delta E_{\epsilon,\beta}}{\delta u} \right) = 0.$$

- Introducing the auxiliary variable

$$w_0 := -\epsilon \Delta u_0 + \beta(1 - 2u_0),$$

[5] Ehrlacher, Marino, and Pietschmann 2021.

Adding a Cahn-Hilliard contribution[5]

- Motivation: to understand the evolution of the moving interface → diffuse interface approach.
- Now modify the free energy into

$$E_{\epsilon,\beta}(u) := \int_\Omega \sum_{i=0}^{n} (u_i \log(u_i) - u_i + 1) + \frac{\epsilon}{2}|\nabla u_0|^2 + \beta u_0(1-u_0),$$

for some positive constants $\epsilon, \beta > 0$, and consider the new system:

$$\partial_t u - \mathrm{div}_x \left(M(u) \nabla_x \frac{\delta E_{\epsilon,\beta}}{\delta u} \right) = 0.$$

- Introducing the auxiliary variable

$$w_0 := -\epsilon \Delta u_0 + \beta(1-2u_0),$$

the scalar form of the system reads, for $i = 1, \dots, n$

$$\partial_t u_i - \mathrm{div} \left(\sum_{0 \leqslant j \neq i \leqslant n} K_{ij}(u_j \nabla u_i - u_i \nabla u_j) - K_{i0} u_i u_0 \nabla w_0 \right) = 0,$$

and

$$\partial_t u_0 - \mathrm{div} \left(\sum_{1 \leqslant i \leqslant n} K_{i0}(u_i \nabla u_0 - u_0 \nabla u_i) + \sum_{i=1}^{n} K_{i0} u_i u_0 \nabla w_0 \right) = 0.$$

[5] Ehrlacher, Marino, and Pietschmann 2021.

Main steps of the analysis[6]

The strategy of the authors is as follows:

- First approximate the system by a time-discrete and regularized system.

[6] Ehrlacher, Marino, and Pietschmann 2021.

Main steps of the analysis[6]

The strategy of the authors is as follows:

- First approximate the system by a time-discrete and regularized system. The problem is that the *Boundedness by entropy method* does not readily apply, since the free energy density reads

$$h(u) := \sum_{i=0}^{n} (u_i \log(u_i) - u_i + 1) + \frac{\epsilon}{2} |\nabla u_0|^2 + \beta u_0 (1 - u_0),$$

  whose partial derivative with respect to u_0 can no longer be explicitly inverted (in consequence no free L^∞ bounds on u_0).

[6] Ehrlacher, Marino, and Pietschmann 2021.

Main steps of the analysis[6]

The strategy of the authors is as follows:

- First approximate the system by a time-discrete and regularized system. The problem is that the *Boundedness by entropy method* does not readily apply, since the free energy density reads

$$h(u) := \sum_{i=0}^{n} (u_i \log(u_i) - u_i + 1) + \frac{\epsilon}{2} |\nabla u_0|^2 + \beta u_0 (1 - u_0),$$

  whose partial derivative with respect to u_0 can no longer be explicitly inverted (in consequence no free L^∞ bounds on u_0). Instead, the authors had to study a system of elliptic PDEs with logarithmic nonlinearities with variational methods.

[6] Ehrlacher, Marino, and Pietschmann 2021.

Main steps of the analysis[6]

The strategy of the authors is as follows:

- First approximate the system by a time-discrete and regularized system. The problem is that the *Boundedness by entropy method* does not readily apply, since the free energy density reads

$$h(u) := \sum_{i=0}^{n} (u_i \log(u_i) - u_i + 1) + \frac{\epsilon}{2} |\nabla u_0|^2 + \beta u_0 (1 - u_0),$$

  whose partial derivative with respect to u_0 can no longer be explicitly inverted (in consequence no free L^∞ bounds on u_0). Instead, the authors had to study a system of elliptic PDEs with logarithmic nonlinearities with variational methods.

- Derive enough estimates on the approximate system to pass to the limit. The difficulty is that, contrary to classical CH, only u_0 will enjoy H^2 regularity. In consequence the convergence of the additional CH term for the equations of the other u_i in the approximate system is not straightforward and requires to be carefully analyzed.

[6] Ehrlacher, Marino, and Pietschmann 2021.

Main steps of the analysis[6]

The strategy of the authors is as follows:

- First approximate the system by a time-discrete and regularized system. The problem is that the *Boundedness by entropy method* does not readily apply, since the free energy density reads

$$h(u) := \sum_{i=0}^{n} (u_i \log(u_i) - u_i + 1) + \frac{\epsilon}{2} |\nabla u_0|^2 + \beta u_0 (1 - u_0),$$

  whose partial derivative with respect to u_0 can no longer be explicitly inverted (in consequence no free L^∞ bounds on u_0). Instead, the authors had to study a system of elliptic PDEs with logarithmic nonlinearities with variational methods.

- Derive enough estimates on the approximate system to pass to the limit. The difficulty is that, contrary to classical CH, only u_0 will enjoy H^2 regularity. In consequence the convergence of the additional CH term for the equations of the other u_i in the approximate system is not straightforward and requires to be carefully analyzed.

Theorem (Ehrlacher, Marino, Pietschmann, '21)

Let Ω be a regular domain of $\mathbb{R}^d$, with $d = 1, 2, 3$. Let $u^0 := (u_0^0, \dots, u_n^0) \in H^1(\Omega, \mathbb{R}^{n+1})$ be an initial condition satisfying the volume-filling constraints. Then there exists at least one weak solution to the CDCH system.

[6] Ehrlacher, Marino, and Pietschmann 2021.

Outline of the talk

Finite volume numerical approximation

- Two Point Finite Volume approximation with mesh $(\mathcal{T}, \mathcal{E}, (x_K)_{K\in\mathcal{T}})$ that satisfies the orthogonality condition. m_K is the measure of cell K, m_σ the measure of face σ. $\sigma = K|L$ may denote the face between cells L and K. $\mathcal{E}_{K,\mathrm{int}}$ is the set of faces of K that are not on the boundary. For a face $\sigma \in \mathcal{E}_{K,\mathrm{int}}$, we may write $\sigma = K|L$, meaning that $\sigma = \overline{K} \cap \overline{L}$, where $L \in \mathcal{T}$. We also define $d_\sigma := |x_K - x_L|$ and $\tau_\sigma = \frac{m_\sigma}{d_\sigma}$.

Finite volume numerical approximation

- Two Point Finite Volume approximation with mesh $(\mathcal{T}, \mathcal{E}, (x_K)_{K\in\mathcal{T}})$ that satisfies the orthogonality condition. m_K is the measure of cell K, m_σ the measure of face σ. $\sigma = K|L$ may denote the face between cells L and K. $\mathcal{E}_{K,\mathrm{int}}$ is the set of faces of K that are not on the boundary. For a face $\sigma \in \mathcal{E}_{K,\mathrm{int}}$, we may write $\sigma = K|L$, meaning that $\sigma = \overline{K} \cap \overline{L}$, where $L \in \mathcal{T}$. We also define $d_\sigma := |x_K - x_L|$ and $\tau_\sigma = \frac{m_\sigma}{d_\sigma}$.
- Discrete gradients are defined as

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

where $v_{K\sigma}$ is the mirror value of v_K across σ.

Finite volume numerical approximation

- Two Point Finite Volume approximation with mesh $(\mathcal{T}, \mathcal{E}, (x_K)_{K\in\mathcal{T}})$ that satisfies the orthogonality condition. m_K is the measure of cell K, m_σ the measure of face σ. $\sigma = K|L$ may denote the face between cells L and K. $\mathcal{E}_{K,\mathrm{int}}$ is the set of faces of K that are not on the boundary. For a face $\sigma \in \mathcal{E}_{K,\mathrm{int}}$, we may write $\sigma = K|L$, meaning that $\sigma = \overline{K} \cap \overline{L}$, where $L \in \mathcal{T}$. We also define $d_\sigma := |x_K - x_L|$ and $\tau_\sigma = \frac{m_\sigma}{d_\sigma}$.
- Discrete gradients are defined as

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

  where $v_{K\sigma}$ is the mirror value of v_K across σ.
- Assume that $\boldsymbol{u}^p = \left(u_{i,K}^p\right)_{K\in\mathcal{T},0\leqslant i\leqslant n}$ is given for some $p \in \mathbb{N}$, then we have to define how to compute the discrete volume fractions $\boldsymbol{u}^{p+1} = \left(u_{i,K}^{p+1}\right)_{K\in\mathcal{T},0\leqslant i\leqslant n}$ and the discrete fluxes $\boldsymbol{J}^{p+1} = \left(J_{i,K\sigma}^{p+1}\right)_{\sigma\in\mathcal{E},0\leqslant i\leqslant n}$.

Finite volume numerical approximation

- Two Point Finite Volume approximation with mesh $(\mathcal{T}, \mathcal{E}, (x_K)_{K\in\mathcal{T}})$ that satisfies the orthogonality condition. m_K is the measure of cell K, m_σ the measure of face σ. $\sigma = K|L$ may denote the face between cells L and K. $\mathcal{E}_{K,\mathrm{int}}$ is the set of faces of K that are not on the boundary. For a face $\sigma \in \mathcal{E}_{K,\mathrm{int}}$, we may write $\sigma = K|L$, meaning that $\sigma = \overline{K} \cap \overline{L}$, where $L \in \mathcal{T}$. We also define $d_\sigma := |x_K - x_L|$ and $\tau_\sigma = \frac{m_\sigma}{d_\sigma}$.
- Discrete gradients are defined as

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

  where $v_{K\sigma}$ is the mirror value of v_K across σ.
- Assume that $\boldsymbol{u}^p = \left(u_{i,K}^p\right)_{K\in\mathcal{T}, 0\leqslant i\leqslant n}$ is given for some $p \in \mathbb{N}$, then we have to define how to compute the discrete volume fractions $\boldsymbol{u}^{p+1} = \left(u_{i,K}^{p+1}\right)_{K\in\mathcal{T}, 0\leqslant i\leqslant n}$ and the discrete fluxes $\boldsymbol{J}^{p+1} = \left(J_{i,K\sigma}^{p+1}\right)_{\sigma\in\mathcal{E}, 0\leqslant i\leqslant n}$.
- Conservative laws:

$$m_K \frac{u_{i,K}^{p+1} - u_{i,K}^p}{\Delta t_p} + \sum_{\sigma\in\mathcal{E}_{K,\mathrm{int}}} J_{i,K\sigma}^{p+1} = 0, \quad \forall K \in \mathcal{T},\ \forall 0 \leqslant i \leqslant n.$$

The semi-implicit scheme: extension of the PVD scheme[8]

- The edge values $u_{i,\sigma}^{p+1}$ are defined through a logarithmic mean as follows:

$$u_{i,\sigma}^{p+1} = \begin{cases} 0 & \text{if } \min(u_{i,K}^{p+1}, u_{i,K\sigma}^{p+1}) \leqslant 0, \\ u_{i,K}^{p+1} & \text{if } 0 < u_{i,K}^{p+1} = u_{i,K\sigma}^{p+1}, \\ \dfrac{u_{i,K}^{p+1} - u_{i,K\sigma}^{p+1}}{\log(u_{i,K}^{p+1}) - \log(u_{i,K\sigma}^{p+1})} & \text{otherwise,} \end{cases} \tag{1}$$

[7] Eyre 1997.

[8] Cancès and Gaudeul 2020.

The semi-implicit scheme: extension of the PVD scheme[8]

- The edge values $u_{i,\sigma}^{p+1}$ are defined through a logarithmic mean as follows:

$$u_{i,\sigma}^{p+1} = \begin{cases} 0 & \text{if } \min(u_{i,K}^{p+1}, u_{i,K\sigma}^{p+1}) \leqslant 0, \\ u_{i,K}^{p+1} & \text{if } 0 < u_{i,K}^{p+1} = u_{i,K\sigma}^{p+1}, \\ \dfrac{u_{i,K}^{p+1} - u_{i,K\sigma}^{p+1}}{\log(u_{i,K}^{p+1}) - \log(u_{i,K\sigma}^{p+1})} & \text{otherwise,} \end{cases} \tag{1}$$

so that the discrete chain rule holds: if $u_{i,K}^{p+1}, u_{i,K\sigma}^{p+1} > 0$ then

$$D_{K\sigma} \boldsymbol{u}_i^{p+1} = u_{i,\sigma}^{p+1} D_{K\sigma} \log(\boldsymbol{u}_i^{p+1}).$$

[7] Eyre 1997.

[8] Cancès and Gaudeul 2020.

The semi-implicit scheme: extension of the PVD scheme[8]

- The edge values $u_{i,\sigma}^{p+1}$ are defined through a logarithmic mean as follows:

$$u_{i,\sigma}^{p+1} = \begin{cases} 0 & \text{if } \min(u_{i,K}^{p+1}, u_{i,K\sigma}^{p+1}) \leqslant 0, \\ u_{i,K}^{p+1} & \text{if } 0 < u_{i,K}^{p+1} = u_{i,K\sigma}^{p+1}, \\ \dfrac{u_{i,K}^{p+1} - u_{i,K\sigma}^{p+1}}{\log(u_{i,K}^{p+1}) - \log(u_{i,K\sigma}^{p+1})} & \text{otherwise,} \end{cases} \tag{1}$$

  so that the discrete chain rule holds: if $u_{i,K}^{p+1}, u_{i,K\sigma}^{p+1} > 0$ then

$$D_{K\sigma} \boldsymbol{u}_i^{p+1} = u_{i,\sigma}^{p+1} D_{K\sigma} \log(\boldsymbol{u}_i^{p+1}).$$

- The variable w_0 is discretized as: for any $K \in \mathcal{T}$,

$$w_{0,K}^{p+\frac{1}{2}} = -\frac{\epsilon}{m_K} \sum_{\sigma \in \mathcal{E}_{K,\mathrm{int}}} \tau_\sigma D_{K\sigma} \boldsymbol{u}_0^{p+1} + \beta(1 - 2u_{0,K}^p),$$

[7] Eyre 1997.

[8] Cancès and Gaudeul 2020.

The semi-implicit scheme: extension of the PVD scheme[8]

- The edge values $u_{i,\sigma}^{p+1}$ are defined through a logarithmic mean as follows:

$$u_{i,\sigma}^{p+1} = \begin{cases} 0 & \text{if } \min(u_{i,K}^{p+1}, u_{i,K\sigma}^{p+1}) \leqslant 0, \\ u_{i,K}^{p+1} & \text{if } 0 < u_{i,K}^{p+1} = u_{i,K\sigma}^{p+1}, \\ \dfrac{u_{i,K}^{p+1} - u_{i,K\sigma}^{p+1}}{\log(u_{i,K}^{p+1}) - \log(u_{i,K\sigma}^{p+1})} & \text{otherwise,} \end{cases} \tag{1}$$

  so that the discrete chain rule holds: if $u_{i,K}^{p+1}, u_{i,K\sigma}^{p+1} > 0$ then

$$D_{K\sigma} \boldsymbol{u}_i^{p+1} = u_{i,\sigma}^{p+1} D_{K\sigma} \log(\boldsymbol{u}_i^{p+1}).$$

- The variable w_0 is discretized as: for any $K \in \mathcal{T}$,

$$w_{0,K}^{p+\frac{1}{2}} = -\frac{\epsilon}{m_K} \sum_{\sigma \in \mathcal{E}_{K,\mathrm{int}}} \tau_\sigma D_{K\sigma} \boldsymbol{u}_0^{p+1} + \beta(1 - 2u_{0,K}^p),$$

  Remark that the convex part of the free energy $\frac{\epsilon}{2}|\nabla u_0|^2$ is discretized implicitly while the concave part $\beta u_0(1-u_0)$ is discretized explicitly.[7]

[7] Eyre 1997.

[8] Cancès and Gaudeul 2020.

The semi-implicit scheme: extension of the PVD scheme

Additionally a parameter $K^\star > 0$ is introduced to avoid unphysical solutions when the volumic fractions reach 0.[9]

[9] Cancès and Gaudeul 2020.

The semi-implicit scheme: extension of the PVD scheme

Additionally a parameter $K^\star > 0$ is introduced to avoid unphysical solutions when the volumic fractions reach 0.[9] Finally the fluxes are discretized as:

$$J_{i,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_i^{p+1} - \tau_\sigma \sum_{0\leqslant j\neq i\leqslant n} (K_{ij} - K^\star)\left(u_{j,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1} - u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_j^{p+1}\right)$$

$$+ \tau_\sigma K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}},\ 1 \leqslant i \leqslant n,$$

[9] Cancès and Gaudeul 2020.

The semi-implicit scheme: extension of the PVD scheme

Additionally a parameter $K^\star > 0$ is introduced to avoid unphysical solutions when the volumic fractions reach 0.[9] Finally the fluxes are discretized as:

$$J_{i,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_i^{p+1} - \tau_\sigma \sum_{0\leqslant j\neq i\leqslant n} (K_{ij} - K^\star)\left(u_{j,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1} - u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_j^{p+1}\right)$$

$$+ \tau_\sigma K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}},\ 1 \leqslant i \leqslant n,$$

$$J_{0,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_0^{p+1} - \tau_\sigma \sum_{i=1}^{n} (K_{i0} - K^\star)\left(u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_0^{p+1} - u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1}\right)$$

$$- \tau_\sigma \sum_{i=1}^{n} K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}}.$$

[9] Cancès and Gaudeul 2020.

The semi-implicit scheme: extension of the PVD scheme

Additionally a parameter $K^\star > 0$ is introduced to avoid unphysical solutions when the volumic fractions reach 0.[9] Finally the fluxes are discretized as:

$$J_{i,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_i^{p+1} - \tau_\sigma \sum_{0\leqslant j\neq i\leqslant n} (K_{ij} - K^\star)\left(u_{j,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1} - u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_j^{p+1}\right)$$

$$+ \tau_\sigma K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}},\ 1 \leqslant i \leqslant n,$$

$$J_{0,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_0^{p+1} - \tau_\sigma \sum_{i=1}^{n} (K_{i0} - K^\star)\left(u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_0^{p+1} - u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1}\right)$$

$$- \tau_\sigma \sum_{i=1}^{n} K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}}.$$

Basic properties of the scheme:

[9] Cancès and Gaudeul 2020.

The semi-implicit scheme: extension of the PVD scheme

Additionally a parameter $K^\star > 0$ is introduced to avoid unphysical solutions when the volumic fractions reach 0.[9] Finally the fluxes are discretized as:

$$J_{i,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_i^{p+1} - \tau_\sigma \sum_{0\leqslant j\neq i\leqslant n} (K_{ij} - K^\star)\left(u_{j,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1} - u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_j^{p+1}\right)$$

$$+ \tau_\sigma K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}},\ 1 \leqslant i \leqslant n,$$

$$J_{0,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_0^{p+1} - \tau_\sigma \sum_{i=1}^{n} (K_{i0} - K^\star)\left(u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_0^{p+1} - u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1}\right)$$

$$- \tau_\sigma \sum_{i=1}^{n} K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}}.$$

Basic properties of the scheme:

- Mass conservation (conservativity).

[9] Cancès and Gaudeul 2020.

The semi-implicit scheme: extension of the PVD scheme

Additionally a parameter $K^\star > 0$ is introduced to avoid unphysical solutions when the volumic fractions reach 0.[9] Finally the fluxes are discretized as:

$$J_{i,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_i^{p+1} - \tau_\sigma \sum_{0\leqslant j\neq i\leqslant n} (K_{ij} - K^\star)\left(u_{j,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1} - u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_j^{p+1}\right)$$

$$+ \tau_\sigma K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}},\ 1 \leqslant i \leqslant n,$$

$$J_{0,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_0^{p+1} - \tau_\sigma \sum_{i=1}^{n} (K_{i0} - K^\star)\left(u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_0^{p+1} - u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1}\right)$$

$$- \tau_\sigma \sum_{i=1}^{n} K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}}.$$

Basic properties of the scheme:

- Mass conservation (conservativity).
- Preservation of volume-filling constraints (sum the equations).

[9] Cancès and Gaudeul 2020.

The semi-implicit scheme: extension of the PVD scheme

Additionally a parameter $K^\star > 0$ is introduced to avoid unphysical solutions when the volumic fractions reach 0.[9] Finally the fluxes are discretized as:

$$J_{i,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_i^{p+1} - \tau_\sigma \sum_{0\leqslant j\neq i\leqslant n} (K_{ij} - K^\star)\left(u_{j,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1} - u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_j^{p+1}\right)$$

$$+ \tau_\sigma K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}},\ 1 \leqslant i \leqslant n,$$

$$J_{0,K\sigma}^{p+1} = -\tau_\sigma K^\star D_{K\sigma}\boldsymbol{u}_0^{p+1} - \tau_\sigma \sum_{i=1}^{n} (K_{i0} - K^\star)\left(u_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_0^{p+1} - u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{u}_i^{p+1}\right)$$

$$- \tau_\sigma \sum_{i=1}^{n} K_{i0} u_{i,\sigma}^{p+1} u_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{w}_0^{p+\frac{1}{2}}.$$

Basic properties of the scheme:

- Mass conservation (conservativity).
- Preservation of volume-filling constraints (sum the equations).
- Strong positivity property (thanks to $K^\star > 0$).

[9] Cancès and Gaudeul 2020.

Free energy dissipation

Define the discrete free energy as $E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{v}) = E_{\mathrm{conv},\mathcal{T}}(\boldsymbol{v}) + E_{\mathrm{conc},\mathcal{T}}(\boldsymbol{v})$ with

$$E_{\mathrm{conv},\mathcal{T}}(\boldsymbol{v}) = \sum_{i=0}^{n} \sum_{K\in\mathcal{T}} m_K (v_{i,K} \log(v_{i,K}) - v_{i,k} + 1) + \frac{\epsilon}{2} \sum_{\sigma\in\mathcal{E}_{\mathrm{int}},\ \sigma=K|L} \tau_\sigma |D_{K\sigma} \boldsymbol{v}_0|^2$$

and

$$E_{\mathrm{conc},\mathcal{T}}(\boldsymbol{v}) = \beta \sum_{K\in\mathcal{T}} m_K v_{0,K}(1 - v_{0,K})$$

Free energy dissipation

Define the discrete free energy as $E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{v}) = E_{\mathrm{conv},\mathcal{T}}(\boldsymbol{v}) + E_{\mathrm{conc},\mathcal{T}}(\boldsymbol{v})$ with

$$E_{\mathrm{conv},\mathcal{T}}(\boldsymbol{v}) = \sum_{i=0}^{n} \sum_{K\in\mathcal{T}} m_K (v_{i,K} \log(v_{i,K}) - v_{i,k} + 1) + \frac{\epsilon}{2} \sum_{\sigma\in\mathcal{E}_{\mathrm{int}},\ \sigma=K|L} \tau_\sigma |D_{K\sigma} \boldsymbol{v}_0|^2$$

and

$$E_{\mathrm{conc},\mathcal{T}}(\boldsymbol{v}) = \beta \sum_{K\in\mathcal{T}} m_K v_{0,K}(1 - v_{0,K})$$

Lemma (Free energy dissipation)

Let $p \in \mathbb{N}$ and let $\boldsymbol{u}^p \in \mathbb{A}^{|\mathcal{T}|}$. Then any solution $\boldsymbol{u}^{p+1}$ to the scheme satisfies $(\bar{w}_i^{p+1} := w_i^{p+1} - w_0^{p+1} = \log(u_i^{p+1}) - \log(u_0^{p+1} - w_0^{p+1})$

$$\frac{1}{\Delta t_p} \left(E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{u}^{p+1}) - E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{u}^p)\right) + \sum_{\sigma\in\mathcal{E}_{\mathrm{int}}} (D_{K\sigma}\bar{\boldsymbol{w}}^{p+1})^T M(\boldsymbol{u}_\sigma^{p+1}) D_{K\sigma}\bar{\boldsymbol{w}}^{p+1} \leqslant 0. \qquad (2)$$

In particular, since M is a positive semi-definite matrix, $E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{u}^{p+1}) \leqslant E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{u}^p) \leqslant E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{u}^0)$.

Free energy dissipation

Define the discrete free energy as $E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{v}) = E_{\mathrm{conv},\mathcal{T}}(\boldsymbol{v}) + E_{\mathrm{conc},\mathcal{T}}(\boldsymbol{v})$ with

$$E_{\mathrm{conv},\mathcal{T}}(\boldsymbol{v}) = \sum_{i=0}^{n} \sum_{K\in\mathcal{T}} m_K (v_{i,K} \log(v_{i,K}) - v_{i,k} + 1) + \frac{\epsilon}{2} \sum_{\sigma\in\mathcal{E}_{\mathrm{int}},\ \sigma=K|L} \tau_\sigma |D_{K\sigma} \boldsymbol{v}_0|^2$$

and

$$E_{\mathrm{conc},\mathcal{T}}(\boldsymbol{v}) = \beta \sum_{K\in\mathcal{T}} m_K v_{0,K}(1 - v_{0,K})$$

Lemma (Free energy dissipation)

Let $p \in \mathbb{N}$ and let $\boldsymbol{u}^p \in \mathbb{A}^{|\mathcal{T}|}$. Then any solution $\boldsymbol{u}^{p+1}$ to the scheme satisfies $(\bar{w}_i^{p+1} := w_i^{p+1} - w_0^{p+1} = \log(u_i^{p+1}) - \log(u_0^{p+1} - w_0^{p+1})$

$$\frac{1}{\Delta t_p} \left(E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{u}^{p+1}) - E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{u}^p)\right) + \sum_{\sigma\in\mathcal{E}_{\mathrm{int}}} (D_{K\sigma}\bar{\boldsymbol{w}}^{p+1})^T M(\boldsymbol{u}_\sigma^{p+1}) D_{K\sigma}\bar{\boldsymbol{w}}^{p+1} \leqslant 0. \tag{2}$$

In particular, since M is a positive semi-definite matrix, $E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{u}^{p+1}) \leqslant E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{u}^p) \leqslant E_{\mathrm{tot},\mathcal{T}}(\boldsymbol{u}^0)$.

Proof is based on the one hand on the discrete chain rule and on the other hand on the convex-concave splitting of the free energy.

Outline of the talk

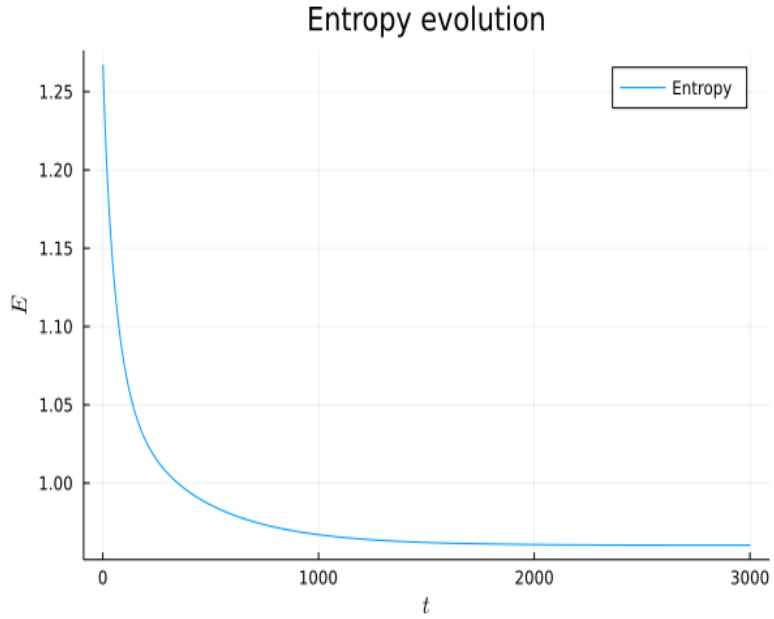
- Numerical scheme implemented in Julia in $1d$ and $2d$ on structured meshes.

- Numerical scheme implemented in Julia in $1d$ and $2d$ on structured meshes.
- Nonlinear system solved with a Newton algorithm to satisfy the volume-filling constraints and adaptive time step. Automatic differentiation is used to compute jacobians.

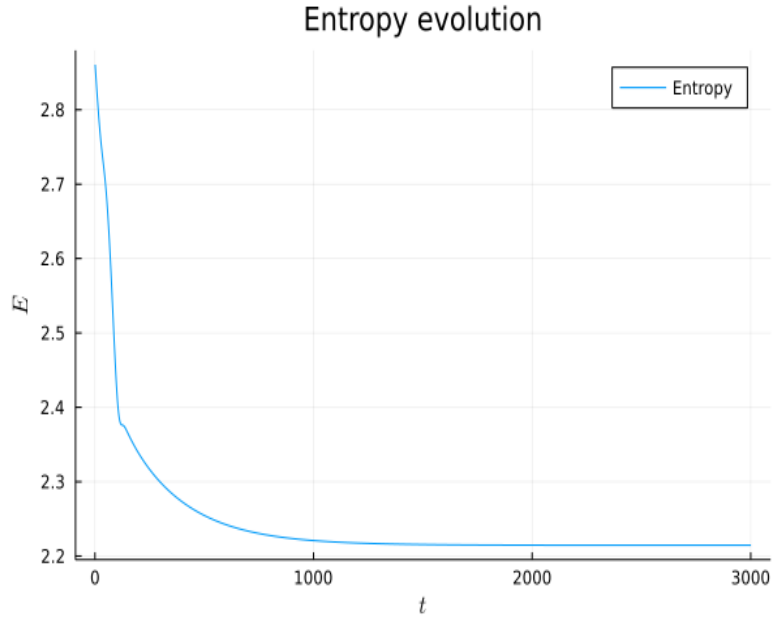
- Numerical scheme implemented in Julia in $1d$ and $2d$ on structured meshes.
- Nonlinear system solved with a Newton algorithm to satisfy the volume-filling constraints and adaptive time step. Automatic differentiation is used to compute jacobians.
- Simulations with parameters $T = 3,\ \epsilon = 0.1,\ \beta = \frac{1}{\epsilon}$. The diffusion matrix is given by

$$A = \begin{pmatrix} 0 & 0.2 & 1 \\ 0.2 & 0 & 0.1 \\ 1 & 0.1 & 0 \end{pmatrix}$$

$T = 3, \epsilon = 0, dt = 1e-3, k^\star = 0.1$

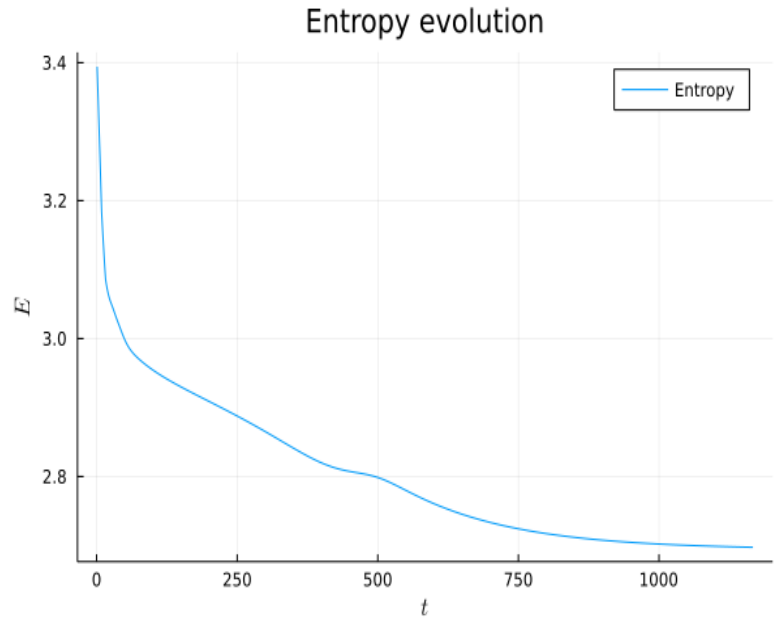


$T = 3, \epsilon = 0.1, dt = 1e-3, k^\star = 0.1$



Species 1

Species 3



Species 2

Perspectives

- Ongoing work: full numerical analysis of the scheme. Proving existence of a discrete solution to the nonlinear system and convergence of the scheme.

Perspectives

- Ongoing work: full numerical analysis of the scheme. Proving existence of a discrete solution to the nonlinear system and convergence of the scheme.
- Perspective: sharp interface limit $\epsilon \longrightarrow 0$ to derive a geometric evolution law.

Perspectives

- Ongoing work: full numerical analysis of the scheme. Proving existence of a discrete solution to the nonlinear system and convergence of the scheme.
- Perspective: sharp interface limit $\epsilon \longrightarrow 0$ to derive a geometric evolution law.
- **Let's talk if you have experience in Cahn-Hilliard simulations !**

References

Bakhta, Athmane and Virginie Ehrlacher (July 2018). "Cross-Diffusion Systems with Non-Zero Flux and Moving Boundary Conditions". In: *ESAIM: Mathematical Modelling and Numerical Analysis* 52.4, pp. 1385–1415. ISSN: 0764-583X, 1290-3841. DOI: 10.1051/m2an/2017053.

Cancès, Clément and Benoît Gaudeul (Jan. 2020). "A Convergent Entropy Diminishing Finite Volume Scheme for a Cross-Diffusion System". In: *SIAM Journal on Numerical Analysis* 58.5, pp. 2684–2710. ISSN: 0036-1429, 1095-7170. DOI: 10.1137/20M1316093.

Ehrlacher, G. Marino, and J.-F. Pietschmann (2021). "Existence of Weak Solutions to a Cross-Diffusion Cahn-Hilliard Type System". In: *Journal of Differential Equations* 286, pp. 578–623. ISSN: 00220396. DOI: 10.1016/j.jde.2021.02.025.

Eyre, David J (1997). "An Unconditionally Stable One-Step Scheme for Gradient Systems". In: p. 15.

Jüngel, Ansgar (June 2015). "The Boundedness-by-Entropy Principle for Cross-Diffusion Systems". In: *Nonlinearity* 28.6, pp. 1963–2001. ISSN: 0951-7715, 1361-6544. DOI: 10.1088/0951-7715/28/6/1963. arXiv: 1403.5419.

Otto, Felix (Jan. 2001). "The Geometry of Dissipative Evolution Equations: The Porous Medium Equation". In: *Communications in Partial Differential Equations* 26.1-2, pp. 101–174. ISSN: 0360-5302, 1532-4133. DOI: 10.1081/PDE-100002243.