

Discrete Duality Finite Volumes scheme for Cahn-Hilliard equations with surfactants

CJC 2024

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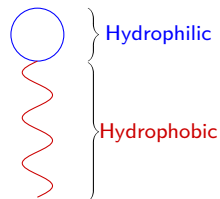
28th of October 2024

PhD supervisors: Ludovic Goudenège and Flore Nabet



Surfactants

- Amphipathic structure
- Examples of surfactants: soap, cell membrane



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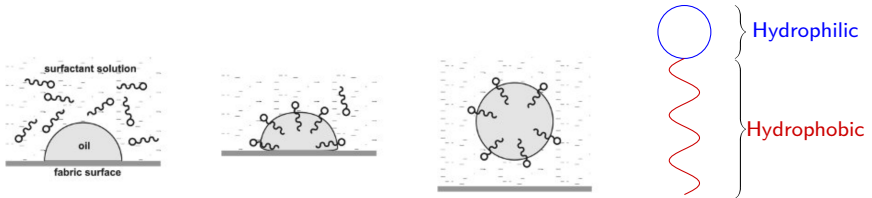


Figure: Essential Chemical Industry 2024

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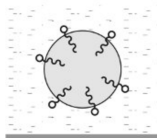
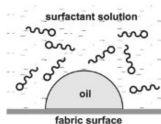


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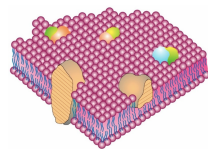
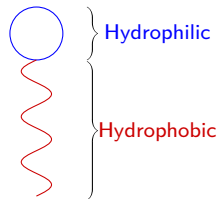


Figure: Nicolson and Mattos 2021



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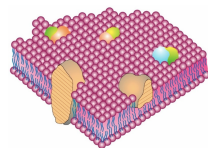
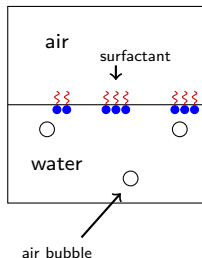
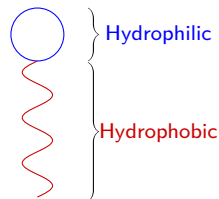


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- Amphipathic structure
- Examples of surfactants: soap, cell membrane

Use of surfactants:

- Applications in microfluidics (Liu and Zhang 2010)
 - Micro-cellular imaging
 - Drug delivery
- Controlled release or protection of certain ingredients (probiotics) (Zychowski 2015)
- Modeling the spread of cancer cells (Cahn Hilliard + Navier Stokes) (Elbar and Poulain 2023)

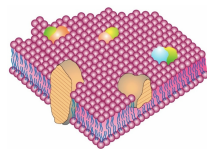
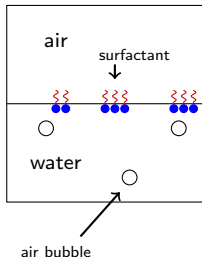
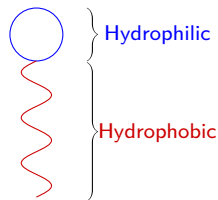


Figure: Nicolson and Mattos 2021



The model

We seek $\phi : (0, T) \times \Omega \rightarrow \mathbb{R}$ that satisfies

$$\begin{cases} \partial_t \phi = \Delta \mu, & \text{in } (0, T) \times \Omega \\ \mu = -\epsilon_\phi \Delta \phi + \frac{1}{\epsilon_\phi} f'_\phi(\phi), & \text{in } (0, T) \times \Omega \\ \nabla \phi \cdot \vec{n} = \nabla \mu \cdot \vec{n} = 0, & \text{on } (0, T) \times \partial \Omega \end{cases}$$

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We seek $\phi : (0, T) \times \Omega \rightarrow \mathbb{R}$ and $c : (0, T) \times \Omega \rightarrow \mathbb{R}$, such that

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where f_ϕ and f_c are the classical Cahn-Hilliard double well potential,

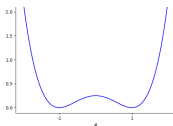


Figure: ϕ potential

$$f_\phi(\phi) = \frac{1}{4}(\phi^2 - 1)^2, \quad f_c(c) = c^2(1 - c)^2.$$

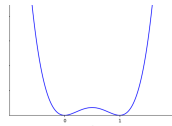


Figure: c potential

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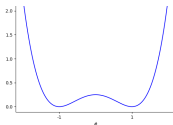


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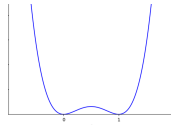


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where F is the coupling potential,

$$F(\phi, c) = \beta \phi^2 c - \gamma \phi^3 c - \alpha |\nabla \phi|^2 c + \delta |\nabla \phi|^4.$$

$$\hookrightarrow \partial_\phi F(\phi, c) = 2\beta \phi c - 3\gamma \phi^2 c + 2\alpha \nabla \cdot (c \nabla \phi) - \delta \nabla \cdot (\nabla \phi)^3,$$

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Energy of the system

Definition of the free energy

$$\mathcal{E} : H^1(\Omega) \times H^1(\Omega) \longrightarrow \mathbb{R}$$

$$\begin{aligned} (\phi, c) \longmapsto & \int_{\Omega} \left(\frac{\epsilon_{\phi}}{2} |\nabla \phi|^2 + \frac{\epsilon_c}{2} |\nabla c|^2 \right) + \int_{\Omega} \left(\frac{1}{\epsilon_{\phi}} f_{\phi}(\phi) + \frac{1}{\epsilon_c} f_c(c) \right) \\ & + \int_{\Omega} F(\phi, c). \end{aligned}$$

Dissipation of energy over time

$$\frac{d}{dt} \mathcal{E}(\phi, c) = -M_0 \int_{\Omega} |\nabla \mu|^2 - N_0 \int_{\Omega} |\nabla \eta|^2 \leq 0$$

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not bounded from below!

$$-\alpha |\nabla \phi|^2 c + \delta |\nabla \phi|^4 = \delta (|\nabla \phi|^2 - \frac{\alpha}{\delta} c)^2 - \frac{\alpha^2 c^2}{\delta}$$

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Dissipativity hypothesis:

$$f_c(c) \geq \tau_1 c^2 - \tau_2, \quad \tau_1 > 0, \tau_2 \geq 0.$$

Discrete duality finite volumes (DDFV): why this method?

- 1 Good approximation of the gradient
- 2 Definition of a discrete divergence operator in duality
- 3 Possibility of non conforming mesh

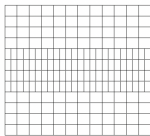


Figure: Mesh with two interfaces

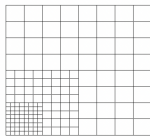


Figure: Locally refined mesh

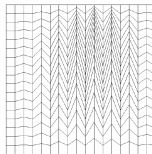


Figure: Mesh with deformed quadrangles

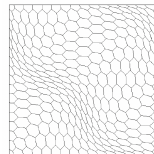
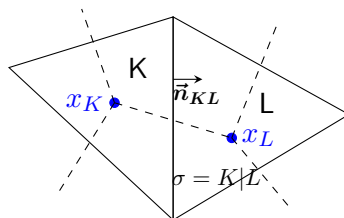


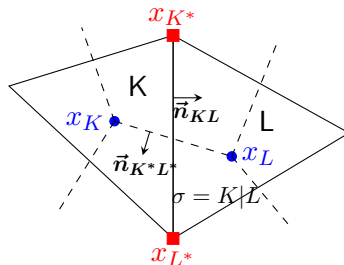
Figure: Mesh with hexagons

Discrete Duality Finite Volumes (DDFV)



The unknowns are piece-wise constant functions.
Unknowns at the **centers** of the control volumes

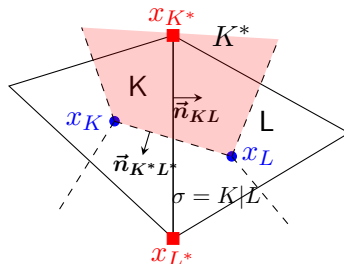
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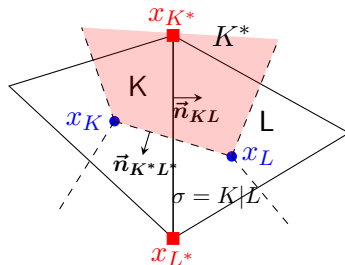
- Primal mesh: $\mathcal{M}$

Vector of unknowns:

- Dual mesh: $\mathcal{M}^*$

$$u_{\mathcal{T}} = \begin{pmatrix} (u_K)_{K \in \mathcal{M}} \\ (u_{K^*})_{K^* \in \mathcal{M}^*} \end{pmatrix} \in \mathbb{R}^{N_{\mathcal{T}}}, \text{ with } \mathcal{T} = \mathcal{M} \cup \mathcal{M}^*.$$

Discrete Duality Finite Volumes (DDFV)



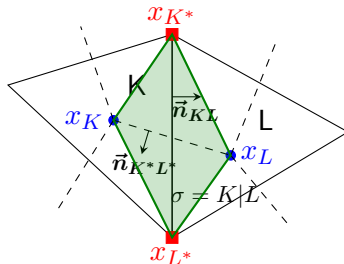
The unknowns are piece-wise constant functions.

Unknowns at the **centers** of the control volumes and on the **vertices**.

Approximate solution:

$$u_h := \frac{1}{2} \sum_{K \in \mathcal{M}} u_K \mathbb{1}_K + \frac{1}{2} \sum_{K \in \mathcal{M}^*} u_{K^*} \mathbb{1}_{K^*}.$$

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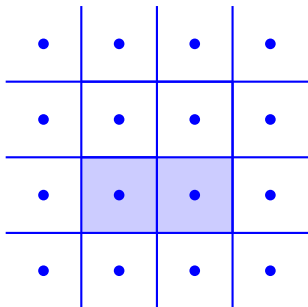


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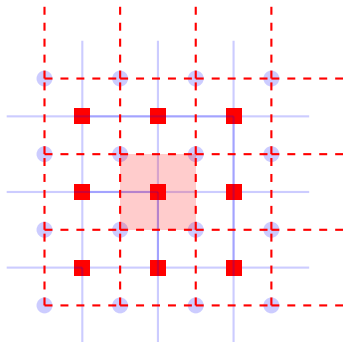
The discrete gradient $\nabla^{\mathcal{D}} u_{\mathcal{T}}$ is defined on the diamond mesh $\mathcal{D}$.

Definition of the meshes



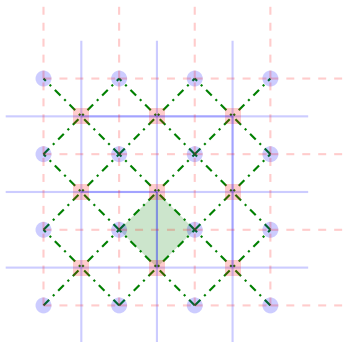
- Primal unknown $\mathbf{u}_\kappa$
- Primal control vol. $\kappa \in \mathcal{M}$

Definition of the meshes



- Primal unknown $\mathbf{u}_\kappa$
- Primal control vol. $\kappa \in \mathcal{M}$
- Dual unknown $\mathbf{u}_{\kappa^*}$
- Dual control vol. $\kappa^* \in \mathcal{M}^*$

Definition of the meshes



- Primal unknown $\mathbf{u}_\kappa$
- Primal control vol. $\kappa \in \mathcal{M}$
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- Dual control vol. $\kappa^* \in \mathcal{M}^*$
- Diamond cells $D \in \mathcal{D}$

Discrete gradient of a scalar field

$$\nabla^{\mathfrak{D}} : \mathbb{R}^{N_{\mathcal{T}}} \rightarrow (\mathbb{R}^2)^{\mathfrak{D}}, \quad \text{where } \mathcal{T} = \mathcal{M} \cup \mathcal{M}^*$$

$$\nabla^{\mathfrak{D}} u_{\mathcal{T}} = (\nabla^D u_{\mathcal{T}})_{D \in \mathfrak{D}}$$

We define $(\nabla^D u_{\mathcal{T}})_{D \in \mathfrak{D}}$ such that
$$\begin{cases} \nabla^D u_{\mathcal{T}} \cdot (x_L - x_K) = u_L - u_K, \\ \nabla^D u_{\mathcal{T}} \cdot (x_{L^*} - x_{K^*}) = u_{L^*} - u_{K^*}. \end{cases}$$

Discrete divergence of a vector field

$$\int_K \operatorname{div} \xi_{\mathcal{D}} = \int_{\partial K} \xi_{\mathcal{D}} \cdot \vec{n} = \sum_{D \in \mathcal{D}_K} m_{\sigma} \xi_D \cdot \vec{n}_{KL} \quad \forall K.$$

$$\operatorname{div}^{\mathcal{T}} : (\mathbb{R}^2)^{\mathcal{D}} \rightarrow \mathbb{R}^{N_{\mathcal{T}}}$$

$$\operatorname{div}^{\mathcal{T}} \xi_{\mathcal{D}} = ((\operatorname{div}^K \xi_{\mathcal{D}})_{K \in \mathcal{M}}, (\operatorname{div}^{K^*} \xi_{\mathcal{D}})_{K^* \in \mathcal{M}^*})$$

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Definition

$$\forall K \in \mathcal{M}, \quad \operatorname{div}^K \xi_{\mathcal{D}} = \frac{1}{m_K} \sum_{D \in \mathcal{D}_K} m_{\sigma} \xi_D \cdot \vec{n}_{KL},$$

$$\forall K^* \in \mathcal{M}^*, \quad \operatorname{div}^{K^*} \xi_{\mathcal{D}} = \frac{1}{m_{K^*}} \sum_{D \in \mathcal{D}_{K^*}} m_{\sigma^*} \xi_D \cdot \vec{n}_{K^*L^*}.$$

Green's theorem (homogeneous Neumann B.C.)

Discrete duality property

Theorem

For all $(\xi_{\mathfrak{D}}, u_{\mathcal{T}}) \in (\mathbb{R}^2)^{\mathfrak{D}} \times \mathbb{R}^{N_{\mathcal{T}}}$, we have

$$\int_{\Omega} \operatorname{div}^{\mathcal{T}} \xi_{\mathfrak{D}} u_{\mathcal{T}} = \llbracket \operatorname{div}^{\mathcal{T}} \xi_{\mathfrak{D}}, u_{\mathcal{T}} \rrbracket_{\mathcal{T}} = -(\xi_{\mathfrak{D}}, \nabla^{\mathfrak{D}} u_{\mathcal{T}})_{\mathfrak{D}} = - \int_{\Omega} \xi_{\mathfrak{D}} \cdot \nabla^{\mathfrak{D}} u_{\mathcal{T}}.$$

- Scalar product on $\mathbb{R}^{N_{\mathcal{T}}}$:

$$\llbracket u_{\mathcal{T}}, v_{\mathcal{T}} \rrbracket_{\mathcal{T}} = \frac{1}{2} \left(\sum_{K \in \mathcal{M}} m_K u_K v_K + \sum_{K^* \in \mathcal{M}^*} m_{K^*} u_{K^*} v_{K^*} \right)$$
- Scalar product on $\mathbb{R}^{\mathfrak{D}}$: $(\xi_{\mathfrak{D}}, \psi_{\mathfrak{D}})_{\mathfrak{D}} = \sum_{D \in \mathfrak{D}} m_D \xi_D \cdot \psi_D.$

The discrete problem

Knowing $(\phi_{\mathcal{T}}^n, c_{\mathcal{T}}^n) \in \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}}$, find
 $(\phi_{\mathcal{T}}^{n+1}, \mu_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}, \eta_{\mathcal{T}}^{n+1}) \in \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}}$, such that

$$\left\{ \begin{array}{l} \phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n = M_{\phi} \Delta t \operatorname{div}^{\mathcal{T}}(\nabla^{\mathfrak{D}} \mu_{\mathcal{T}}^{n+1}), \\ \mu_{\mathcal{T}}^{n+1} = -\frac{3\epsilon_{\phi}}{2} \operatorname{div}^{\mathcal{T}}(\nabla^{\mathfrak{D}} \phi_{\mathcal{T}}^{n+1}) + \frac{12}{\epsilon_{\phi}} d_{\phi}^{f_{\phi}}(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}) \\ \quad + d_{\phi}^F(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}), \\ c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n = M_c \Delta t \operatorname{div}^{\mathcal{T}}(\nabla^{\mathfrak{D}} \eta_{\mathcal{T}}^{n+1}), \\ \eta_{\mathcal{T}}^{n+1} = -\theta \epsilon_c \operatorname{div}^{\mathcal{T}}(\nabla^{\mathfrak{D}} c_{\mathcal{T}}^{n+1}) + \frac{1}{\epsilon_c} d_c^{f_c}(c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}) + d_c^F(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}). \\ + \text{discrete } B.C. \end{array} \right.$$

Discrete energy estimation

Proposition (Discrete energy estimation)

Let $\phi_{\mathcal{T}}^n \in \mathbb{R}^{N_{\mathcal{T}}}$, $c_{\mathcal{T}}^n \in \mathbb{R}^{N_{\mathcal{T}}}$. Suppose there exists a solution $(\phi_{\mathcal{T}}^{n+1}, \mu_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}, \eta_{\mathcal{T}}^{n+1}) \in \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}}$ to the discrete problem. Then, for all time step Δt , the following equality holds

$$\begin{aligned}
 & M_{\phi} \Delta t \|\nabla^{\mathfrak{D}} \mu_{\mathcal{T}}^{n+1}\|_{\mathfrak{D}}^2 + M_c \Delta t \|\nabla^{\mathfrak{D}} \eta_{\mathcal{T}}^{n+1}\|_{\mathfrak{D}}^2 + \mathcal{E}_{\mathcal{T}}(\phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}) - \mathcal{E}_{\mathcal{T}}(\phi_{\mathcal{T}}^n, c_{\mathcal{T}}^n) \\
 & + \frac{3\epsilon_{\phi}}{4} \|\nabla^{\mathfrak{D}} (\phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n)\|_{\mathfrak{D}}^2 + \frac{\theta\epsilon_c}{2} \|\nabla^{\mathfrak{D}} (c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n)\|_{\mathfrak{D}}^2 \\
 & + \frac{12}{\epsilon_{\phi}} \left(\llbracket d^f_{\phi}(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}), \phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} - \llbracket f_{\phi}(\phi_{\mathcal{T}}^{n+1}), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} + \llbracket f_{\phi}(\phi_{\mathcal{T}}^n), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} \right) \\
 & + \frac{1}{\epsilon_c} \left(\llbracket d^f_c(c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}), c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} - \llbracket f_c(c_{\mathcal{T}}^{n+1}), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} + \llbracket f_c(c_{\mathcal{T}}^n), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} \right) \\
 & + \left(\llbracket d^F_{\phi}(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}), \phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} + \llbracket d^F_c(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}), c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} \right. \\
 & \left. + \llbracket -F(\phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}) + F(\phi_{\mathcal{T}}^n, c_{\mathcal{T}}^n), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} \right) = 0.
 \end{aligned}$$

Discrete energy estimation

Proposition (Discrete energy estimation)

Let $\phi_{\mathcal{T}}^n \in \mathbb{R}^{N_{\mathcal{T}}}$, $c_{\mathcal{T}}^n \in \mathbb{R}^{N_{\mathcal{T}}}$. Suppose there exists a solution $(\phi_{\mathcal{T}}^{n+1}, \mu_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}, \eta_{\mathcal{T}}^{n+1}) \in \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}}$ to the discrete problem. Then, for all time step Δt , the following equality holds

$$\begin{aligned}
 & M_{\phi} \Delta t \|\nabla^{\mathfrak{D}} \mu_{\mathcal{T}}^{n+1}\|_{\mathfrak{D}}^2 + M_c \Delta t \|\nabla^{\mathfrak{D}} \eta_{\mathcal{T}}^{n+1}\|_{\mathfrak{D}}^2 + \mathcal{E}_{\mathcal{T}}(\phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}) - \mathcal{E}_{\mathcal{T}}(\phi_{\mathcal{T}}^n, c_{\mathcal{T}}^n) \\
 & + \frac{3\epsilon_{\phi}}{4} \|\nabla^{\mathfrak{D}} (\phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n)\|_{\mathfrak{D}}^2 + \frac{\theta\epsilon_c}{2} \|\nabla^{\mathfrak{D}} (c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n)\|_{\mathfrak{D}}^2 \\
 & + \frac{12}{\epsilon_{\phi}} \left(\llbracket d^f_{\phi}(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}), \phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} - \llbracket f_{\phi}(\phi_{\mathcal{T}}^{n+1}), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} + \llbracket f_{\phi}(\phi_{\mathcal{T}}^n), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} \right) \\
 & + \frac{1}{\epsilon_c} \left(\llbracket d^f_c(c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}), c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} - \llbracket f_c(c_{\mathcal{T}}^{n+1}), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} + \llbracket f_c(c_{\mathcal{T}}^n), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} \right) \\
 & + \left(\llbracket d^F_{\phi}(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}), \phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} + \llbracket d^F_c(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}), c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} \right. \\
 & \left. + \llbracket -F(\phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}) + F(\phi_{\mathcal{T}}^n, c_{\mathcal{T}}^n), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} \right) = 0.
 \end{aligned}$$

Discretization of the derivatives of the potentials

We define, for any $K \in \mathcal{T} = \mathcal{M} \cup \mathcal{M}^*$,

$$d_{\phi}^{f_{\phi}}(\phi_K^n, \phi_K^{n+1}) = \frac{f_{\phi}(\phi_K^{n+1}) - f_{\phi}(\phi_K^n)}{(\phi_K^{n+1} - \phi_K^n)}, \quad d_c^{f_c}(c_K^n, c_K^{n+1}) = \frac{f_c(c_K^{n+1}) - f_c(c_K^n)}{(c_K^{n+1} - c_K^n)},$$

$$\rightsquigarrow d_{\phi}^{f_{\phi}}(\phi_K^n, \phi_K^{n+1})(\phi_K^{n+1} - \phi_K^n) - f_{\phi}(\phi_K^{n+1}) + f_{\phi}(\phi_K^n) = 0$$

$$\rightsquigarrow d_c^{f_c}(c_K^n, c_K^{n+1})(c_K^{n+1} - c_K^n) - f_c(c_K^{n+1}) + f_c(c_K^n) = 0.$$

Discretization of the derivatives of the potentials

We define, for any $K \in \mathcal{T} = \mathcal{M} \cup \mathcal{M}^*$,

$$\rightsquigarrow d_\phi^f(\phi_K^n, \phi_K^{n+1})(\phi_K^{n+1} - \phi_K^n) - f_\phi(\phi_K^{n+1}) + f_\phi(\phi_K^n) = 0$$

$$\rightsquigarrow d_c^f(c_K^n, c_K^{n+1})(c_K^{n+1} - c_K^n) - f_c(c_K^{n+1}) + f_c(c_K^n) = 0.$$

$$\begin{aligned} & d_\phi^F(\phi_K^n, \phi_K^{n+1}, c_K^n, c_K^{n+1})(\phi_K^{n+1} - \phi_K^n) + d_c^F(\phi_K^n, \phi_K^{n+1}, c_K^n, c_K^{n+1})(c_K^{n+1} - c_K^n) \\ & - F(\phi_K^{n+1}, c_K^{n+1}) + F(\phi_K^n, c_K^n) \\ & = \frac{\delta}{4m_K} \sum_{D \in \mathfrak{D}_K} m_D (|\nabla^D \phi_K^{n+1}|^2 - |\nabla^D \phi_K^n|^2)^2 \\ & + \frac{\delta}{2m_K} \sum_{D \in \mathfrak{D}_K} m_D |\nabla^D \phi_K^{n+1}|^2 |\nabla^D \phi_K^{n+1} - \nabla^D \phi_K^n|^2. \end{aligned}$$

Discretization of the derivatives of the potentials

We define, for any $K \in \mathcal{T} = \mathcal{M} \cup \mathcal{M}^*$,

$$\rightsquigarrow d_\phi^f(\phi_K^n, \phi_K^{n+1})(\phi_K^{n+1} - \phi_K^n) - f_\phi(\phi_K^{n+1}) + f_\phi(\phi_K^n) = 0$$

$$\rightsquigarrow d_c^f(c_K^n, c_K^{n+1})(c_K^{n+1} - c_K^n) - f_c(c_K^{n+1}) + f_c(c_K^n) = 0.$$

$$\begin{aligned} & d_\phi^F(\phi_K^n, \phi_K^{n+1}, c_K^n, c_K^{n+1})(\phi_K^{n+1} - \phi_K^n) + d_c^F(\phi_K^n, \phi_K^{n+1}, c_K^n, c_K^{n+1})(c_K^{n+1} - c_K^n) \\ & - F(\phi_K^{n+1}, c_K^{n+1}) + F(\phi_K^n, c_K^n) \\ & = \frac{\delta}{4m_K} \sum_{D \in \mathfrak{D}_K} m_D (|\nabla^D \phi_K^{n+1}|^2 - |\nabla^D \phi_K^n|^2)^2 \\ & + \frac{\delta}{2m_K} \sum_{D \in \mathfrak{D}_K} m_D |\nabla^D \phi_K^{n+1}|^2 |\nabla^D \phi_K^{n+1} - \nabla^D \phi_K^n|^2 = \delta(T_1 + T_2). \end{aligned}$$

Discrete energy estimation

Proposition (Discrete energy estimation)

Let $\phi_{\mathcal{T}}^n \in \mathbb{R}^{N_{\mathcal{T}}}$, $c_{\mathcal{T}}^n \in \mathbb{R}^{N_{\mathcal{T}}}$. Suppose there exists a solution $(\phi_{\mathcal{T}}^{n+1}, \mu_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}, \eta_{\mathcal{T}}^{n+1}) \in \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}}$ to the discrete problem. Then, for all time step Δt , the following equality holds

$$\begin{aligned}
 & M_{\phi} \Delta t \|\nabla^{\mathcal{D}} \mu_{\mathcal{T}}^{n+1}\|_{\mathcal{D}}^2 + M_c \Delta t \|\nabla^{\mathcal{D}} \eta_{\mathcal{T}}^{n+1}\|_{\mathcal{D}}^2 + \mathcal{E}_{\mathcal{T}}(\phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}) - \mathcal{E}_{\mathcal{T}}(\phi_{\mathcal{T}}^n, c_{\mathcal{T}}^n) \\
 & + \frac{3\epsilon_{\phi}}{4} \|\nabla^{\mathcal{D}} (\phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n)\|_{\mathcal{D}}^2 + \frac{\theta \epsilon_c}{2} \|\nabla^{\mathcal{D}} (c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n)\|_{\mathcal{D}}^2 \\
 & + \frac{12}{\epsilon_{\phi}} \left(\llbracket d^f \phi(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}), \phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} - \llbracket f_{\phi}(\phi_{\mathcal{T}}^{n+1}), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} + \llbracket f_{\phi}(\phi_{\mathcal{T}}^n), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} \right) \\
 & + \frac{1}{\epsilon_c} \left(\llbracket d^c(c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}), c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} - \llbracket f_c(c_{\mathcal{T}}^{n+1}), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} + \llbracket f_c(c_{\mathcal{T}}^n), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} \right) \\
 & + \left(\llbracket d_{\phi}^F(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}), \phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} + \llbracket d_c^F(\phi_{\mathcal{T}}^n, \phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^n, c_{\mathcal{T}}^{n+1}), c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n \rrbracket_{\mathcal{T}} \right. \\
 & \left. + \llbracket -F(\phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}) + F(\phi_{\mathcal{T}}^n, c_{\mathcal{T}}^n), \mathbb{1}_{\mathcal{T}} \rrbracket_{\mathcal{T}} \right) = 0.
 \end{aligned}$$

Discrete energy estimation

Proposition (Discrete energy estimation)

Let $\phi_{\mathcal{T}}^n \in \mathbb{R}^{N_{\mathcal{T}}}$, $c_{\mathcal{T}}^n \in \mathbb{R}^{N_{\mathcal{T}}}$. Suppose there exists a solution $(\phi_{\mathcal{T}}^{n+1}, \mu_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}, \eta_{\mathcal{T}}^{n+1}) \in \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}}$ to the discrete problem. Then, for all time step Δt , the following equality holds

$$M_{\phi} \Delta t \|\nabla^{\mathcal{D}} \mu_{\mathcal{T}}^{n+1}\|_{\mathfrak{D}}^2 + M_c \Delta t \|\nabla^{\mathcal{D}} \eta_{\mathcal{T}}^{n+1}\|_{\mathfrak{D}}^2 + \mathcal{E}_{\mathcal{T}}(\phi_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}) - \mathcal{E}_{\mathcal{T}}(\phi_{\mathcal{T}}^n, c_{\mathcal{T}}^n) \\ + \frac{3\epsilon_{\phi}}{4} \|\nabla^{\mathcal{D}}(\phi_{\mathcal{T}}^{n+1} - \phi_{\mathcal{T}}^n)\|_{\mathfrak{D}}^2 + \frac{\theta\epsilon_c}{2} \|\nabla^{\mathcal{D}}(c_{\mathcal{T}}^{n+1} - c_{\mathcal{T}}^n)\|_{\mathfrak{D}}^2 + \delta(T_1 + T_2) = 0.$$

Existence of discrete solutions

Proposition (Existence of a discrete solution)

Let $(\phi_{\mathcal{T}}^n, c_{\mathcal{T}}^n) \in \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}}$. We suppose that

- $f_{\phi}(\phi)$ and $f_c(c)$ satisfy the dissipativity condition: $\lim_{|x| \rightarrow \infty} \inf f''(x) > 0$,
- $d_{\phi}^{f_{\phi}}, d_c^{f_c}, d_{\phi}^{F_2}$ and $d_c^{F_2}$ satisfy the polynomial growth hypothesis,
- the following conditions on the parameters hold,

$$\frac{\tau_1}{2\epsilon_c} - \frac{2\alpha^2}{\delta} \geq 0, \quad \epsilon_{\phi} \leq \frac{4}{\gamma}, \quad \text{and} \quad \epsilon_c \leq \frac{2}{\gamma}.$$

Then, there exists at least one solution

$(\phi_{\mathcal{T}}^{n+1}, \mu_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}, \eta_{\mathcal{T}}^{n+1}) \in \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}} \times \mathbb{R}^{N_{\mathcal{T}}}$ to the discrete problem.

Topological Degree

$\mathcal{P}$: Find $\mathbf{u} \in \mathcal{W}$ such that $\mathcal{F}(\mathbf{u}) = 0$.

For any $\rho \in [0, 1]$, let $\mathcal{P}_\rho$ be such that:

- ① $\mathcal{P}_1 = \mathcal{P}$;
- ② for $\rho = 0$, the problem $\mathcal{P}_0$ has a solution in $\mathcal{W}$;
- ③ $\exists R > 0$ such that, for all $\rho \in [0, 1]$,

$\mathbf{w}$ is a solution of $\mathcal{P}_\rho$ and $\|\mathbf{w}\|_{\mathcal{W}} \leq R \Rightarrow \|\mathbf{w}\|_{\mathcal{W}} \neq R$.

$\rightsquigarrow$ *A priori* estimates.

Then, there exists at least one solution to problem $\mathcal{P}_1$.

A priori estimates

To bound the solutions, we need the **stability term**

$$\begin{aligned}
 & -\alpha\rho \sum_{D\in\mathfrak{D}} m_D c_D^{n+1} |\nabla^D \phi_{\mathcal{T}}^{n+1}|^2 + \frac{\delta\rho}{4} \sum_{D\in\mathfrak{D}} m_D |\nabla^D \phi_{\mathcal{T}}^{n+1}|^4 \\
 & = \frac{\delta\rho}{4} \sum_{D\in\mathfrak{D}} m_D \left(|\nabla^D \phi_{\mathcal{T}}^{n+1}|^2 - \frac{2\alpha}{\delta} c_D^{n+1} \right)^2 - \frac{\rho\alpha^2}{\delta} \sum_{D\in\mathfrak{D}} m_D (c_D^{n+1})^2,
 \end{aligned}$$

we can bound this thanks to the dissipativity hypothesis: $\exists \tau_1 > 0$, $\tau_2 \geq 0$, such that $f_c(c) \geq \tau_1 c^2 - \tau_2$. The following condition arises

$$\frac{\tau_1}{2\epsilon_c} - \frac{2\alpha^2}{\delta} \geq 0.$$

Convergence

(Work in progress)

First step:

Proposition (Existence of the limits)

- 1 *There exist functions ϕ , μ , c , and $\eta \in L^2(\Omega)$ such that (up to a subsequence) we have $\phi_{\mathcal{T}} \rightarrow \phi$, $\mu_{\mathcal{T}} \rightharpoonup \mu$, $c_{\mathcal{T}} \rightarrow c$, and $\eta_{\mathcal{T}} \rightharpoonup \eta$.*
- 2 *Moreover, these functions are in $H^1(\Omega)$, and we have the following convergence for the gradients: $\nabla \phi_{\mathcal{T}} \rightarrow \nabla \phi$, $\nabla \mu_{\mathcal{T}} \rightharpoonup \nabla \mu$, $\nabla c_{\mathcal{T}} \rightarrow \nabla c$, and $\nabla \eta_{\mathcal{T}} \rightharpoonup \nabla \eta$, in $(L^2(\Omega))^d$.*

Convergence

(Work in progress)

First step:

Proposition (Existence of the limits)

- 1 *There exist functions ϕ , μ , c , and $\eta \in L^2(\Omega)$ such that (up to a subsequence) we have $\phi_{\mathcal{T}} \rightarrow \phi$, $\mu_{\mathcal{T}} \rightarrow \mu$, $c_{\mathcal{T}} \rightarrow c$, and $\eta_{\mathcal{T}} \rightarrow \eta$.*
- 2 *Moreover, these functions are in $H^1(\Omega)$, and we have the following convergence for the gradients: $\nabla \phi_{\mathcal{T}} \rightarrow \nabla \phi$, $\nabla \mu_{\mathcal{T}} \rightarrow \nabla \mu$, $\nabla c_{\mathcal{T}} \rightarrow \nabla c$, and $\nabla \eta_{\mathcal{T}} \rightarrow \nabla \eta$, in $(L^2(\Omega))^d$.*

Second step: passing to the limit

- ↪ For the classical Cahn-Hilliard terms, ok.
- ↪ Difficulty: coupling terms.

Convergence of the coupling terms

Passing to the limit for the coupling terms:

$$\partial_\phi F(\phi, c) = 2\beta\phi c - 3\gamma\phi^2 c + 2\alpha\nabla \cdot (c\nabla\phi) - \delta\nabla \cdot (\nabla\phi|\nabla\phi|^2),$$

$$\partial_c F(\phi, c) = -\alpha|\nabla\phi|^2 + \beta\phi^2 - \gamma\phi^3.$$

Convergence of the coupling terms

Passing to the limit for the coupling terms:

$$\begin{aligned}\partial_\phi F(\phi, c) &= 2\beta\phi c - 3\gamma\phi^2 c + \boxed{2\alpha\nabla \cdot (c\nabla\phi)} - \delta\nabla \cdot (\nabla\phi|\nabla\phi|^2), \\ \partial_c F(\phi, c) &= -\alpha|\nabla\phi|^2 + \beta\phi^2 - \gamma\phi^3.\end{aligned}$$

For $\psi \in \mathcal{C}_c^\infty$

$$\begin{aligned}\left| \int_{\Omega} c_{\mathcal{T}} \nabla \phi_{\mathcal{T}} \cdot \nabla \psi - \int_{\Omega} c \nabla \phi \cdot \nabla \psi \right| &= \left| \int_{\Omega} (c_{\mathcal{T}} - c) \nabla \phi \cdot \nabla \psi + \int_{\Omega} c_{\mathcal{T}} (\nabla \phi_{\mathcal{T}} - \nabla \phi) \cdot \nabla \psi \right| \\ &\leq \underbrace{\|\nabla \psi\|_{\infty} \left(\int_{\Omega} |c_{\mathcal{T}}|^2 \right)^{1/2}}_{\leq c} \left(\int_{\Omega} |\nabla \phi_{\mathcal{T}} - \nabla \phi|^2 \right)^{1/2} \longrightarrow 0 \\ &\quad + \underbrace{\|\nabla \psi\|_{\infty} \left(\int_{\Omega} |\nabla \phi|^2 \right)^{1/2}}_{\leq c} \left(\int_{\Omega} (c_{\mathcal{T}} - c)^2 \right)^{1/2} \longrightarrow 0\end{aligned}$$

Convergence of the coupling terms

Passing to the limit for the coupling terms:

$$\partial_\phi F(\phi, c) = 2\beta\phi c - 3\gamma\phi^2 c + 2\alpha\nabla \cdot (c\nabla\phi) - \delta\nabla \cdot (\nabla\phi|\nabla\phi|^2),$$

$$\partial_c F(\phi, c) = \boxed{-\alpha|\nabla\phi|^2} + \beta\phi^2 - \gamma\phi^3.$$

For $\psi \in \mathcal{C}_c^\infty$

$$\left| \int_{\Omega} \nabla\phi_{\mathcal{T}} \cdot \nabla\phi_{\mathcal{T}} \psi - \int_{\Omega} \nabla\phi \cdot \nabla\phi \psi \right| \leq \|\psi\|_{\infty} \left(\underbrace{\|\nabla\phi_{\mathcal{T}}\|_{L^2(\Omega)}^2 - \|\nabla\phi\|_{L^2(\Omega)}^2}_{\longrightarrow 0} \right).$$

Convergence of the coupling terms

Passing to the limit for the coupling terms:

$$\begin{aligned}\partial_\phi F(\phi, c) &= 2\beta\phi c - 3\gamma\phi^2 c + 2\alpha\nabla \cdot (c\nabla\phi) \boxed{-\delta\nabla \cdot (\nabla\phi|\nabla\phi|^2)}, \\ \partial_c F(\phi, c) &= -\alpha|\nabla\phi|^2 + \beta\phi^2 - \gamma\phi^3.\end{aligned}$$

L^4 bound (energy estimation): $\exists C > 0$ s.t. $\|\nabla\phi\|_{L^4(\Omega)}, \|\nabla\phi_{\mathcal{T}}\|_{L^4(\Omega)} \leq C$

For $\psi \in \mathcal{C}_c^\infty$

$$\begin{aligned}& \left| \int_{\Omega} |\nabla\phi_{\mathcal{T}}|^2 \nabla\phi_{\mathcal{T}} \cdot \nabla\psi - \int_{\Omega} |\nabla\phi|^2 \nabla\phi \cdot \nabla\psi \right| \\&= \left| \int_{\Omega} |\nabla\phi_{\mathcal{T}}|^2 (\nabla\phi_{\mathcal{T}} - \nabla\phi) \cdot \nabla\psi + \int_{\Omega} (|\nabla\phi_{\mathcal{T}}|^2 - |\nabla\phi|^2) \nabla\phi \cdot \nabla\psi \right| \\&\leq \|\nabla\psi\|_{\infty} \left[\underbrace{\|\nabla\phi\|_{L^4}}_{\leq C} \underbrace{\|\nabla\phi_{\mathcal{T}} - \nabla\phi\|_{L^4(\Omega)}}_{\leq C} \xrightarrow{\quad\quad\quad} 0 \right] + \|\nabla\psi\|_{\infty} \underbrace{\|\nabla\phi_{\mathcal{T}}\|_{L^4}}_{\leq C} \xrightarrow{\quad\quad\quad} 0\end{aligned}$$

Numerical simulations - spinodal decomposition



Figure: Water - air separation, model without surfactants



Figure: Water - air separation, model with surfactants



Numerical simulations - one air bubble in water

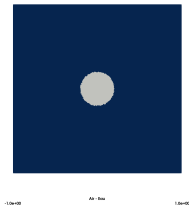


Figure: An air bubble in water

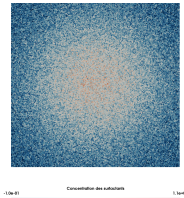


Figure: Surfactants dynamics around an air bubble

Numerical simulations - air bubbles in water

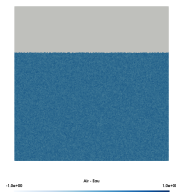


Figure: Phase separation, water with bubbles

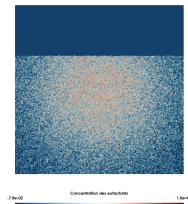


Figure: Surfactants dynamics in water with bubbles