Convergence analysis of a finite volume scheme for a phase-field model of a ternary mixture with surfactants

CANUM, June 2026

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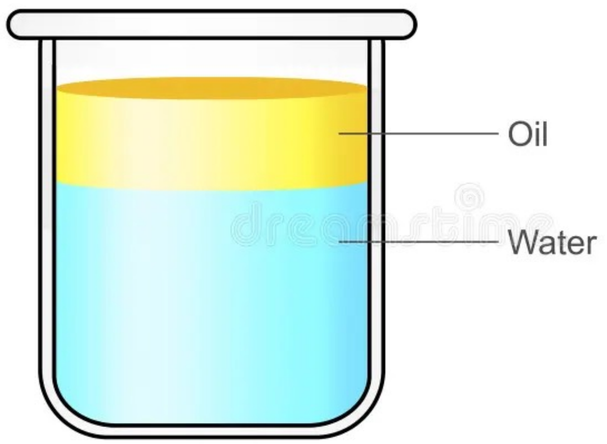
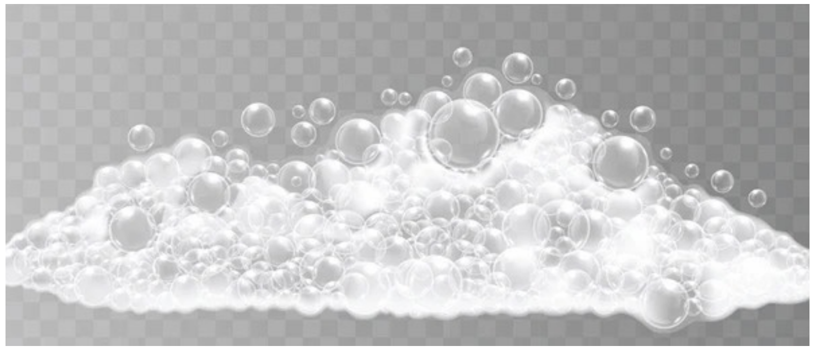
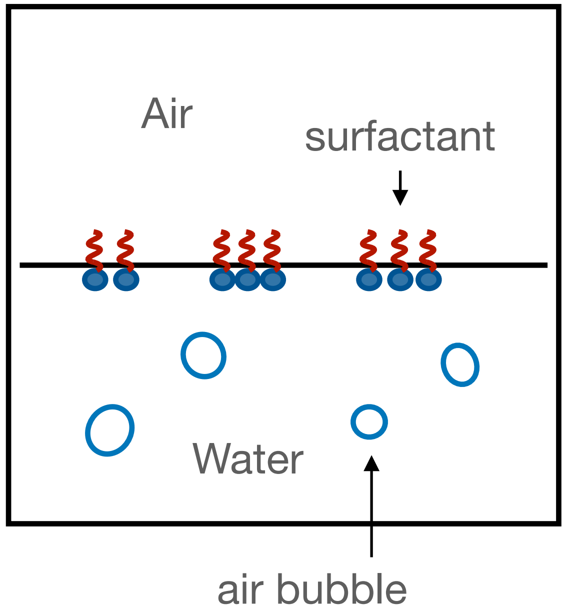
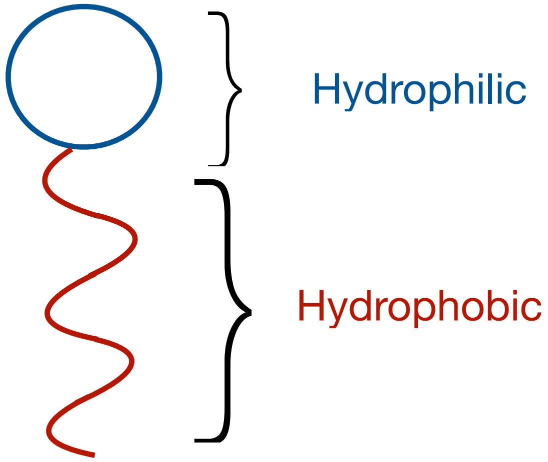
What are surfactants





- Molecules with amphipatic structure
- Common examples: soap, cell membrane.





Constructing the model

Regions occupied by the fluids

$$\phi(t,x) = \begin{cases} 1 & \text{fluid 1 (water)}, \\ -1 & \text{fluid 2 (air)}. \end{cases}$$

Interface between the two fluids: $\{x \in \Omega : \phi(t,x) = 0\}$, interface thickness: ϵ_ϕ.

Regions occupied by surfactants

$$c(t,x) = \begin{cases} 1 & \text{saturated with surfactants}, \\ 0 & \text{absence of surfactants}. \end{cases}$$

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$$\mathscr{E}(\phi, c) = \int_\Omega \frac{\epsilon_\phi}{2}|\nabla \phi|^2 + \frac{\epsilon_c}{2}|\nabla c|^2 + \frac{1}{\epsilon_\phi} f_\phi(\phi) + \frac{1}{\epsilon_c} f_c(c) + F(\phi, c)dx$$

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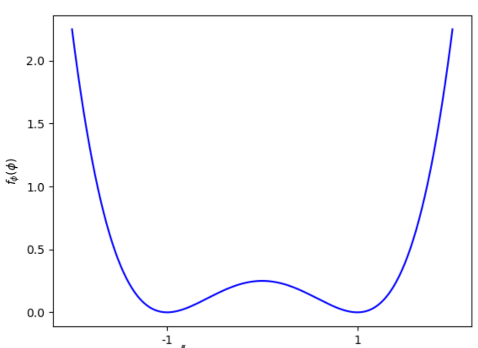
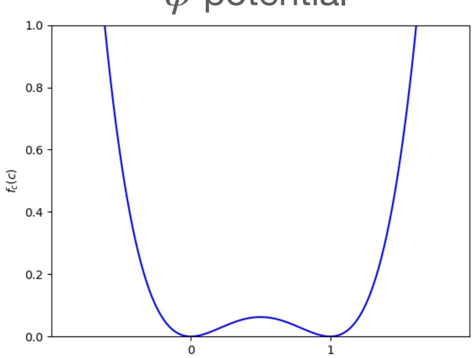


ϕ potential

$$f_\phi(\phi) = \frac{1}{16}(\phi^2 - 1)^2$$



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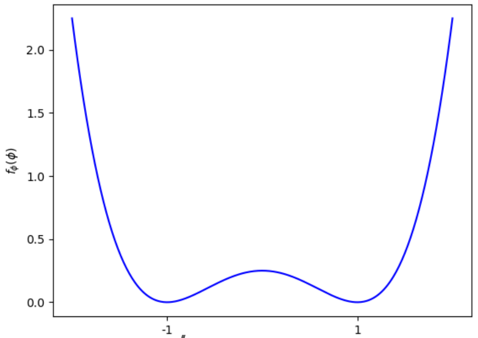

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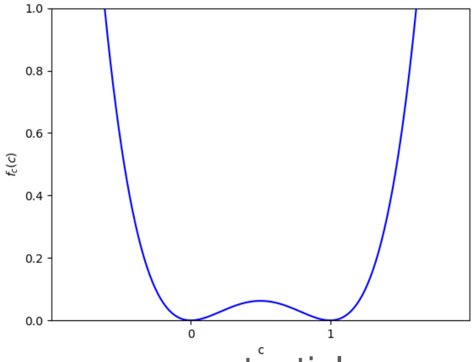

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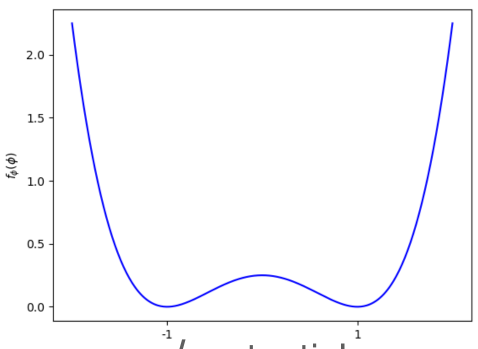

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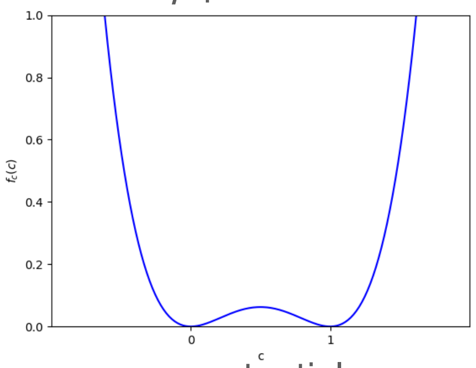

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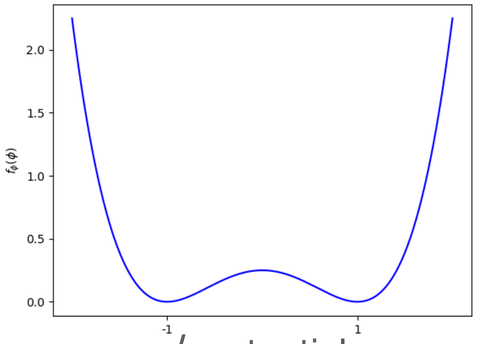

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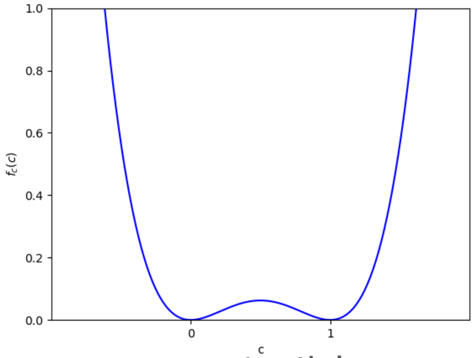

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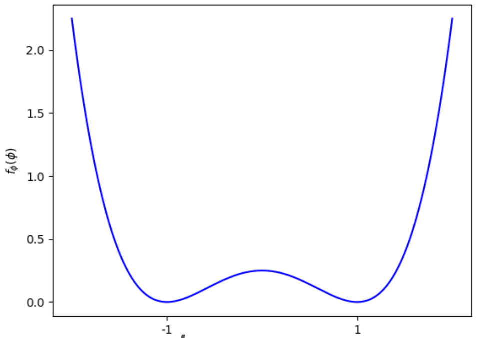

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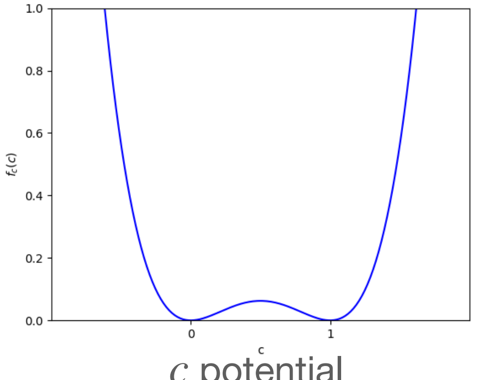

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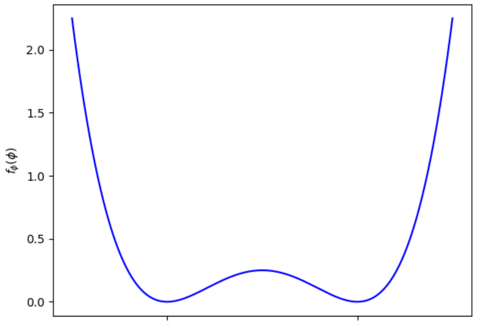

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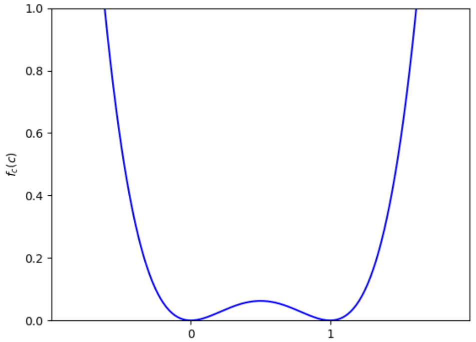

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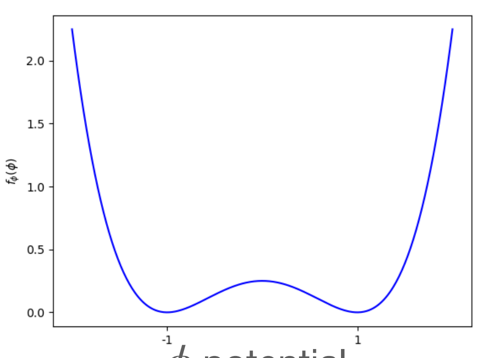

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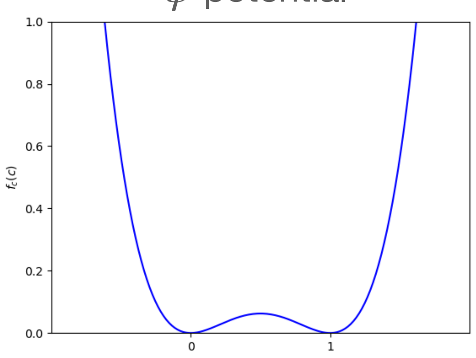

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$$\longrightarrow \quad -\alpha|\nabla\phi|^2 c + \delta|\nabla\phi|^4$$

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

Constructing the model

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

$$\begin{cases} \partial_t \phi = \Delta \mu, & \text{in } (0,T) \times \Omega \\ \mu = -\epsilon_\phi \Delta \phi + \dfrac{1}{\epsilon_\phi} f'_\phi(\phi) + \partial_\phi F(\phi, c), & \text{in } (0,T) \times \Omega \\ \partial_t c = \Delta \eta, & \text{in } (0,T) \times \Omega \\ \eta = -\epsilon_c \Delta c + \dfrac{1}{\epsilon_c} f'_c(c) + \partial_c F(\phi, c), & \text{in } (0,T) \times \Omega \\ \nabla \phi \cdot \overrightarrow{\boldsymbol{n}} = \nabla c \cdot \overrightarrow{\boldsymbol{n}} = \nabla \mu \cdot \overrightarrow{\boldsymbol{n}} = \nabla \eta \cdot \overrightarrow{\boldsymbol{n}} = 0 & \text{on } \partial(0,T) \times \Omega \end{cases}$$

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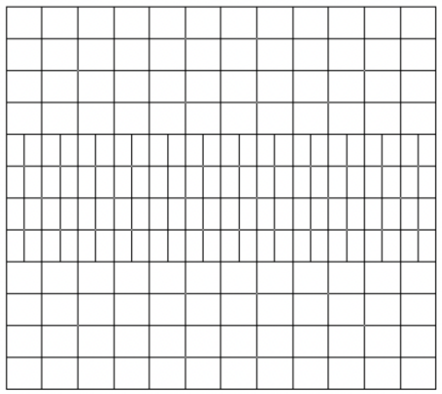
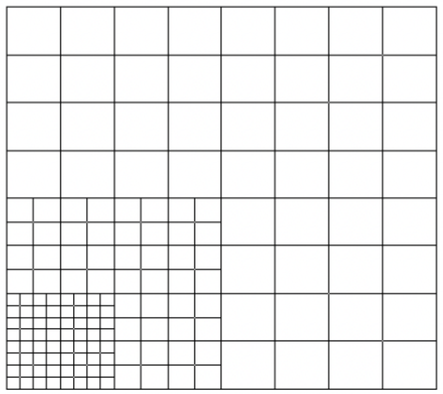
Energy dissipation over time: $\dfrac{d}{dt}\mathscr{E}(\phi, c) = -\int_\Omega |\nabla \mu|^2 - \int_\Omega |\nabla \eta|^2 \leq 0$

Discrete Duality Finite volumes

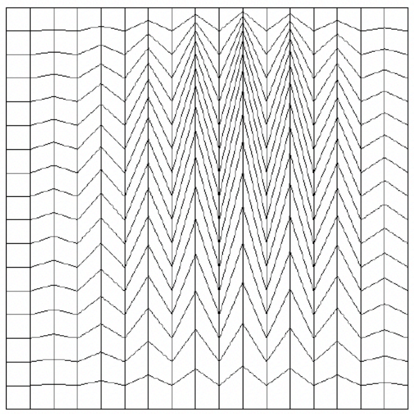
1. Good approximation of the gradient
2. Definition of a discrete divergence in duality
3. Possibility of non-conforming mesh
4. Works for Navier-Stokes coupling



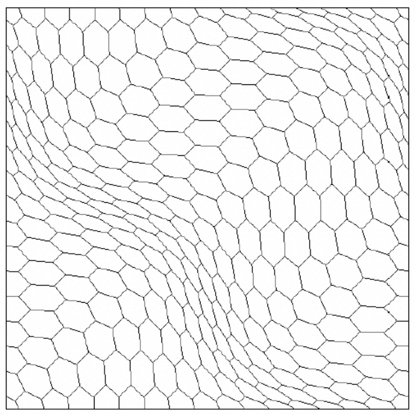
Mesh with two interfaces



Locally refined mesh



Mesh with deformed quadrangles

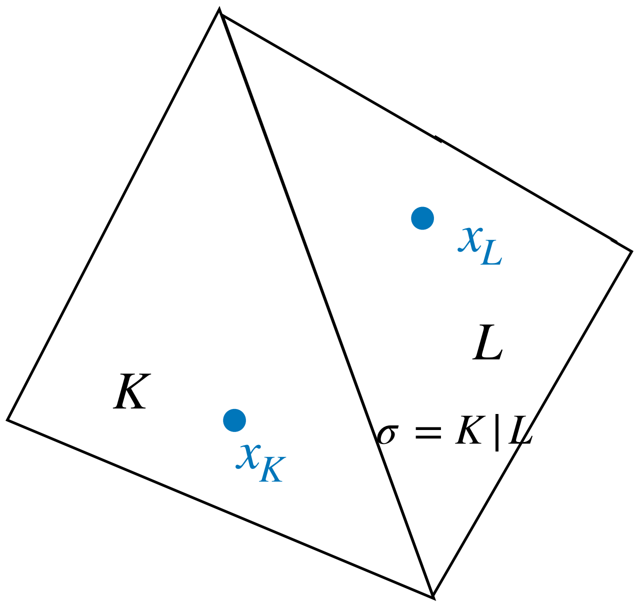


Mesh with hexagons

Discrete Duality Finite volumes

Unknowns are piece-wise constant functions,

defined at the centers and at the vertexes of the controls volumes.



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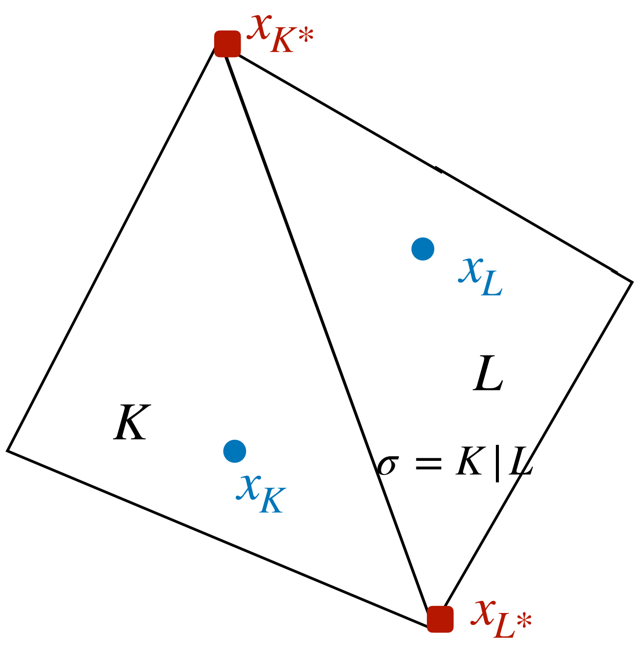

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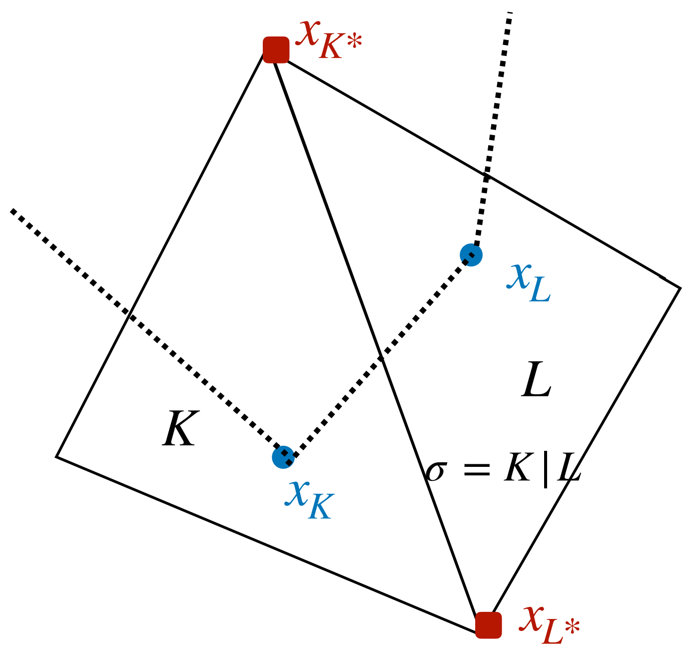

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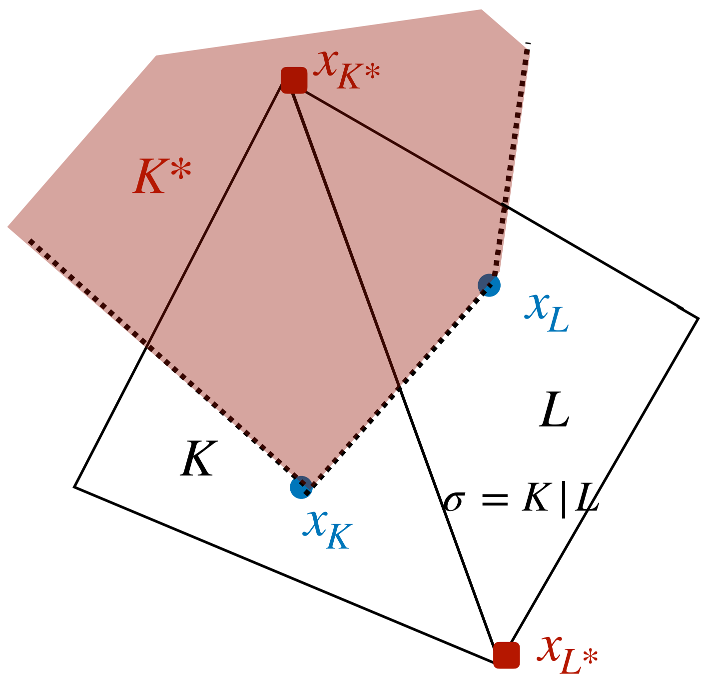

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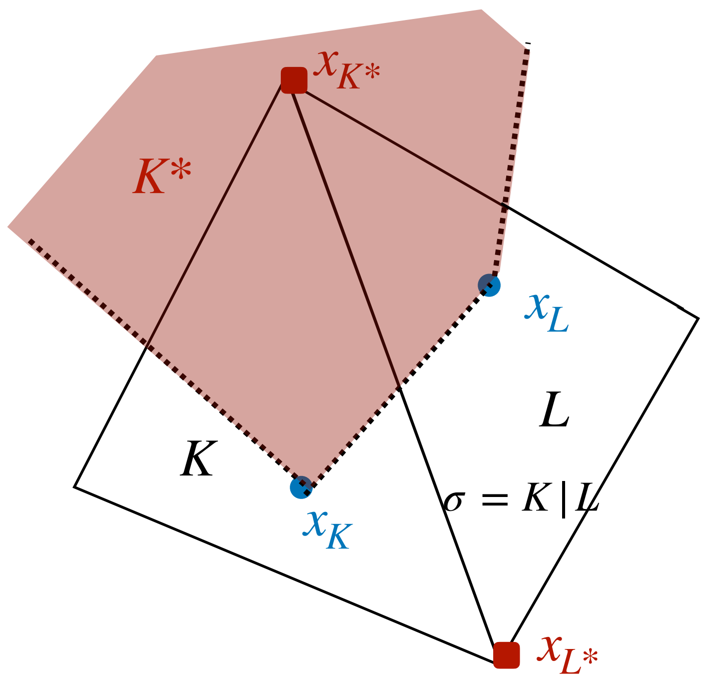

Vector of unknowns:

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

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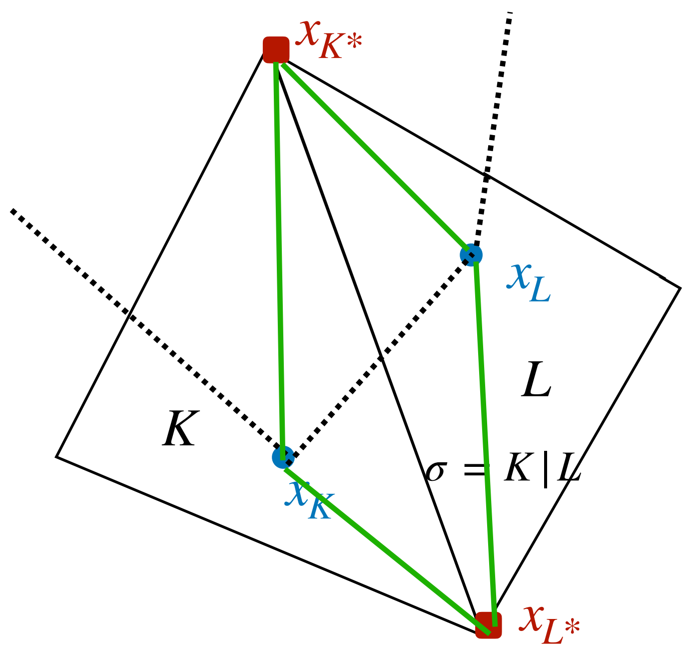

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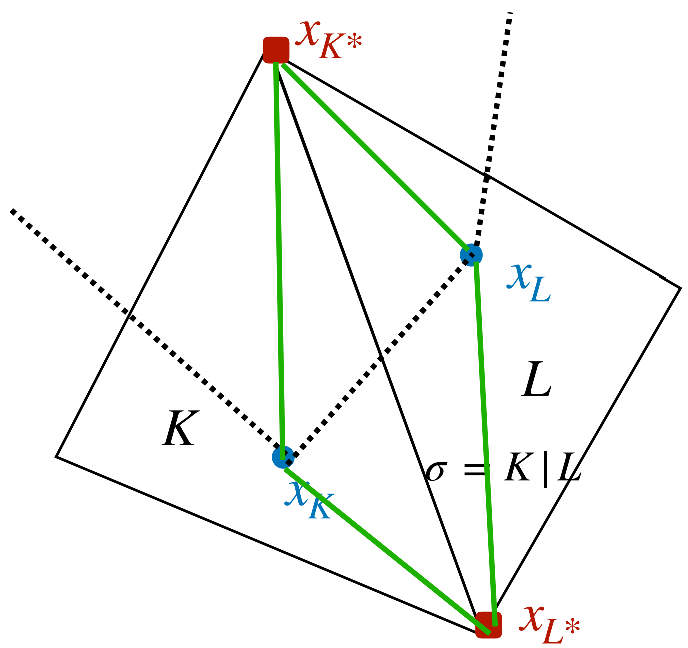

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The discrete gradient $\nabla^{\mathcal{D}} u_T$ is defined on the diamond mesh $\mathcal{D}$.

Discrete gradient and discrete divergence

<u>The discrete gradient:</u>

$$\nabla^{\mathscr{D}} : \mathbb{R}^{N_T} \to (\mathbb{R}^2)^{\mathscr{D}},$$

$$(\nabla^D u_T)_{D\in\mathscr{D}} \text{ such that } \begin{cases} \nabla^D u_T \cdot (x_L - x_K) = u_L - u_K, \\ \nabla^D u_T \cdot (x_{L*} - x_{K*}) = u_{L*} - u_{K*} \,. \end{cases}$$

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Stokes formula

$$\int_K \text{div}\, \xi_{\mathcal{D}} = \int_{\partial K} \xi_{\mathcal{D}} \cdot \boldsymbol{n} = \sum_{D\in\mathcal{D}_K} m_\sigma \xi_D \cdot \boldsymbol{n_{KL}} \quad \forall K\,.$$

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

$$\int_\Omega div^T(\xi_{\mathcal{D}}) u_T = -\int_\Omega \xi_{\mathcal{D}} \cdot \nabla^{\mathcal{D}} u_T$$

The discrete problem

Knowing (ϕ_T^n, c_T^n) *find* $(\phi_T^{n+1}, \mu_T^{n+1}, c_T^{n+1}, \eta_T^{n+1})$ *such that*

$$
\begin{cases}
\phi_T^{n+1} - \phi_T^n = \Delta t \, \mathrm{div}^T(\nabla^{\mathcal{D}} \mu_T^{n+1}), \\
\mu_T^{n+1} = -\epsilon_\phi \, \mathrm{div}^T(\nabla^{\mathcal{D}} \phi_T^{n+1}) + \frac{1}{\epsilon_\phi} d_\phi^{f_\phi}(\phi_T^n, \phi_T^{n+1}) + d_\phi^p(\phi_T^n, \phi_T^{n+1}, c_T^{n+1}) \underbrace{+2\alpha \mathrm{div}^T\left(c_{\mathcal{D}}^{n+1} \nabla^{\mathcal{D}}\left(\frac{\phi_T^{n+1} + \phi_T^n}{2}\right)\right)}_{\approx \partial_\phi(c|\nabla\phi|^2)} + \Pi^T \phi_T^{n+1} \\
\qquad - \delta \mathrm{div}^T(\nabla^{\mathcal{D}} \phi_T^{n+1} |\nabla^{\mathcal{D}} \phi_T^{n+1}|^2) \\
c_T^{n+1} - c_T^n = \Delta t \mathrm{div}^T(\nabla^{\mathcal{D}} \eta_T^{n+1}), \\
\eta_T^{n+1} = -\epsilon_c \mathrm{div}^T(\nabla^{\mathcal{D}} c_T^{n+1}) + \frac{1}{\epsilon_c} d_c^{f_c}(c_T^n, c_T^{n+1}) + d_c^p(\phi_T^n) \underbrace{-\alpha \mathcal{P}_T(\nabla^{\mathcal{D}} \phi_T^n)}_{\approx \partial_c(c|\nabla\phi|^2)} + \Pi^T c_T^{n+1}
\end{cases}
$$

The discrete problem

Knowing (ϕ_T^n, c_T^n) *find* $(\phi_T^{n+1}, \mu_T^{n+1}, c_T^{n+1}, \eta_T^{n+1})$ *such that*

$$\begin{cases} \phi_T^{n+1} - \phi_T^n = \Delta t \, \mathrm{div}^T(\nabla^{\mathcal{D}} \mu_T^{n+1}), \\ \mu_T^{n+1} = -\epsilon_\phi \, \mathrm{div}^T(\nabla^{\mathcal{D}} \phi_T^{n+1}) + \frac{1}{\epsilon_\phi} d_\phi^{f_\phi}(\phi_T^n, \phi_T^{n+1}) + d_\phi^p(\phi_T^n, \phi_T^{n+1}, c_T^{n+1}) \overbrace{+2\alpha \mathrm{div}^T\left(c_{\mathcal{D}}^{n+1} \nabla^{\mathcal{D}}\left(\frac{\phi_T^{n+1} + \phi_T^n}{2}\right)\right)}^{\approx \partial_\phi(c|\nabla\phi|^2)} + \Pi^T \phi_T^{n+1} \\ \qquad -\delta \mathrm{div}^T(\nabla^{\mathcal{D}} \phi_T^{n+1} |\nabla^{\mathcal{D}} \phi_T^{n+1}|^2) \\ c_T^{n+1} - c_T^n = \Delta t \mathrm{div}^T(\nabla^{\mathcal{D}} \eta_T^{n+1}), \\ \eta_T^{n+1} = -\epsilon_c \mathrm{div}^T(\nabla^{\mathcal{D}} c_T^{n+1}) + \frac{1}{\epsilon_c} d_c^{f_c}(c_T^n, c_T^{n+1}) + d_c^p(\phi_T^n) \underbrace{-\alpha \mathscr{P}_T(\nabla^{\mathcal{D}} \phi_T^n)}_{\approx \partial_c(c|\nabla\phi|^2)} + \Pi^T c_T^{n+1} \end{cases}$$

Primal & Dual mesh → Diamond mesh

We define for any $D \in \mathcal{D}$,

$$c_D = \frac{1}{m_D} \int_D c_h(x) dx$$

The discrete problem

Knowing (ϕ_T^n, c_T^n) *find* $(\phi_T^{n+1}, \mu_T^{n+1}, c_T^{n+1}, \eta_T^{n+1})$ *such that*

$$
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\phi_T^{n+1} - \phi_T^n = \Delta t \, \mathrm{div}^T(\nabla^{\mathfrak{D}} \mu_T^{n+1}), \\
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c_T^{n+1} - c_T^n = \Delta t \mathrm{div}^T(\nabla^{\mathfrak{D}} \eta_T^{n+1}), \\
\eta_T^{n+1} = -\epsilon_c \mathrm{div}^T(\nabla^{\mathfrak{D}} c_T^{n+1}) + \dfrac{1}{\epsilon_c} d_c^{f_c}(c_T^n, c_T^{n+1}) + d_c^p(\phi_T^n) \underbrace{-\alpha \mathscr{P}_T(\nabla^{\mathfrak{D}} \phi_T^n)}_{\approx \partial_c(c|\nabla\phi|^2)} + \Pi^T c_T^{n+1}
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Primal & Dual mesh ⟶ Diamond mesh

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Diamond mesh ⟶ Primal & Dual mesh

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Diamond mesh ⟶ Primal & Dual mesh

$$\mathscr{P}_T(\nabla^{\mathscr{D}} \phi_T) \approx \int_\Omega |\nabla \phi|^2$$

Link Primal & Dual mesh (for convergence)

$$\forall u_T \in \mathbb{R}^{N_{\mathscr{T}}}, \quad [\![\Pi^T u_T, u_T]\!]_T = \frac{1}{2h^\beta} \|u_{h,M} - u_{h,M^*}\|_{L^2(\Omega)}^2$$

Discrete results

Proposition: Unconditionally stable energy estimate

Let (ϕ_T^n, c_T^n) be given. Suppose there exists a solution $(\phi_T^{n+1}, \mu_T^{n+1}, c_T^{n+1}, \eta_T^{n+1})$ to the discrete problem. Then, for all time step $\Delta t,$ a discrete energy equality holds.

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⟶ *A priori* bounds on the solutions:

- $L^\infty(0,T; H^1(\Omega))$ bound on ϕ_T^n, c_T^n
- $L^\infty(0,T; L^4(\Omega))$ bound on $\nabla^{\mathcal{D}}\phi_T^n$
- $L^2(0,T; H^1(\Omega))$ bound on μ_T^n, η_T^n
- $L^2(0,T; H^1(\Omega))$ bound on $\partial_t\phi_T^n$, $\partial_t c_T^n$

Discrete results

Proposition: Unconditionally stable energy estimate

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

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- $L^2(0,T;H^1(\Omega))$ bound on $\partial_t\phi_{\mathcal{T}}^n$, $\partial_t c_{\mathcal{T}}^n$

Proposition: Existence of a discrete solution

Let $(\phi_{\mathcal{T}}^n, c_{\mathcal{T}}^n)$ be given. Suppose that $f_\phi(\phi)$ and $f_c(c)$ satisfy a dissipativity condition, and that the polynomial terms satisfy the polynomial growth hypothesis.

Then, there exists at least one solution $(\phi_{\mathcal{T}}^{n+1}, \mu_{\mathcal{T}}^{n+1}, c_{\mathcal{T}}^{n+1}, \eta_{\mathcal{T}}^{n+1})$ to the discrete problem.

Proof. Topological degree (Brouwer fixed point).

Convergence of the numerical scheme

Convergence theorem

Let $\Delta t, h \to 0$ with $\mathrm{reg}(T)$ bounded. Assume

$$c_{\mathscr{D}}^{\Delta t} \leq M \quad \text{a.e. in } (0,T)\times\Omega . \qquad (\star)$$

Then, up to a subsequence, the approximate solutions converge to a weak solution (ϕ, c, μ, η) of the continuous problem:

- $\phi_h^{\Delta t} \to \phi$ strongly in $L^2(0,T;L^2(\Omega))$, $\quad \nabla^h \phi_h^{\Delta t} \to \nabla\phi$ strongly in $L^2(0,T;L^4(\Omega))^2$
- $c_h^{\Delta t} \to c$ strongly in $L^2(0,T;L^2(\Omega))$, $\quad \nabla^h c_h^{\Delta t} \rightharpoonup \nabla c$ weakly in $L^2(0,T;L^2(\Omega))^2$
- $\mu_h^{\Delta t} \rightharpoonup \mu$, $\quad \eta_h^{\Delta t} \rightharpoonup \eta$ weakly in $L^2(0,T;H^1(\Omega))$

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- $\mu_h^{\Delta t} \rightharpoonup \mu, \quad \eta_h^{\Delta t} \rightharpoonup \eta$ weakly in $L^2(0,T;H^1(\Omega))$

Proof. Three-step strategy

STEP 1: Existence of limits (ϕ, μ, c, η)
STEP 2: Pass to the limit in the system: 2 non identified limits — ξ, χ
STEP 3: Identify ξ, χ via Minty's trick and convergence of norms

Step 1: existence of limits

1)

Proposition: Existence of the limits

There exist $\phi, c, \mu, \eta \in L^2(0,T; H^1(\Omega))$, such that (up to a subsequence)

- $\phi_h^{\Delta t} \to \phi, \quad c_h^{\Delta t} \to c$ strongly in $L^2(0,T; L^2(\Omega))$
- $\nabla^h \phi_h^{\Delta t} \rightharpoonup \nabla \phi, \quad \nabla^h c_h^{\Delta t} \rightharpoonup \nabla c$ weakly in $L^2(0,T; L^2(\Omega))^2$
- $\mu_h^{\Delta t} \rightharpoonup \mu, \quad \eta_h^{\Delta t} \rightharpoonup \eta$

Primal and dual approximations share the same limits

Proof. Discrete Aubin–Simon lemma *(Gallouët–Latché)* + Penalization term

Step 1: existence of limits

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There exist $\phi, c, \mu, \eta \in L^2(0,T; H^1(\Omega))$, such that (up to a subsequence)

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Primal and dual approximations share the same limits

Proof. Discrete Aubin–Simon lemma *(Gallouët–Latché)* + Penalization term

2) Since $\nabla^h \phi_h^{\Delta t}$ is bounded in $L^\infty(0,T; L^4)$, we get $\nabla^h \phi_h^{\Delta t} \rightharpoonup \nabla \phi$ weakly in $L^2(0,T; L^4(\Omega))^2$.

Step 2: limit equations (with unidentified terms)

Proposition: Limit equations

$$\int_0^T \int_\Omega (-\partial_t \psi \phi + \nabla \mu \cdot \nabla \psi) = \int_\Omega \phi^0 \psi(0,\cdot)$$

$$\int_0^T \int_\Omega \left(-\mu + \frac{1}{\epsilon_\phi} f'_\phi(\phi) + \partial_\phi p(\phi, c)\right)\psi + \left(\epsilon_\phi \nabla \phi - 2\alpha c \nabla \phi\right) \cdot \nabla \psi = -\delta \int_0^T \int_\Omega \vec{\xi} \cdot \nabla \psi$$

$$\int_0^T \int_\Omega (-\partial_t \psi, c + \nabla \eta \cdot \nabla \psi) = \int_\Omega c^0 \psi(0,\cdot)$$

$$\int_0^T \int_\Omega \left(-\eta + \frac{1}{\epsilon_c} f'_c(c) + \partial_c p(\phi, c)\right)\psi + \epsilon_c \nabla c \cdot \nabla \psi = \alpha \int_0^T \int_\Omega \chi \psi$$

Convergence of the non-linear polynomial terms thanks to the **penalization term.**

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Convergence of the non-linear polynomial terms thanks to the **penalization term.**

⟶ $\vec{\xi} \; ? = |\nabla \phi|^2 \nabla \phi, \qquad \chi \; ? = |\nabla \phi|^2$

Only weak gradient convergence ⟹ cannot identify cubic and quadratic limits directly.

Step 3a: identifying $\vec{\xi} = |\nabla \phi|^2 \nabla \phi$

We use Minty's trick

1) Under (★): $M - c_{\mathscr{D}}^{n+1} \geq 0$

⟶ **Minty inequality:** $\int_0^T \int_\Omega 2\alpha(M-c)|\nabla\psi - \nabla\phi|^2 + \delta(|\nabla\psi|^2\nabla\psi - \xi)\cdot(\nabla\psi - \nabla\phi) \geq 0$

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2) Take $\psi = \phi \pm t\omega,\, t \to 0$ $\Longrightarrow$ $\nabla \cdot \xi = \nabla \cdot (|\nabla\phi|^2 \nabla\phi)$

Step 3b: identifying $\chi = |\nabla\phi|^2$

Strong convergence of the gradient

Identified by Minty

$$(\star) \qquad \int_0^T \int_\Omega \left(-\mu + \frac{1}{\epsilon_\phi} f_\phi'(\phi) + \partial_\phi F(\phi, c)\right)\psi + \left(\epsilon_\phi \nabla\phi - 2\alpha c \nabla\phi\right) \cdot \nabla\psi = -\delta \int_0^T \int_\Omega |\nabla\phi|^2 \nabla\phi \cdot \nabla\psi$$

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1) Test $(\star)$ with $\psi = \phi$: $$\limsup_{h,\Delta t\to 0}\left(\sum_{n=1}^N \Delta t\|\nabla^{\mathcal{D}}\phi_T^n\|^4_{L^4(\Omega)}\right) \le \int_0^T \|\nabla\phi\|^4_{L^4(\Omega)}dt\,.$$

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2) Weak lower semicontinuity $\quad \liminf_{h,\Delta t\to 0}\Big(\sum_{n=1}^N \Delta t\|\nabla^{\mathcal{D}}\phi_T^n\|^4_{L^4(\Omega)}\Big) \ge \int_0^T \|\nabla\phi\|^4_{L^4(\Omega)}dt.$

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$$\liminf_{h,\Delta t\to 0}\Big(\sum_{n=1}^N \Delta t\|\nabla^{\mathcal{D}}\phi_T^n\|^4_{L^4(\Omega)}\Big) \ge \int_0^T \|\nabla\phi\|^4_{L^4(\Omega)}dt.$$

$$\Longrightarrow \quad \boxed{\lim_{h,\Delta t\to 0}\Big(\sum_{n=1}^N \Delta t\|\nabla^{\mathcal{D}}\phi_T^n\|^4_{L^4(\Omega)}\Big) = \int_0^T \|\nabla\phi\|^4_{L^4(\Omega)}dt.}$$

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Strong convergence of the gradient

Identified by Minty

$$(\star) \qquad \int_0^T \int_\Omega \left(-\mu + \frac{1}{\epsilon_\phi} f'_\phi(\phi) + \partial_\phi F(\phi, c)\right)\psi + \left(\epsilon_\phi \nabla \phi - 2\alpha c \nabla \phi\right) \cdot \nabla \psi = -\delta \int_0^T \int_\Omega |\nabla \phi|^2 \nabla \phi \cdot \nabla \psi$$

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1) Test $(\star)$ with $\psi = \phi$: $\quad \limsup_{h,\Delta t \to 0} \left(\sum_{n=1}^{N} \Delta t \|\nabla^{\mathcal{D}} \phi_{\mathcal{T}}^n\|_{L^4(\Omega)}^4 \right) \leq \int_0^T \|\nabla \phi\|_{L^4(\Omega)}^4 dt.$

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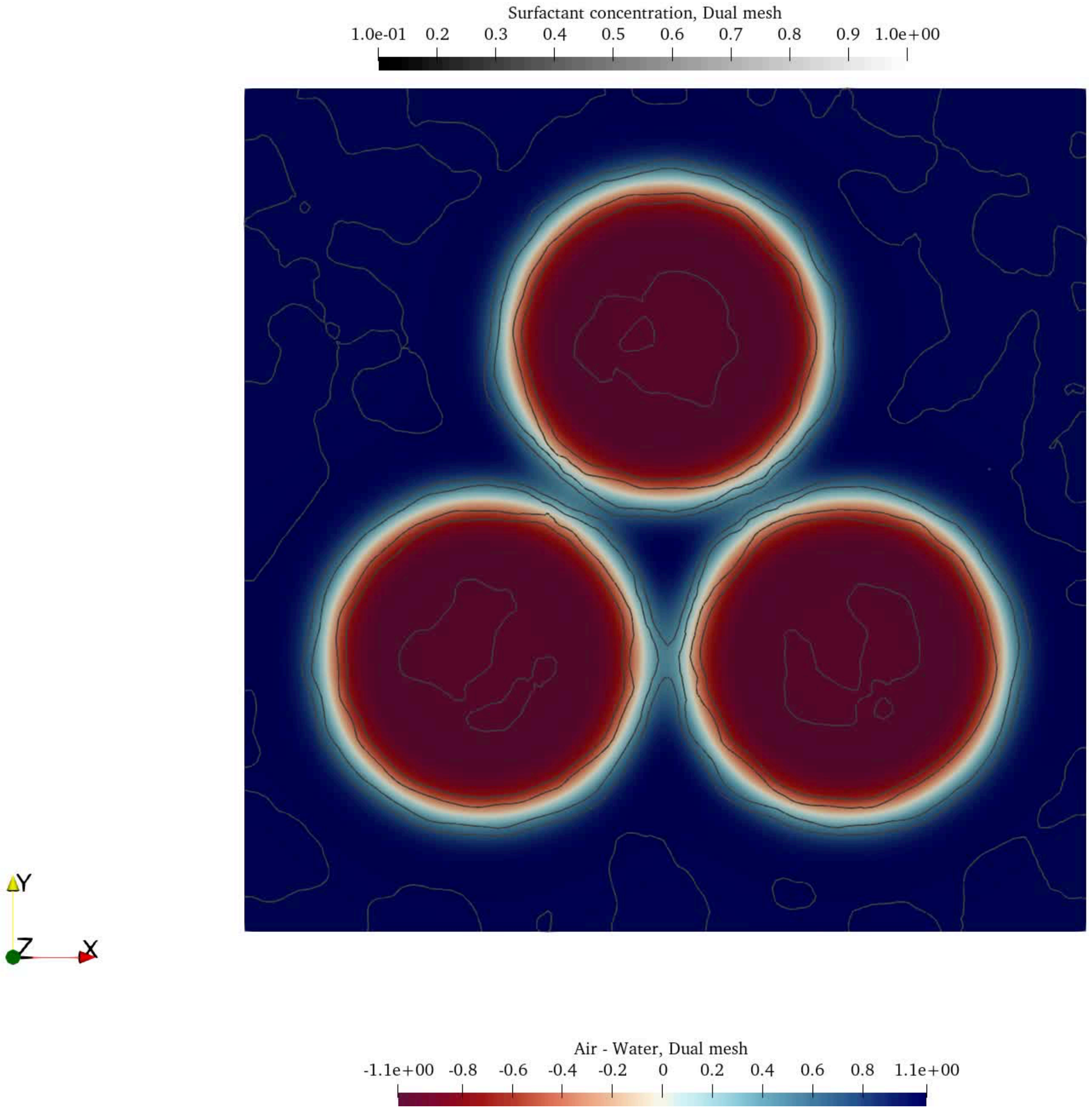
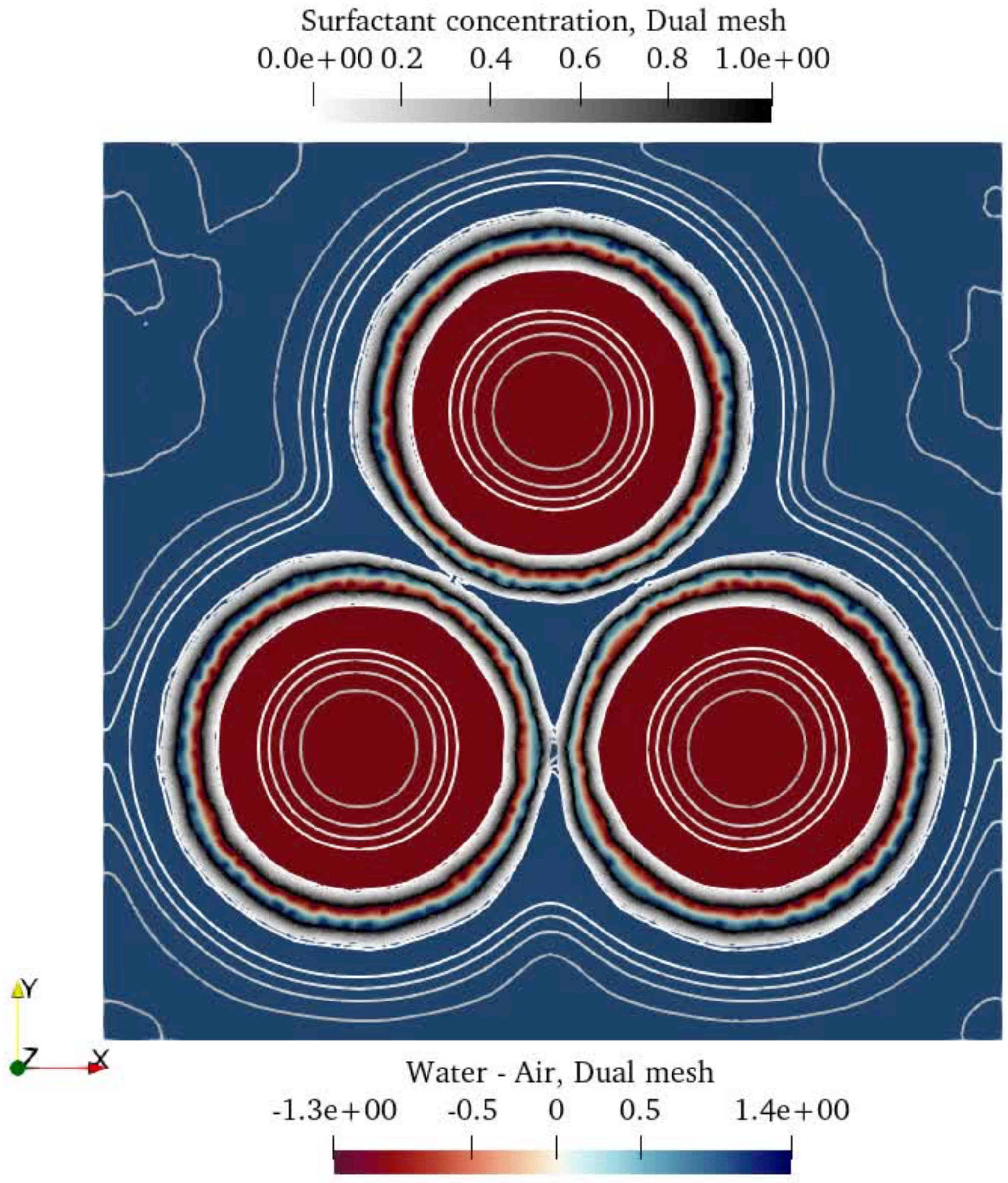
$$\Longrightarrow \quad \boxed{\lim_{h,\Delta t \to 0} \left(\sum_{n=1}^{N} \Delta t \|\nabla^{\mathcal{D}} \phi_{\mathcal{T}}^n\|_{L^4(\Omega)}^4 \right) = \int_0^T \|\nabla \phi\|_{L^4(\Omega)}^4 dt.}$$

Weak convergence + Convergence of the norms
= Strong convergence

$$\Longrightarrow \quad \boxed{\chi = |\nabla \phi|^2}$$

Numerical simulations - surfactants stabilizing bubbles





Numerical coupling with Navier-Stokes equations

Time splitting

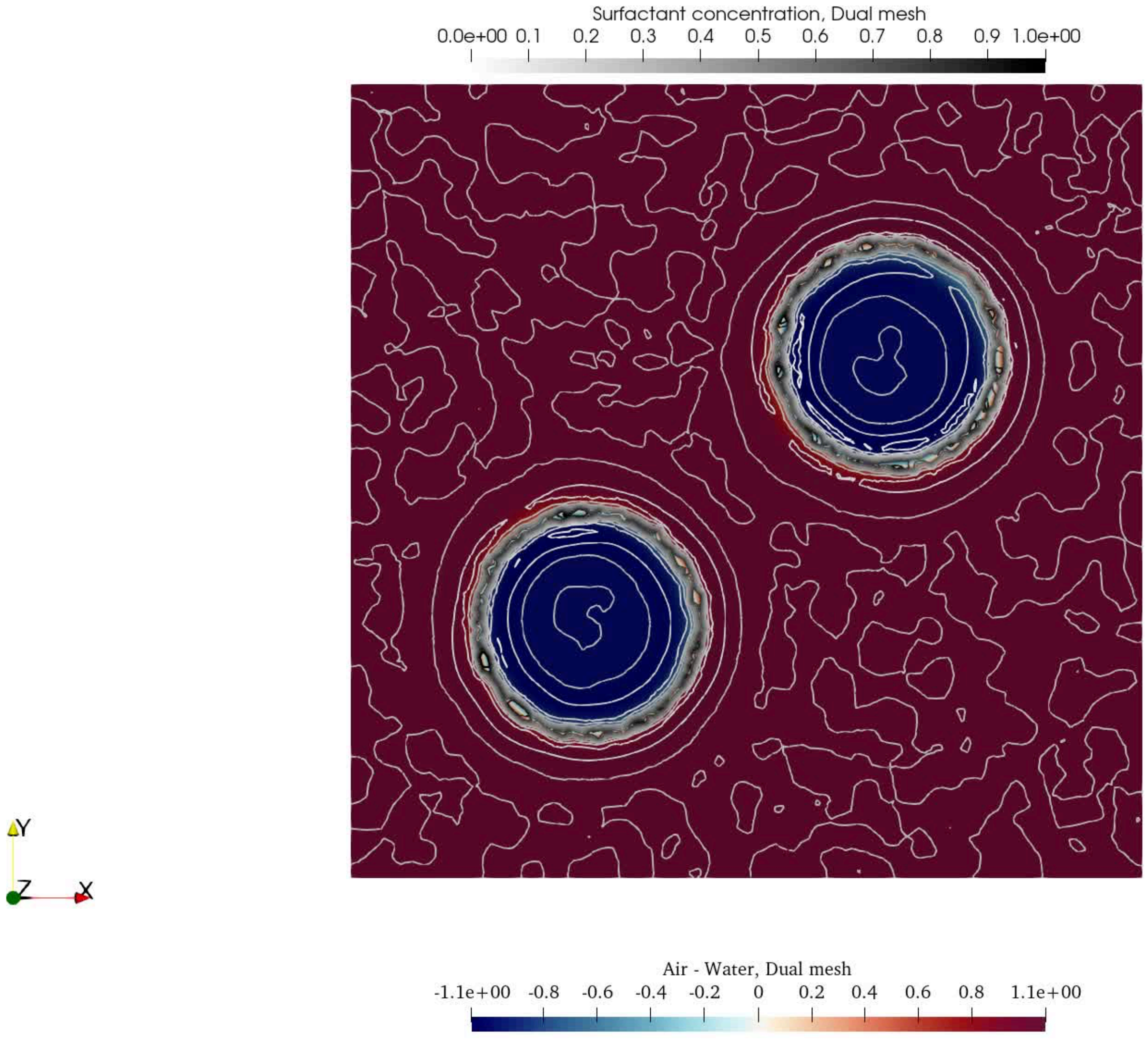
Step 1 — Let (ϕ_T^n, c_T^n, u_T^n) be given, solve Cahn-Hilliard

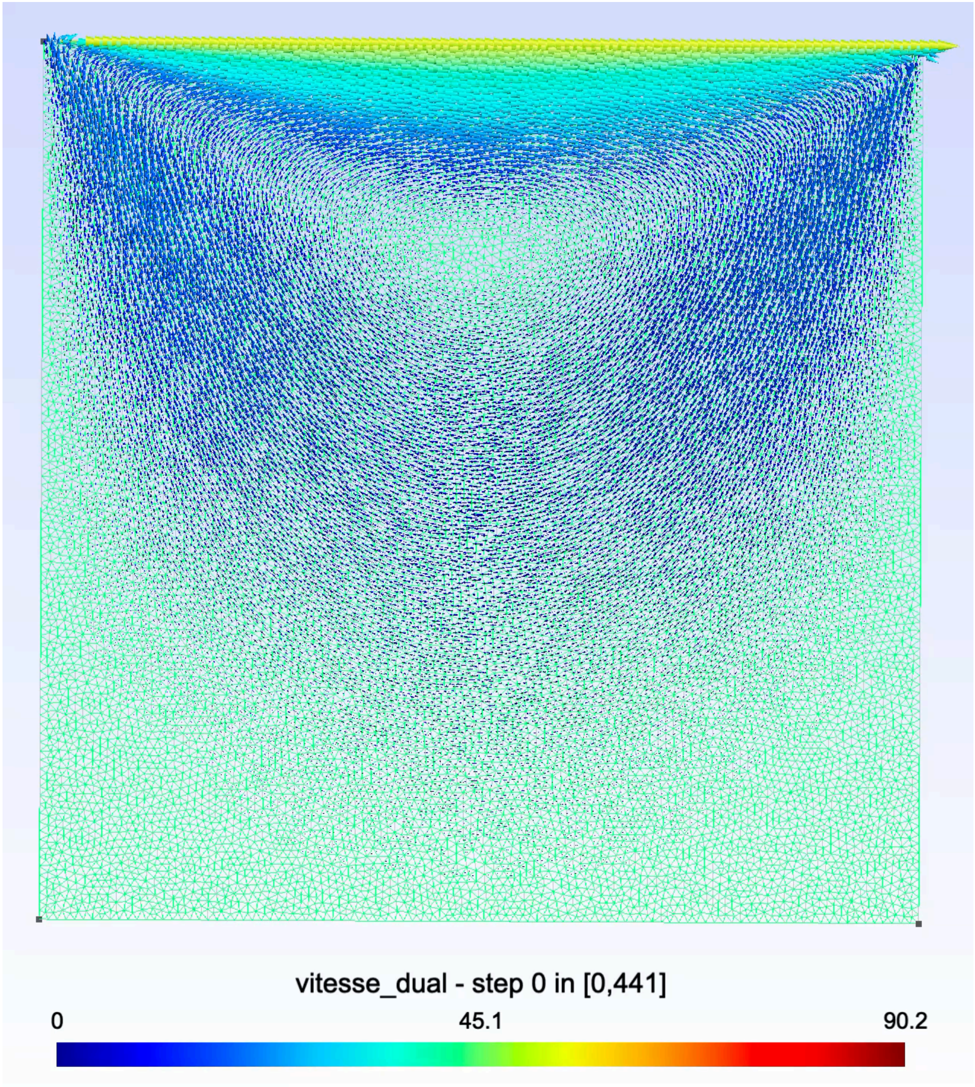
$$\begin{cases} \partial_t \phi + \nabla \cdot (u^n \phi) = \Delta \mu, \\ \mu = -\epsilon_\phi \Delta \phi + \dfrac{1}{\epsilon_\phi} f'_\phi(\phi) + \partial_\phi F(\phi, c), \\ \partial_t c + \nabla \cdot (u^n \phi) = \Delta \eta, \\ \eta = -\epsilon_c \Delta c + \dfrac{1}{\epsilon_c} f'_c(c) + \partial_c F(\phi, c), \end{cases}$$

Step 2 — Let $(\phi_T^{n+1}, c_T^{n+1}, u_T^n)$ be given, solve Navier-Stokes

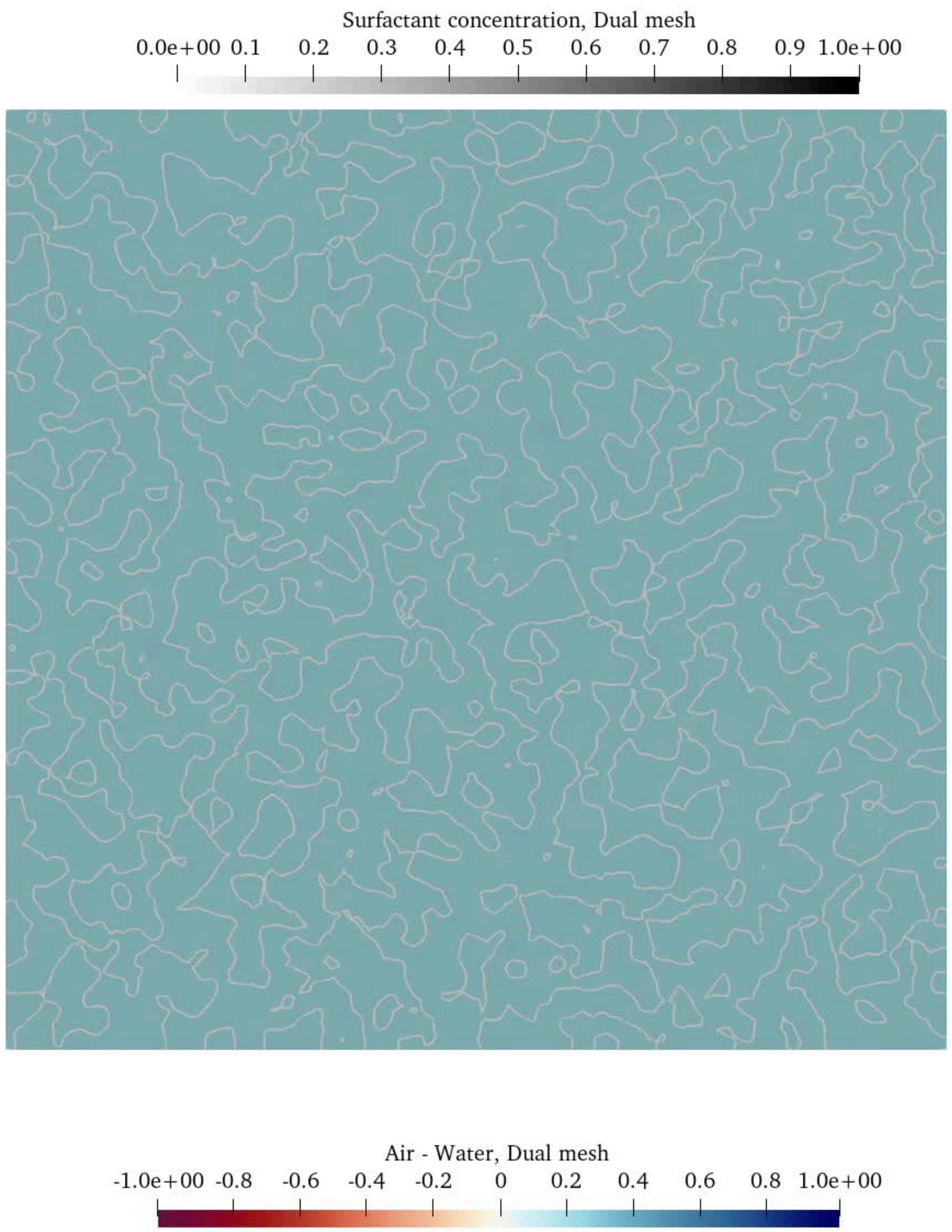
$$\begin{cases} \partial_t u + (u \cdot \nabla) u + \nabla p - \nu \Delta u = -\phi^{n+1} \nabla \mu^{n+1} - c^{n+1} \nabla \eta^{n+1}, \\ \nabla \cdot u = 0 \end{cases}$$

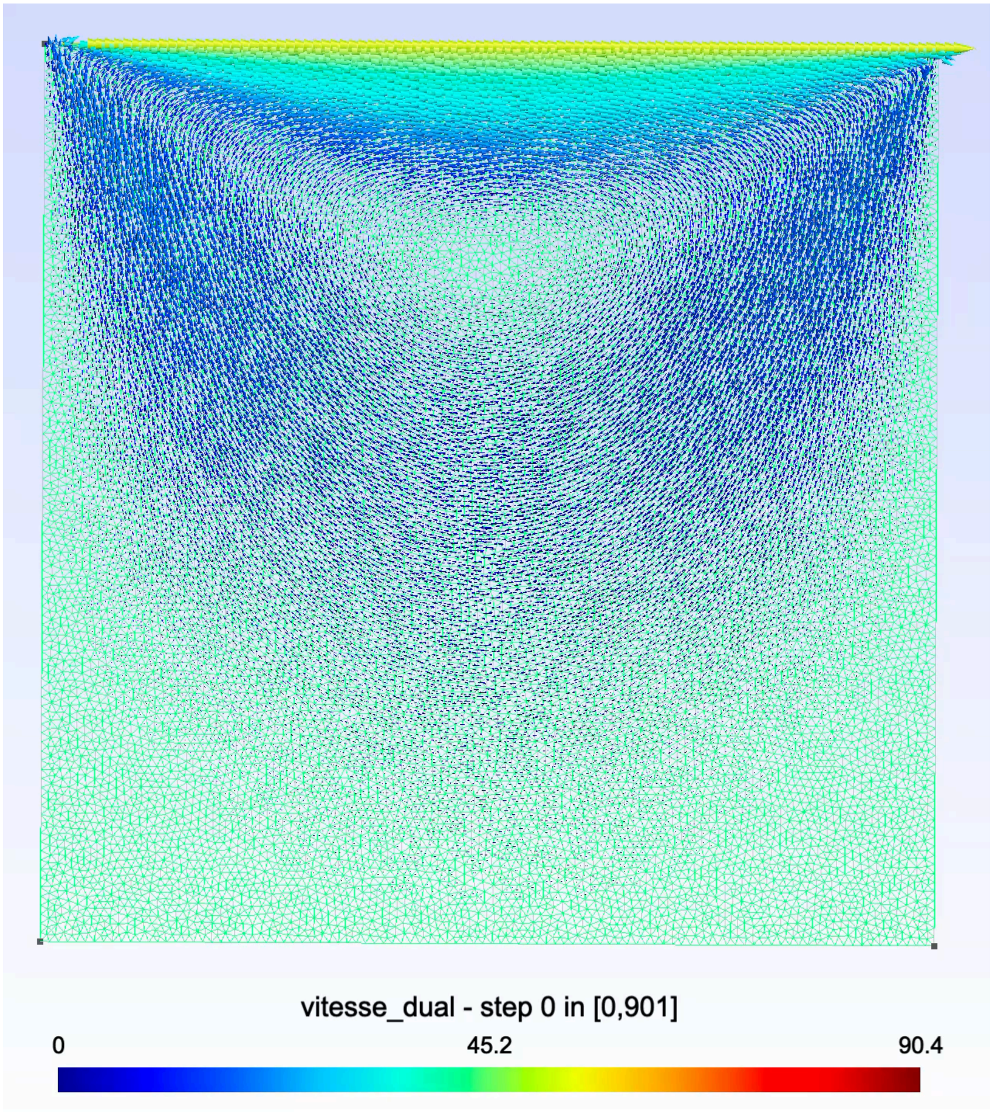
Numerical simulations - surfactants around air bubbles with NS





Numerical simulations - surfactants around air bubbles with NS





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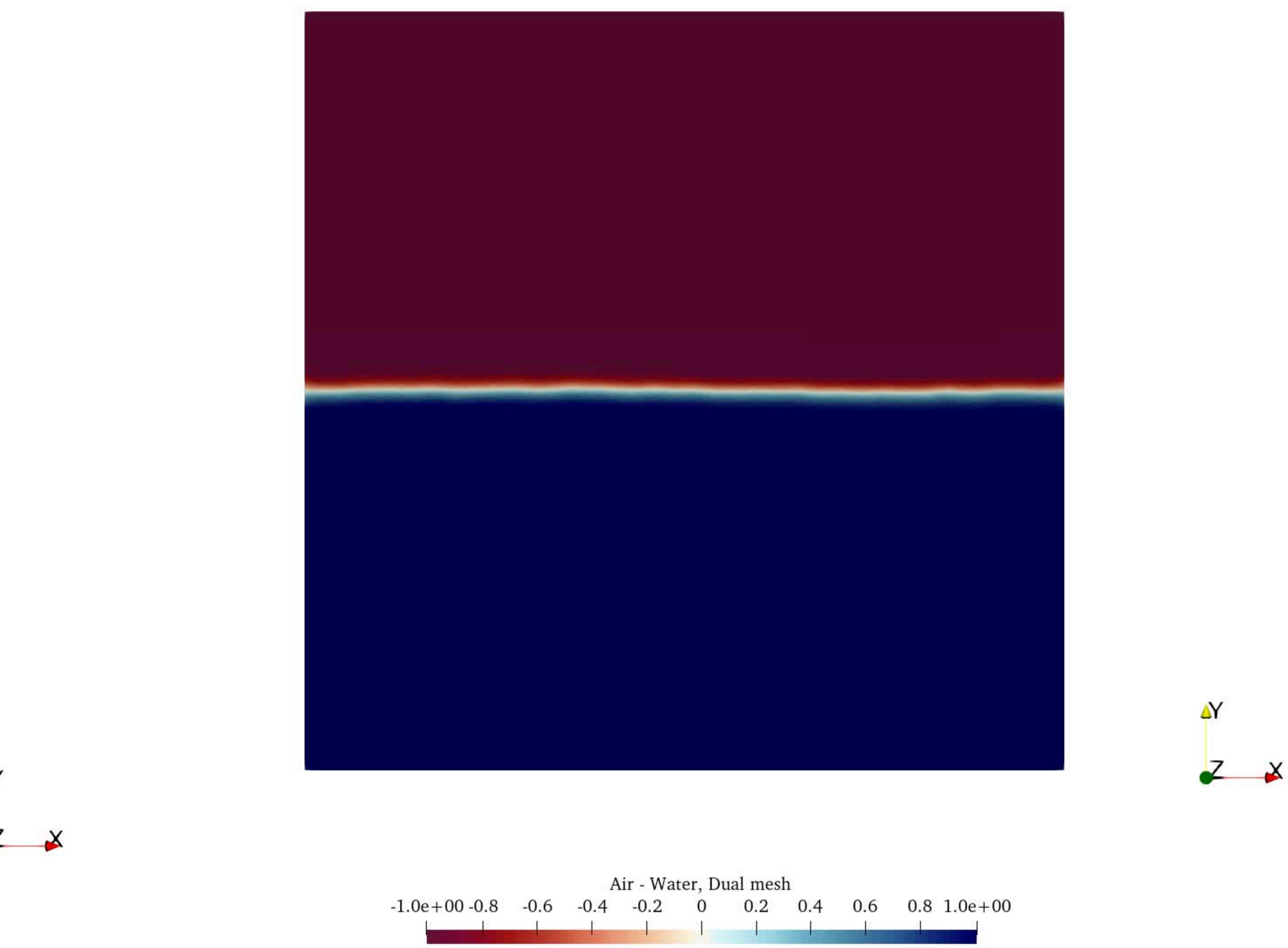

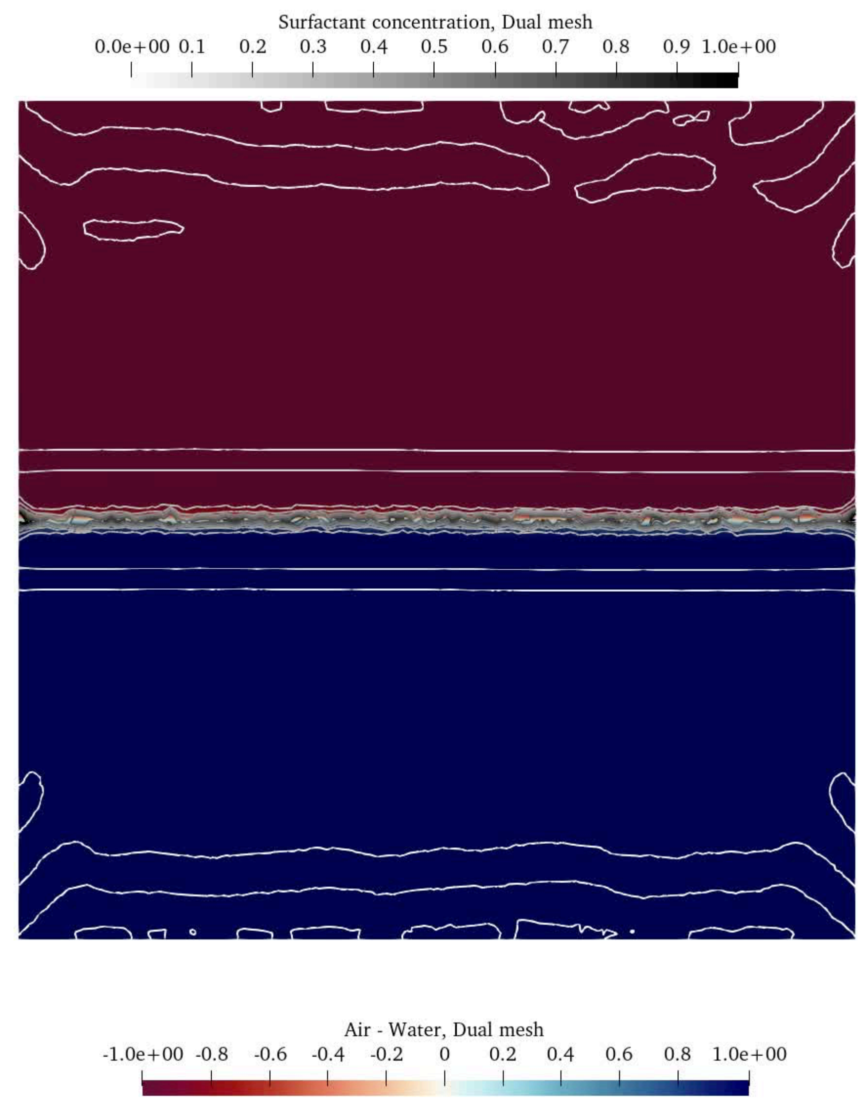

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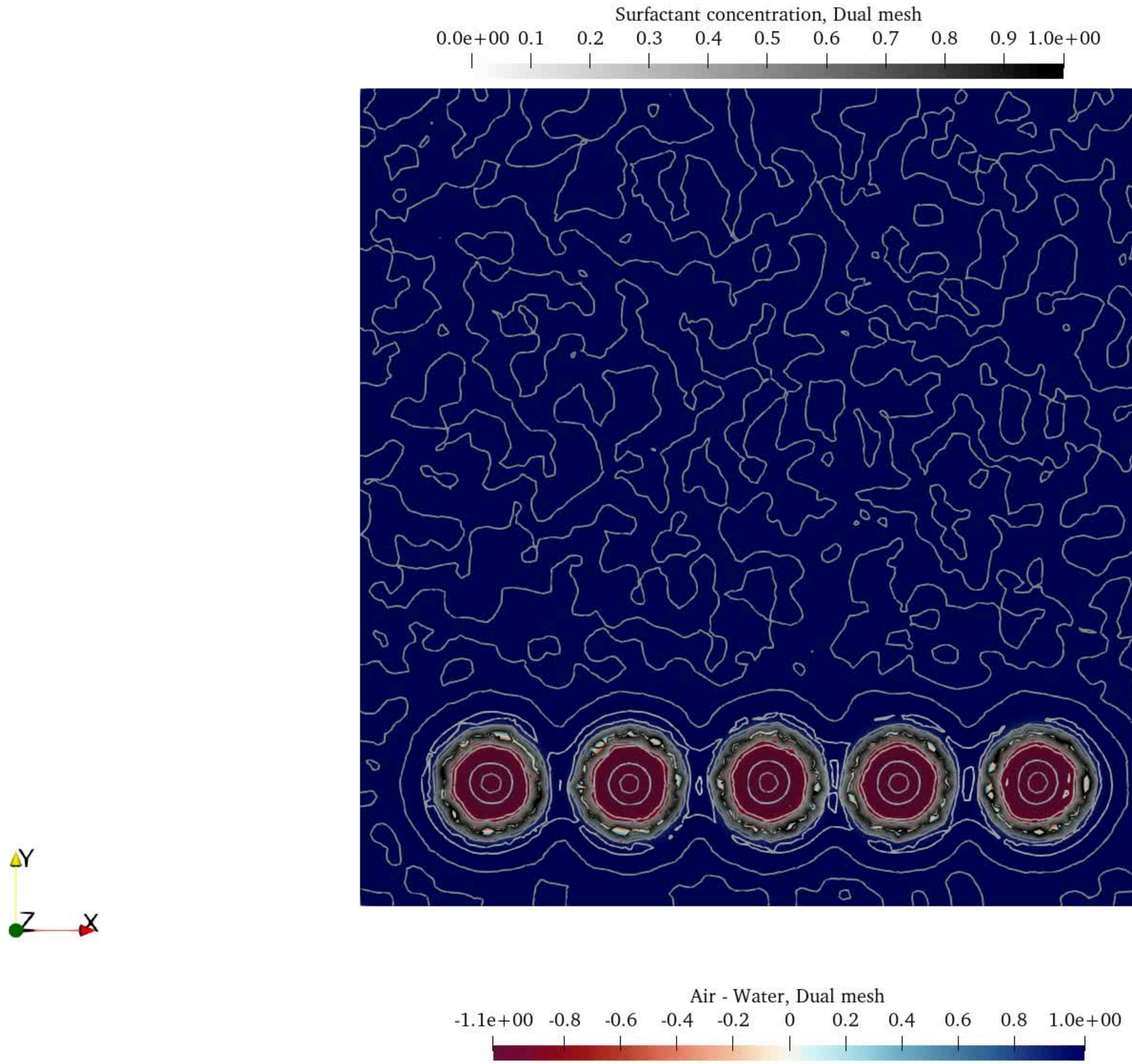

Conclusion and perspectives

Conclusion

- Construction of an unconditionally energy-stable DDFV scheme
- Existence and a priori estimates of the discrete solution
- First convergence result for the Chan-Hilliard model with surfactants
- Numerical coupling with Navier-Stokes and energy estimate

Perspectives

- Existence of a discrete solution for the coupled Chan-Hilliard model with surfactants
- Existence proof for the continuous model