Finite volume method for the Cahn-Hilliard equation with dynamic boundary condition

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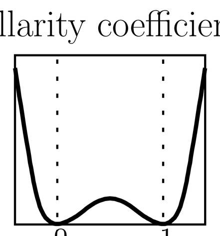
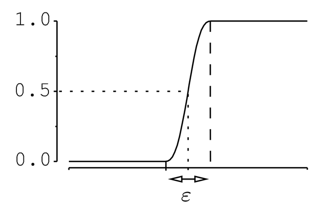
We study the evolution of binary mixtures taking into account the effective interaction between the wall (i.e the boundary Γ) and two mixture components. This phenomenon is described by the Cahn-Hilliard equation with non-linear dynamic boundary condition: Find $c : (0,T) \times \Omega \to \mathbb{R}$,

$$(\mathcal{P}) \begin{cases} \partial_t c = \Gamma_b \Delta\mu, & \text{in } (0,T)\times\Omega; \\ \mu = -\frac{3}{2}\varepsilon\sigma_b\Delta c + \frac{12}{\varepsilon}\sigma_b f_b'(c), & \text{in } (0,T)\times\Omega; \\ \partial_t c_{|\Gamma} = \frac{\Gamma_s\Gamma_b}{\varepsilon^3}\left[\sigma_s\sigma_b\varepsilon^2\Delta_{\|}c_{|\Gamma} - 3\sqrt{2}\sigma_b f_s'(c_{|\Gamma}) - \frac{3}{2}\varepsilon\sigma_b\partial_n c\right], & \text{in } (0,T)\times\Gamma; \\ \partial_n\mu = 0 & \text{in } (0,T)\times\Gamma; \\ c(0,.) = c_0, & \text{in } \Omega; \end{cases}$$

where c is called the order parameter and μ the chemical potential.
$\Omega \subset \mathbb{R}^2$ is a smooth connected bounded domain, Γ_b is a bulk mobility, σ_b is the fluid-fluid surface tension, Γ_s defines a surface kinetic coefficient, σ_s a surface capillarity coefficient and f_s is the surface free energy density.



Bulk free energy density f_b



Interface thickness ε

The free energy functional associated with this problem is the following:

$$\mathcal{F}(c) = \int_\Omega \left(\frac{3}{4}\varepsilon\sigma_b|\nabla c|^2 + \frac{12}{\varepsilon}\sigma_b f_b(c)\right) + \int_\Gamma \left(\frac{\varepsilon^2}{2}\sigma_s\sigma_b\left|\nabla_{\|}c\right|^2 + 3\sqrt{2}\sigma_b f_s(c)\right),$$

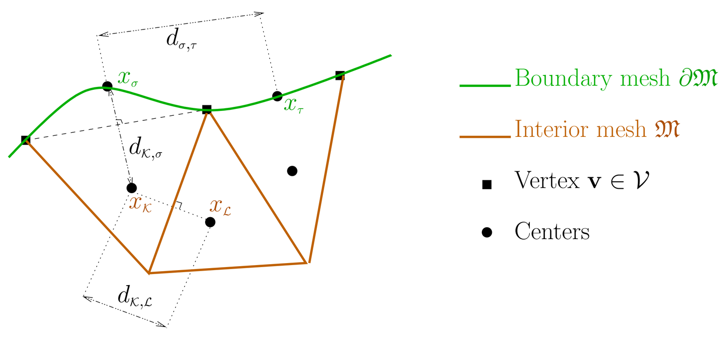
and formally verifies:

$$\frac{d}{dt}\mathcal{F}[c(t,.)] = -\Gamma_b\int_\Omega|\nabla\mu|^2 - \frac{\varepsilon^3}{\Gamma_s\Gamma_b}\int_\Gamma|\partial_t c_{|\Gamma}|^2.$$

Remark: The standard Neumann boundary condition $\partial_n c = 0$ can be recovered by setting $\Gamma_s = +\infty$, $\sigma_s = 0$ and $f_s = 0$.

1. FV framework

- **Space discretization:** $\mathcal{T} = (\mathfrak{M}, \partial\mathfrak{M})$



- **Time discretization:** Let $N \in \mathbb{N}^*$ and $T \in]0,+\infty[$.
  Time step: $\Delta t = \frac{T}{N} \Rightarrow t_n = n\Delta t, \quad \forall n \in [\![0,N]\!]$.

- **Discrete unknowns:** For $n \in [\![0,N]\!]$,
  $\mu_\mathfrak{M}^n = (\mu_\mathcal{K}^n)_{\mathcal{K}\in\mathfrak{M}}$ and $c_\mathcal{T}^n = (c_\mathfrak{M}^n, c_{\partial\mathfrak{M}}^n)$ where $c_\mathfrak{M}^n = (c_\mathcal{K}^n)_{\mathcal{K}\in\mathfrak{M}}$, $c_{\partial\mathfrak{M}}^n = (c_\sigma^n)_{\sigma\in\partial\mathfrak{M}}$.
- **Discrete H^1 seminorms:** For $u_\mathcal{T} \in \mathbb{R}^\mathcal{T}$ and $v_{\partial\mathfrak{M}} \in \mathbb{R}^{\partial\mathfrak{M}}$,

$$|u_\mathcal{T}|_{1,\mathcal{T}}^2 \stackrel{def}{=} \sum_{\sigma\subset\Omega} m_\sigma d_{\mathcal{K},\mathcal{L}}\left(\frac{u_\mathcal{K} - u_\mathcal{L}}{d_{\mathcal{K},\mathcal{L}}}\right)^2 + \sum_{\sigma\in\partial\mathfrak{M}} m_\sigma d_{\mathcal{K},\sigma}\left(\frac{u_\mathcal{K} - u_\sigma}{d_{\mathcal{K},\sigma}}\right)^2$$

  where $u_\sigma = u_\mathcal{K}$ if $u_\mathcal{T}$ satisfies Neumann boundary condition.

$$|v_{\partial\mathfrak{M}}|_{1,\partial\mathfrak{M}}^2 \stackrel{def}{=} \sum_{\mathbf{v}\in\mathcal{V}} d_{\sigma,\tau}\left(\frac{v_\sigma - v_\tau}{d_{\sigma,\tau}}\right)^2.$$

- **Discrete projection:** For $u \in \mathcal{C}^0([0,T]\times\overline{\Omega})$ and $n \in [\![0,N]\!]$ fixed,

$$\mathbb{P}_\mathcal{T}^c u(t^n) \stackrel{def}{=} (\mathbb{P}_\mathfrak{M}^c u(t^n), \mathbb{P}_{\partial\mathfrak{M}}^c u(t^n)) \stackrel{def}{=} (u(t^n, x_\mathcal{K})_{\mathcal{K}\in\mathfrak{M}}, u(t^n, x_\sigma)_{\sigma\in\partial\mathfrak{M}}).$$

- **Discrete free energy** :

$$\mathcal{F}_\mathcal{T}(c_\mathcal{T}) \stackrel{def}{=} \mathcal{F}_\mathfrak{M}^b(c_\mathcal{T}) + \mathcal{F}_{\partial\mathfrak{M}}^s(c_{\partial\mathfrak{M}}),$$

  where

$$\begin{cases} \mathcal{F}_\mathfrak{M}^b(c_\mathcal{T}) \stackrel{def}{=} \frac{12}{\varepsilon}\sigma_b\sum_{\mathcal{K}\in\mathfrak{M}} m_\mathcal{K} f_b(c_\mathcal{K}) + \frac{3}{4}\varepsilon\sigma_b|c_\mathcal{T}|_{1,\mathcal{T}}^2, \\ \mathcal{F}_{\partial\mathfrak{M}}^s(c_{\partial\mathfrak{M}}) \stackrel{def}{=} 3\sqrt{2}\sigma_b\sum_{\sigma\in\partial\mathfrak{M}} m_\sigma f_s(c_\sigma) + \frac{\varepsilon^2}{2}\sigma_b\sigma_s|c_{\partial\mathfrak{M}}|_{1,\partial\mathfrak{M}}^2. \end{cases}$$

2. FV scheme

- Consistent two point flux approximation for Laplace operators in Ω.
- Consistent two point flux approximation for Laplace-Beltrami op. on Γ.
- Semi implicit approximation in time $\Rightarrow$ Newton method.
- **Coupling between interior and surface evolution equations through flux terms.**

Find $(c_\mathcal{T}^n, \mu_\mathfrak{M}^n)_n$ such that $c_\mathcal{T}^0 = \mathbb{P}_\mathcal{T}^c c_0$ and for all n:

$$(\mathcal{S}) \begin{cases} m_\mathcal{K}\frac{c_\mathcal{K}^{n+1} - c_\mathcal{K}^n}{\Delta t} = -\Gamma_b\sum_{\sigma\subset\partial\mathcal{K}\cap\Omega} m_\sigma\left(\frac{\mu_\mathcal{K}^{n+1} - \mu_\mathcal{L}^{n+1}}{d_{\mathcal{K},\mathcal{L}}}\right), & \forall\mathcal{K}\in\mathfrak{M} \\ \frac{3}{2}\varepsilon\sigma_b\left(\sum_{\sigma\subset\partial\mathcal{K}\cap\Omega} m_\sigma\left(\frac{c_\mathcal{K}^{n+1} - c_\mathcal{L}^{n+1}}{d_{\mathcal{K},\mathcal{L}}}\right) + \boxed{\sum_{\sigma\subset\partial\mathcal{K}\cap\partial\mathfrak{M}} m_\sigma\left(\frac{c_\mathcal{K}^{n+1} - c_\sigma^{n+1}}{d_{\mathcal{K},\sigma}}\right)}\right) & \\ \quad + m_\mathcal{K}\frac{12}{\varepsilon}\sigma_b d^{f_b}(c_\mathcal{K}^n, c_\mathcal{K}^{n+1}) = m_\mathcal{K}\mu_\mathcal{K}^{n+1}, & \forall\mathcal{K}\in\mathfrak{M} \\ \frac{\varepsilon^3 m_\sigma}{\Gamma_b\Gamma_s}\frac{c_\sigma^{n+1} - c_\sigma^n}{\Delta t} = -\varepsilon^2\sigma_b\sigma_s\sum_{\mathbf{v}\in\mathcal{V}_\sigma}\frac{c_\sigma^{n+1} - c_\tau^{n+1}}{d_{\sigma,\tau}} & \\ \quad - \frac{3}{2}\varepsilon\sigma_b m_\sigma\boxed{\frac{c_\sigma^{n+1} - c_\mathcal{K}^{n+1}}{d_{\mathcal{K},\sigma}}} - 3\sqrt{2}\sigma_b m_\sigma d^{f_s}(c_\sigma^n, c_\sigma^{n+1}), & \forall\sigma\in\partial\mathfrak{M} \end{cases}$$

where $d^{f_*} = (f_*(b) - f_*(a))/(b-a)$.

3. Theoretical results

Theorem : Discrete energy equality
For $c_\mathcal{T}^n \in \mathbb{R}^\mathcal{T}$ given if there exists a solution $(c_\mathcal{T}^{n+1}, \mu_\mathfrak{M}^{n+1})$ of $(\mathcal{S})$, then:

$$\mathcal{F}_\mathcal{T}(c_\mathcal{T}^{n+1}) + \Delta t\Gamma_b\left|\mu_\mathfrak{M}^{n+1}\right|_{1,\mathcal{T}}^2 + \frac{1}{\Delta t}\frac{\varepsilon^3}{\Gamma_b\Gamma_s}\left\|c_{\partial\mathfrak{M}}^{n+1} - c_{\partial\mathfrak{M}}^n\right\|_{0,\partial\mathfrak{M}}^2 + \frac{3}{4}\varepsilon\sigma_b\left|c_\mathcal{T}^{n+1} - c_\mathcal{T}^n\right|_{1,\mathcal{T}}^2 + \frac{\varepsilon^2}{2}\sigma_b\sigma_s\left|c_{\partial\mathfrak{M}}^{n+1} - c_{\partial\mathfrak{M}}^n\right|_{1,\partial\mathfrak{M}}^2 = \mathcal{F}_\mathcal{T}(c_\mathcal{T}^n).$$

Theorem : Existence of a discrete solution
For all $c_\mathcal{T}^0$, there exists at least one solution $((c_\mathcal{T}^n, \mu_\mathfrak{M}^n))_n$ of $(\mathcal{S})$.

Main tool: Topological degree theory.

Theorem : Convergence
Consider the problem $(\mathcal{P})$ on a bounded domain Ω. Then, for all $c_0 \in H^1(\Omega)$ such that $\gamma(c_0) \in H^1(\Gamma)$ there exists a weak solution (c,μ) on $[0,T[$ such that:

$$c \in L^\infty(0,T;H^1(\Omega)), \quad \gamma(c) \in L^\infty(0,T;H^1(\Gamma)), \quad \mu \in L^2(0,T;H^1(\Omega)),$$

and for all $q \geq 1$, there exists a subsequence such that

$$c_\mathcal{T}^{\Delta t} \xrightarrow[\text{size}(\mathcal{T}),\Delta t\to 0]{} c \text{ in } L^2(0,T;L^q(\Omega)) \text{ strong},$$
$$c_{\partial\mathfrak{M}}^{\Delta t} \xrightarrow[\text{size}(\mathcal{T}),\Delta t\to 0]{} \gamma(c) \text{ in } L^2(0,T;L^q(\Gamma)) \text{ strong},$$
$$\text{and } \mu_\mathfrak{M}^{\Delta t} \xrightarrow[\text{size}(\mathcal{T}),\Delta t\to 0]{} \mu \text{ in } L^2(0,T;L^q(\Omega)) \text{ weak}.$$

Main tools: Bounds on discrete solutions - Uniform estimates of time and space translates on Ω and Γ - Kolmogorov theorem - Discrete H^1 compactness.

Theorem : Error estimate (Neumann boundary condition)
Assume that the solution (c,μ) of $(\mathcal{P})$ satisfy $c \in \mathcal{C}^2([0,T],H^2(\Omega))$ and $\mu \in \mathcal{C}^1([0,T],H^2(\Omega))$, then:

$$\max_{0\leq n\leq N}|\mathbb{P}_\mathfrak{M}^c c(t^n) - c_\mathfrak{M}^n|_{1,\mathcal{T}} \leq C\left(\Delta t + \text{size}(\mathcal{T})\right).$$

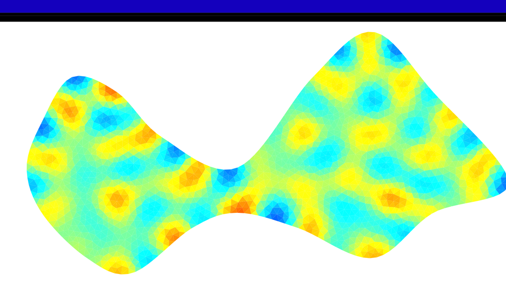
Remark: These results are true with a fully implicit method with $\Delta t \leq \Delta t_0$.

Work in progress: Error estimate for dynamic boundary conditions.

4. Numerical results

Case 1: Phase separation dynamics

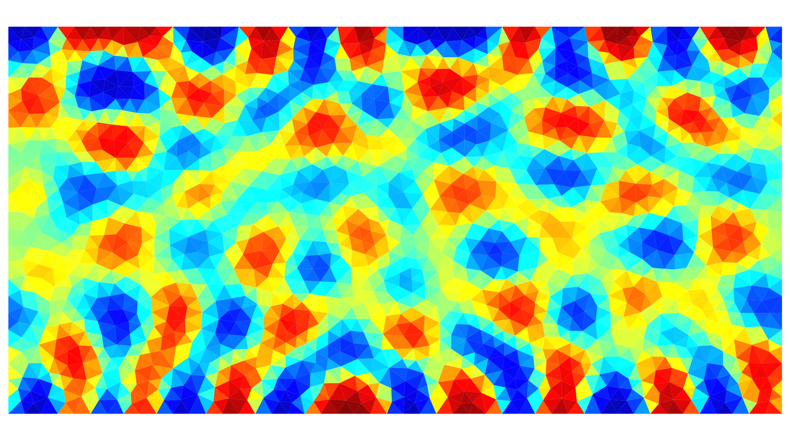
Neumann case parameters:
- Bulk: $\varepsilon = 0.1$, $\Gamma_b = \sigma_b = 0.1$
- Time: $T = 0.03$, $dt = 0.005$.



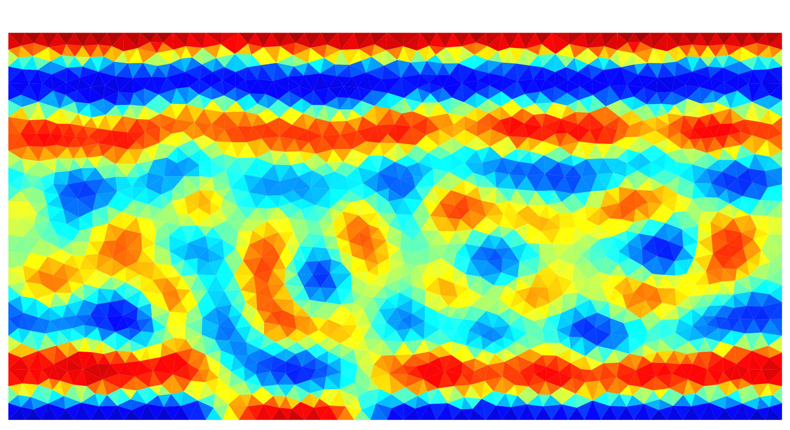
Subcase 1: $f_s = f_b$ $\rightsquigarrow$ In accordance with [1]

Parameters: Domain size 8×4
- Bulk: $\varepsilon = 0.3$, $\Gamma_b = \sigma_b = 0.1$
- Surface: $\Gamma_s = 10$
- Time: $T = 0.75$, $dt = 0.05$.

$\sigma_s = 0$

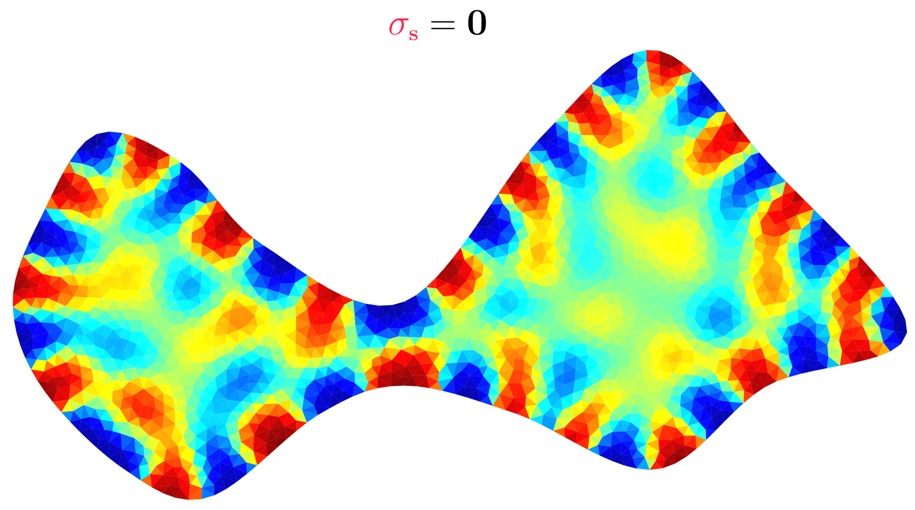


$\sigma_s = 5$

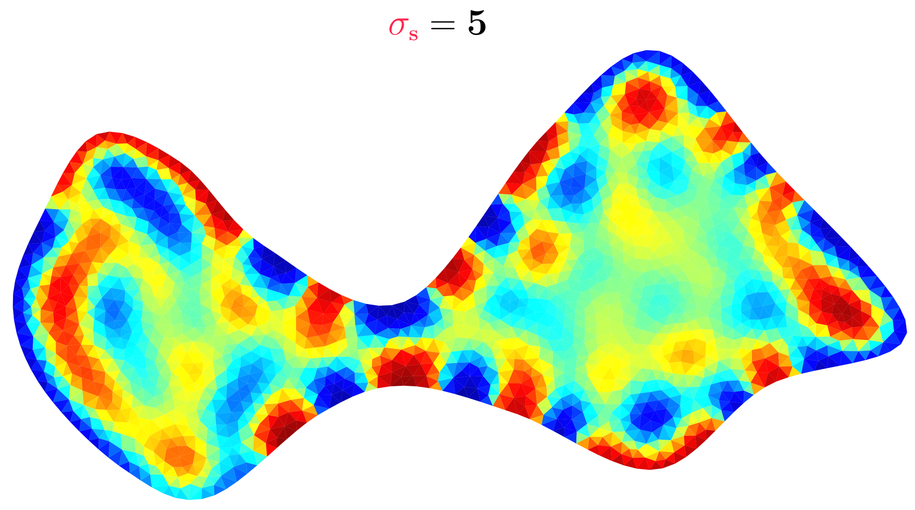


Parameters: Lateral domain size ~ 2
- Bulk: $\varepsilon = 0.1$, $\Gamma_b = \sigma_b = 0.1$
- Surface: $\Gamma_s = 10$
- Time: $T = 0.025$, $dt = 0.005$.

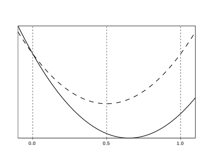
$\sigma_s = 0$



$\sigma_s = 5$



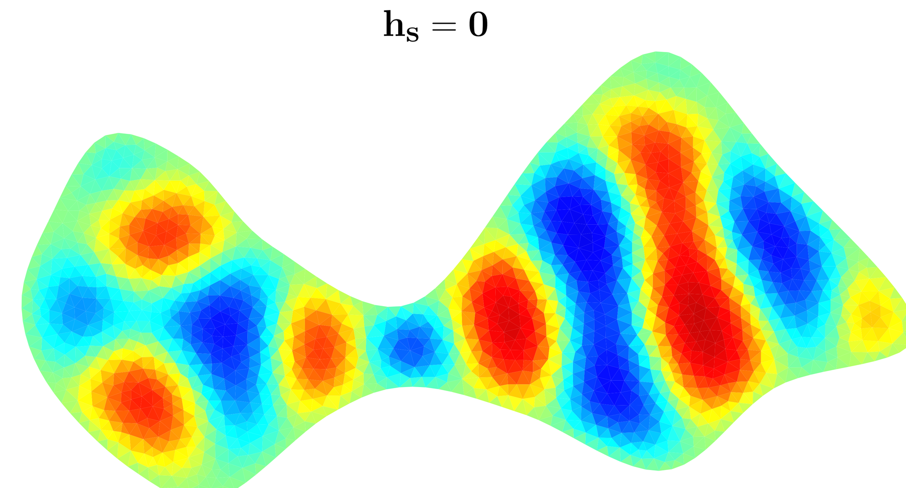
Subcase 2: $f_s(c) = g_s c^2 - (h_s + g_s)c$
$\rightsquigarrow$ In accordance with [3]



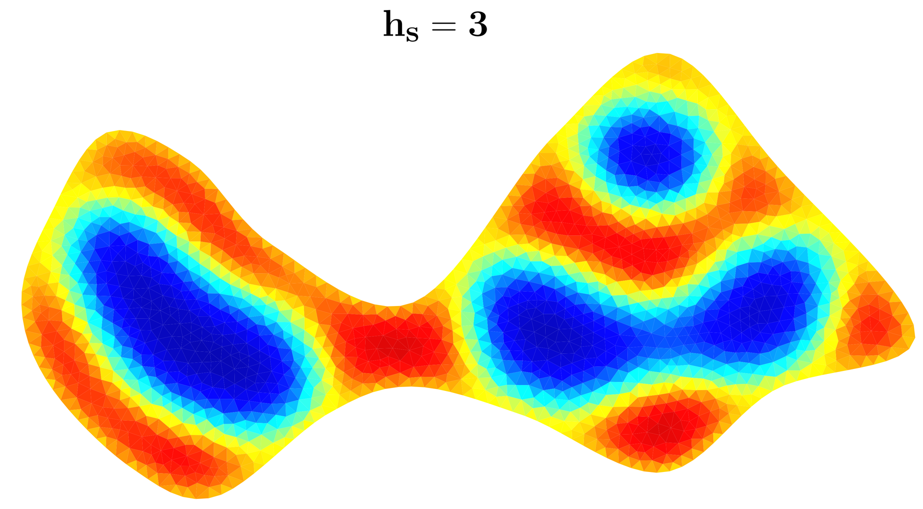
- $h_s = 3$
- - $h_s = 0$

Parameters:
- Bulk: $\varepsilon = 0.2$, $\Gamma_b = \sigma_b = 0.1$
- Surface: $\Gamma_s = 10$, $\sigma_s = 0$, $g_s = 10$
- Time: $dt = 0.001$, $T = 0.37$.

$\mathbf{h_s = 0}$



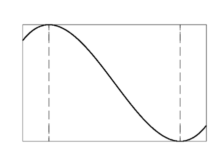
$\mathbf{h_s = 3}$



Case 2: Interface dynamics contact-angle

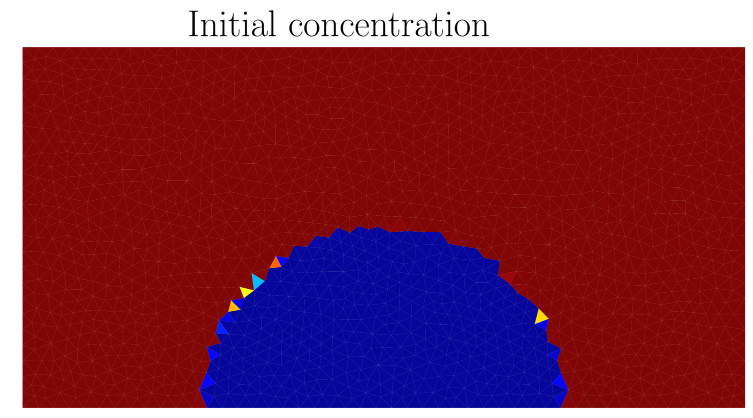
Density: $f_s(c) = \cos(\theta_s)c^2(\frac{2}{3}c - 1)$
$\rightsquigarrow$ In accordance with [4]

Parameters:

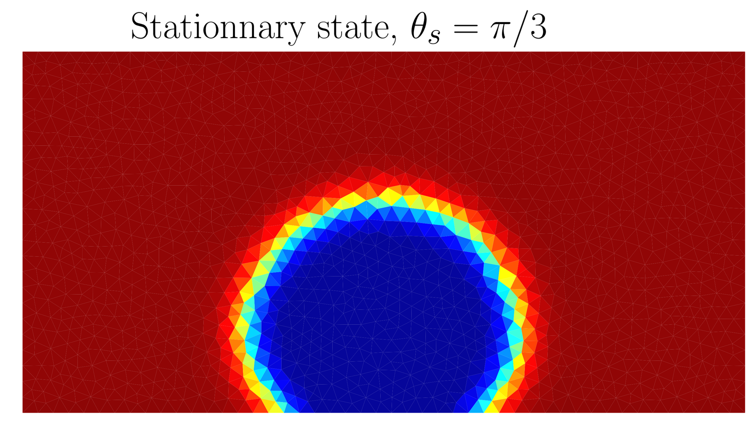


- Bulk: $\varepsilon = 0.4$, $\Gamma_b = \sigma_b = 0.1$
- Surface: $\Gamma_s = 10^7$, $\sigma_s = 0$
- Time: $T = 100$, $dt = 0.1$

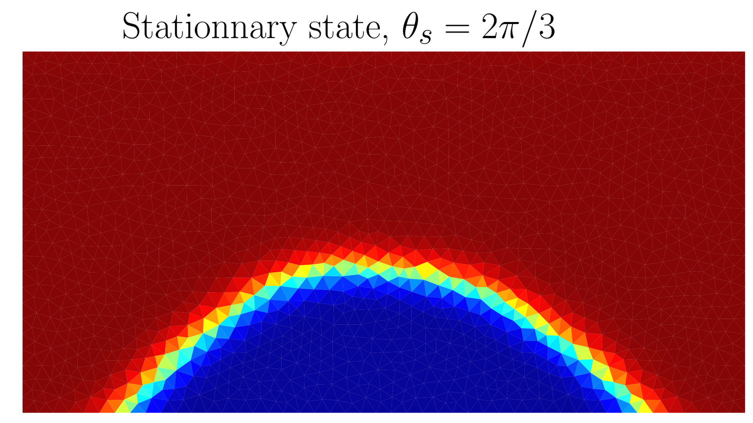
Initial concentration



Stationary state, $\theta_s = \pi/3$



Stationary state, $\theta_s = 2\pi/3$



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