Extensions of the Cahn–Hilliard equation: modelling and simulation of coupled phase-separation processes

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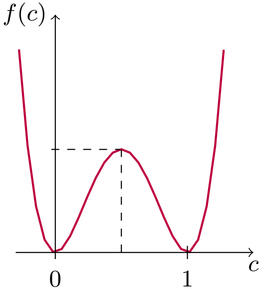
Phase separation

With the Cahn–Hilliard equation we can descibe the separation of a binary mixture:

$$\partial_t c = \nabla \cdot \Big(M \nabla \big(f'(c) - \lambda \Delta c \big) \Big) \quad \text{in } \Omega \times (0, T).$$

- order parameter $c \in [0, 1]$ describes the relative concentration ($c = 0$ and $c = 1$ denotes pure phases)
- total free energy:

  $F(c) \simeq \int_\Omega f(c) + \frac{\lambda}{2} |\nabla c|^2 \, \mathrm{d}x$
- $f(c)$: local free energy
- λ: line tension



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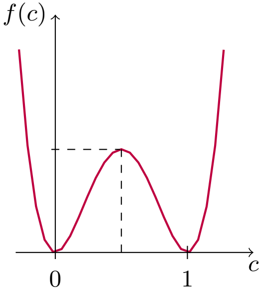


We complete the model with periodic boundary conditions and an initial condition with small local fluctuations.

Mixed finite-element method for Cahn–Hilliard

- split Cahn–Hilliard equation into two 2nd order equations:

$$\partial_t c - \nabla \cdot \big(M \nabla \mu\big) = 0$$
$$\mu - \big(f'(c) - \lambda \Delta c\big) = 0$$

- linear periodic Lagrange elements for discretisation in space (V_h)

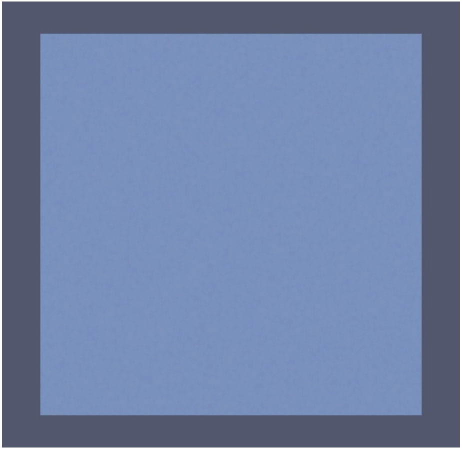
Find $c_h, \mu_h \colon [0,T] \to V_h$ such that

$$(c_h', \varphi_1)_\Omega + (M \nabla \mu_h, \nabla \varphi_1)_\Omega = 0,$$
$$(\mu_h, \varphi_2)_\Omega - (f'(c_h), \varphi_2)_\Omega - (\lambda \nabla c_h, \nabla \varphi_2)_\Omega = 0,$$

for all $\varphi_1, \varphi_2 \in V_h$.

[G. Wells, E. Kuhl and K. Garikipati, 2006]

- backward Euler for discretisation in time



Cahn–Hilliard–Stokes

We use the linear Stokes equation to take flow effects into account.

$$\partial_t c + v \cdot \nabla c - \nabla \cdot (M \nabla \mu) = 0$$
$$\mu - (f'(c) - \lambda \Delta c) = 0$$

$$\partial_t v - \nu \Delta v + \rho^{-1} \nabla p - \rho^{-1} \mu \nabla c = 0$$
$$\nabla \cdot v = 0$$

[C. Eck, M. Fontelos, G. Grün, F. Klingbeil and O. Vantzos, 2009]

Cahn–Hilliard–Stokes

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$$\begin{aligned} \partial_t c + v \cdot \nabla c - \nabla \cdot (M \nabla \mu) &= 0 \\ \mu - (f'(c) - \lambda \Delta c) &= 0 \\ \partial_t v - \nu \Delta v + \rho^{-1} \nabla p - \rho^{-1} \mu \nabla c &= 0 \\ \nabla \cdot v &= 0 \end{aligned}$$

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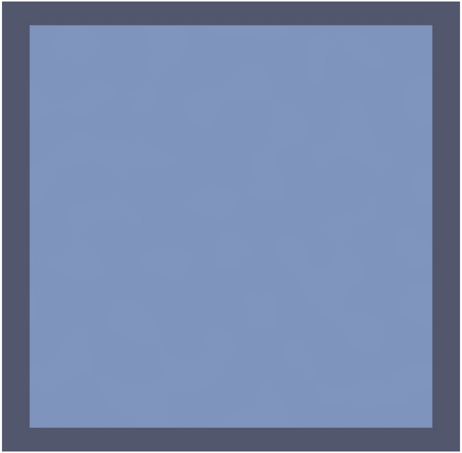
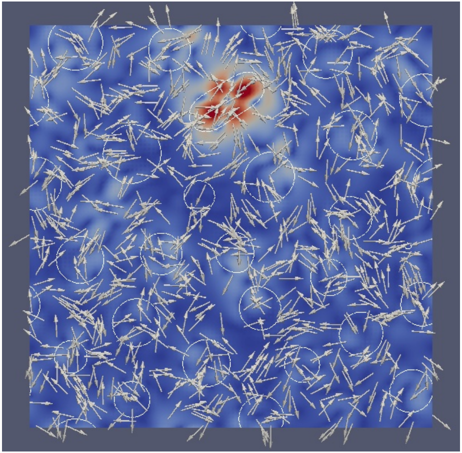
Notes on the numerics:

- periodic boundary conditions
- Taylor-Hood element (P_2, P_1) for discretisation

Cahn–Hilliard–Stokes: separation process





Cahn–Hilliard–Stokes–Poisson

We model electrostatic charge effects with the Poisson equation.

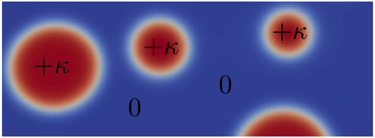
$$\partial_t c + v \cdot \nabla c - \nabla \cdot (M \nabla \mu) = 0$$
$$\mu - (f'(c) - \lambda \Delta c) = 0$$

$$\partial_t v - \nu\, \Delta v + \rho^{-1} \nabla p - \rho^{-1} \mu \nabla c + \rho^{-1} \sigma_{\text{in}} \nabla \phi = 0$$
$$\nabla \cdot v = 0$$

$$-\nabla \cdot (\epsilon \nabla \phi) = \sigma_{\text{in}} + \sigma_{\text{ex}}$$

[C. Eck, M. Fontelos, G. Grün, F. Klingbeil and O. Vantzos, 2009]

- the internal charge density σ_{in}



$$\sigma_{\text{in}}(c) = \kappa\, c, \quad \text{with } \kappa > 0$$

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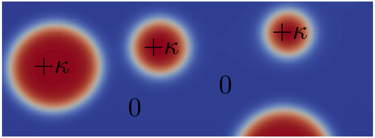
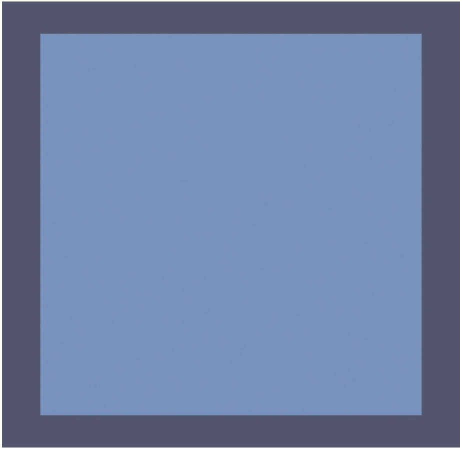


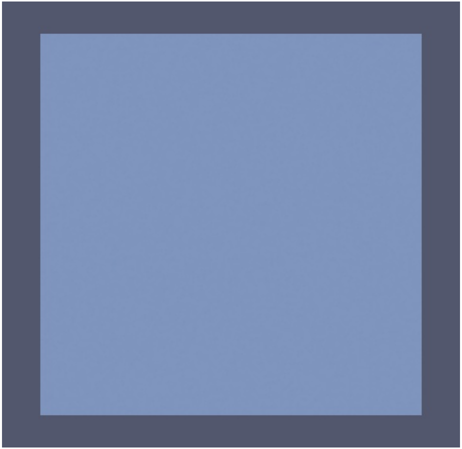
$$\sigma_{\text{in}}(c) = \kappa\, c, \quad \text{with } \kappa > 0$$

- Notes on the numerics:
  - periodic boundary conditions for the electrostatic potential ϕ
  - linear Langrange elements for discretisation in space

Phase separation with one charged phase



Phase separation with external potential



Numerical experiments...