

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

Margherita CASTELLANO, CMAP - Palaiseau

Ludovic GOUDENÈGE, LaMME - Évry

Flore NABET, CMAP - Palaiseau

This work studies the numerical analysis of a phase field model with surfactants introduced by Laradji et al. [2]. The model describes phase separation between water and air in the presence of surfactants (Surface Active Agents), which interact actively with the interface. We model this dynamics using two coupled Cahn-Hilliard equations. The first equation describes phase separation between water and air through an order parameter  $\phi$ , while the second captures how surfactants (concentration  $c$ ) migrate to and accumulate at the interface. We seek  $\phi : (0, T) \times \Omega \rightarrow \mathbb{R}$  and  $c : (0, T) \times \Omega \rightarrow \mathbb{R}$  satisfying

$$\left\{ \begin{array}{ll} \partial_t \phi = M_\phi \Delta \mu, & \forall (t, x) \in (0, T) \times \Omega, \\ \mu = -\epsilon_\phi \Delta \phi + \frac{1}{\epsilon_\phi} f'_\phi(\phi) + \partial_\phi W(\phi, c), & \forall (t, x) \in (0, T) \times \Omega, \\ \partial_t c = M_c \Delta \eta, & \forall (t, x) \in (0, T) \times \Omega, \\ \eta = -\epsilon_c \Delta c + \frac{1}{\epsilon_c} f'_c(c) + \partial_c W(\phi, c), & \forall (t, x) \in (0, T) \times \Omega, \\ \nabla \phi \cdot \vec{n} = \nabla c \cdot \vec{n} = \nabla \mu \cdot \vec{n} = \nabla \eta \cdot \vec{n} = 0, & \forall (t, x) \in (0, T) \times \partial \Omega, \end{array} \right.$$

where  $\Omega$  is a bounded open set of  $\mathbb{R}^d$  ( $d = 2$  or  $3$ ),  $\epsilon_\phi$  and  $\epsilon_c$  represent interface thicknesses associated with  $\phi$  and  $c$ , respectively, and the diffusion coefficients  $M_\phi$  and  $M_c$  are physical parameters called mobilities. The potentials  $f_\phi(\phi)$  and  $f_c(c)$  are classical fourth-order polynomial double-well potentials that ensure phase separation. We rely on the coupling potential  $W(\phi, c) = -\alpha |\nabla \phi|^2 c + \beta \phi^2 c - \gamma \phi^3 c + \delta |\nabla \phi|^4$  introduced by [3], where the first three terms model the interaction between air, water, and surfactants, and the last term guarantees stability. We propose a Discrete Duality Finite Volume (DDFV) scheme to approximate the system, and prove the convergence of the discrete solution towards a weak solution of the continuous problem. From a mathematical perspective, this is particularly challenging due to the strong nonlinearities in the coupling potential, which require the strong convergence of the discrete gradient. This motivates the choice of the DDFV method. The convergence is established using discrete results, such as energy estimates, *a priori* bounds on the discrete solutions, and compactness arguments (including in particular the discrete Aubin-Simon lemma [1]). The strong convergence of the discrete gradient is obtained using Minty's trick, allowing us to pass to the limit in the most nonlinear terms. Finally, we validate the model through numerical simulations.

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