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A Cahn-Hilliard type equation with degenerate mobility and single-well potential. Part I: convergence analysis of a continuous Galerkin finite element discretization.

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Abstract

We consider a Cahn-Hilliard type equation with degenerate mobility and single-well potential of Lennard-Jones type. This equation models the evolution and growth of biological cells such as solid tumors. The degeneracy set of the mobility and the singularity set of the cellular potential do not coincide, and the absence of cells is an unstable equilibrium configuration of the potential. This feature introduces a nontrivial difference with respect to the Cahn-Hilliard equation analyzed in the literature. We formulate a continuous finite element approximation of the problem, where the positivity of the solution is enforced through a discrete variational inequality. We prove the existence and uniqueness of the discrete solution together with the convergence to the weak solution. We present simulation results in one and two space dimensions. We also study the dynamics of the spinodal decomposition and the growth and scaling laws of phase ordering dynamics. In this case we find similar results to the ones obtained in standard phase ordering dynamics and we highlight the fact that the asymptotic behavior of the solution is dominated by the mechanism of growth by bulk diffusion.

1 Introduction

The Cahn-Hilliard equation has originally been proposed as a phenomenological model for phase separation in binary solutions due to cooling processes in [9, 10]. In this phenomenon the two phases spontaneously separate to form domains where pure components dominate (see, for instance, [27, 33] and their references). Under suitable assumptions, the Cahn-Hilliard equation can be written as a mass continuity equation with a flux J, namely,

$$\frac{\partial c}{\partial t} + \mathrm{div} J = 0, \tag{1}$$

where $c \in [0, 1]$ is the (relative) concentration of one component of the binary solution and J is given by

$$J = -b(c)\nabla \frac{\delta F}{\delta c},$$

where $b(c)$ is the mobility and F is the total Helmholtz free energy defined by

$$F(c) = \int_\Omega \Big(\frac{\gamma}{2}|\nabla c|^2 + \psi(c)\Big)\, dx.$$

Here γ is a positive material parameter related to the thickness of the diffuse interface separating the two phases and $\psi(c)$ is the homogeneous Helmholtz free energy density defined by

$$\psi(c) = \frac{\theta}{2}\big((1+c)\log(1+c) + (1-c)\log(1-c)\big) - \frac{\theta_*}{2}c^2,$$

where $0 < \theta < \theta_*$, θ being the absolute temperature and θ_* a given critical temperature below which the phase separation takes place. We recall that this logarithmic potential is often approximated by a smooth double-well potential defined on the whole real line.

Consequently equation (1) can be written as a fourth-order nonlinear evolution equation as follows

$$\frac{\partial c}{\partial t} = \mathrm{div}(\mathrm{b(c)}\nabla(-\gamma\Delta \mathrm{c} + \psi'(\mathrm{c}))). \tag{2}$$

The theoretical aspects of equation (2) has been investigated in many contributions. Especially in the case where the mobility is a positive constant and ψ is a smooth double-well potential. Regarding the latter, we just mention the pioneering results obtained in [18], while for the logarithmic potential the reader is referred to the review paper [13]. If the mobility is degenerate at the pure phases, namely $b(c) = c(1-c)$, and ψ is of logarithmic type, then the only known result is the existence of a suitably weak solution, which has been established in [17] (see also [8] for the interpretation of the sharp interface limit).

Cahn Hilliard type equations have been used in several different contexts. From the original one (i.e. binary alloys) introduced in [2], to multicomponent polymeric systems in [32], and lithium-ion batteries in [42], but also in modeling nanoporosity during dealloying in [19], or inpainting of binary images in [5], and even the formation of Saturn rings in [37]. Further generalizations include extensions to deformable elastic continua, as in [22], binary fluids (see, e.g., [23, 30]). In the last years, Cahn-Hilliard type equations have also been employed to model pattern formation in biological systems (see, for instance, [26, 29]). Moreover, a Cahn-Hilliard equation with degenerate mobility results from the application of mixture theory to solid tumors, which are modeled as elastic fluids with a free energy functional characterized by a double-well potential ψ, as described in [40].

The standard initial and boundary value problem associated with (2) is the following

Problem P Find $c(\mathbf{x}, t)$ such that

$$\frac{\partial c}{\partial t} = \operatorname{div}(b(c)\nabla(-\gamma\Delta c + \psi'(c))) \quad \text{in } \Omega_{\mathrm{T}} := \Omega \times (0, \mathrm{T}), \tag{3}$$

$$c(\mathbf{x}, 0) = c_0(\mathbf{x}) \qquad \forall \mathbf{x} \in \Omega, \tag{4}$$

$$\nabla c \cdot \nu = b(c)\nabla(-\gamma\Delta c + \psi'(c)) \cdot \nu = 0 \quad \text{on } \partial\Omega \times (0, \mathrm{T}), \tag{5}$$

where $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$ is a given bounded domain with a Lipschitz boundary $\partial\Omega$, ν is the unit normal vector pointing outward to $\partial\Omega$ and c_0 is a given initial concentration.

Finite element discretizations of **Problem P** using continuous elements have been studied first in [15] for a constant mobility and in [3] for degenerate mobility (for more recent contributions see, e.g., [21, 28], where an isogeometric analysis of the C-H equation has been carried out, and [24, 39, 41], where a finite element discretization with discontinuous elements has been studied). In these papers ψ is always a double-well logarithmic type potential. However, in modeling tumor growth such a choice seems unphysical for biological cells, since it has been observed that cell-cell interactions are attractive at a moderate cell volume fraction (for $c < c*$), where $c* \in \mathbb{R}$, $0 < c* < 1$, and repulsive at a high volume fraction (for $c > c*$), with a zero for $c = 0$ and an infinite cell-cell repulsion as $c \to 1$, (see, e.g., [7]). We recall that c stands for the volume fraction of cancerous cells.

Accordingly, in this work we propose a finite element approximation of **Problem P**, using a single-well potential of Lennard-Jones type, as introduced in [12] (cf. also [14]). More precisely, we take

$$\psi(c) = \psi_1(c) + \psi_2(c), \tag{6}$$

where

$$\begin{aligned} \psi_1(c) &= -(1 - c*)\log(1 - c), \\ \psi_2(c) &= -\frac{c^3}{3} - (1 - c*)\frac{c^2}{2} - (1 - c*)c + k. \end{aligned} \tag{7}$$

Here $c*$ is the volume fraction at which the cells would naturally be at mutual equilibrium and $k > 0$. The spinodal decomposition can be triggered if $c < \bar{c}$, where $\psi''(\bar{c}) = 0$. Moreover, we have

$$\psi'(c) = \frac{c^2(c - c*)}{1 - c}. \tag{8}$$

Correspondingly, the mobility is given by

$$b(c) = c(1 - c)^2. \tag{9}$$

Note that ψ_1 is a convex function defined on $[0, 1)$ while ψ_2 is concave. Also, the product $b\psi''$ is a continuous function in $[0, 1]$.

Therefore the Cahn-Hilliard equation we want to analyze degenerates on the set $\{c = 0; c = 1\}$, but the singularity is concentrated on the set $\{c = 1\}$ only. This feature introduces a nontrivial difference with respect to the Cahn-Hilliard equation analyzed in the literature. For instance, in the degenerate case studied in [3], the degeneracy and the singularity sets coincide. A technical consequence is that we cannot exploit the relationship between b and ψ at 0 in order to ensure that $c \geq 0$. Therefore we impose this condition at a discrete level as a constraint and formulate a variational inequality.

The paper is organized as follows. In Sections 2 and 3 we introduce a continuous Galerkin finite element approximation of (3)−(8), we show its well-posedness and we prove its convergence in one spatial dimension. In particular, in order to handle the singular cellular potential, we introduce and study a regularized problem in Subsection 2.1 as an intermediate step. Section 3 is devoted to the convergence analysis in one space dimension. In Section 4 we present the iterative scheme we have used to solve the discrete variational inequality and we present some numerical experiments in dimensions one and two. We also discuss the growth of the coarsening domains in two dimensions. The final Section 5 contains a discussion of the main results.

1.1 Notation and functional setting

For a given domain $\omega \subset \Omega$, $d = 1, 2, 3$, we indicate with $L^p(\omega)$, $W^{m,p}(\omega)$, $H^m(\omega) = W^{m,2}(\omega)$ and $L^p((0, T); V)$ the usual Banach and Sobolev spaces and spaces with values in Sobolev spaces, (see, e.g., [1]), for a $p \in [1, \infty]$ and $m \in \mathbb{N}$, endowed with the corresponding norms and seminorms $||\cdot||_{m,p,\omega}$, $||\cdot||_{m,\omega}$, $|\cdot|_{m,p,\omega}$ and $|\cdot|_{m,\omega}$, respectively. Throughout, $(\cdot, \cdot)_\omega$ denotes the standard L^2 inner product over ω, and $< \cdot, \cdot >_\omega$ denotes the duality pairing between $(H^1(\omega))'$ and $(H^1(\omega))$. We omit the index ω when $\omega = \Omega$. With $C(\bar{\Omega})$, $C^n(I_1, I_2)$, $n \geq 0$, and $C^{s_1,s_2}_{x,t}(\bar{\Omega}_T)$, $0 < s_1, s_2 < 1$, we indicate the space of continuous functions from $\bar{\Omega}$ to $\mathbb{R}$, the space of C^n continuous functions from interval $I_1 \subset \mathbb{R}$ to interval $I_2 \subset \mathbb{R}$, and the space of Hölder continuous functions from $\bar{\Omega}_T$ to $\mathbb{R}$ with Hölder exponents s_1 and s_2 in the arguments x and t, respectively.

Given a function $c : \Omega_T \to \mathbb{R}$, we indicate with $c(t) : \Omega \to \mathbb{R}$, for a fixed value $t \in (0, T)$, the corresponding function such that $c(t)(\cdot) = c(t, \cdot)$.

Furthermore, C denotes throughout a generic positive constant independent of the unknown variables, the discretization and the regularization parameters, the value of which might change from line to line; $C_1, C_2, \ldots$ indicate generic positive constants whose particular value must be tracked through the calculations; $C(a)$ denotes a constant depending on the non-negative parameter a, such that, for $C_1 > 0$, if $a \leq C_1$, there exists a $C_2 > 0$ such that $C(a_1) \leq C_2$.

It is useful to introduce the "inverse Laplacian" operator $\mathcal{G} : \mathcal{F} \to V$ such that

$$(\nabla \mathcal{G} v, \nabla \eta) =< v, \eta > \quad \forall \eta \in H^1(\Omega), \tag{10}$$

where $\mathcal{F} = \{v \in (H^1(\Omega))' :< v, 1 >= 0\}$ and $V = \{v \in H^1(\Omega) : (v, 1) = 0\}$. The existence and uniqueness of an element $\mathcal{G}v \in V$, for any $v \in \mathcal{F}$, follows from the Lax-Milgram theorem and the Poincaré inequality.
We can define a norm on $\mathcal{F}$ by setting

$$||v||_{\mathcal{F}} := |\mathcal{G}v|_1 \equiv < v, \mathcal{G}v >^{1/2} \quad \forall v \in \mathcal{F} \tag{11}$$

We will use the following Sobolev interpolation result, (see, e.g., [1]). Let $p \in [1, \infty]$, $m \geq 1$, we set

$$r \in \begin{cases} [p, \infty] & \text{if } m - \frac{d}{p} > 0, \\ [p, \infty) & \text{if } m - \frac{d}{p} = 0, \\ [p, -\frac{d}{m-(d/p)}] & \text{if } m - \frac{d}{p} < 0, \end{cases}$$

and $\mu = \frac{d}{m}\left(\frac{1}{p} - \frac{1}{r}\right)$. Then, there is a constant C such that

$$||v||_{0,r} \leq C ||v||_{0,p}^{1-\mu} ||v||_{m,p}^{\mu} \quad \forall v \in W^{m,p}(\Omega). \tag{12}$$

Let $\mathcal{T}_h$ be a quasi-uniform conforming decomposition of Ω into $d-$simplices K, $d = 1, 2, 3$, and let us introduce the following finite element spaces:

$$\begin{aligned} S^h &:= \{\chi \in C(\bar{\Omega}) : \chi|_K \in P^1(K) \; \forall K \in \mathcal{T}_h\} \subset H^1(\Omega), \\ K^h &:= \{\chi \in S^h : \chi \geq 0 \text{ in } \Omega\} \end{aligned}$$

where $\mathbb{P}_1(K)$ indicates the space of polynomials of total order one on K.

Let J be the set of nodes of $\mathcal{T}_h$ and $\{x_j\}_{j \in J}$ be the set of their coordinates. Moreover, let $\{\phi_j\}_{j \in J}$ be the Lagrangian basis functions associated with each node $j \in J$. Denoting by $\pi^h : C(\bar{\Omega}) \to S^h$ the standard Lagrangian interpolation operator we define the lumped scalar product as

$$(\eta_1, \eta_2)^h = \int_\Omega \pi^h(\eta_1(x)\eta_2(x))dx \equiv \sum_{j \in J} (1, \chi_j)\eta_1(x_j)\eta_2(x_j), \tag{13}$$

for all $\eta_1, \eta_2 \in C(\bar{\Omega})$. We also introduce the L^2 projection operator $P^h : L^2(\Omega) \to S^h$ and its lumped version $\hat{P}^h : L^2(\Omega) \to S^h$ defined by

$$
\begin{aligned}
(P^h \eta, \chi) &= (\eta, \chi) \quad \forall \chi \in S^h, \qquad (14)\\
(\hat{P}^h \eta, \chi)^h &= (\eta, \chi) \quad \forall \chi \in S^h.
\end{aligned}
$$

We recall the following well-known results, (see, e.g., [36]).

Lemma 1.1 *The following properties hold*

$$
\begin{aligned}
&|\chi|_{m,p_2} \le Ch^{-d(\frac{1}{p_1}-\frac{1}{p_2})}|\chi|_{m,p_1} \quad \forall \chi \in S^h,\ 1 \le p_1 \le p_2 \le \infty,\ m = 0, 1; \qquad (15)\\
&|\chi|_{1,p} \le Ch^{-1}||\chi||_{0,p} \quad \forall \chi \in S^h,\ 1 \le p \le \infty; \qquad (16)
\end{aligned}
$$

$$
\begin{aligned}
&\lim_{h\to 0} ||(I - \pi^h)\eta||_{0,\infty} = 0 \qquad \forall \eta \in C(\bar{\Omega}); \qquad (17)\\
&||(I - P^h)\eta||_0 + h|(I - P^h)\eta|_1 \le Ch^m|\eta|_m \quad \forall \eta \in H^m(\Omega),\ m = 1, 2; \qquad (18)
\end{aligned}
$$

$$
\begin{aligned}
&||\chi||_0^2 \le (\chi, \chi)^h \le (d + 2)||\chi||_0^2 \qquad \forall \chi \in S^h \qquad (19)\\
&|(v^h, \chi)^h - (v^h, \chi)| \le Ch^{1+m}||v^h||_m||\chi||_1 \quad \forall v^h, \chi \in S^h,\ m = 0, 1; \qquad (20)
\end{aligned}
$$

$$
|(I - \pi^h)\eta|_{m,r} \le Ch^{1-m}|\eta|_{1,r} \quad \forall \eta \in W^{1,r}(\Omega),\ m = 0, 1,\ r \in [1, \infty] \text{ if } d = 1; \qquad (21)
$$

$$
\lim_{h\to 0} ||(I - \pi^h)\eta||_1 = 0 \quad \forall \eta \in H^1(\Omega) \text{ if d} = 1. \qquad (22)
$$

Similarly to (10), we define the operators $\mathcal{G}^h : \mathcal{F} \to V^h$ and $\hat{\mathcal{G}}^h : \mathcal{F}^h \to V^h$ as follows

$$
\begin{aligned}
(\nabla \mathcal{G}^h v, \nabla \chi) &=< v, \chi > \quad \forall \chi \in S^h, \qquad (23)\\
(\nabla \hat{\mathcal{G}}^h v, \nabla \chi) &= (v, \chi)^h \quad \forall \chi \in S^h, \qquad (24)
\end{aligned}
$$

where $\mathcal{F}^h = \{v \in \bar{C}(\Omega) : (v, 1) = 0\}$ and $V^h = \{v^h \in S^h : (v^h, 1) = 0\}$.

2 Continuous Galerkin Finite Element approximation

In this section we introduce the finite element and time discretization of (3)-(5). We set $\Delta t = T/N$ for a $N \in \mathbb{N}$ and $t_n = n\Delta t$, $n =, ..., N$. For $d = 1, 2, 3$, starting from a datum $c_0 \in H^1(\Omega)$ and $c_h^0 = \pi^h c_0$ (if $d = 1$) or $c_h^0 = \hat{P}^h c_0$ (if $d = 2, 3$), with $0 \le c_h^0 < 1$, we consider the following fully discretized problem:

Problem $\mathbf{P}^h$. For $n = 1, \ldots, N$, given $c_h^{n-1} \in K^h$, find $(c_h^n, w_h^n) \in K^h \times S^h$ such that for all $(\chi, \phi) \in S^h \times K^h$,

$$\begin{cases} \left(\dfrac{c_h^n - c_h^{n-1}}{\Delta t}, \chi \right)^h + (b(c_h^{n-1}) \nabla w_h^n, \nabla \chi) = 0, \\ \gamma(\nabla c_h^n, \nabla(\phi - c_h^n)) + (\psi_1'(c_h^n), \phi - c_h^n)^h \geq (w_h^n - \psi_2'(c_h^{n-1}), \phi - c_h^n)^h. \end{cases} \tag{25}$$

Remark 2.1 *Choosing $\phi \equiv 0$ and $\phi \equiv 2c_h^n$ in (25) yields, for all $j \in J$, that either $|c_h^n(x_j)| = 0$ or $|c_h^n(x_j)| > 0$ and $\gamma(\nabla c_h^n, \nabla \chi_j) + (\psi_1'(c_h^n) + \psi_2'(c_h^{n-1}) - w_h^n, \chi_j)^h = 0$.*

Defining the discrete energy functional $F_1 : K^h \to \mathbb{R}^+$ as

$$F_1[c_h^n] = \int_\Omega \left\{ \frac{\gamma}{2} |\nabla c_h^n|^2 + \psi_1(c_h^n) + \chi_{\mathbb{R}^+}(c_h^n) \right\} dx, \tag{26}$$

where $\chi_{\mathbb{R}^+}(\cdot)$ is the indicator function of the closed and convex set $\mathbb{R}^+$, and endowing the space K^h with the lumped scalar product (13), we can rewrite the second equation of system (25) as

$$(w_h^n - \psi_2'(c_h^{n-1}), \phi - c_h^n)^h + F_1[c_h^n] \leq F_1[\phi], \tag{27}$$

which is equivalent to

$$w_h^n - \psi_2'(c_h^{n-1}) \in \partial F_1[c_h^n], \tag{28}$$

where ∂ is the subdifferential of the convex and lower semi-continuous function F_1. We note that the formulation (28) represents the generalized discrete analogous of the subdifferential approach to the standard Cahn-Hilliard equation with constraints introduced in [25]. Here that approach is generalized to the our case. Inequality (27) will be used in (64) and (74) in order to study the convergence of a suitable regularized problem to the original one. In particular, using the properties of convex and lower semi-continuous functions and of subdifferential calculus, we avoid the necessity to bound the first derivative of the potential $\psi_1(\cdot)$, like in [3], which requires to introduce the hypothesis of acuteness of the partition of the domain.

Remark 2.2 *Given the assumption $0 \leq c_h^0 < 1$, the term $(\psi_1'(c_h^n), \chi - c_h^n)^h$ in the second equation of (25) is well defined, since we will show that $|c_h^0|_{0,\infty} < 1$ implies that $|c_h^n|_{0,\infty} < 1$ for all $n \geq 1$ (see Lemma 2.3). From now on, we assume that $0 \leq c_h^0 < 1$. Notice that this is a physically-consistent assumption, since subregions in the domains where the cellular phase concentrates against infinite cell-cell repulsion are unphysical.*

We introduce now the discrete Green operator of the first degenerate elliptic equation in (25), which will be used to express the chemical potential w_h^n in terms of $\frac{c_h^n - c_h^{n-1}}{\Delta t}$ and to show the well posedness of **Problem $\mathbf{P}^h$**. We follow

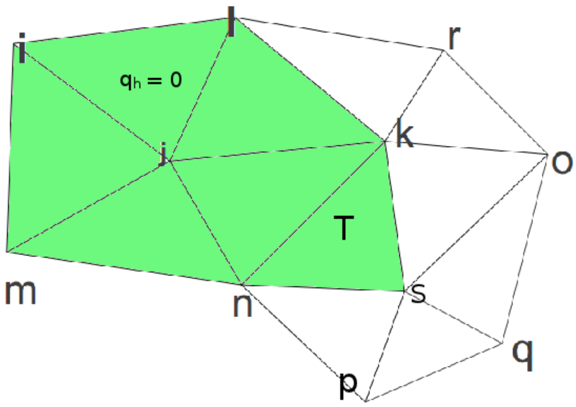


Figure 1: A partition of the domain Ω into regions where $q_h \equiv 0$ (the colored region) and $q_h \neq 0$.

the approach in [3] to invert the degenerate elliptic form on a proper closed and convex subset of S^h.

In order to introduce the subset of S^h on which we can invert the degenerate elliptic form $(b(c_h^{n-1})\nabla w_h^n, \nabla\chi)$, we must subdivide the partition $\mathcal{T}^h$ of Ω into elements on which $c_h^{n-1} \equiv 0$ and elements on which $c_h^{n-1} \neq 0$. Given $q^h \in K^h$ with $⨍ q^h \in (0,1)$, where $⨍ q^h = \frac{1}{|\Omega|}(q^h, 1)$, we define the set of passive nodes $J_0(q^h) \subset J$ by

$$j \in J_0(q^h) \Leftrightarrow \hat{P}^h q^h(x_j) = 0 \Leftrightarrow (q^h, \chi_j) = 0. \tag{29}$$

The nodes in the set $J_+(q^h) = J \setminus J_0(q^h)$ are called active nodes; these nodes can be partitioned into mutually disjoint and maximally connected subsets $I_m(q^h)$ such that $J_+(q^h) \equiv \bigcup_{m=1}^M I_m(q^h)$. In Figure 1 we show a possible partition of the domain in regions where $q_h \equiv 0$ (the colored region) and $q_h \neq 0$. We note that the node $j \in J_0(q^h)$, and all other nodes are in $J_+(q^h)$.

Defining

$$\Sigma_m(q^h) = \sum_{j \in I_m(q^h)} \chi_j,$$

we note that

$$\Sigma_m(q^h) \equiv 1 \quad \text{on each element on which } q^h \neq 0, \tag{30}$$

since all the vertices of this elements belong to $I_m(q^h)$. Note that there are also elements on which $q^h \equiv 0$ and $\Sigma_m(q^h) \equiv 1$, like the element T in Figure 1. Hence, on each element $K \in \mathcal{T}^h$, we have that $q^h \equiv 0$ or $\Sigma_m(q^h) \equiv 1$ for some m, except for those elements on which both $q^h \equiv 0$ and $\Sigma_m(q^h) \equiv 1$. We define the following sets:

$$\Omega_m(q^h) = \{ \bigcup_{K \in \mathcal{T}^h} \bar{K} : \Sigma_m(q^h)(x) = 1 \; \forall x \in K \},$$

i.e. the union of the maximally connected elements on which $q^h \neq 0$, or $q^h \equiv 0$ and the indexes of the vertices of the elements belong to $I_m(q^h)$ for a given m. We also set

$$\Gamma_m(q^h) = \text{supp}\{\Sigma_m(q^h)\} \setminus \Omega_m(q^h).$$

Finally, we introduce the space

$$V^h(q^h) = \{v^h \in S^h : v^h(x_j) = 0\, \forall j \in J_0(q^h) \text{ and } (v^h, \Sigma_m(q^h))^h = 0,\ m = 1, \dots, M\}, \tag{31}$$

that consists of all $v^h \in S^h$ which are orthogonal (with respect to the lumped discrete scalar product (13)) to χ_j, for $j \in J_0(q^h)$, (see the definition (29)), and which have zero average (again with respect to the scalar product (13)) on each element which does not contain any passive node.

We recall from [3] that any $v^h \in S^h$ can be written as

$$v^h \equiv \bar{v}^h + \sum_{j \in J_0(q^h)} v^h(x_j)\chi_j + \sum_{m=1}^{M} \left[⨍_{\Omega_m(q^h)} v^h \right] \Sigma_m(q^h), \tag{32}$$

where $\bar{v}^h$ is the $\hat{P}^h$ projection of v^h onto $V^h(q^h)$, and

$$⨍_{\Omega_m(q^h)} v^h := \frac{(v^h, \Sigma_m(q^h))^h}{(1, \Sigma_m(q^h))}. \tag{33}$$

We can now define, for all $q^h \in K^h$ with $q^h < 1$, the discrete anisotropic Green's operator $\hat{G}^h_{q^h} : V^h(q^h) \to V^h(q^h)$ as

$$(b(q^h)\nabla \hat{G}^h_{q^h} v^h, \nabla \chi) = (v^h, \chi)^h \quad \forall \chi \in S^h. \tag{34}$$

The well posedness of $\hat{G}^h_{q^h}$ can be shown as in [3] (see in particular formula (2.23) and (2.24) in [3]), choosing $\chi = \chi_j$ for $j \in J_0(q^h)$ and $\chi = \Sigma_m(q^h)$, for $m = 1, \dots, M$, and using the fact that $||b(q^h)||_{0,\infty} \leq C$ for all $q^h \in S^h$.

Finally, we give an explanation of the construction of the space $V^h(q^h)$. The properties that $v^h(x_j) = 0\ \forall j \in J_0(q^h)$ and $(v^h, 1)^h = 0$ on $\Omega_m(q^h)$ ensure that (34) is satisfied for all $\chi \in S^h$. Using the L^2 scalar product $(\cdot, \cdot)$ instead of its lumped counterpart (13) in (34), choosing $\chi \equiv \chi_i$, $i \in J_0(q^h)$, and noting that $b(q^h) = 0$ on suppχ_i, (34) would be satisfied only if $v^h(x_j) = 0$ for all the nodes in the closure of the support of χ_i. From the first equation in (25) we observe that, in the case in which $v^h = \frac{c_h^n - c_h^{n-1}}{\Delta t}$ and $q^h = c_h^{n-1}$, this should mean that $c_h^n(x_j) = 0$ for all the nodes in the closure of the support of χ_i, $i \in J_0(c_h^{n-1})$, causing all the regions where $c_h^{n-1} \equiv 0$ on the support of a basis function to remain fixed regions of zero values for the variable c_h^n. This locking phenomenon for the discrete solution would be in contrast with analytical results for a solution of (3), obtained, e.g., in [4], which show the property of a moving support with finite speed of velocity in an unstationary regime. The presence of these unphysical discrete solutions with fixed support is linked to the non-unicity of the solution of (3), described e.g. in [4]. The use of the lumped mass scalar product (13) in (25) introduces the requirement that only the values of v^h on the nodes $x_j \in J_0(q^h)$ are set to zero, leaving the values on the other nodes where $q^h \equiv 0$ free to take non-zero values. When $v^h = \frac{c_h^n - c_h^{n-1}}{\Delta t}$ and $q^h = c_h^{n-1}$, this introduces the property of a moving support of the discrete solution of (25) with a finite speed of velocity, since the support can expand at most of a length proportional to h at each time step.

We now study a regularized version of Problem (25), in order to deal with the singularity in the cellular potential and to show the well posedness of Problem (25) when the regularization parameter tends to zero.

2.1 Regularized problem

We introduce the following regularization of the cellular potential near $c_h^n = 1$: for $\epsilon > 0$, we set

$$\psi''_{1,\epsilon}(c_h^n) := \begin{cases} \psi''_1(1-\epsilon) & \text{for } c_h^n \geq 1-\epsilon, \\ \psi''_1(c_h^n) & \text{for } c_h^n < 1-\epsilon. \end{cases} \tag{35}$$

By expanding $\psi_1(c_h^n)$ in (7) in a neighborhood of $(1-\epsilon)$ when $c_h^n \geq 1-\epsilon$, we obtain $\psi_{1,\epsilon}$, i.e.

$$\psi_{1,\epsilon}(c_h^n) := \begin{cases} -(1-c*)\log\epsilon + & \frac{3}{2}(1-c*) - \frac{2}{\epsilon}(1-c*)(1-c_h^n) + \frac{1-c*}{2\epsilon^2}(1-c_h^n)^2 \\ & \text{for } c_h^n \geq 1-\epsilon, \\ \psi_1(c_h^n) & \text{for } c_h^n < 1-\epsilon, \end{cases} \tag{36}$$

and $\psi'_{1,\epsilon}$, i.e.

$$\psi'_{1,\epsilon}(c_h^n) := \begin{cases} \frac{2}{\epsilon}(1-c*) - \frac{1-c*}{\epsilon^2}(1-c_h^n) & \text{for } c_h^n \geq 1-\epsilon, \\ \psi'_1(c_h^n) & \text{for } c_h^n < 1-\epsilon, \end{cases} \tag{37}$$

respectively. From the convexity property of the function $\psi_{1,\epsilon}$ we have the following property:

$$\psi'_{1,\epsilon}(s)(r-s) \leq \psi_{1,\epsilon}(r) - \psi_{1,\epsilon}(s), \quad \forall r, s \in \mathbb{R}. \tag{38}$$

Furthermore, expanding $\psi_{1,\epsilon}(\cdot)$ in the Taylor series around $(1-\epsilon)$, with an argument $s > 1$ and with $\epsilon < 1$, using (35), (36) and (37) we obtain

$$\begin{aligned} \psi_{1,\epsilon}(s) &= \psi_{1,\epsilon}(1-\epsilon) + \psi'_{1,\epsilon}(1-\epsilon)(s-(1-\epsilon)) + \frac{1}{2}\psi''_{1,\epsilon}(1-\epsilon)(s-(1-\epsilon))^2 \\ &= -(1-c*)\log\epsilon + \frac{1-c*}{\epsilon}(s-(1-\epsilon)) + \frac{1-c*}{2\epsilon^2}(s-(1-\epsilon))^2 \\ &\geq \frac{1-c*}{2\epsilon^2}(s-1)^2. \end{aligned}$$

Hence we have that

$$\psi_{1,\epsilon}(s) \geq \frac{1-c*}{2\epsilon^2}([s-1]_+)^2 \quad \forall s \in \mathbb{R}, \tag{39}$$

where $[\cdot]_+ = \max\{\cdot, 0\}$. Introducing the concave preserving extension $\bar{\psi}_2 \in C^1(\mathbb{R})$ of $\psi_2 \in C^1([0,1])$,

$$\bar{\psi}_{2,}(c_h^n) := \begin{cases} \psi_2(1) + (c_h^n - 1)\psi_2'(1) & \text{for } c_h^n \geq 1, \\ \psi_2(c_h^n) & \text{for } c_h^n \leq 1, \end{cases} \tag{40}$$

and setting $\psi_\epsilon(c_h^n) := \psi_{1,\epsilon}(c_h^n) + \bar{\psi}_2(c_h^n)$, we obtain from (39) and (40) that, given $\epsilon_0 < 1$, it holds that

$$\psi_\epsilon(s) \geq \frac{1-c*}{2\epsilon^2}([s-1]_+)^2 - C \geq -C \quad \forall s \in \mathbb{R},\ \epsilon \leq \epsilon_0. \tag{41}$$

In order to show the well posedness of **Problem** $\mathbf{P}^h$, we introduce the following regularized version of (25):

Problem $\mathbf{P}^h_\epsilon$**.** For $n = 1, \ldots, N$, given $c_h^{n-1} \in K^h$, with $c_h^{n-1} < 1$ and $|c_h^{n-1}|_1 \leq C$, find $(c_{h,\epsilon}^n, w_{h,\epsilon}^n) \in K^h \times S^h$ such that for all $(\chi, \phi) \in S^h \times K^h$,

$$\begin{cases} \left(\dfrac{c_{h,\epsilon}^n - c_h^{n-1}}{\Delta t}, \chi\right)^h + (b(c_h^{n-1})\nabla w_{h,\epsilon}^n, \nabla\chi) & = 0, \\ \gamma(\nabla c_{h,\epsilon}^n, \nabla(\phi - c_{h,\epsilon}^n)) + (\psi_{1,\epsilon}'(c_{h,\epsilon}^n), \phi - c_{h,\epsilon}^n)^h & \geq (w_{h,\epsilon}^n - \hat{\psi}_2'(c_h^{n-1}), \phi - c_{h,\epsilon}^n)^h. \end{cases} \tag{42}$$

The following result shows that **Problem** $\mathbf{P}^h_\epsilon$ is well posed.

Lemma 2.1 *There exists a solution* $(c_{h,\epsilon}^n, w_{h,\epsilon}^n)$ *to* ***Problem*** $\mathbf{P}^h_\epsilon$*. Moreover, the solution* $\{c_{h,\epsilon}^n\}_{n=1}^N$ *is unique, and* $w_{h,\epsilon}^n$ *is unique on* $\Omega_m(c_h^{n-1})$*, for* $m = 1, \ldots, M$ *and* $n = 1, \ldots, N$*.*

Proof. From the first equation in (42) and from (34) it follows that, given $c_h^{n-1} \in K^h$, $c_h^{n-1} < 1$, we search for $c_{h,\epsilon}^n \in K^h(c_h^{n-1})$, where

$$K^h(c_h^{n-1}) = \{\chi \in K^h \,:\, \chi - c_h^{n-1} \in V^h(c_h^{n-1})\}. \tag{43}$$

Moreover, a solution $w_{h,\epsilon}^n \in S^h$ can be expressed in terms of $c_{h,\epsilon}^n - c_h^{n-1}$ through the discrete anisotropic Green operator (34), recalling (32), as

$$w_{h,\epsilon}^n = -\hat{\mathcal{G}}^h_{c_h^{n-1}}\left[\frac{c_{h,\epsilon}^n - c_h^{n-1}}{\Delta t}\right] + \sum_{j \in J_0(c_h^{n-1})} \mu_{j,\epsilon}^n \chi_j + \sum_{m=1}^M \lambda_{m,\epsilon}^n \Sigma_m(c_h^{n-1}), \tag{44}$$

where $\{\mu_{j,\epsilon}^n\}_{j \in J_0(c_h^{n-1})}$ and $\{\lambda_{m,\epsilon}^n\}_{m=1}^M$ are constants which express the values of $w_{h,\epsilon}^n$ on the passive nodes and its "average" value on $\Omega_m(c_h^{n-1})$, respectively. Hence, **Problem** $\mathbf{P}^h_\epsilon$ can be restated as follows: given $c_h^{n-1} \in K^h$, with $c_h^{n-1} < 1$, find $c_{h,\epsilon}^n \in K^h(c_h^{n-1})$

and constant Lagrange multipliers $\{\mu^n_{j,\epsilon}\}_{j\in J_0(c_h^{n-1})}$ and $\{\lambda^n_{m,\epsilon}\}_{m=1}^M$ such that, for all $\chi \in K^h$,

$$\gamma(\nabla c^n_{h,\epsilon}, \nabla(\chi - c^n_{h,\epsilon})) + \left(\hat{\mathcal{G}}^h_{c_h^{n-1}}\left[\frac{c^n_{h,\epsilon} - c_h^{n-1}}{\Delta t}\right] + \psi'_{1,\epsilon}(c^n_{h,\epsilon}), \chi - c^n_{h,\epsilon}\right)^h$$
$$\geq \left(\sum_{j\in J_0(c_h^{n-1})} \mu^n_{j,\epsilon}\chi_j + \sum_{m=1}^M \lambda^n_{m,\epsilon}\Sigma_m(c_h^{n-1}) - \hat{\psi}'_2(c_h^{n-1}), \chi - c^n_{h,\epsilon}\right)^h. \quad (45)$$

We note that (45) represents, together with $c^n_{h,\epsilon} \in K^h(c_h^{n-1})$, the Karush-Kuhn-Tucker optimality conditions, (see, e.g., [16]), of the minimization problem

$$\inf_{v_{h,\epsilon}\in S^h} \sup_{\mu_{j,\epsilon},\lambda_{m,\epsilon},\nu_\epsilon\geq 0} \Bigg\{\gamma|v_{h,\epsilon}|_1^2 + \frac{1}{\Delta t}||[b(c_h^{n-1})]^{1/2}\nabla\hat{\mathcal{G}}^h_{c_h^{n-1}}(v_{h,\epsilon} - c_h^{n-1})||_0^2$$
$$+ 2(\psi_{1,\epsilon}(v_{h,\epsilon}) + \hat{\psi}'_2(c_h^{n-1})v_{h,\epsilon}, 1)^h - \sum_{j\in J_0(c_h^{n-1})} \mu_{j,\epsilon}(\chi_j, v_{h,\epsilon})^h - \sum_{m=1}^M \lambda_{m,\epsilon}(\Sigma_m(c_h^{n-1}), v_{h,\epsilon})^h$$
$$- (\nu_\epsilon, v_{h,\epsilon})^h\Bigg\}, \quad (46)$$

being $\nu_\epsilon \in K^h$ the Lagrange multiplier of the inequality constraint. Noting the convexity of $\psi_{1,\epsilon}(\cdot)$ and the fact that $c_h^{n-1} \in K^h$, the primal form associated to the Lagrangian (46) is a convex, proper, lower semi continuous and coercive function from the closed and convex set $K^h(c_h^{n-1})$ to $\mathbb{R}$, and the primal problem is stable. Hence, from the Kuhn-Tucker theorem, (see, e.g., [16]), there exist $c^n_{h,\epsilon} \in K^h(c_h^{n-1})$, solution of the primal problem, and Lagrange multipliers $\{\mu^n_{j,\epsilon}\}_{j\in J_0(c_h^{n-1})}$, $\{\lambda^n_{m,\epsilon}\}_{m=1}^M$ and $\nu_\epsilon(x_i) \in -\partial\chi_{\mathbb{R}^+}(c^n_{h,\epsilon}(x_i))$, for each $i \in J$ and each n. Therefore, from (44) we have the existence of a solution $(c^n_{h,\epsilon}, w^n_{h,\epsilon})_{n=1}^N$ to **Problem** $\mathbf{P}^h_\epsilon$.

Let us now prove uniqueness. If, for fixed $n \geq 1$, (45) has two solutions $(c^{n,i}_{h,\epsilon}, \{\mu^{n,i}_{j,\epsilon}\}_{j\in J_0(c_h^{n-1})}, \{\lambda^{n,i}_{m,\epsilon}\}_{m=1}^M)$, $i = 1, 2$, by taking $\chi = c^{n,2}_{h,\epsilon}$ in the inequality for $c^{n,1}_{h,\epsilon}$ and $\chi = c^{n,1}_{h,\epsilon}$ in the inequality for $c^{n,2}_{h,\epsilon}$ and taking the difference between the two inequalities, setting $c^{n,1}_{h,\epsilon} - c^{n,2}_{h,\epsilon} = d^n_{h,\epsilon} \in V^h(c_h^{n-1})$ and thanks to (31), we have

$$\gamma|d^n_{h,\epsilon}|_1^2 + \frac{1}{\Delta t}||[b(c_h^{n-1})]^{1/2}\nabla\hat{\mathcal{G}}^h_{c_h^{n-1}} d^n_{h,\epsilon}||_0^2 + (\psi'_{1,\epsilon}(c^{n,1}_{h,\epsilon}) - \psi'_{1,\epsilon}(c^{n,2}_{h,\epsilon}), d^n_{h,\epsilon})^h \leq 0,$$

and therefore

$$\gamma|d^n_{h,\epsilon}|_1^2 + \frac{1}{\Delta t}||[b(c_h^{n-1})]^{1/2}\nabla\hat{\mathcal{G}}^h_{c_h^{n-1}} d^n_{h,\epsilon}||_0^2 \leq 0,$$

where we have used the monotonicity of $\psi'_{1,\epsilon}(\cdot)$ in the second step. Therefore the uniqueness of $c^n_{h,\epsilon}$ follows from the Poincaré inequality and the fact that $\fint c^n_{h,\epsilon} = \fint c^0_{h,\epsilon}$. Choosing $\chi = c^n_{h,\epsilon} \pm \delta\pi_h[c^n_{h,\epsilon}\Sigma_m(c_h^{n-1})]$ in (45), for any $\delta \in (0, 1)$ and $m = 1, \ldots, M$, yields uniqueness of the Lagrange multiplier $\lambda^n_{m,\epsilon}$. Hence the uniqueness of $w^n_{h,\epsilon}$ follows from (44). The proof is complete. □

In order to pass to the limit as $\epsilon \to 0$ in system (42), we need to deduce suitable $\epsilon-$independent bounds for the solution $(c^n_{h,\epsilon}, w^n_{h,\epsilon})$. The following result holds.

Lemma 2.2 *For every sequence $\epsilon \to 0$, there exist a subsequence $\epsilon' \to 0$ and a $c_h^n \in K^h$ such that*

$$c_{h,\epsilon'}^n \to c_h^n \quad \text{and} \quad \nabla c_{h,\epsilon'}^n \to \nabla c_h^n \quad \text{for } \epsilon' \to 0. \tag{47}$$

For every sequence $\epsilon \to 0$, there exist a subsequence $\epsilon' \to 0$ and a $w_h^n \in S^h$ such that

$$w_{h,\epsilon'}^n \to w_h^n \quad \text{on} \quad \Omega_{m,*}(c_h^{n-1}) \quad \text{and} \quad \nabla w_{h,\epsilon'}^n \to \nabla w_h^n \quad \text{on } \Omega_{m,*}(c_h^{n-1}) \quad \text{for } \epsilon' \to 0, \tag{48}$$

where $\Omega_{m,*}(c_h^{n-1})$ is the set of those elements of $\Omega_m(c_h^{n-1})$ on which $c_h^{n-1} \not\equiv 0$.

Proof. We start by proving stability bounds for the regularized Problem (42). Choosing $\chi = w_{h,\epsilon}^n$ in the first equation of (42) and $\phi = c_h^{n-1}$ in the second equation of (42), we get

$$\gamma(\nabla c_{h,\epsilon}^n, \nabla(c_{h,\epsilon}^n - c_h^{n-1})) + (\psi_{1,\epsilon}'(c_{h,\epsilon}^n) + \hat{\psi}_2'(c_h^{n-1}), c_{h,\epsilon}^n - c_h^{n-1})^h + \Delta t||[b(c_h^{n-1})]^{1/2}\nabla w_{h,\epsilon}^n||_0^2 \le 0.$$

Using now the identity $2s(s-r) = s^2 - r^2 + (s-r)^2$, $\forall r, s \in \mathbb{R}$, and the convexity and the concavity properties of $\psi_{1,\epsilon}(\cdot)$ and $\hat{\psi}_2(\cdot)$, it follows that

$$\frac{\gamma}{2}|c_{h,\epsilon}^n|_1^2 + \frac{\gamma}{2}|c_{h,\epsilon}^n - c_h^{n-1}|_1^2 + (\psi_\epsilon(c_{h,\epsilon}^n), 1)^h + \Delta t||[b(c_h^{n-1})]^{1/2}\nabla w_{h,\epsilon}^n||_0^2 \le (\psi_\epsilon(c_h^{n-1}), 1)^h + \frac{\gamma}{2}|c_h^{n-1}|_1^2 \le C. \tag{49}$$

From (49) and (41) we deduce that

$$([c_{h,\epsilon}^n - 1]_+^2, 1)^h \le C\epsilon^2. \tag{50}$$

Hence, from (50), (15) and (19) it follows that

$$||[c_{h,\epsilon}^n - 1]_+||_{0,\infty} \le Ch^{-d/2}\epsilon. \tag{51}$$

From the fact that $\psi_{1,\epsilon}(c_{h,\epsilon}^n) \ge 0$ for all $c_{h,\epsilon}^n \ge 0$ (see (36)) and from (49) we have that

$$C_1(\psi_{1,\epsilon}(c_{h,\epsilon}^n), \psi_{1,\epsilon}(c_{h,\epsilon}^n))^h \le (\psi_\epsilon(c_{h,\epsilon}^n), 1)^h \le C. \tag{52}$$

Therefore, from (15) and (19) we have a uniform bound on $\psi_{1,\epsilon}(c_{h,\epsilon}^n)$, independent on ϵ, i.e.

$$||\psi_{1,\epsilon}(c_{h,\epsilon}^n)||_{0,\infty} \le Ch^{-d/2}. \tag{53}$$

From (49), the fact that $(c_{h,\epsilon}^n, 1)^h = (c_h^{n-1}, 1)^h$ and (20), from the Poincaré inequality and the Bolzano-Weierstrass theorem it follows that there exists a subsequence $\{c_{h,\epsilon'}^n\}$ and a $c_h^n \in K^h$ such that (47) holds.

We next show (48). Using the Poincaré inequality on $\Omega_{m,*}(c_h^{n-1})$, (19) and (49) leads to

$$
\begin{aligned}
&((([(I - ⨍_{\Omega_{m,*}(c_h^{n-1})})w_{h,\epsilon}^n]\Sigma_m^*(c_h^{n-1}))^2, 1)^h \\
&\le C \int_{\Omega_{m,*}(c_h^{n-1})} \nabla |w_{h,\epsilon}^n|^2 dx \\
&\le C[b_{min}(c_h^{n-1})]^{-1} \int_{\Omega_{m,*}(c_h^{n-1})} b(c_h^{n-1}) \nabla |w_{h,\epsilon}^n|^2 dx \\
&\le C((\Delta t)^{-1})[b_{min}(c_h^{n-1})]^{-1},
\end{aligned} \tag{54}
$$

where $\Sigma_m^*(c_h^{n-1}) := \sum_{j \in I_m^*(c_h^{n-1})} \chi_j$, with $I_m^*(c_h^{n-1})$ the subset of nodes of $I_m(c_h^{n-1})$ which are in $\Omega_{m,*}(c_h^{n-1})$. We now bound $⨍_{\Omega_{m,*}(c_h^{n-1})} w_{h,\epsilon}^n$. Let us take

$$K^h \ni \phi = c_{h,\epsilon}^n + \Sigma_m^*(c_h^{n-1})$$

in the second equation of system (42). We get

$$
\begin{aligned}
(w_{h,\epsilon}^n, \Sigma_m^*(c_h^{n-1}))^h \le \gamma(\nabla c_{h,\epsilon}^n, \nabla \Sigma_m^*(c_h^{n-1})) + (\psi_{1,\epsilon}'(c_{h,\epsilon}^n), \Sigma_m^*(c_h^{n-1}))^h \\
+ (\hat{\psi}_2'(c_h^{n-1}), \Sigma_m^*(c_h^{n-1}))^h.
\end{aligned}
$$

Observing that $\Sigma_m^*(c_h^{n-1}) \equiv 1$ on $\Omega_{m,*}(c_h^{n-1})$ and that $\hat{\psi}_2'(c_h^{n-1})$ is bounded, using moreover (49) we obtain

$$
\begin{aligned}
&|(w_{h,\epsilon}^n, \Sigma_m^*(c_h^{n-1}))^h| \\
&\le \gamma \left| \int_{\Gamma_m^*(c_h^{n-1})} \nabla c_{h,\epsilon}^n \cdot \nabla \Sigma_m^*(c_h^{n-1}) \, dx \right| + |(\psi_{1,\epsilon}'(c_{h,\epsilon}^n), \Sigma_m^*(c_h^{n-1}))^h| + C||\Sigma_m^*(c_h^{n-1})||_{0,\infty} \\
&\le \gamma |\Gamma_m^*(c_h^{n-1})|^{1/2} ||\nabla \Sigma_m^*(c_h^{n-1})||_{0,\infty} |c_{h,\epsilon}^n|_1 + |(\psi_{1,\epsilon}'(c_{h,\epsilon}^n), \Sigma_m^*(c_h^{n-1}))^h| + C||\Sigma_m^*(c_h^{n-1})||_{0,\infty} \\
&\le Ch^{-1} + C + |(\psi_{1,\epsilon}'(c_{h,\epsilon}^n), \Sigma_m^*(c_h^{n-1}))^h|,
\end{aligned} \tag{55}
$$

where $\Gamma_m^*(c_h^{n-1}) := \mathrm{supp}\{\Sigma_m^*(c_h^{n-1})\} \setminus \Omega_{m,*}(c_h^{n-1})$.

In order to control the last term in the last line of (55) we take

$$K^h \ni \phi = \Sigma_m^*(c_h^{n-1}) ⨍_{\Omega_{m,*}(c_h^{n-1})} c_{h,\epsilon}^n$$

in the second equation of system (42). Using the boundedness of $\hat{\psi}_2'(c_h^{n-1})$, the facts that, from (51) and since $\epsilon \in [0, 1)$, $c_{h,\epsilon}^n$ is uniformly bounded with respect to ϵ, and that $⨍_{\Omega_{m,*}(c_h^{n-1})}(c_{h,\epsilon}^n) \in (0, 1)$, the definition (33) and the Cauchy-Schwarz inequality, we obtain

$$
\begin{aligned}
&\left| \left(\psi_{1,\epsilon}'(c_{h,\epsilon}^n) \Sigma_m^*(c_h^{n-1}), 1 - ⨍_{\Omega_{m,*}(c_h^{n-1})} c_{h,\epsilon}^n \right)^h \right| \le \\
&C + |(\psi_{1,\epsilon}'(c_{h,\epsilon}^n), \Sigma_m^*(c_h^{n-1}) - c_{h,\epsilon}^n)^h| + \gamma |\Gamma_m^*(c_h^{n-1})|^{1/2} ||\nabla \Sigma_m^*(c_h^{n-1})||_{0,\infty} |c_{h,\epsilon}^n|_1 \\
&+ \gamma |c_{h,\epsilon}^n|_1^2 + \left(w_{h,\epsilon}^n, c_{h,\epsilon}^n - \Sigma_m^*(c_h^{n-1}) \frac{(c_{h,\epsilon}^n, \Sigma_m^*(c_h^{n-1}))^h}{(1, \Sigma_m^*(c_h^{n-1}))} \right)^h.
\end{aligned} \tag{56}
$$

From the fact that $\Sigma_m(c_h^{n-1})(x_j) = c_{h,\epsilon}^n(x_j) = 0$ for $j \in J_0(c_h^{n-1})$ and $\Sigma_m(c_h^{n-1})(x_j) = 1$ for $j \in I_m(c_h^{n-1})$, we deduce the identity

$$
\begin{aligned}
(c_{h,\epsilon}^n, w_{h,\epsilon}^n)^h &= (c_{h,\epsilon}^n, w_{h,\epsilon}^n \Sigma_m(c_h^{n-1}))^h \\
&= (c_{h,\epsilon}^n, w_{h,\epsilon}^n \Sigma_m^*(c_h^{n-1}))^h + (c_{h,\epsilon}^n, w_{h,\epsilon}^n \Sigma_m(c_h^{n-1}) - \Sigma_m^*(c_h^{n-1}))^h.
\end{aligned} \tag{57}
$$

Using now in (56) the convexity property of $\psi_{1,\epsilon}(\cdot)$, the identity (57), the estimate (49) and the definition (33), we get

$$
\begin{aligned}
&\left| \left(\psi_{1,\epsilon}'(c_{h,\epsilon}^n) \Sigma_m^*(c_h^{n-1}), 1 - \fint_{\Omega_{m,*}(c_h^{n-1})} c_{h,\epsilon}^n \right)^h \right| \leq \\
&\psi_{1,\epsilon}(\Sigma_m^*(c_h^{n-1})) - \psi_{1,\epsilon}(c_{h,\epsilon}^n) + C + Ch^{-1} + (c_{h,\epsilon}^n, [(I - \fint_{\Omega_{m,*}(c_h^{n-1})}) w_{h,\epsilon}^n] \Sigma_m^*(c_h^{n-1}))^h \\
&+ (c_{h,\epsilon}^n, w_{h,\epsilon}^n [\Sigma_m(c_h^{n-1}) - \Sigma_m^*(c_h^{n-1})])^h.
\end{aligned}
$$

Then, from the uniform bound (53), the Cauchy-Schwarz and Young inequalities and the estimate (54), we obtain

$$
\begin{aligned}
&\left| \left(\psi_{1,\epsilon}'(c_{h,\epsilon}^n) \Sigma_m^*(c_h^{n-1}), 1 - \fint_{\Omega_{m,*}(c_h^{n-1})} c_{h,\epsilon}^n \right)^h \right| \\
&\leq C + Ch^{-1} + (([-\fint_{\Omega_{m,*}(c_h^{n-1})}) w_{h,\epsilon}^n] \Sigma_m^*(c_h^{n-1}))^2, 1)^h + C(c_{h,\epsilon}^n, c_{h,\epsilon}^n)^h \\
&+ (c_{h,\epsilon}^n, w_{h,\epsilon}^n [\Sigma_m(c_h^{n-1}) - \Sigma_m^*(c_h^{n-1})])^h \\
&\leq C + Ch^{-1} + C((\Delta t)^{-1})[b_{min}(c_h^{n-1})]^{-1} + (c_{h,\epsilon}^n, w_{h,\epsilon}^n [\Sigma_m(c_h^{n-1}) - \Sigma_m^*(c_h^{n-1})])^h.
\end{aligned} \tag{58}
$$

In order to bound the last term in the last line of (58), we note that

$$
(c_{h,\epsilon}^n, w_{h,\epsilon}^n [\Sigma_m(c_h^{n-1}) - \Sigma_m^*(c_h^{n-1})])^h = \sum_{j \in K_j} c_{h,\epsilon}^n(x_j) w_{h,\epsilon}^n(x_j)(1, \chi_j),
$$

in the case in which $c_{h,\epsilon}^n(x_j) > 0$ for at least one node j in an element $K_j \subset \Gamma_m^*(c_h^{n-1})$. We choose $\chi \equiv w_{h,\epsilon}^n \sum_{l \in K_j} \chi_l$, with $c_{h,\epsilon}^n(x_j) > 0$ for some $j \in K_j$, in the first equation of system (42). Using the fact that $c_h^{n-1} \equiv 0$ on K_j, using moreover (49), the Cauchy-Schwarz and the Young inequalities and (19), writing only the lowest order terms in Δt, we get

$$
\begin{aligned}
\sum_{j \in K_j} c_{h,\epsilon}^n(x_j) w_{h,\epsilon}^n(x_j)(1, \chi_j) &\leq C \Delta t (b(c_h^{n-1}) \nabla w_{h,\epsilon}^n, \nabla w_{h,\epsilon}^n) + \frac{1}{2} |(w_{h,\epsilon}^n, \Sigma_m^*(c_h^{n-1}))^h| \\
&\leq C + \frac{1}{2} |(w_{h,\epsilon}^n, \Sigma_m^*(c_h^{n-1}))^h|.
\end{aligned} \tag{59}
$$

Finally, observing that $\fint_{\Omega_{m,*}(c_h^{n-1})}(c_{h,\epsilon}^n) \in (0, 1)$ and using (59) in (58) and Young inequality, we get

$$
\begin{aligned}
|(\psi_{1,\epsilon}'(c_{h,\epsilon}^n), \Sigma_m^*(c_h^{n-1}))^h| \leq C + Ch^{-1} + C((\Delta t)^{-1})[b_{min}(c_h^{n-1})]^{-1} \\
+ \frac{1}{2} |(w_{h,\epsilon}^n, \Sigma_m^*(c_h^{n-1}))^h|,
\end{aligned} \tag{60}
$$

Using (60) in (55) leads to

$$|(w^n_{h,\epsilon}, \Sigma^*_m(c_h^{n-1}))^h| \le C + Ch^{-1} + C((\Delta t)^{-1})[b_{min}(c_h^{n-1})]^{-1}. \tag{61}$$

Now, combining (54) with (61), recalling the definition (33) and using the Poincaré inequality, we obtain

$$(w^n_{h,\epsilon}\Sigma^*_m(c_h^{n-1}), w^n_{h,\epsilon}\Sigma^*_m(c_h^{n-1}))^h \le C + Ch^{-1} + C((\Delta t)^{-1})[b_{min}(c_h^{n-1})]^{-1}. \tag{62}$$

Finally, from (62), (49), (20) and the Bolzano-Weierstrass theorem it follows that there exists a subsequence $\{w^n_{h,\epsilon'}\}$ and a $w^n_h \in S^h$ such that (48) holds. The proof is complete. □

Lemma 2.3 *The limit point c^n_h of Lemma 2.2 satisfies the property $0 \le c^n_h < 1$.*

Proof. Due to the logarithmic term in $\psi_{1,\epsilon}(\cdot)$, (52) and (19) imply that the elements $c^n_{h,\epsilon}$ are less than one in magnitude, uniformly in ϵ and h. As a consequence, we have that $||\psi_{1,\epsilon}(c^n_{h,\epsilon})||_{0,\infty} \le C$. Passing to the limit for $\epsilon' \to 0$ in (52), using the convergence property (47), the uniform boundedness of $\psi_{1,\epsilon}(c^n_{h,\epsilon})$ and considering the logarithmic term in $\psi_1(\cdot)$, we obtain that the limit point is such that $0 \le c^n_h < 1$. □

2.2 Well-posedness of Problem $\mathbf{P}^h$

We now have all the ingredients to show the well-posedness of **Problem $\mathbf{P}^h$**.

Theorem 2.1 *Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, and let $c^0_h \in K^h$ with $c^0_h < 1$ and $|c^0_h|_1 \le C$. Then, there exists a solution (c^n_h, w^n_h) to Problem (25) for any $n = 1, \dots, N$.*

Moreover, the solution $\{c^n_h\}_{n=1}^N$ is unique, while the solution w^n_h is unique on $\Omega_m(c_h^{n-1})$, for $m = 1, \dots, M$ and $n = 1, \dots, N$.

Proof. Recalling the definition (26) and noting the convexity of $\psi_{1,\epsilon}(\cdot)$, we can introduce a regularized lower semi continuous convex energy functional defined as

$$F_{1,\epsilon}[c^n_{h,\epsilon}] = \int_\Omega \left\{ \frac{\gamma}{2}|\nabla c^n_{h,\epsilon}|^2 + \psi_{1,\epsilon}(c^n_{h,\epsilon}) + \chi_{\mathbb{R}^+}(c^n_{h,\epsilon}) \right\} dx, \tag{63}$$

and rewrite system (42) as

$$\begin{cases} \left(\dfrac{c^n_{h,\epsilon} - c_h^{n-1}}{\Delta t}, \chi \right)^h + (b(c_h^{n-1})\nabla w^n_{h,\epsilon}, \nabla \chi) & = 0, \\ (w^n_{h,\epsilon} - \hat{\psi}'_2(c_h^{n-1}), \phi - c^n_{h,\epsilon})^h + F_{1,\epsilon}[c^n_{h,\epsilon}] & \le F_{1,\epsilon}[\phi]. \end{cases} \tag{64}$$

We can now pass to the limit in (64), considering the convergence properties (47) and (48) of Lemma 2.2. For any $(\chi, \phi) \in S^h \times K^h$, we have

$$\lim_{\epsilon \to 0} \left(\frac{c^n_{h,\epsilon} - c_h^{n-1}}{\Delta t}, \chi \right)^h = \left(\frac{c^n_h - c_h^{n-1}}{\Delta t}, \chi \right)^h; \tag{65}$$

$$\lim_{\epsilon \to 0} (b(c_h^{n-1})\nabla w^n_{h,\epsilon}, \nabla \chi) = (b(c_h^{n-1})\nabla w^n_h, \nabla \chi); \tag{66}$$

$$\lim_{\epsilon \to 0} (w^n_{h,\epsilon} - \hat{\psi}'_2(c_h^{n-1}), \phi - c^n_{h,\epsilon})^h \ge (w^n_h - \psi'_2(c_h^{n-1}), \phi - c^n_h)^h, \tag{67}$$

In order to derive the last limit (67), we use the convergence properties (47) and (48) of Lemma 2.2, the relation (28) written for the regularized discrete solutions and the monotonicity of the operators in $\partial F_{1,\epsilon}(\cdot)$. At first we take $\phi = 2c^n_{h,\epsilon} - c^n_h$ in the second equation of (64). Noting that, since $c^n_{h,\epsilon} \geq 0$ and $c^n_h \geq 0$, there exists a $\bar{\epsilon} > 0$ such that, for all $\epsilon \leq \bar{\epsilon}$, $\phi \geq 0$. Hence we obtain

$$(w^n_{h,\epsilon} - \hat{\psi}'_2(c^{n-1}_h), c^n_{h,\epsilon} - c^n_h)^h \leq F_{1,\epsilon}[2c^n_{h,\epsilon} - c^n_h] - F_{1,\epsilon}[c^n_{h,\epsilon}].$$

Considering the convergence property (47) and taking the limit for $\epsilon \to 0$ in the previous inequality, we get

$$\limsup_{\epsilon\to 0}(w^n_{h,\epsilon}, c^n_{h,\epsilon} - c^n_h)^h \leq 0. \tag{68}$$

From (44) and the convergence properties (47) and (48) of Lemma 2.2 we note that we can rewrite $w^n_{h,\epsilon}$ as

$$w^n_{h,\epsilon} \equiv -\hat{\mathcal{G}}^h_{c^{n-1}_h}\left[\frac{c^n_{h,\epsilon} - c^{n-1}_h}{\Delta t}\right] + \sum_{j\in J_0(c^{n-1}_h)} \mu^n_{j,\epsilon}\chi_j + \sum_{m=1}^{M} \lambda^n_{m,\epsilon}\Sigma_m(c^{n-1}_h) \tag{69}$$

and the limit point w^n_h as

$$w^n_h \equiv -\hat{\mathcal{G}}^h_{c^{n-1}_h}\left[\frac{c^n_h - c^{n-1}_h}{\Delta t}\right] + \sum_{j\in J_0(c^{n-1}_h)} \alpha^n_j\chi_j + \sum_{m=1}^{M} \lambda^n_m\Sigma_m(c^{n-1}_h). \tag{70}$$

Analogously to (28), we can write

$$w^n_{h,\epsilon} - \psi'_2(c^{n-1}_h) \in \partial F_{1,\epsilon}[c^n_{h,\epsilon}], \tag{71}$$

which define a monotone map $c^n_{h,\epsilon} \to w^n_{h,\epsilon} - \psi'_2(c^{n-1}_h)$ from S^h to S^h. Let us introduce the quantity $f_\lambda = (1+\lambda)c^n_h - \lambda\phi$, with $\lambda \in \mathbb{R}$, $0 < \lambda < 1$ and $\phi \in K^h$ with $\phi(x_j) = 0$ if $c^n_h(x_j) = 0$. It is clear that there exists a $\bar{\lambda} < 1$ such that, for all $\lambda \leq \bar{\lambda}$, $f_\lambda \geq 0$. We moreover introduce the quantity

$$w^n_{h,\lambda} \equiv -\hat{\mathcal{G}}^h_{c^{n-1}_h}\left[\frac{f_\lambda - c^{n-1}_h}{\Delta t}\right] + \sum_{j\in J_0(c^{n-1}_h)} \alpha^n_{j,\lambda}\chi_j + \sum_{m=1}^{M} \lambda^n_{m,\lambda}\Sigma_m(c^{n-1}_h).$$

From the monotonicity property of the map $c^n_{h,\epsilon} \to w^n_{h,\epsilon} - \psi'_2(c^{n-1}_h)$ and from the facts that $\phi(x_j) = 0$ and $c^n_h(x_j) = 0$ for $j \in J_0(c^{n-1}_h)$, it follows

$$(w^n_{h,\epsilon} - w^n_{h,\lambda}, c^n_{h,\epsilon} - ((1+\lambda)c^n_h - \lambda\phi))^h \geq 0. \tag{72}$$

On the other hand, from (72) it follows

$$\lambda(w^n_{h,\epsilon}, \phi - c^n_{h,\epsilon})^h \geq -(1+\lambda)(w^n_{h,\epsilon}, c^n_{h,\epsilon} - c^n_h)^h - (w^n_{h,\lambda}, c^n_{h,\epsilon} - c^n_h)^h + \lambda(w^n_{h,\lambda}, \phi - c^n_h)^h. \tag{73}$$

Taking now the limit for $\epsilon \to 0$ in (73), using (68), dividing by λ and taking the limit for $\lambda \to 0$, we obtain

$$\liminf_{\epsilon\to 0}(w^n_{h,\epsilon} - \hat{\psi}'_2(c^{n-1}_h), \phi - c^n_{h,\epsilon})^h \geq (w^n_h - \psi'_2(c^{n-1}_h), \phi - c^n_h)^h,$$

which is (67) for all $\phi \in K^h$ with $\phi(x_j) = 0$ if $c^n_h(x_j) = 0$.

Due to the uniform boundedness of $\psi_{1,\epsilon}$ and the facts that $0 \leq c^n_{h,\epsilon} < 1$, that $\psi_{1,\epsilon}(\cdot) \to \psi_1(\cdot)$ uniformly for $\epsilon \to 0$, the convergence property (47), and from the semi continuity property of the indicator function $\chi_{\mathbb{R}^+}(\cdot)$, we have that

$$\lim_{\epsilon\to 0} F_{1,\epsilon}[c^n_{h,\epsilon}] \geq F_1[c^n_h],$$
$$\lim_{\epsilon\to 0} F_{1,\epsilon}[\phi] = F_1[\phi].$$

Hence, the limit point (c^n_h, w^n_h) satisfies, for each $(\chi,\phi) \in S^h \times K^h$, with $\phi(x_j) = 0$ if $c^n_h(x_j) = 0$,

$$\begin{cases} \left(\dfrac{c^n_h - c^{n-1}_h}{\Delta t}, \chi\right)^h + (b(c^{n-1}_h)\nabla w^n_h, \nabla\chi) = 0, \\ (w^n_h - \psi_2'(c^{n-1}_h), \phi - c^n_h)^h + F_1[c^n_h] \leq F_1[\phi]. \end{cases} \tag{74}$$

Finally, since $c^n_h < 1$ (see Lemma 2.3) and $\psi_1(c^n_h)$ is convex and Lipschitz continuous for $c^n_h < 1$, system (74) is equivalent to system (25) (see (27)), hence the limit point (c^n_h, w^n_h) is the unique solution of **Problem $\mathbf{P}^h$**. Note from Remark 2.1 that if (25) is valid for each $(\chi,\phi) \in S^h \times K^h$, with $\phi(x_j) = 0$ if $c^n_h(x_j) = 0$, it is also valid for each for each $(\chi,\phi) \in S^h \times K^h$. □

We now proceed to obtain the energy estimates.

Lemma 2.4 (Energy estimates) *Let (c^n_h, w^n_h), $n = 1,\dots,N$, be the solution of **Problem** $\mathbf{P}^h$. Then, the following stability bound holds:*

$$\max_{n=1\to N} ||c^n_h||_1^2 + (\Delta t)^2 \sum_{n=1}^N \left|\frac{c^n_h - c^{n-1}_h}{\Delta t}\right|_1^2 + \Delta t \sum_{n=1}^N ||[b(c^{n-1}_h)]^{1/2}\nabla w^n_h||_0^2$$
$$+ \Delta t \sum_{n=1}^N [b^{n-1}_{\max}]^{-1} \left|\hat{\mathcal{G}}^h\left[\frac{c^n_h - c^{n-1}_h}{\Delta t}\right]\right|_1^2 \leq C(|c^0_h|_1^2), \tag{75}$$

where $b_{max} \geq \max_{n=1\to N} ||b(c^{n-1}_h)||_{0,\infty}$.

Proof. Taking the limit for $\epsilon \to 0$ in (49) we get

$$\frac{\gamma}{2}|c^n_h|_1^2 + \frac{\gamma}{2}|c^n_h - c^{n-1}_h|_1^2 + (\psi(c^n_h), 1)^h + \Delta t||[b(c^{n-1}_h)]^{1/2}\nabla w^n_h||_0^2 \leq (\psi(c^{n-1}_h), 1)^h + \frac{\gamma}{2}|c^{n-1}_h|_1^2. \tag{76}$$

Summing from $n = 1 \to m$, for $m = 1 \to N$, noting that $0 \leq c^0_h < 1$ and $\psi(c^0_h) \leq C$, that $|c^0_h|_1 \leq C$, that $c^n_h < 1$, and using the Poincaré inequality (note that $\fint c^n_h = \fint c^0_h$), we get the bound for the first three terms in (75).

Choosing now $\chi = \hat{\mathcal{G}}^h\left[\frac{c^n_h - c^{n-1}_h}{\Delta t}\right]$ in the first equation of system (25), using (24) and Cauchy-Schwarz and Young inequalities, we get

$$\left(\frac{c^n_h - c^{n-1}_h}{\Delta t}, \hat{\mathcal{G}}^h\left[\frac{c^n_h - c^{n-1}_h}{\Delta t}\right]\right)^h = \left|\hat{\mathcal{G}}^h\left[\frac{c^n_h - c^{n-1}_h}{\Delta t}\right]\right|_1$$
$$= -\left(b(c^{n-1}_h)\nabla w^n_h, \nabla\hat{\mathcal{G}}^h\left[\frac{c^n_h - c^{n-1}_h}{\Delta t}\right]\right) \leq \frac{1}{2}|b(c^{n-1}_h)\nabla w^n_h|_0^2 + \frac{1}{2}\left|\hat{\mathcal{G}}^h\left[\frac{c^n_h - c^{n-1}_h}{\Delta t}\right]\right|_1^2$$
$$\leq b^{n-1}_{\max}||[b(c^{n-1}_h)]^{1/2}\nabla w^n_h||_0^2.$$

Summing from $n = 1 \to N$ and using the bound for the third term in (75) we get the bound for the last term in (75). $\square$

Remark 2.3 *We note from* (76) *that the function* $\frac{\gamma}{2}|c_h^n|_1^2 + (\psi(c_h^n), 1)^h$ *is a decreasing (Lyapunov) function for the discrete solutions. Hence the finite element and time discretization* (25) *has the gradient stability property in the sense of Eyre, described in [20]. We will check this dissipative behavior of the discrete solution in the numerical tests (see Section* 4*).*

3 Convergence analysis

In this section we present the convergence analysis for the discrete scheme (25) in the case $d = 1$ (see Remark 3.1).

To the sequence of discrete solutions c_h^n to **Problem** $\mathbf{P}^h$ we associate the following continuous in time approximation:

$$C_h(t) := \frac{t - t_{n-1}}{\Delta t} c_h^n + \frac{t_n - t}{\Delta t} c_h^{n-1}, \tag{77}$$

for $t \in [t_{n-1}, t_n]$, $n = 1, \ldots, N$, which is a family of linear time interpolants that depend on the parameters h and Δt. We also define the piecewise constant-in-time functions

$$\begin{aligned} C_h^+(t) &:= c_h^n, \quad C_h^-(t) := c_h^{n-1}, \\ W_h^+(t) &:= w_h^n, \quad W_h^-(t) := w_h^{n-1}, \end{aligned} \tag{78}$$

for $t \in (t_{n-1}, t_n]$, $n = 1, \ldots, N$.
By multiplying system (25) by a $C_0^\infty([0,T])$ function, and integrating in time from 0 to T, we obtain that (C_h, W_h) satisfies the following weak formulation:
Find $(C_h, W_h) \in L^2(0,T;K^h) \times L^2(0,T;S^h)$ such that, for all $(\chi, \phi) \in L^2(0,T;S^h) \times L^2(0,T;K^h)$

$$\begin{cases} \displaystyle\int_0^T \left[\left(\frac{\partial C_h}{\partial t}, \chi \right)^h + (b(C_h^-) \nabla W_h^+, \nabla \chi) \right] dt & = 0, \\ \displaystyle\int_0^T [\gamma(\nabla C_h^+, \nabla(\phi - C_h^+)) + (\psi_1'(C_h^+), \phi - C_h^+)^h] dt & \geq \int_0^T (W_h^+ - \psi_2'(C_h^-), \phi - C_h^+)^h, \end{cases} \tag{79}$$

with $C_h(0) = c_h^0$.
In order to pass to the limit in (79) as $(h, \Delta t) \to (0,0)$ and identify the system satisfied by the limit points, we need the following result, whose proof is similar to those presented in [3], and therefore has been reported in Appendix.

Lemma 3.1 *Let* $d = 1$ *and* $c_h^0 = \pi_h(c_0)$*, with* $0 \leq c_0 < 1$ *and* $|c_0|_1 \leq C$*. There exist a subsequence of continuous and piecewise constant in time interpolants* (77) *and* (78)*, and functions* $c \in L^\infty(0,T;H^1(\Omega)) \cap H^1(0,T;(H^1(\Omega))') \cap$

$C^{\frac{1}{2},\frac{1}{8}}_{x,t}(\bar{\Omega}_T)$ *and* $w \in L^2_{\mathrm{loc}}(0 < c < 1)$ *with* $\frac{\partial w}{\partial x} \in L^2_{\mathrm{loc}}(0 < c < 1)$*, such that, for* $(h, \Delta t) \to 0$*,*

$$C_h, C_h^{\pm} \rightharpoonup c \text{ weakly in } \mathrm{L}^2(0, \mathrm{T}; \mathrm{H}^1(\Omega)), \tag{80}$$
$$C_h, C_h^{\pm} \to c \text{ uniformly on } \bar{\Omega}_{\mathrm{T}}, \tag{81}$$
$$W_h^+ \rightharpoonup w, \quad \frac{\partial W_h^+}{\partial x} \rightharpoonup \frac{\partial w}{\partial x} \quad \text{weakly in } \mathrm{L}^2_{\mathrm{loc}}(0 < \mathrm{c} < 1), \tag{82}$$

where $\{0 < q < 1\} := \{(x, t) \in \Omega_T : 0 < q(x, t) < 1\}$*.*

Remark 3.1 *In the case* $d = 1$ *the uniform convergence* (81)*, together with the convergence result* (82)*, allows to take the limit as* $(h, \Delta t) \to (0, 0)$ *of the degenerate elliptic term in the first equation of system* (79) *on the set* $\{0 < c < 1\}$*. To the best of our knowledge, in the case* $d > 1$ *it does not exist in the literature a convergence result which shows the convergence of the discrete solution of* (79) *to the continuous solution of a weak formulation of* (3)*.*

In order to proceed, let us introduce the following sets. For any $\delta > 0$, we define

$$D_\delta^+ = \{(x, t) \in \bar{\Omega}_T \, : \delta < c(x, t) < 1\}, \qquad D_\delta^+(t) = \{x \in \bar{\Omega} \, : \delta < c(x, t) < 1\}.$$

From uniform convergence (81) it follows that, for a fixed $\delta > 0$, there exists a $h(\delta) \in \mathbb{R}^+$ such that, for all $h \le h(\delta)$,

$$\begin{aligned} &0 \le C_h^{\pm}(x, t) < \min\{2\delta, 1\} \quad \forall (x, t) \notin D_\delta^+, \\ &\frac{1}{8}\delta \le C_h^{\pm}(x, t) < 1 \quad \forall (x, t) \in D^+_{\frac{\delta}{4}}. \end{aligned} \tag{83}$$

We can now obtain the limit equations of system (79) as $(h, \Delta t) \to (0, 0)$. Indeed, setting $\int_{0<c<1}(\, , \,)dt := \int_0^T (\, , \,)_{D_0^+(t)} dt$, we have

Theorem 3.1 *The limit point* (c, w) *of Lemma 3.1 satisfies the weak formulation*

$$\begin{cases} \displaystyle\int_0^T \left\langle \frac{\partial c}{\partial t}, \eta \right\rangle dt + \int_{0<c<1} \left(b(c) \frac{\partial w}{\partial x}, \frac{\partial \eta}{\partial x} \right) dt = 0, \quad \forall \eta \in L^2(0, T; H^1(\Omega)), \\ \displaystyle\int_{0<c<1} \gamma \left(\frac{\partial c}{\partial x}, \frac{\partial \theta}{\partial x} \right) dt + \int_{0<c<1} (\psi'(c), \theta) dt - \int_{0<c<1} (w, \theta) dt = 0, \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall \theta \in L^2(0, T; H^1(\Omega)), \end{cases} \tag{84}$$

with $c(\cdot, 0) = c_0(\cdot)$*, and with* $\mathrm{supp}(\theta) \subset \{0 < \mathrm{c} < 1\}$*.*

Proof. Let us choose $\eta \in H^1(0,T;H^1(\Omega))$ and $\theta \in L^2(0,T;H^1(\Omega))$, with $\mathrm{supp}(\theta) \subset \mathrm{D}_\delta^+$. Taking $\chi = \pi^h\eta$, $\psi = \pi^h\theta$ in (79) and considering (107), we rewrite (79) as

$$\left\{\begin{array}{l} \displaystyle\int_0^T \left(\frac{\partial C_h}{\partial t}, \eta\right) dt + \int_0^T \left(b(C_h^-)\frac{\partial W_h^+}{\partial x}, \frac{\partial \eta}{\partial x}\right) dt = \\ \displaystyle\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \left[\left(\frac{\partial C_h}{\partial t}, \pi^h\eta\right) - \left(\frac{\partial C_h}{\partial t}, \pi^h\eta\right)^h\right] dt + \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \left(\frac{\partial C_h}{\partial t}, (\eta - \pi^h\eta)\right) dt + \\ \displaystyle\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \left(b(C_h^-)\frac{\partial W_h^+}{\partial x}, \frac{\partial}{\partial x}(\eta - \pi^h\eta)\right) dt = \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3, \\ \\ \displaystyle\int_0^T \gamma\left(\frac{\partial C_h^+}{\partial x}, \frac{\partial \theta}{\partial x}\right) dt + \int_0^T ([\psi_1'(C_h^+) + \psi_2'(C_h^-)], \theta) dt - \int_0^T (W_h^+, \theta) dt = \\ \displaystyle\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \gamma\left(\frac{\partial C_h^+}{\partial x}, \frac{\partial}{\partial x}(\theta - \pi^h\theta)\right) dt + \\ \displaystyle\sum_{n=1}^N \int_{t_{n-1}}^{t_n} [(\psi_1'(C_h^+) + \psi_2'(C_h^-), \pi^h\theta) - (\psi_1'(C_h^+) + \psi_2'(C_h^-), \pi^h\theta)^h] dt + \\ \displaystyle\sum_{n=1}^N \int_{t_{n-1}}^{t_n} (\psi_1'(C_h^+) + \psi_2'(C_h^-), \theta - \pi^h\theta) dt - \sum_{n=1}^N \int_{t_{n-1}}^{t_n} [(W_h^+, \pi^h\theta) - (W_h^+, \pi^h\theta)^h] dt - \\ \displaystyle\sum_{n=1}^N \int_{t_{n-1}}^{t_n} (W_h^+, \theta - \pi^h\theta) dt = \mathcal{I}_4 + \mathcal{I}_5 + \mathcal{I}_6 + \mathcal{I}_7 + \mathcal{I}_8. \end{array}\right. \tag{85}$$

Consider the first equation of system (85). The left hand side converges, for $(h, \Delta t) \to (0,0)$, to

$$(c(\cdot,T), \eta(\cdot,T)) - (c(\cdot,0), \eta(\cdot,0)) - \int_0^T (c, \frac{\partial \eta}{\partial t}) dt + \int_{0<c<1} \left(b(c)\frac{\partial w}{\partial x}, \frac{\partial \eta}{\partial x}\right) dt \tag{86}$$

Indeed, for the first term in (85) we have

$$\int_0^T \left(\frac{\partial C_h}{\partial t}, \eta\right) dt = -\int_0^T \left(C_h, \frac{\partial \eta}{\partial t}\right) dt + (C_h(\cdot,T), \eta(\cdot,T)) - (C_h(\cdot,0), \eta(\cdot,0)). \tag{87}$$

From the uniform convergence (81) and the regularity of η we deduce the first limit term in (86). Note that the further regularity in time of $\eta \in H^1(0,T;H^1(\Omega))$ makes it possible to take an integration by part in time in (87) and use the convergence properties of C_h in the limit process. For the second term, we denote the domain of integration by $\Omega_T = (\Omega_T \setminus D_\delta^+) \cup D_\delta^+$. On account of the third bound in (103) and (105), we get

$$\begin{aligned} &\left| \int_{\Omega_T \setminus D_\delta^+} \left(b(C_h^-)\frac{\partial W_h^+}{\partial x}, \frac{\partial \eta}{\partial x}\right) dx dt \right| \\ &\le ||(b(C_h^-))^{1/2}||_{L^\infty(\Omega_T \setminus D_\delta^+)} \left|\left| (b(C_h^-))^{1/2}\frac{\partial W_h^+}{\partial x} \right|\right|_{L^2(\Omega_T)} ||\eta||_{L^2(0,T;H^1(\Omega))} \\ &\le C(b_{\max}(2\delta))^{1/2} ||\eta||_{L^2(0,T;H^1(\Omega))}, \end{aligned} \tag{88}$$

where $b_{\max}(2\delta) = \max_{0\le z\le 2\delta} b(z)$ for all $h \le h(\delta)$. Next, we write

$$\int_{D_\delta^+}\left(b(C_h^-)\frac{\partial W_h^+}{\partial x}, \frac{\partial \eta}{\partial x}\right)dxdt = \int_{D_\delta^+}\left(b(c)\frac{\partial W_h^+}{\partial x}, \frac{\partial \eta}{\partial x}\right)dxdt$$
$$+ \int_{D_\delta^+}\left([b(C_h^-) - b(c)]\frac{\partial W_h^+}{\partial x}, \frac{\partial \eta}{\partial x}\right)dxdt. \quad (89)$$

For the second term on the right hand side of equation (89), due to the uniform convergence (81) and the bound (106), we have that

$$\left|\int_{D_\delta^+}\left([b(C_h^-) - b(c)]\frac{\partial W_h^+}{\partial x}, \frac{\partial \eta}{\partial x}\right)dxdt\right|$$
$$\le ||b(C_h^-) - b(c)||_{L^\infty(\Omega_T)}\left|\left|\frac{\partial W_h^+}{\partial x}\right|\right|_{L^2(D_\delta^+)}||\eta||_{L^2(0,T;H^1(\Omega))}$$
$$\le C[b_{\min}(\frac{\delta}{8})]^{-1}||b(C_h^-) - b(c)||_{L^\infty(\Omega_T)}||\eta||_{L^2(0,T;H^1(\Omega))} \to 0 \quad \text{for } h, \Delta t \to 0. \quad (90)$$

Hence, from (112), (89) and (90), we obtain

$$\int_{D_\delta^+}\left(b(C_h^-)\frac{\partial W_h^+}{\partial x}, \frac{\partial \eta}{\partial x}\right)dxdt \to \int_{D_\delta^+}\left(b(c)\frac{\partial w}{\partial x}, \frac{\partial \eta}{\partial x}\right)dxdt \quad \text{for } h, \Delta t \to 0. \quad (91)$$

Considering (88) and (91) for all $\delta > 0$, and noting that $b_{\max}(2\delta) \to 0$ as $\delta \to 0$, we get (86). We now show that the terms in the right hand side of the first equation of system (85) converge to zero as $(h, \Delta t) \to (0, 0)$. We denote these terms by $\mathcal{I}_1, \cdots, \mathcal{I}_3$.
Integrating by parts in time, considering (20), (81), the regularity of η and the Cauchy-Schwarz inequality we get

$$|\mathcal{I}_1| \le Ch\left(\int_0^T ||C_h||^2 dt\right)^{1/2}\left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} ||\frac{\partial \pi^h \eta}{\partial t}||_1^2 dt\right)^{1/2}$$
$$+ Ch||C_h(\cdot, T)||\,||\pi^h\eta(\cdot, T)||_1 + Ch||C_h(\cdot, 0)||\,||\pi^h\eta(\cdot, 0)||_1$$
$$\le Ch||\pi^h\eta||_{H^1(0,T;H^1(\Omega))} \to 0. \quad (92)$$

Similarly, we obtain $|\mathcal{I}_2| \to 0$ by considering (81) and (21).
Using the third bound in (103), (22) and the Cauchy-Schwarz inequality we can write

$$|\mathcal{I}_3| \le$$
$$||(b(C_h^-)^{1/2})||_{L^\infty(\Omega_T)}\left|\left|(b(C_h^-))^{1/2}\frac{\partial W_h^+}{\partial x}\right|\right|_{L^2(\Omega_T)}\left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n}\left|\left|\frac{\partial}{\partial x}(\eta - \pi^h\eta)\right|\right|^2 dt\right)^{1/2}$$
$$\le C||\eta - \pi^h\eta||_{L^2(0,T;H^1(\Omega))} \to 0. \quad (93)$$

Hence, the first equation of system (85) converges to the limit, for $h, \Delta t \to 0$,

$$(c(\cdot, T), \eta(\cdot, T)) - (c(\cdot, 0), \eta(\cdot, 0)) - \int_0^T (c, \frac{\partial \eta}{\partial t})dt + \int_{0<c<1}\left(b(c)\frac{\partial w}{\partial x}, \frac{\partial \eta}{\partial x}\right)dt = 0. \quad (94)$$

Since, from the third bound in (103), we have that $b(c)\frac{\partial w}{\partial x} \in L^2(0 < c < 1)$, from (94) we deduce that $c \in H^1(0, T; (H^1(\Omega))')$, and the first equation in (84) is valid. Moreover, due to the uniform convergence (81), $c(\cdot, 0) = c_0(\cdot)$.

Consider now the second equation in (85). The left hand side converges to the limit, for $h, \Delta t \to 0$,

$$\int_{0<c<1} \gamma\left(\frac{\partial c}{\partial x}, \frac{\partial \theta}{\partial x}\right)dt + \int_{0<c<1} (\psi'(c), \theta)dt - \int_{0<c<1} (w, \theta)dt,$$
$$\forall \theta \in L^2(0,T; H^1(\Omega)) \,\text{with}\, \text{supp}(\theta) \subset \mathrm{D}_0^+. \tag{95}$$

For the first and the third term of the second equation in (85) this is a direct consequence of the convergence results (80) and (82). From the facts that $\psi_1(\cdot) \in C^1([0,1))$, $\psi_2(\cdot) \in C^1([0,1])$, that $0 \leq C_h^{\pm} < 1$, $0 \leq c < 1$, and from the uniform convergence (81), we have that

$$\left| \int_0^T ([\psi_1'(C_h^+) + \psi_2'(C_h^-) - \psi_1'(c) - \psi_2'(c)], \theta)dt \right| \leq$$
$$C||\psi_1'(C_h^+) - \psi_1'(c)||_{L^\infty(\Omega_T)}||\theta||_{L^2(\Omega_T)} + D||\psi_2'(C_h^-) - \psi_2'(c)||_{L^\infty(\Omega_T)}||\theta||_{L^2(\Omega_T)} \to 0.$$

Hence the second term on the left hand side of (85) converges to the second term in (95). Note that, since $\theta \in L^2(0,T; H^1(\Omega))$ and $d = 1$, we could have used the dominated convergence theorem in order to obtain the limit point in the second term of (95).
We now show that the terms in the right hand side of the second equation in (85) converge to zero for $(h, \tau) \to 0$. We denote these terms by $\mathcal{I}_4, \cdots, \mathcal{I}_8$. Given (80) and (22) we deduce, similarly to (93), that $|\mathcal{I}_4| \to 0$. Using the facts that $\psi_1(\cdot) \in C^1([0,1))$, $\psi_2(\cdot) \in C^1([0,1])$, that $0 \leq C_h^{\pm} < 1$, the results (20) and (21), similarly to (92), we deduce that $|\mathcal{I}_5| \to 0$ and $|\mathcal{I}_6| \to 0$. Finally, using (112), (20) and (21), on noting that $\text{supp}(\theta) \subset D_\delta^+$, similarly to (92), we deduce that $|\mathcal{I}_7| \to 0$ and $|\mathcal{I}_8| \to 0$.

Collecting (94) and (95) we finally obtain (84) and the proof is complete. □

4 Numerical results

After proving the existence and uniqueness and the convergence of the discrete solution, we have implemented the numerical algorithm for solving the variational inequality at each time step in **Problem $\mathbf{P}^h$**. Following the splitting procedure proposed in [3], we used the following iterative scheme:

Require: $\mu > 0$ (a relaxation parameter), c_h^{n-1}, w_h^{n-1};
for $k \geq 0$ **do**
Initialization

$$c_h^{n,0} = c_h^{n-1}, w_h^{n,0} = w_h^{n-1};$$

Step 1 Find $Z^{n,k} \in S_h$ such that $\forall q \in S_h$:

$$(Z^{n,k}, q)^h = (c_h^{n,k}, q)^h - \mu[\lambda(\nabla c_h^{n,k}, \nabla q) + (\psi_2'(c_h^{n-1}) - w_h^{n,k}, q)^h];$$

Step 2 Find $c_h^{n,k+1/2} \in K_h$, $\forall r \geq 0$, such that:
if $j \in J_0(c_h^{n-1})$ **then**
$c_h^{n,k+1/2}(x_j) \leftarrow c_h^{n-1}(x_j)$
else

$$(c_h^{n,k+1/2}(x_j) + \mu\psi_1'(c_h^{n,k+1/2})(x_j) - Z^{n,k}(x_j), r - c_h^{n,k+1/2}(x_j)) \geq 0 \tag{96}$$

end if
Step 3 Find $(c_h^{n,k+1}, w_h^{n,k+1}) \in S_h \times S_h$, $\forall q \in S_h$, such that:

$$\begin{cases} \left(\dfrac{c_h^{n,k+1} - c_h^{n-1}}{\Delta t}, q\right)^h + (\nabla w_h^{n,k+1}, \nabla q) = ([1 - b(c_h^{n-1})]\nabla w_h^{n,k}, \nabla q) \\ (c_h^{n,k+1}, q)^h + \mu[\lambda(\nabla c_h^{n,k+1}, \nabla q) + (\psi_2'(c_h^{n-1}) - w_h^{n,k+1}, q)^h = (2c_h^{n,k+1/2} - Z^{n,k}, q)^h. \end{cases}$$

if $||c_h^{n,K+1} - c_h^{n,K}||_{0,\infty} < 10^{-6}$ **then**
$(c_h^n, w_h^n) \leftarrow (c_h^{n,K+1}, w_h^{n,K+1})$; **break**.
end if
end for

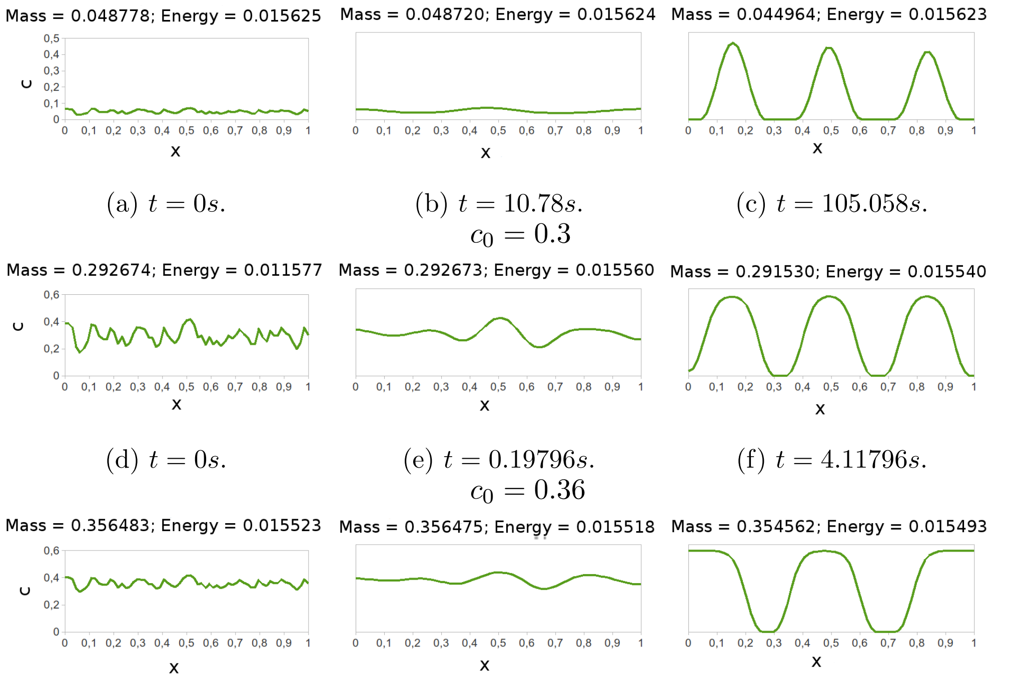
The scalar inequality in (96) is solved using a projected gradient method, introducing an approximative analogue of the set $J_+(c_h^{n-1})$ where $c_h^{n-1} > 10^{-6}$ is meant for $c_h^{n-1} > 0$. We remark that this approximation introduces a small error in the mass conservation of the algorithm.

In order to test the accuracy of the proposed numerical procedure, let us now consider the evolution of a system characterized by an initial concentration with a small uncorrelated white noise over a constant value c_0. Since we set $c_0 < \bar{c}$, the system undergoes a spinodal decomposition and evolves, after a transitory regime, towards an equilibrium state consisting of regions which are rich ($c \sim c*$) or empty ($c = 0$) of cells. The main features of the phase order dynamics are predicted by the classical theory of coarsening in systems with a locally conserved order parameter, described, e.g., in [6, 11].

In the following subsections we will investigate the spinodal decomposition dynamics described by the solution of **Problem** $\mathbf{P}^h$ for different average values of initial concentration and homogeneous Neumann boundary conditions both for the $d = 1$ and $d = 2$ cases. For the latter case, we will also study the coarsening dynamics for long time scale solutions with the same set of average values of initial concentration as that introduced in the study of the spinodal decomposition dynamics and with periodic boundary conditions.

4.1 Test cases in one space dimension

Let us first analyze the system evolution in the one dimensional case. We consider three test cases in which the initial value c_0 is chosen to be a small uniformly distributed random perturbation around the values $c_0 = 0.05$, $c_0 = c*/2 = 0.3$ and $c_0 = 0.36$. We consider homogeneous Neumann boundary conditions as in (5). We set $\gamma = 0.000196$, $c* = 0.6$ and $\Delta t = 10\gamma$. The relaxation parameter is chosen to be $\mu = 1/64$. The domain is $\Omega = (0, 1)$, and a uniform partition with mesh points $x_j = (j - 1)h$, $j = 1, \ldots, 65$, with $h = 1/64$, is introduced. The results are collected in Figure 2, showing that the system exhibits two kinds of subregions after a transitory regime, one empty in cells, i.e. $c = 0$, and the other rich in cells, with $c \sim c*$. The initial separation of the two phases is fast compared to the overall growth timescale of the segregated pattern.



$c_0 = 0.05$

(a) $t = 0s$. (b) $t = 10.78s$. (c) $t = 105.058s$.

$c_0 = 0.3$

(d) $t = 0s$. (e) $t = 0.19796s$. (f) $t = 4.11796s$.

$c_0 = 0.36$

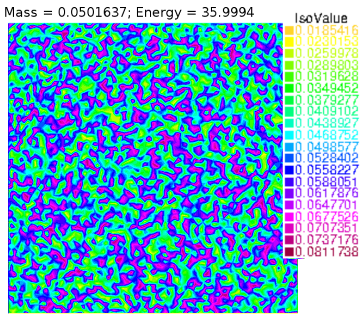
(g) $t = 0s$. (h) $t = 0.392s$. (i) $t = 8.232s$.

Figure 2: Values of $c(x)$ plotted against x for $c_0 = 0.05, 0.3, 0.36$ at different instants of time. The values of mass and energy are reported. The values of the parameters are $\gamma = 0.000196$, $c* = 0.6$ and $\Delta t = 10\gamma$.

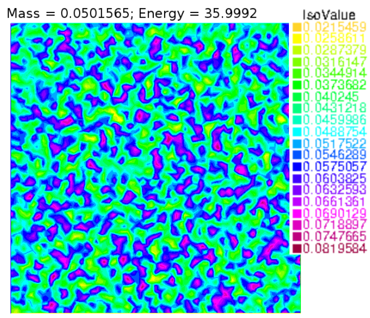
If $c_0 < c*/2$ (resp. $c > c*/2$) then the segregated solution is made of isolated clusters of cells (resp. voids), while if $c_0 = c*/2$ the domain is equally spaced in subregions rich in each phase. We also check that the mass, i.e. the value of $(c_h^n, 1)^h$, is conserved up to a small error, and that the value of the energy F (see Equation (1)) decreases.

4.2 Test cases in two space dimensions

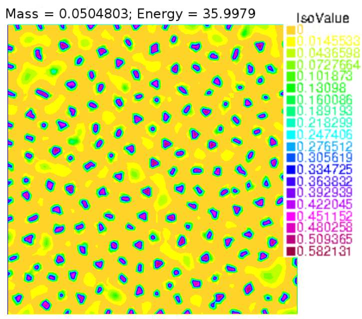
Let us now study the evolution of the system in two space dimensions. The set of initial and boundary values and needed parameters is the same of the 1D case (except for $\mu = 3/64$ here). The domain is $\Omega = (-3, 3) \times (-3, 3)$, and a uniform partition of 64-by-64 triangular elements is introduced. The results are reported in Figure 3, showing the phase separation dynamics for the case $c_0 = 0.05$. As expected, after a transitory regime, the system evolves towards the formation of circular clusters of cells. The initial transitory regime is characterized by the appearance of maze-like patterns. We also check that the mass, i.e. the value of $(c_h^n, 1)^h$, is conserved up to a small error, and that the value of the energy F



(a) $c_0 = 0.05$, $t = 0s$.



(b) $c_0 = 0.05$, $t = 0.392s$.



(c) $c_0 = 0.05$, $t = 9.80196s$.

Figure 3: Values of $c(x, y)$ for $t = 0\,s\,, t = 0.392\,s\,, t = 9.80196\,s$. The values of mass and energy are reported. The values of the parameters are $\gamma = 0.000196$, $c* = 0.6$ and $\Delta t = 10\gamma$.

(see Equation (1)) decreases.

In Figure 4 we compare the simulation results of the degenerate case versus the ones obtained with constant mobility obtained using a $c_0 = 0.05$, $c_0 = 0.3$ and $c_0 = 0.36$. We can observe that in the degenerate case there is little evolution of neighboring maze-like domains, whereas in the constant mobility case such structures grow over time. Moreover, the separation of the two components happens at a faster time scale for the constant mobility case.

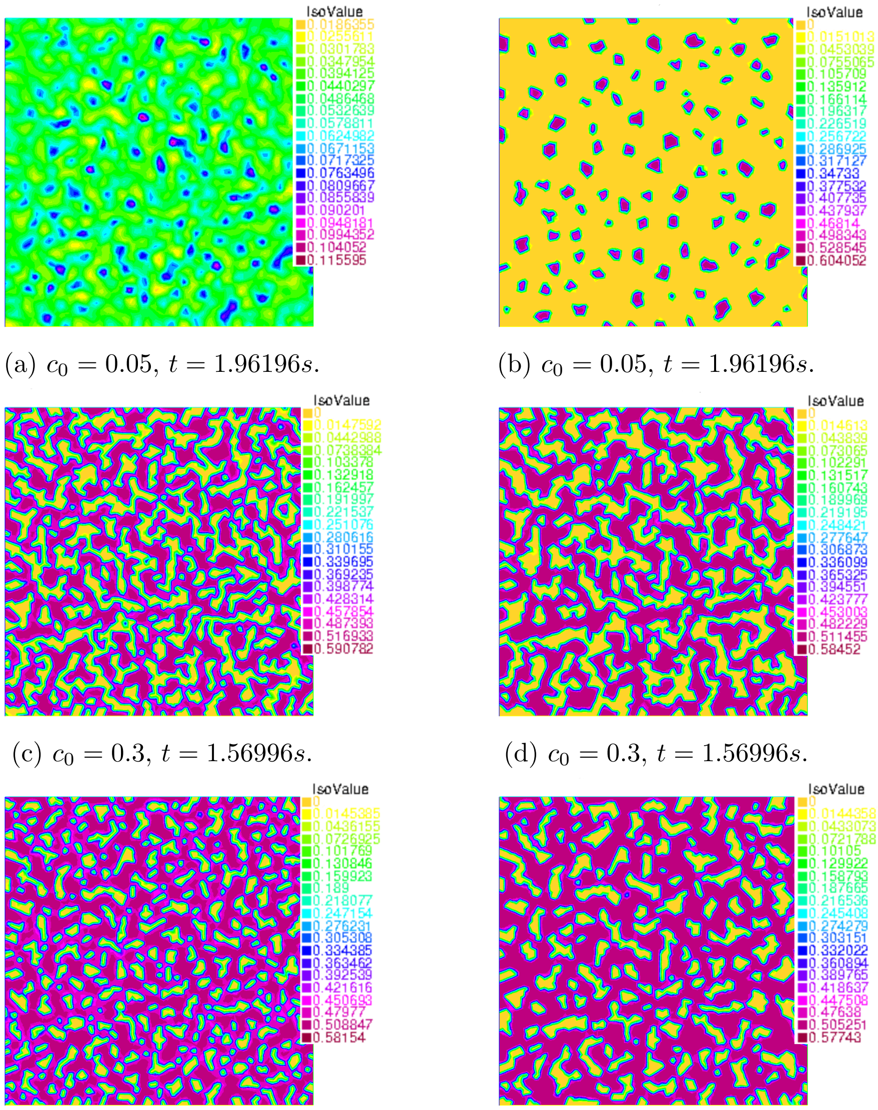
From Figure 4 we can observe that, in the case $c_0 = 0.05$, the system tends to create isolated clusters of cells, whereas the system forms maze-like patterns and cell subdomains tend to occupy half the space in the case $c_0 = c * /2$. Finally, the system tends to form isolated circular domains empty of cells in the case $c_0 = 0.36$.

4.3 Phase-ordering dynamics in two space dimensions

The coarsening domains in Cahn-Hilliard (CH) type models are characterized by a unique time-dependent length scale $L(t)$. For systems with a conserved order parameter and constant mobility (like the classical CH equation), the

Degenerate mobility

Constant mobility



(a) $c_0 = 0.05$, $t = 1.96196s$.

(b) $c_0 = 0.05$, $t = 1.96196s$.

(c) $c_0 = 0.3$, $t = 1.56996s$.

(d) $c_0 = 0.3$, $t = 1.56996s$.

(e) $c_0 = 0.36$, $t = 1.96196s$.

(f) $c_0 = 0.36$, $t = 1.96196s$.

Figure 4: Values of $c(x, y)$ for $c_0 = 0.05$, $c_0 = 0.3$ and $c_0 = 0.36$ for different instant of times during spinodal decomposition, for the degenerate (left panels) and constant mobility (right panels) cases. The values of the parameters are $\gamma = 0.000196$, $c* = 0.6$ and $\Delta t = 10\gamma$.

characteristic domain size obeys the Lifshitz-Slyozov (LS) growth law $L(t) \sim t^{1/3}$, (see, e.g., [6, 35]). The evolution of a single phase subdomain with typical length scale L_i at time $t \geq 0$ can follow two possible paths, as described, e.g., in [6]: either they can shrink by diffusion if $L_i < L(t)$ or grow by absorbing material from the other phase if $L_i > L(t)$. In the standard CH equation with degenerate mobility, two limiting behaviors are typically encountered. If the degeneration set, consisting of pure phases, coincides with the set of stable equilibrium points of the double-well potential, then Mazenko's technique predicts a growth law $L(t) \sim t^{1/4}$, since the surface diffusion mechanism dominates, as described in [35]. Upper bounds on coarsening rates, obtained by interpolation inequalities and energy estimates, which enforce the 1/3 and 1/4 growth laws for the constant and the degenerate mobility cases respectively are obtained in [38, 34]. Conversely, if the degeneration occurs for the unstable equilibrium point $c = 0$, then the LS growth law is recovered, and bulk diffusion dominates, as obtained in [11]. For what concerns the case of the degenerate CH equation with a single-well potential (8), a growth law $L(t) \sim t^{0.37}$ is obtained in [11], which is similar to the LS growth law associated to the standard CH equation with constant mobility. This might be associated to the fact that the stable equilibrium point $c = c*$ of (8) is not a pure phase on which the mobility (9) vanishes, and the pure phase $c = 0$ on which the mobility degenerate is an unstable equilibrium point of (8): the growth driven by bulk diffusion competes with the surface diffusion mechanism. Following [6], it is found that the structure factor exhibits a dynamical scaling,

$$S(k,t) = L(t)^d \mathcal{F}(kL(t)), \tag{97}$$

where $S(k,t)$ is the spherically averaged time dependent structure factor, i.e. the average on the angles of the wave vector of the Fourier transform of the equal time correlation function of the solution, d is the space dimension and $\mathcal{F}(\cdot)$ is a time-independent master function. A definition of the typical length scale of the system at time t is given by the inverse of the first moment of the spherically averaged structure factor, $L(t) =< k >^{-1}$, with

$$< k >= \frac{\int dk\, kS(k,t)}{\int dk\, S(k,t)}.$$

We study three test cases with the same initial data c_0 as in the previous test cases and with periodic boundary conditions. In Figure 5, setting $d = 2$ in (97), we plot the length scale $L(t) :=< k >^{-1}$ in function of time and the spherically averaged scaled structured function $S(k,t) < k >^2$ in function of $kL(t)$ for the late time solutions of the systems evolved from the initial conditions $c_0 = 0.05$, $c_0 = 0.3$ and $c_0 = 0.36$.

The spherically averaged not normalized time dependent structure factor $s(k,t)$ is calculated, following [31], as the average over all wavevectors of magnitude $(k - \Delta k)$ and $(k + \Delta k)$ of the structure factor $S(\mathbf{k},t)$, i.e.

$$s(k,t) = \frac{\sum_{k-\Delta k<|\mathbf{k}|\leq k-\Delta k} S(\mathbf{k},t)}{\sum_{k-\Delta k<|\mathbf{k}|\leq k-\Delta k} 1}, \tag{98}$$

whith

$$S(\mathbf{k},t) = \left\langle \frac{1}{N}\left|\sum_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}}[c(\mathbf{r},t)- < c >]\right|^2 \right\rangle, \tag{99}$$

where in (99) the sum runs over the lattice points positions, $N = L^2$ is the total number of points in the lattice, L is the linear size of the lattice, $< c >$ is the spatial average of c over the lattice and the outer braces $< \cdot >$ stand for ensemble averaging. The summation in $\mathbf{r}$ in Equation (99) is calculated as a Fourier discrete transform, with $\mathbf{k} = 2\pi\mathbf{n}/L$, where the vector $\mathbf{n} = (n_1, n_2)$, $n_1, n_2 = 0, \ldots, \sqrt{N} - 1$, indicates the positions in the dual lattice. We set $\Delta k = (2\pi/L)l$, with l a real value near one for which the plot of the structure function is smooth. For $n_1, n_2 > L/2$, we reassign $n_1 = (L - n_1 - 1)$, $n_2 = (L - n_2 - 1)$. The normalized spherically averaged time dependent structure factor $S(k,t)$ in (97) is then

$$S(k,t) = \frac{s(k,t)}{< c^2 > - < c >^2}.$$

The length scale $L(t)$ is calculated as $L(t) = 1/k_1(t)$, where

$$k_1(t) = \frac{\sum_k ks(k,t)}{\sum_k s(k,t)}$$

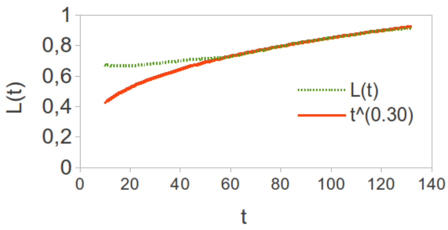
is the first moment of $s(k,t)$.

We observe that the length scale of the systems exhibits a power law evolution $L(t) \sim t^\alpha$ at the late stages of evolution with $\alpha = 0.30$ for $c_0 = 0.05$ and $\alpha = 0.32$ for $c_0 = 0.3$ and $c_0 = 0.36$, close to the LS law. We note that the best coefficient α is calculated using the ordinary Least Squares method in a linear regression analysis of the set of data $\{\log(t), \log(L(t))\}$, starting from a value of the parameter t from which $L(t)$ starts to show a power growth law after an initial plateau. Moreover, we recover the classical result that the structure factors collapse on a time-independent master function, showing that the self-similar scaling behavior (97) for standard phase ordering dynamics.

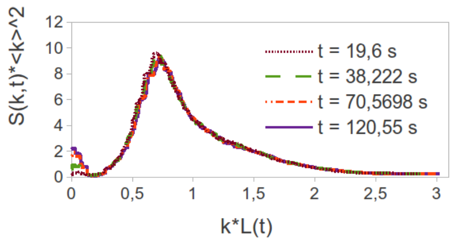
5 Conclusions

In this work we have considered a Cahn-Hilliard type equation with degenerate mobility and single-well potential. In contrast to the model studied in the literature, where the degeneracy and the singularity sets coincide, here we deal with a degeneracy $\{c = 0, c = 1\}$ and a singularity $\{c = 1\}$. This constitutive choice introduces further complications, since $\{c = 0\}$ is an unstable equilibrium point, and the singularity in $c = 1$ does not guarantee that $c \geq 0$. The latter condition has been imposed as a constraint and implemented as a variational inequality.

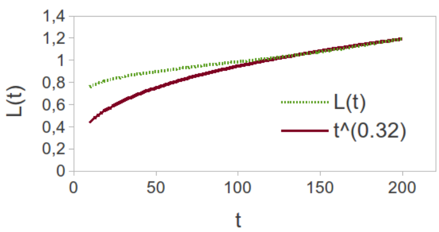
In Section 2 we have formulated a FEM approximation with continuous finite elements where we have enforced the positivity of the solution by means of a discrete variational inequality. We have proved the existence and uniqueness of



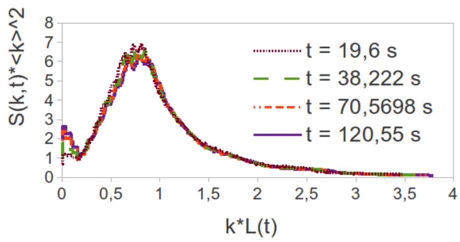
(a) $c_0 = 0.05$, $L(t) \sim t^{0.3}$.



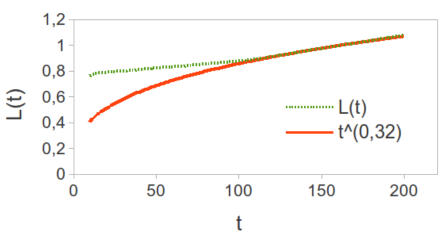
(b) $c_0 = 0.05$.



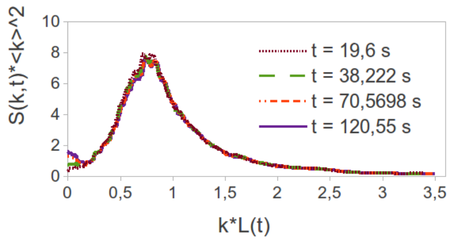
(c) $c_0 = 0.3$, $L(t) \sim t^{0.32}$.



(d) $c_0 = 0.3$.



(e) $c_0 = 0.36$, $L(t) \sim t^{0.32}$.



(f) $c_0 = 0.36$.

Figure 5: *Left panels*: $L(t)$ in function of t superposed to a power growth law t^α for the late stages of time evolution, where the exponent α is obtained by a linear regression analysis, with $\alpha = 0.3$ in the case $c_0 = 0.05$, and $\alpha = 0.32$ in the cases $c_0 = 0.3$ and $c_0 = 0.36$. *Right panels*: spherically averaged scaled structured function $S(k,t) < k >^2$ in function of $kL(t)$ for the late time solutions of the systems evolved from the initial conditions $c_0 = 0.05$, $c_0 = 0.3$ and $c_0 = 0.36$.

the discrete solution, together with the convergence to the weak solution, using a regularization approach. Moreover we have generalized the earlier results of [3] using some properties of subdifferential calculus for avoiding the introduction of an acute partitioning of the domain.

In Section 3 we have established the well-posedness in d spatial dimensions and the convergence in one space dimension. The generalization of convergence analysis to n spatial dimensions will be treated in a forthcoming work.

In Section 4 we have presented the numerical algorithm used for solving the discrete variational inequality and we have performed simulations both in one and two space dimensions. We find that the dynamics of the spinodal decomposition for the solution of **Problem $\mathbf{P}^h$** is, to a certain extent, analogous to the one obtained in standard phase ordering dynamics. In fact the geometry of the segregated domains is driven by the initial value of the concentration, with the appearance of isolated clusters of cells for $c_0 < c*/2$ (see Figure 3) and a maze-like pattern for $c_0 = c*/2$, see Figure 4. A different feature of this model concerns the growth and scaling laws of phase ordering. Whilst the degenerate CH equation with double-well potential is dominated by a surface diffusion mechanism at long time-scales, our model follows a Lifshitz-Slyozov growth law for the characteristic length scale of the emerging patterns. Similarly to the classical CH with constant mobility, this asymptotic behavior highlights the dominance of growth by bulk diffusion. These results on the phase ordering dynamics are finally collected in Figure 5, also showing the existence of a master curve for the structure function.

A further development of this work will concern the error analysis of the discrete solution, which will be presented in a forthcoming paper.

Future work will be focused on the analysis of this model using a finite element approximations with discontinuous elements.

Appendix A. Proof of Lemma 3.1

Proof. From the definition (77) we have

$$||\nabla C_h||_0^2 = ||\nabla c_h^{n-1} + \nabla[c_h^n - c_h^{n-1}]\frac{t - t_{n-1}}{\Delta t}||_0^2$$
$$\leq 2||\nabla c_h^{n-1}||_0^2 + 2\frac{(t-t_{n-1})^2}{(\Delta t)^2}||\nabla[c_h^n - c_h^{n-1}]||_0^2.$$

Hence, using the first bound in (75) and the parallelogram identity, we get

$$||\nabla C_h||_0^2 \leq C, \quad ||\nabla C_h^{\pm}||_0^2 \leq C. \tag{100}$$

From (22) we have that $C_h(0) \to c_0$ strongly in $H^1(\Omega)$ as $h \to 0$. This implies that $⨍ C_h(0) = ⨍ C_h = ⨍ C_h^{\pm} \in (0,1)$. Thus by (100) and the Poincaré inequality we obtain

$$||C_h||^2_{L^\infty(0,T;H^1(\Omega))} \leq C. \tag{101}$$

Furthermore, using (75) and the definition (77), we get

$$\int_0^T |\partial_t C_h|_1^2 dt = \sum_{n=1}^N \int_{t_{n-1}}^{t_n} |\frac{c_h^n - c_h^{n-1}}{\Delta t}|_1^2 dt \le \sum_{n=1}^N \Delta t |\frac{c_h^n - c_h^{n-1}}{\Delta t}|_1^2 \le C(\Delta t)^{-1},$$

$$\int_0^T ||[b(c_h^{n-1})]^{1/2} \nabla w_h^n||_0^2 dt = \sum_{n=1}^N \int_{t_{n-1}}^{t_n} ||[b(c_h^{n-1})]^{1/2} \nabla w_h^n||_0^2 dt$$
$$\le \sum_{n=1}^N \Delta t ||[b(c_h^{n-1})]^{1/2} \nabla w_h^n||_0^2 \le C,$$

$$\int_0^T \left| \hat{\mathcal{G}}^h \left[\frac{c_h^n - c_h^{n-1}}{\Delta t} \right] \right|_1^2 dt = \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \left| \hat{\mathcal{G}}^h \left[\frac{c_h^n - c_h^{n-1}}{\Delta t} \right] \right|_1^2 dt$$
$$\le \sum_{n=1}^N \Delta t \left| \hat{\mathcal{G}}^h \left[\frac{c_h^n - c_h^{n-1}}{\Delta t} \right] \right|_1^2 \le C b_{\max} \le C. \quad (102)$$

Hence, we find

$$||C_h||^2_{L^\infty(0,T;H^1(\Omega))} + \Delta t ||C_h||^2_{H^1(0,T;H^1(\Omega))} + \left|\left| [b(C_h^-)]^{1/2} \frac{\partial W_h^+}{\partial x} \right|\right|_{L^2(\Omega_T)} \le C. \quad (103)$$

In the next step we show that the continuous interpolants C_h are uniformly Hölder continuous. The first bound in (103) gives

$$|C_h(x_2,t) - C_h(x_1,t)| = \left| \int_{x_1}^{x_2} \frac{\partial C_h}{\partial x}(s,t) ds \right| \le |x_2 - x_1|^{1/2} \left(\int_{x_1}^{x_2} \left| \frac{\partial C_h}{\partial x}(s,t) \right|^2 dx \right)^{1/2}$$
$$\le |x_2 - x_1|^{1/2} \left|\left| \frac{\partial C_h}{\partial x} \right|\right|_{L^\infty(0,T;L^2(\Omega))}$$
$$\le C|x_2 - x_1|^{1/2} \quad \forall x_1, x_2 \in \bar{\Omega}, \ \forall t \ge 0.$$

In addition, from (12), the definition (24), (19), the Cauchy-Schwarz inequality and the third bound in (102) it follows that

$$||C_h(\cdot,t_2) - C_h(\cdot,t_1)||_{0,\infty}$$
$$\le C||C_h(\cdot,t_2) - C_h(\cdot,t_1)||_0^{1/2} ||C_h(\cdot,t_2) - C_h(\cdot,t_1)||_1^{1/2}$$
$$\le C(\nabla \hat{\mathcal{G}}^h(C_h(\cdot,t_2) - C_h(\cdot,t_1)), \nabla(C_h(\cdot,t_2) - C_h(\cdot,t_1)))^{1/4} ||C_h(\cdot,t_2) - C_h(\cdot,t_1)||_1^{1/2}$$
$$\le C|\nabla \hat{\mathcal{G}}^h(C_h(\cdot,t_2) - C_h(\cdot,t_1))|_1^{1/4} ||C_h(\cdot,t_2) - C_h(\cdot,t_1)||_1^{3/4}$$
$$\le C \left| \int_{t_1}^{t_2} \hat{\mathcal{G}}^h \frac{\partial C_h}{\partial t}(\cdot,t) dt \right|_1^{1/4} ||C_h||^{3/4}_{L^\infty(0,T;H^1(\Omega))} \le C(t_2 - t_1)^{1/8} \left(\int_{t_1}^{t_2} \left| \hat{\mathcal{G}}^h \frac{\partial C_h}{\partial t}(\cdot,t) \right|_1^2 dt \right)^{1/8}$$
$$\le C(t_2 - t_1)^{1/8} \quad \forall t_2 \ge t_1 \ge 0. \quad (104)$$

From the first bound in (103), the Poincaré inequality and (12), the norm of C_h is uniformly bounded on $\bar{\Omega}_T$ independently on $h, \Delta t$ and T. Moreover, from the previous bounds we have that its $C_{x,t}^{\frac{1}{2},\frac{1}{8}}(\bar{\Omega}_T)$ norm is uniformly bounded independently on $h, \Delta t$ and T. Hence, every sequence C_h is uniformly bounded and equicontinuous on $\bar{\Omega}_T$. Hence the Ascoli-Arzelá Theorem yields a subsequence of C_h such that (81) holds, with

$0 \le c < 1$. Moreover, the first bound in (103) implies that this same subsequence satisfies (80).
From the fact that

$$C_h - C_h^{\pm} = (t - t_n^{\pm})\frac{\partial C_h}{\partial t}, \quad t \in (t_{n-1}, t_n),\ n \ge 1,$$

using the second bound in (103) and taking $t_1 = t_n^{\pm}$ in (104), we deduce that

$$\begin{aligned}
&||C_h - C_h^{\pm}||^2_{L^2(0,T;H^1(\Omega))} \le (\Delta t)^2 ||\frac{\partial C_h}{\partial t}||^2_{L^2(0,T;H^1(\Omega))} \le C\Delta t;\\
&||C_h - C_h^{\pm}||_{L^\infty(\Omega_T)} \le C(\Delta t)^{1/8}.
\end{aligned}$$

Hence, the same convergence results (80) and (81) hold for the piecewise constant interpolants $C_h^{\pm}$.

We now show the boundedness of $\{W_h^+\}_h$ and $\left\{\frac{\partial W_h^+}{\partial x}\right\}_h$ on $L^2_{\text{loc}}(\{0 < c < 1\})$. For any $\delta > 0$, we set

$$\begin{aligned}
D_\delta^+ &= \{(x,t) \in \bar{\Omega}_T \,:\, \delta < c(x,t) < 1\},\\
D_\delta^+(t) &= \{x \in \bar{\Omega} \,:\, \delta < c(x,t) < 1\}.
\end{aligned}$$

On account of the uniform convergence (81), for a fixed $\delta > 0$, it follows that there exists a $h(\delta) \in \mathbb{R}^+$ such that, for all $h \le h(\delta)$,

$$\begin{aligned}
&0 \le C_h^{\pm}(x,t) < \min\{2\delta, 1\} \quad \forall (x,t) \notin D_\delta^+,\\
&\frac{1}{8}\delta \le C_h^{\pm}(x,t) < 1 \quad \forall (x,t) \in D^+_{\frac{\delta}{4}}.
\end{aligned} \tag{105}$$

From the third bound in (103) and from (105) we have

$$b_{\min}(\frac{\delta}{8}) \int_{D^+_{\frac{\delta}{4}}} \left|\frac{\partial W_h^+}{\partial x}\right|^2 dxdt \le \int_{D^+_{\frac{\delta}{4}}} b(C_h^-)\left|\frac{\partial W_h^+}{\partial x}\right|^2 dxdt \le C, \tag{106}$$

where $b_{\min}(\delta) := \min_{\delta \le z < 1} b(z)$. From (105) we have that for all $h \le h(\delta)$ and for almost every $t \in (0,T)$

$$\psi(\cdot,t) \equiv C_h^+(\cdot,t) \pm \frac{1}{8}\delta \frac{\eta^h(\cdot,t)}{||\eta^h(\cdot,t)||_{L^\infty(\Omega)}} \in K^h, \quad \forall \eta^h \in L^2(0,T;S^h) \text{ with } \mathrm{supp}(\eta^h) \subset \mathrm{D}^+_{\frac{\delta}{4}}.$$

Choosing such a ψ in the second equation of system (79) yields, $\forall h < h(\delta)$, that

$$\int_0^T \left[\gamma\left(\frac{\partial C_h^+}{\partial x}, \frac{\partial \eta^h}{\partial x}\right) + (\psi_1'(C_h^+) + \psi_2'(C_h^-), \eta^h)^h\right] dt = \int_0^T (W_h^+, \eta^h)^h dt. \tag{107}$$

We introduce now a cut-off function $\theta_\delta \in C_0^\infty(D^+_{\frac{\delta}{2}})$ such that

$$\theta_\delta(\cdot,t) \equiv 1 \quad \text{on } \mathrm{D}_\delta^+(\mathrm{t}), \quad 0 \le \theta_\delta(\cdot,t) \le 1. \tag{108}$$

Noting that, since $c \in C^{\frac{1}{2},\frac{1}{8}}_{x,t}(\bar{\Omega}_T)$, we have that $C\delta \le |x_2 - x_1|^{1/2}$ for $x_1, x_2 \in D^+_{\frac{\delta}{2}} \setminus D^+_\delta$, we can choose a $\theta_\delta(\cdot,t)$ such that

$$|\nabla \theta_\delta(\cdot,t)| \le C\delta^{-2}. \tag{109}$$

Since $\theta_\delta^2 W_h^+ \in L^2(\Omega)$, and, from definition (14), there exists an $h_1(\delta) \leq h(\delta)$ such that $\mathrm{supp}(\hat{\mathrm{P}}^{\mathrm{h}}(\theta_\delta^2 \mathrm{W}_{\mathrm{h}}^+)) \subset \mathrm{D}_{\frac{\delta}{4}}^+$, for all $h \leq h_1(\delta)$, we can choose $\eta^h = \hat{P}^h(\theta_\delta^2 W_h^+)$ in (107). Using the definition (14), the fact that $C_h^\pm < 1$ and that $\psi_i(\cdot) \in C^1([0,1))$, the estimate (101), and the following inequality (cf. (16), (18) and (20))

$$||(I - \hat{P}^h)\eta||_0 + h|(I - \hat{P}^h)\eta|_1 \leq Ch|\eta|_1 \quad \forall \eta \in H^1(\Omega); \tag{110}$$

we get

$$\begin{aligned}
&\int_0^T (W_h^+, \hat{P}^h(\theta_\delta^2 W_h^+))^h dt = \int_{\Omega_T} \theta_\delta^2 (W_h^+)^2 dx dt \\
&\int_0^T \left[\gamma\left(\frac{\partial C_h^+}{\partial x}, \frac{\partial}{\partial x}(\hat{P}^h(\theta_\delta^2 W_h^+)) \right) + (\psi_1'(C_h^+) + \psi_2'(C_h^-), \hat{P}^h(\theta_\delta^2 W_h^+))^h \right] dt \\
&\leq C||C_h^+||_{L^2(0,T;H^1(\Omega))} \left|\left| \frac{\partial}{\partial x}(\theta_\delta^2 W_h^+) \right|\right|_{L^2(\Omega_T)} + D||\theta_\delta W_h^+||_{L^2(\Omega_T)} \\
&\leq C(1+\delta^{-2})||\theta_\delta W_h^+||_{L^2(\Omega_T)} + D \left|\left| \frac{\partial W_h^+}{\partial x} \right|\right|_{L^2(D^+_{\frac{\delta}{4}})}.
\end{aligned}$$

Using now Young's inequality and bound (106), we infer

$$\int_{\Omega_T} \theta_\delta^2 (W_h^+)^2 dx dt \leq C(\delta)^{-1}. \tag{111}$$

Therefore, combining (111) and (106) and recalling the definition of $\theta_\delta(\cdot, t)$, we have that, for all $\delta > 0$,

$$||W_h^+||_{L^2(0,T;H^1(D_\delta^+(t)))} \leq C(\delta^{-1}) \quad \forall h \leq h_1(\delta). \tag{112}$$

Applying (112) on compact subsets of the set $\{0 < c < 1\} \equiv D_0^+$ we eventually obtain (82). $\square$

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