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A POSITIVITY-PRESERVING FINITE ELEMENT SCHEME FOR THE RELAXED CAHN-HILLIARD EQUATION WITH SINGLE-WELL POTENTIAL AND DEGENERATE MOBILITY

FEDERICA BUBBA* AND ALEXANDRE POULAIN*

ABSTRACT. We propose and analyse a finite element approximation of the Cahn-Hilliard equation regularised in space [15] with single-well potential of Lennard-Jones type and degenerate mobility. The Cahn-Hilliard model has recently been applied to model evolution and growth for living tissues: although the choices of degenerate mobility and singular potential are biologically relevant, they induce difficulties regarding the design of a numerical scheme. We propose a finite element scheme in one and two dimensions and we show that it preserves the physical bounds of the solutions thanks to an upwind approach adapted to the finite elements method. Moreover, we show well-posedness, energy stability properties and convergence of solutions to the numerical scheme. Finally, numerical simulations in one and two dimensions are presented.

1. INTRODUCTION

The Cahn-Hilliard equation [9, 10], proposed originally to describe phase separation occurring in binary alloys, has recently found application in biological contexts, for example in modelling cancer growth [17] and buds formation in *in vitro* cultures of cells undergoing attraction and repulsion effects [4]. In a regular bounded domain $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$ and for $T > 0$, the model writes

$$(1) \quad \partial_t n = \nabla \cdot (b(n) \nabla (\psi'(n) - \gamma \Delta n)), \quad x \in \Omega, t \in (0, T],$$

where $n(t, x)$ represents the (relative) density or volume fraction of cancer cells. The Cahn-Hilliard equation (1) is a conservation law for the cell density

$$\partial_t n + \nabla \cdot \mathbf{J} = 0,$$

with a flux defined by

$$\mathbf{J} = -b(n) \nabla \left(\frac{\delta \mathcal{E}[n]}{\delta n} \right),$$

where $\mathcal{E}[n]$ is the total Helmholtz free energy

$$\mathcal{E}[n](t) := \int_{\Omega} \left(\frac{\gamma}{2} |\nabla n|^2 + \psi(n) \right) dx,$$

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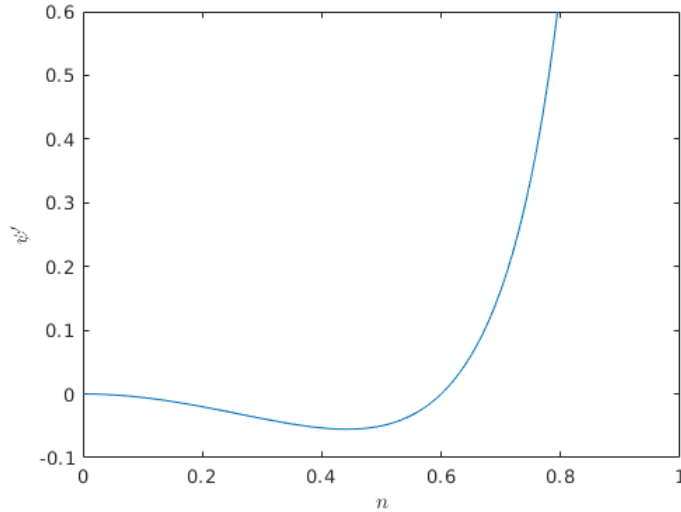


FIGURE 1. Single-well potential of Lennard-Jones type.

and $\psi(n)$ is the homogeneous free energy which accounts for repulsing phenomena occurring in a mixture. In most applications, this functional is a double-well logarithmic potential, often approximated by a smooth polynomial function, with minima located at the two attraction points that represent pure phases (usually $n = -1$ and $n = 1$). The pure phases are linked by a diffuse interface of thickness proportional to γ .

In the context of tumor growth, the choice of a double-well potential appears to be unphysical: as suggested by Byrne and Preziosi in [8], a single-well potential of Lennard-Jones type enables to be more biologically relevant in the description of the attractive and repulsive forces between cells. Following this suggestion, Agosti *et al.* [3] employ a potential $\psi : [0, 1) \rightarrow \mathbb{R}$ defined as (cf. Figure 1)

$$(2) \quad \psi(n) = -(1 - n^*) \log(1 - n) - \frac{n^3}{3} - (1 - n^*) \frac{n^2}{2} - (1 - n^*)n + k,$$

with k constant. With this choice, cells undergo attractive forces when the cell density is small ($\psi'(\cdot) < 0$ for $n \leq n^*$) and repulsive ones in overcrowded zones ($\psi'(\cdot) > 0$ for $n \geq n^*$). The value $n^* > 0$ represents the cell density for which attractive and repulsive forces are at equilibrium. In the case of a single-well potential, the pure phases are represented by the states $n = 0$ and $n = 1$. The Cahn-Hilliard equation with the logarithmic single-well potential defined in (2) and a mobility function $b(\cdot)$ that degenerates at pure phases, *i.e.*

$$(3) \quad b(n) := n(1 - n)^2,$$

has been studied by Agosti *et al.* in [3], where existence of weak solutions was proved for $d \leq 3$.

When studying the Cahn-Hilliard equation from a numerical point of view, a common practice is to consider the second-order splitting

$$(4) \quad \begin{aligned} \partial_t n &= \nabla \cdot (b(n)\nabla w), \\ w &= -\gamma\Delta n + \psi'(n), \end{aligned}$$

as proposed, for example, in [3, 5, 12]. In the context of material science w is called chemical potential.

In this paper, we propose a different technique to overcome the resolution of a fourth-order equation based on the spatial relaxation suggested and studied in [15]. We will present and analyse a finite element approximation of the relaxed degenerate Cahn-Hilliard system (RDCH in short) that writes

$$(5) \quad \begin{aligned} \partial_t n &= \nabla \cdot (b(n)\nabla (\varphi + \psi'_+(n))), \quad x \in \Omega, t \in (0, T], \\ -\sigma\Delta\varphi + \varphi &= -\gamma\Delta n + \psi'_-(n - \frac{\sigma}{\gamma}\varphi), \end{aligned}$$

with nonnegative initial conditions

$$n(0, x) = n_0(x), \quad x \in \Omega,$$

and equipped with zero-flux boundary conditions

$$\frac{\partial(n - \frac{\sigma}{\gamma}\varphi)}{\partial\nu} = \frac{b(n)\partial(\varphi + \psi'_+(n))}{\partial\nu} = 0, \quad x \in \partial\Omega, t \in (0, T],$$

where ν is the unit normal pointing outward the boundary surface $\partial\Omega$. In System (5), the mobility $b(\cdot)$ is defined as in (3), σ is the relaxation parameter that satisfies $0 < \sigma < \gamma$ and, as in Eyre [14], the potential (2) was split into a convex part ψ_+ and a non-convex one ψ_- , in our case defined as

$$(6) \quad \psi_+(n) = -(1 - n^*) \log(1 - n) - \frac{n^3}{3},$$

$$(7) \quad \psi_-(n) = -(1 - n^*) \frac{n^2}{2} - (1 - n^*)n + k.$$

Notice that $\psi_+(\cdot)$ is convex for $n^* \leq 0.7$.

The main idea is to replace the chemical potential w by its regularised diffuse approximation φ . In [15], authors proved that, for $\sigma \rightarrow 0$, weak solutions to the relaxed System (5) converge to the ones of the original Cahn-Hilliard equation (1), both with a single-well potential and a degenerate mobility. The proof relies in particular on *a priori* estimates based on the energy functional

$$(8) \quad \mathcal{E}[n](t) := \int_{\Omega} \left\{ \frac{\gamma}{2} \left| \nabla \left(n - \frac{\sigma}{\gamma}\varphi \right) \right|^2 + \frac{\sigma}{2\gamma} |\varphi|^2 + \psi_+(n) + \psi_- \left(n - \frac{\sigma}{\gamma}\varphi \right) \right\} dx,$$

that is proved to be decreasing in time because

$$\frac{d\mathcal{E}[n]}{dt} = - \int_{\Omega} b(n) |\nabla (\varphi + \psi'_+(n))|^2 dx.$$

We observe that the relaxed Cahn-Hilliard system recalls the Keller-Segel model with additional cross diffusion, proposed and studied by Carrillo *et al.* [11].

The aim of this paper is to propose a finite element scheme to solve the relaxed Cahn-Hilliard system in one and two dimensions. We will study well-posedness of the scheme as well as the positivity of discrete solutions, ensured (under a restriction condition on the time-step) thanks to an adaptation of the upwind technique to the finite element approximation method.

A review of numerical methods for the Cahn-Hilliard equation. Numerous numerical methods have been developed for the Cahn-Hilliard equation featuring smooth and logarithmic double-well potential as well as constant and degenerate mobilities. Elliott and Songmu [13] proposed a finite element Galerkin method for the Cahn-Hilliard equation with constant mobility and a smooth double-well potential. In the more challenging case of a degenerate mobility and singular potentials, Barrett *et al.* [5] proposed a finite element scheme which employs the convex/non-convex splitting of the potential function. They proved well posedness of the scheme, the convergence of numerical solutions in the one-dimensional case and presented some numerical experiments in one and two dimensions. Numerical methods to solve the Cahn-Hilliard equation without the splitting technique (4) have also been suggested. For example, Brenner *et al.* [7] designed a C^0 interior penalty method which is a class of discontinuous Galerkin method.

Even though a single-well potential seems more relevant for biological applications of the Cahn-Hilliard equation, very few works considered this particular case. As previously cited, Agosti *et al.* [2] proposed a continuous finite element method to solve this particular version of the equation, describing the main issues while working with single-well logarithmic potential and degenerate mobility of forms (2) and (3) respectively. In fact, in this case the positivity of the solution is not ensured at the discrete level due to the fact that the degeneracy set $\{0; 1\}$ does not coincide with the singularity set $\{1\}$. Therefore the absence of cells represents a unstable equilibrium of the potential. Agosti *et al.* designed a scheme which preserves positivity using a discrete variational inequality, as also suggested in [5]. The resulting scheme is highly non-linear and goes through Newton iterations. Recently, Agosti [1] presented a discontinuous Galerkin finite element discretisation of the equation. Again the positivity is ensured by imposing a discrete variational inequality.

This paper is organised as follows. In Section 2, we introduce the finite element approximation of the relaxed Cahn-Hilliard equation (5) in one and two dimensions. As said above, the main issue is to suitably adapt the upwind method to the finite elements setting in order to obtain a positivity-preserving scheme. Well-posedness and positivity of solutions

are analysed in Section 3. In Section 4, we prove a discrete energy stability result that provides *a priori* estimates which enable to prove convergence of discrete solutions. Finally, in Section 5, we present one and two dimensional simulations of the relaxed Cahn-Hilliard equation.

2. NUMERICAL SCHEME

Notations. Let $\Omega \subset \mathbb{R}^d$ with $d = 1, 2, 3$ be a regular domain with Lipschitz boundary $\partial\Omega$. We indicate the usual Banach and Sobolev spaces by respectively $L^p(\Omega)$, $W^{m,p}(\Omega)$ with $H^m(\Omega) = W^{m,2}(\Omega)$, where $1 \leq p \leq +\infty$ and $m \in \mathbb{N}$. The previous spaces are endowed with the corresponding norms $\|\cdot\|_{m,p,\Omega}$, $\|\cdot\|_{m,\Omega}$ and semi-norms $|\cdot|_{m,p,\Omega}$, $|\cdot|_{m,\Omega}$. The standard L^2 inner product will be denoted by $(\cdot, \cdot)_\Omega$ and the duality pairing between $(H^1(\Omega))'$ and $H^1(\Omega)$ by $\langle \cdot, \cdot \rangle_\Omega$.

Let \mathcal{T}^h , $h > 0$, be a quasi-uniform partitioning of the domain Ω into N_h disjoint open simplices K . Let $h_K := \text{diam}(K)$ and $h = \max_K h_K$. Therefore, $\bar{\Omega} = \sum_{K \in \mathcal{T}^h} \bar{K}$. We assume that the partitioning is acute, *i.e.* for $d = 2$ the angles of the triangles can not exceed $\frac{\pi}{2}$ and for $d = 3$ the angle between two faces of the same tetrahedron can not exceed $\frac{\pi}{2}$. We introduce the finite element space associated with \mathcal{T}^h

$$S^h := \{\chi \in C(\bar{\Omega}) : \chi|_K \in \mathbb{P}^1(K), \quad \forall K \in \mathcal{T}^h\} \subset H^1(\Omega),$$

where $\mathbb{P}^1(K)$ denotes the space of polynomials of order 1 on K . For later convenience, we set

$$K^h := \{\chi \in S^h : \chi \geq 0 \quad \text{in } \Omega\}.$$

Let J be the set of nodes of \mathcal{T}^h and $\{x_j\}_{j \in J}$ the set of their coordinates. We call $\{\chi_j\}_{j \in J}$ the standard lagrangian basis functions associated with the spatial mesh. We will refer to the standard lagrangian interpolation function through the function $\pi^h : C(\bar{\Omega}) \rightarrow S^h$ and define the lumped scalar

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

2.1. Description of the scheme. Given $N_T \in \mathbb{N} - \{0\}$, let $\Delta t := T/N_T$ be the time-step and $t_k := k\Delta t$, $k = 0, \dots, N_T - 1$ be the temporal mesh. We introduce the following finite element approximation of System (5): for each $k = 0, \dots, N_T - 1$, find $\{n_h^{k+1}, \varphi_h^{k+1}\}$ in $K^h \times S^h$ such that

(9a)

$$\left(\frac{n_h^{k+1} - n_h^k}{\Delta t}, \chi \right)^h + \left(b^{\text{upw}}(n_h^k) \nabla \varphi_h^{k+1}, \nabla \chi \right) + \left(b(n_h^k) \nabla \psi'_+(n_h^{k+1}), \nabla \chi \right) = 0, \quad \forall \chi \in K^h,$$

(9b)

$$\sigma \left(\nabla \varphi_h^{k+1}, \nabla \chi \right) + \left(\varphi_h^{k+1}, \chi \right)^h = \gamma \left(\nabla n_h^{k+1}, \nabla \chi \right) + \left(\psi'_-(n_h^k - \frac{\sigma}{\gamma} \varphi_h^k), \chi \right)^h, \quad \forall \chi \in S^h,$$

where $n_h^0 \in K^h$ is a suitable approximation in the finite element space of the initial condition $n_0(x)$. The finite element approximations of n and φ are defined as usual by

$$n_h^k(x) := \sum_{j \in J} n_j^k \chi_j(x), \quad \text{and} \quad \varphi_h^k(x) := \sum_{j \in J} \varphi_j^k \chi_j(x),$$

where $\{n_j^k\}_{j \in J}$ and $\{\varphi_j^k\}_{j \in J}$ are unknowns and $\{\chi_j\}_{j \in J}$ is the finite element basis.

Matrix form. For $k = 0, \dots, N_T - 1$, let \underline{n}^k and $\underline{\varphi}^k$ be the vectors of the unknowns

$$\underline{n}^k := [n_1^k, \dots, n_{N_h}^k]^T, \quad \underline{\varphi}^k := [\varphi_1^k, \dots, \varphi_{N_h}^k]^T.$$

Then, we can rewrite Eq. (9a)-(9b) in the matrix form

$$(10a) \quad M \underline{n}^{k+1} = M \underline{n}^k - \Delta t D \underline{n}^{k+1} - \Delta t U \underline{\varphi}^{k+1},$$

$$(10b) \quad (\sigma A + M) \underline{\varphi}^{k+1} = \gamma A \underline{n}^{k+1} + \underline{\psi}'^k.$$

In (10a), M and A are, respectively, the standard finite element mass and stiffness matrices, U is the finite element matrix of elements

$$(11) \quad U_{ij} = \int_{\Omega} [b^{upw}(n_h^k)]_j \nabla \chi_j \nabla \chi_i \, dx, \quad \text{for } i, j = 1, \dots, N_h,$$

and D is the finite element matrix with elemental submatrices

$$(12) \quad D_{ij} = \int_{\Omega} b(n_h^k) \psi_+''(n_h^k) \nabla \chi_j \nabla \chi_i \, dx, \quad \text{for } i, j = 1, \dots, N_h.$$

Finally, $[\underline{\psi}'^k]_j := \psi'_- \left(n_j^k - \frac{\sigma}{\gamma} \varphi_j^k \right)$.

Upwind numerical scheme. In order to preserve the nonnegativity of discrete solutions, we split the flux into a diffusive and convective part, and handle the latter with an upwind scheme adapted to the finite element setting as follows. For $j \in J$ we set

$$(13) \quad [b^{upw}(n_h^k)]_j := \begin{cases} b(n_i^k), & \text{if } \varphi_j^{k+1} - \varphi_i^{k+1} < 0, \\ b(n_j^k), & \text{otherwise.} \end{cases}$$

As we will see later, a necessary condition to ensure the positivity-preserving property is to use a lumped mass matrix M_L , defined element-wise as

$$M_{L,ii} := \sum_{j=1}^{N_h} M_{ij}.$$

Thus, the lumped mass matrix is the diagonal matrix with each term being the row sum of M . In the following of the paper, the mass matrix is replaced by M_L . Furthermore, since U has zero row sum, we can rewrite equation (10a) for each node i

$$(14) \quad M_{L,ii} n_i^{k+1} = M_{L,ii} n_i^k - \Delta t \sum_{j \neq i} \left[D_{ij} (n_j^{k+1} - n_i^{k+1}) + U_{ij} (\varphi_j^{k+1} - \varphi_i^{k+1}) \right].$$

3. EXISTENCE AND NONNEGATIVITY OF DISCRETE SOLUTIONS

In this section, we follow [6] to prove existence and nonnegativity of discrete solutions to (9a) and (9b) using the Brouwer fixed point theorem. We introduce

$$\tilde{K}^h := \{\chi \in K^h : \|\chi\|_{L^1(\Omega)} \leq \|n_0\|_{L^1(\Omega)}\},$$

that is a finite-dimensional, convex and compact set. We define the fixed-point operator $\mathcal{F} : \tilde{K}^h \rightarrow \tilde{K}^h$ that at each n_h^k associates the quantity \tilde{n} , solution of a linearised problem that we now describe. First, given $k \geq 0$ and $n_h^k \in \tilde{K}$, we set $\varphi_h^k := \Delta_h n_h^k$, where Δ_h is a discrete version of the Laplace operator (for example, computed with finite differences). Next, we search for $\tilde{\varphi} \in S^h$, solution to

$$(15) \quad \sigma(\nabla \tilde{\varphi}, \nabla \chi) + (\tilde{\varphi}, \chi)^h = \gamma \left(\nabla n_h^k, \nabla \chi \right) + \left(\psi'_-(n_h^k - \frac{\sigma}{\gamma} \varphi_h^k), \chi \right)^h.$$

Finally, we find the solution $\tilde{n} \in \tilde{K}^h$ to the linearised equation

$$(16) \quad (\tilde{n}, \chi)^h + \Delta t \left(b(n_h^k) \psi''_+(n_h^k) \nabla \tilde{n}, \nabla \chi \right) = \left(n_h^k, \chi \right)^h - \Delta t \left(b^{\text{upw}}(n_h^k) \nabla \tilde{\varphi}, \nabla \chi \right),$$

for all $\chi \in K^h$.

In order to prove our existence result, we first need to prove that, thanks to the upwind method presented above, the right-hand side of (16) is nonnegative.

Proposition 1 (Positivity-preserving property, 1D). *For $k = 0, \dots, N_T - 1$, let $\{n_h^k, \varphi_h^k\} \in K^h \times S^h$ be such that $0 \leq n_h^k < 1$. The one-dimensional numerical scheme (15)–(16) with b^{upw} defined as in (13) preserves the positivity, i.e.*

$$0 \leq n_h^{k+1} < 1 \text{ in } \Omega.$$

Proof. 1. Positivity: The proof of the positivity ensuring property relies on the analysis of the equation (16) which can be rewritten into a matrix system

$$(17) \quad \tilde{n} = (M_L + \Delta t D)^{-1} \left(M_L n^k - \Delta t U \tilde{\varphi} \right).$$

Since the matrix $(M_L + \Delta t D)$ is a M-matrix (cf. appendix A), we need to ensure that the vector $M_L n^k - \Delta t U \tilde{\varphi}$ is positive element-wise to preserve the positivity of \tilde{n} .

Using the formulation (14), we need to satisfy the inequality

$$M_{L,ii} n_i^k \geq \sum_{j \neq i} U_{ij} (\tilde{\varphi}_j - \tilde{\varphi}_i).$$

where the coefficient U_{ij} are given by

$$U_{ij} = -\frac{1}{\Delta x} [b^{\text{upw}}(n_h^k)]_j.$$

and

$$M_{L,ii} = \Delta x.$$

Thus, we obtain

$$n_i^k \geq -\frac{\Delta t}{\Delta x^2} \sum_{j \neq i} \left[b(n_i^k) \min(0, \tilde{\varphi}_j - \tilde{\varphi}_i) + b(n_j^k) \max(0, \tilde{\varphi}_j - \tilde{\varphi}_i) \right].$$

Since $\min(0, \tilde{\varphi}_j - \tilde{\varphi}_i) \leq 0$, we have

$$\begin{aligned} n_i^k &\geq \frac{\Delta t}{\Delta x^2} \sum_{j \neq i} b(n_i^k) \max(0, \tilde{\varphi}_i - \tilde{\varphi}_j), \\ &\geq -\frac{\Delta t}{\Delta x^2} \sum_{j \neq i} \left[b(n_i^k) \min(0, \tilde{\varphi}_j - \tilde{\varphi}_i) + b(n_j^k) \max(0, \tilde{\varphi}_j - \tilde{\varphi}_i) \right]. \end{aligned}$$

Since $b(n_i^k) = n_i^k(1 - n_i^k)^2$, we have

$$n_i^k \geq \frac{\Delta t}{\Delta x^2} n_i^k (1 - n_i^k)^2 \sum_{j \neq i} \max(0, \tilde{\varphi}_i - \tilde{\varphi}_j).$$

The distance $|\tilde{\varphi}_j - \tilde{\varphi}_i|$ is bounded from above by $\frac{\Delta x}{\sqrt{\sigma}}$ because $\tilde{\varphi}$ is solution of a diffusion equation with σ as diffusion coefficient. Also, since the maximum number of nodes connected to i is 2 and $(1 - n_i^k)^2 < 1$, we obtain the condition for positivity in one dimension

$$(18) \quad \frac{2\Delta t}{\Delta x \sqrt{\sigma}} \leq 1.$$

2. *Upper bound:* We want to prove

$$\|\tilde{n}\|_\infty = \left\| \left(\frac{M_L}{\Delta t} + D \right)^{-1} \left(\frac{M_L}{\Delta t} n_h^k - U \tilde{\varphi} \right) \right\|_\infty < 1.$$

Using the property of the $\|\cdot\|_\infty$,

$$\left\| \left(\frac{M_L}{\Delta t} + D \right)^{-1} \left(\frac{M_L}{\Delta t} n_h^k - U \tilde{\varphi} \right) \right\|_\infty \leq \left\| \left(\frac{M_L}{\Delta t} + D \right)^{-1} \right\|_\infty \left\| \left(\frac{M_L}{\Delta t} n_h^k - U \tilde{\varphi} \right) \right\|_\infty.$$

The Varah [16] bound gives

$$\left\| \left(\frac{M_L}{\Delta t} + D \right)^{-1} \right\|_\infty \leq \frac{1}{\min_i \{ |\frac{\Delta x}{\Delta t} + D_{ii}| - \sum_{i \neq j} |D_{ij}| \}} = \frac{\Delta t}{\Delta x}.$$

Therefore, we want to prove that

$$\begin{aligned} 1 &> \frac{\Delta t}{\Delta x} \left| \frac{\Delta x}{\Delta t} n_i - \sum_{j \neq i} U_{ij} (\tilde{\varphi}_j - \tilde{\varphi}_i) \right|, \\ &= \frac{\Delta t}{\Delta x} \left| \frac{\Delta x}{\Delta t} n_i + \frac{1}{\Delta x} \sum_{j \neq i} b(n_i^k) \min(0, \tilde{\varphi}_j - \tilde{\varphi}_i) + b(n_j^k) \max(0, \tilde{\varphi}_j - \tilde{\varphi}_i) \right|. \end{aligned}$$

Which is ensured if

$$\begin{aligned} 1 &> n_i + \frac{\Delta t}{\Delta x^2} \sum_{j \neq i} b(n_j^k) \max(0, \tilde{\varphi}_j - \tilde{\varphi}_i), \\ &> n_i + \frac{\Delta t}{\Delta x \sqrt{\sigma}} \sum_{j \neq i} b(n_j^k). \end{aligned}$$

Since $\|b\|_{L^\infty((0,1])} = \frac{4}{27}$, we have

$$n_i + \frac{\Delta t}{\Delta x \sqrt{\sigma}} \sum_{j \neq i} b(n_j^k) \leq n_i + \frac{8\Delta t}{27\Delta x \sqrt{\sigma}}.$$

The condition which needs to be satisfied at each time step to preserve the upper bound is

$$(19) \quad 1 - \left\| n_h^k \right\|_\infty > \frac{8\Delta t}{27\Delta x \sqrt{\sigma}}.$$

□

Proposition 2 (Positivity-preserving property, 2D). *Starting from a solution $\{n_h^k, \varphi_h^k\} \in K^h \times S^h$ and $0 \leq n_h^k < 1$, the two-dimensional residual distribution scheme (16)–(15) preserves the positivity, i.e.*

$$0 \leq n_h^{k+1} < 1 \text{ in } \Omega.$$

Proof. 1. Positivity: The outline of the proof for the two dimensional case is close to the one dimensional case. In fact, using the argument that $M_L + \Delta t D$ is a M-matrix (cf. appendix A), the only thing left to prove is that

$$\frac{M_L}{\Delta t} n_h^k - U \tilde{\varphi} \geq 0.$$

Using the formulation (14) and calculating $M_{L,ii} = \sum_{n \in T_i} \frac{2}{12} |K_n|$, where T_i represents the set of elements connected to the node i and $|K_n|$ the surface of the element n . To make the proof clearer, we consider a uniform mesh in the following. If the mesh is not uniform the calculations remain the same but the surface of each element needs to be taken into account in the calculation of the calculation of U_{ij} . Therefore, we have

$$U_{ij} = b_j^{\text{upw}} \int_K \nabla \chi_i \chi_j dx = -\frac{b_j^{\text{upw}}}{4|K|} (D_K^T D_K)_{ij}.$$

Where $D_K = \begin{pmatrix} y_1 - y_2 & y_2 - y_0 & y_0 - y_1 \\ x_2 - x_1 & x_0 - x_2 & x_1 - x_0 \end{pmatrix}$. Using the calculation of the mobility coefficients (13), we have

$$\sum_{n \in T_i} \frac{2}{12} |K| n_i^k \geq - \sum_{n \in T_i} \Delta t \sum_{j \neq i} \frac{1}{4|K|} (D_K^T D_K)_{ij} (b(n_i^k) \min(0, \tilde{\varphi}_j - \tilde{\varphi}_i) + b(n_j^k) \max(0, \tilde{\varphi}_j - \tilde{\varphi}_i)).$$

This inequality is satisfied if

$$n_i^k \sum_{n \in T_i} \frac{2}{12} |K| \geq \Delta t \sum_{n \in T_i} \sum_{j \neq i} \frac{1}{4|K|} (D_K^T D_K)_{ij} b(n_i^k) \max(0, \tilde{\varphi}_i - \tilde{\varphi}_j).$$

For an interior node i , the condition of positivity reads

$$(20) \quad 1 \geq \frac{24\Delta t}{\Delta x \sqrt{\sigma}}.$$

2. *Upper bound:* The proof follows the same outline than in the one-dimensional case. Starting from the Varah bound we obtain the inequality

$$\left(\left(\frac{M_L}{\Delta t} + D \right)^{-1} \left(\frac{M_L}{\Delta t} n_h^k - U \tilde{\varphi} \right) \right)_i \leq n_i^k + \sum_{n \in T_i} \frac{3\Delta t}{2|K_n|^2} \sum_{j \neq i} (D_K^T D_K)_{ij} b(n_j^k) \max(0, \tilde{\varphi}_j - \tilde{\varphi}_i)$$

If we assume an uniform mesh, we have the following maximum values for each term of the r.h.s: we have $\max\{(D_K^T D_K)_{ij}\} = 2\Delta x^2$, $\max\{b(n_j^k)\} = \frac{4}{27}$ and we know that $|\varphi_j - \varphi_i| \leq \frac{\Delta x}{\sqrt{\sigma}}$. Altogether, we obtain the following condition such that $n_h^{k+1} \leq 1$.

$$(21) \quad \frac{8\Delta t}{3\Delta x \sqrt{\sigma}} \leq 1 - \|n_h^k\|_\infty$$

□

Remark 3. *The conditions (19) and (21) are derived assuming the worst case possible. Obviously, in practice these conditions can be relaxed while the numerical scheme preserves the upper bound.*

We can now prove the existence of nonnegative, discrete solutions to (9a) and (9b).

Theorem 4 (Existence of discrete solutions). *There exists a solution $\{n_h^{k+1}, \varphi_h^{k+1}\} \in K^h \times S^h$ to the finite element approximation of the regularised Cahn-Hilliard equation (9a), (9b) that satisfies the bounds*

$$0 \leq n_h^{k+1} < 1, \quad k = 0, \dots, N_T - 1.$$

Proof. We rewrite (15) in the following matrix form

$$(22) \quad (\sigma A + M_L) \tilde{\varphi} = \gamma A n_h^k + \underline{\psi}'_{-}{}^k,$$

where the matrices and the vectors are defined as in (10b). Thanks to the properties of the finite element basis $\{\chi_j\}_{j \in J}$, the matrix $\sigma A + M_L$ is diagonally dominant for $\sigma > 0$. This ensures the existence of a unique $\tilde{\varphi}$. In the same manner, we rewrite (16) as

$$(23) \quad (M_L + \Delta t D) \tilde{n} = M_L n_h^k - \Delta t U \tilde{\varphi}.$$

As showed in Appendix A, the matrix $M_L + \Delta t D$ is an M-matrix. This, together with the nonnegativity of the right-hand side of (23), ensures the existence of a unique $\tilde{n} \in \tilde{K}^h$.

In order to apply the Brouwer fixed-point theorem, we need to show that the operator

$$\mathcal{F} : \tilde{K}^h \rightarrow \tilde{K}^h$$

$$n_h^k \rightarrow \tilde{n}$$

is continuous. This is obvious observing that, thanks to the definition of ψ_- , both equations (15) and (16) are linear in $\tilde{\varphi}$ and \tilde{n} . Thus, the Brouwer fixed-point theorem ensures the existence of $\{n_h^{k+1}, \varphi_h^{k+1}\} \in K^h \times S^h$ solutions to the finite element scheme (9a),(9b). □

4. ENERGY AND CONVERGENCE ANALYSIS

4.1. Dissipation of the discrete energy. Before starting to analyse the numerical properties of the scheme (9a), (9b), we show in this section that there exists a discrete energy that is preserved in the discretisation. In order to prove this, we rewrite (9a) in a more compact form:

$$\left(\frac{n_h^{k+1} - n_h^k}{\Delta t}, \chi \right)^h + \left(b(n_h^k) \nabla \left(\varphi_h^{k+1} + \psi'_+(n_h^{k+1}) \right), \nabla \chi \right) = 0, \quad \forall \chi \in K^h.$$

This can be done since, as we will show in the proof of the next theorem, the choice of the discretization for b does not have a role in the discrete energy, as long as it is non-negative.

Theorem 5 (Energy stability). *Let $\{n_h^{k+1}, \varphi_h^{k+1}\} \in K^h \times S^h$ be the solution of system (9a),(9b). Let the discrete energy be defined as*

$$(24) \quad E_h(n_h^k, \varphi_h^k) := \int_{\Omega} \left\{ \frac{\gamma}{2} |\nabla n_h^k|^2 + \frac{\sigma^2}{2\gamma} |\nabla \varphi_h^k|^2 - \sigma \nabla n_h^k \nabla \varphi_h^k + \frac{\sigma}{2\gamma} |\varphi_h^k|^2 + \psi'_+(n_h^k) + \psi'_-\left(n_h^k - \frac{\sigma}{\gamma} \varphi_h^k\right) \right\}.$$

Then for $k = 0, \dots, N_T - 1$ we have

$$(25) \quad E_h(n_h^{k+1}, \varphi_h^{k+1}) + \Delta t \int_{\Omega} b(n_h^k) |\nabla(\varphi_h^{k+1} + \psi'_+(n_h^{k+1}))|^2 dx \leq E_h(n_h^k, \varphi_h^k) + C\sigma,$$

where C is a constant that does not depend on the spatio-temporal mesh.

Proof. By choosing $\chi = \varphi_h^{k+1} + (\psi'_+(n_h^{k+1}))$ in (9a) we obtain

$$\int_{\Omega} \left(n_h^{k+1} - n_h^k \right) \left(\varphi_h^{k+1} + \psi'_+(n_h^{k+1}) \right) dx = -\Delta t \int_{\Omega} b(n_h^k) |\nabla(\varphi_h^{k+1} + \psi'_+(n_h^{k+1}))|^2 dx.$$

The idea is to find (25) by controlling from below the left-hand side in the above equation. To this end, we first observe that, for a convex function g , the following property holds:

$$g(y) - g(x) \leq g'(y)(y - x).$$

Thus, since $\psi_+(\cdot)$ is a convex function, we write

$$(26) \quad \int_{\Omega} \left(n_h^{k+1} - n_h^k \right) \psi'_+(n_h^{k+1}) dx \geq \int_{\Omega} \left(\psi_+(n_h^{k+1}) - \psi_+(n_h^k) \right) dx.$$

We need now to control from below the term $\int_{\Omega} \left(n_h^{k+1} - n_h^k \right) \varphi_h^{k+1} dx$. To do this, we choose $\chi = n_h^{k+1} - n_h^k$ and $\chi = \varphi_h^{k+1} - \varphi_h^k$ in (9b) and, after integration by parts, we obtain respectively,

$$(27) \quad \begin{aligned} \sigma \int_{\Omega} \nabla \varphi_h^{k+1} \nabla \left(n_h^{k+1} - n_h^k \right) dx + \int_{\Omega} \varphi_h^{k+1} \left(n_h^{k+1} - n_h^k \right) dx = \\ \gamma \int_{\Omega} \nabla n_h^{k+1} \nabla \left(n_h^{k+1} - n_h^k \right) dx + \int_{\Omega} (\psi'_-)^k \left(n_h^{k+1} - n_h^k \right) dx \end{aligned}$$

and

(28)

$$\begin{aligned} \sigma \int_{\Omega} \nabla \varphi_h^{k+1} \nabla (\varphi_h^{k+1} - \varphi_h^k) dx + \int_{\Omega} \varphi_h^{k+1} (\varphi_h^{k+1} - \varphi_h^k) dx = \\ \gamma \int_{\Omega} \nabla n_h^{k+1} \nabla (\varphi_h^{k+1} - \varphi_h^k) dx + \int_{\Omega} (\psi'_-)^k (\varphi_h^{k+1} - \varphi_h^k) dx, \end{aligned}$$

where we wrote $(\psi'_-)^k$ for $\psi'_- \left(n_h^k - \frac{\sigma}{\gamma} \varphi_h^k \right)$. From (27), using the elementary property

$$(29) \quad a(a-b) \geq \frac{1}{2} (a^2 - b^2),$$

we get

$$\begin{aligned} \int_{\Omega} \varphi_h^{k+1} (n_h^{k+1} - n_h^k) dx &\geq -\sigma \int_{\Omega} \nabla \varphi_h^{k+1} \nabla (n_h^{k+1} - n_h^k) dx \\ &\quad + \frac{\gamma}{2} \int_{\Omega} (|\nabla n_h^{k+1}|^2 - |\nabla n_h^k|^2) dx + \int_{\Omega} (\psi'_-)^k (n_h^{k+1} - n_h^k) dx \\ &\geq -\sigma \int_{\Omega} (\nabla \varphi_h^{k+1} \nabla n_h^{k+1} - \nabla \varphi_h^k \nabla n_h^k) dx \\ &\quad - \sigma \int_{\Omega} \nabla (n_h^{k+1} - n_h^k) \nabla (\varphi_h^{k+1} - \varphi_h^k) dx \\ &\quad + \sigma \int_{\Omega} \nabla n_h^{k+1} \nabla (\varphi_h^{k+1} - \varphi_h^k) dx + \frac{\gamma}{2} \int_{\Omega} (|\nabla n_h^{k+1}|^2 - |\nabla n_h^k|^2) dx \\ &\quad + \int_{\Omega} (\psi'_-)^k (n_h^{k+1} - n_h^k) dx. \end{aligned}$$

From (28) and using again the inequality (29), we get

$$\begin{aligned} \sigma \int_{\Omega} \nabla n_h^{k+1} \nabla (\varphi_h^{k+1} - \varphi_h^k) dx &\geq \frac{\sigma^2}{2\gamma} \int_{\Omega} (|\nabla \varphi_h^{k+1}|^2 - |\nabla \varphi_h^k|^2) dx + \frac{\sigma}{2\gamma} \int_{\Omega} (|\varphi_h^{k+1}|^2 - |\varphi_h^k|^2) dx \\ &\quad - \frac{\sigma}{\gamma} \int_{\Omega} (\psi'_-)^k (\varphi_h^{k+1} - \varphi_h^k) dx. \end{aligned}$$

Gathering the last two inequalities, we obtain

$$\begin{aligned} \int_{\Omega} \varphi_h^{k+1} (n_h^{k+1} - n_h^k) dx &\geq -\sigma \int_{\Omega} (\nabla \varphi_h^{k+1} \nabla n_h^{k+1} - \nabla \varphi_h^k \nabla n_h^k) dx \\ &\quad - \sigma \int_{\Omega} \nabla (n_h^{k+1} - n_h^k) \nabla (\varphi_h^{k+1} - \varphi_h^k) dx \\ &\quad + \frac{\sigma^2}{2\gamma} \int_{\Omega} (|\nabla \varphi_h^{k+1}|^2 - |\nabla \varphi_h^k|^2) dx + \frac{\sigma}{2\gamma} \int_{\Omega} (|\varphi_h^{k+1}|^2 - |\varphi_h^k|^2) dx \\ &\quad + \frac{\gamma}{2} \int_{\Omega} (|\nabla n_h^{k+1}|^2 - |\nabla n_h^k|^2) dx + \int_{\Omega} ((\psi_-)^{k+1} - (\psi_-)^k) dx, \end{aligned}$$

where we used the fact that ψ_- is concave and wrote $(\psi_-)^k$ for $\psi_- \left(n_h^k - \frac{\sigma}{\gamma} \varphi_h^k \right)$. Summing up the last inequality with (26) and using the definition of the discrete energy (24) yields

$$\begin{aligned} \int_{\Omega} \left(n_h^{k+1} - n_h^k \right) \left(\varphi_h^{k+1} + \psi'_+(n_h^{k+1}) \right) dx &\geq E_h(n_h^{k+1}, \varphi_h^{k+1}) - E_h(n_h^k, \varphi_h^k) \\ &\quad - \sigma \int_{\Omega} \nabla \left(n_h^{k+1} - n_h^k \right) \nabla \left(\varphi_h^{k+1} - \varphi_h^k \right) dx. \end{aligned}$$

The last inequality, together with the existence result that ensures that $n_h^{k+1}, \varphi_h^{k+1} \in S^h \subset H^1(\Omega)$, terminates the proof. \square

In the following Corollary, we gather all the *a priori* estimates we obtained so far.

Corollary 6. *Let $\{n_h^{k+1}, \varphi_h^{k+1}\}$ be a solution to the scheme (9a), (9b). Then for $k = 0, \dots, N_T - 1$ there exists a constant $C > 0$ independent on $\sigma, h, \Delta t$ such that*

$$(30a) \quad 0 \leq n_h^{k+1} < 1,$$

$$(30b) \quad \left\| n_h^{k+1} \right\|_{L^2(0,T;H^1(\Omega))} + \left\| \varphi_h^{k+1} \right\|_{L^2(0,T;H^1(\Omega))} \leq CT,$$

$$(30c) \quad \Delta t \int_{\Omega} b(n_h^k) \left\| \nabla \left(\varphi_h^{k+1} + \psi'_+(n_h^{k+1}) \right) \right\| dx \leq E_h^0 + N_T C \sigma.$$

4.2. Convergence analysis. In order to study the convergence of the scheme, we follow [5] and define for $k = 0, \dots, N_T - 1$

$$N_h(t, x) := \frac{t - t_k}{\Delta t} n_h^{k+1} + \frac{t_{k+1} - t}{\Delta t} n_h^k, \quad t \in (t_k, t_{k+1}].$$

First we remark that, thanks to (30b), $N_h \in L^2(0, T; H^1(\Omega))$. Moreover simple calculations show that for $t \in (t_k, t_{k+1}]$

$$\frac{\partial N_h}{\partial t} = \frac{n_h^{k+1} - n_h^k}{\Delta t},$$

and

$$N_h - n_h^{k+1} = (t - t_{k+1}) \frac{\partial N_h}{\partial t}, \quad \text{as well as} \quad N_h - n_h^k = (t - t_k) \frac{\partial N_h}{\partial t}.$$

Finally, again using (30b) we recover

$$(31) \quad \left\| N_h - n_h^{k+1} \right\|_{L^2(0,T;L^2(\Omega))}, \left\| N_h - n_h^k \right\|_{L^2(0,T;L^2(\Omega))} \leq (\Delta t)^2 \left\| \frac{\partial N_h}{\partial t} \right\|_{L^2(0,T;L^2(\Omega))} \leq C \Delta t,$$

where $C > 0$ does not depend on h and Δt . We can now state the convergence result.

Theorem 7 (Convergence of discrete solutions). *Let $\{\mathcal{T}^h, \Delta t\}_{h>0}$ be a family of admissible spatio-temporal discretizations. Let $n_h^0 \in K^h$ such that $n_h^0 \rightarrow n_0$ in $H^1(\Omega)$*

as $h \rightarrow 0$. Then there exists a subsequence $\{n_h^{k+1}, \varphi_h^{k+1}\}_{h>0}$ and a pair of functions $\{n, \varphi\} \in (L^2(0, T; H^1(\Omega)))^2$ such that as $h, \Delta t \rightarrow 0$,

$$(32a) \quad N_h, n_h^{k+1}, n_h^k \rightarrow n \quad \text{strongly in } L^2(0, T; L^2(\Omega)),$$

$$(32b) \quad \varphi_h^{k+1} \rightarrow \varphi \quad \text{strongly in } L^2(\Omega),$$

$$(32c) \quad \nabla \varphi_h^{k+1} \rightharpoonup \nabla \varphi \quad \text{weakly in } L^2(\Omega).$$

Moreover, $\{n, \varphi\}$ satisfy the RDCH in the following sense: for all $T > 0$, $\chi \in L^2(0, T; H^1(\Omega))$

$$\begin{aligned} & \int_0^T \left\langle \frac{\partial n}{\partial t}, \chi \right\rangle dt + \int_0^T \int_{\Omega} b(n) \nabla (\varphi + \psi'_+(n)) \nabla \chi \, dx dt = 0, \\ \sigma \int_0^T \int_{\Omega} \nabla \varphi \nabla \chi \, dx dt + \int_0^T \int_{\Omega} \varphi \chi \, dx dt &= \int_0^T \int_{\Omega} \nabla n \nabla \chi \, dx dt + \int_0^T \int_{\Omega} \psi'_- \left(n - \frac{\sigma}{\gamma} \varphi \right) \chi \, dx dt, \end{aligned}$$

and $n(0, \cdot) = n_0(\cdot)$.

Proof. Since the convergence of φ_h^{k+1} follows immediately from the existence result and (30b), we only need to prove strong convergence of n_h^{k+1}, n_h^k . To this end, we use the definition of N_h to rewrite (9a) as

$$\int_{\Omega} \frac{\partial N(t)}{\partial t} \chi dx + \int_{\Omega} b(n_h^k) \nabla (\varphi_h^{k+1} + \psi'_+(n_h^{k+1})) \nabla \chi dx = 0,$$

for all $\chi \in S^h$ and for $t \in (t_k, t_{k+1}]$, $k = 0, \dots, N_T - 1$. Taking $\chi = \pi_h \eta$ with $\eta \in H^1(0, T; H^1(\Omega))$ and integrating in time we get

$$\left| \int_{t_k}^{t_{k+1}} \int_{\Omega} \frac{\partial N_h(t)}{\partial t} \pi^h \eta \, dx dt \right| \leq \int_{t_k}^{t_{k+1}} \int_{\Omega} \left| b(n_h^k) \nabla (\varphi_h^{k+1} + \psi'_+(n_h^{k+1})) \nabla \pi^h \eta \right| \, dx dt.$$

Using first the L^∞ bound on n_h^k (30a) and then the a priori estimate (30c) yields

$$\begin{aligned} & \left| \int_{t_k}^{t_{k+1}} \int_{\Omega} \frac{\partial N_h(t)}{\partial t} \pi^h \eta \, dx dt \right| \\ & \leq \left\| \sqrt{b(n_h^k)} \right\|_{L^\infty((t_k, t_{k+1}) \times \Omega)} \int_{t_k}^{t_{k+1}} \int_{\Omega} \sqrt{b(n_h^k)} \left| \nabla (\varphi_h^{k+1} + \psi'_+(n_h^{k+1})) \nabla \pi^h \eta \right| \, dx dt \\ & \leq \left\| \sqrt{b(n_h^k)} \right\|_{L^\infty((t_k, t_{k+1}) \times \Omega)} (E_h^0 + N_T C \sigma) \left\| \nabla \pi^h \eta \right\|_{L^2((t_k, t_{k+1}) \times \Omega)} \\ & \leq C \left\| \nabla \pi^h \eta \right\|_{L^2((t_k, t_{k+1}) \times \Omega)}, \end{aligned}$$

where $C > 0$ does not depend on $h, \Delta t$. Summing over $k = 0, \dots, N_T - 1$ enables to conclude that

$$\frac{\partial N_h}{\partial t} \in L^2(0, T; (H^1(\Omega))').$$

TABLE 1. Parameters of the test case

	Parameters
γ	0.001
Δt	10^{-4}
δx	1/64
n^0	0.3
n^*	0.6
T	2
σ	10^{-5}

The Lions-Aubin Lemma, together with the fact that $N_h \in L^2(0, T; H^1(\Omega))$ from its definition, implies that there exists $n \in L^2(0, T; L^2(\Omega))$ such that

$$N_h \rightarrow n, \quad \text{strongly in } L^2(0, T; L^2(\Omega)), \quad \frac{\partial N_h}{\partial t} \rightharpoonup \frac{\partial n}{\partial t} \quad \text{weakly in } L^2(0, T; (H^1(\Omega))').$$

Furthermore, from (31) we obtain the strong convergence of both n_h^{k+1} and n_h^k as $\Delta t \rightarrow 0$ and independently on $h > 0$:

$$n_h^{k+1}, n_h^k \rightarrow n, \quad \text{strongly in } L^2(0, T; L^2(\Omega)).$$

From the above convergences and the definition of N_h , we can pass to the limit $\Delta t, h \rightarrow 0$ in the discrete scheme to recover RDCH system. \square

5. NUMERICAL SIMULATIONS

1D Numerical results. The table 1 summarizes the values of the parameters for this test case. The initial condition is taken to a small random noise around the cell density n_0 for each node. The noise is taken to be 5% of a random value between -1 and 1 . Figure 2 shows the evolution in time of the solution n_h . We can clearly observe that the positivity of the solution is ensured at all iterations and especially for the steady state solution. The mass is conserved. The figure 3 represents the evolution of the energy during the simulation. Clearly, the energy decreases through time and tends to stabilize showing that the system encounters a stable or meta-stable state.

2D Numerical results. For the two-dimensional test case, the domain is a square of length $L = 1$. We use an uniform triangular mesh. The initial condition is chosen in the same way as for the one-dimensional test case. The summary of the values of parameters can be found in table 2. Figure 4 shows the evolution of the solution through time. The mass is constant and the figure shows that the energy is monotonically decreasing until it reaches a plateau.

6. CONCLUSIONS

In this work, we described and studied a finite element scheme to solve the relaxed degenerate Cahn-Hilliard equation with single-well logarithmic potential. The spatial relaxation

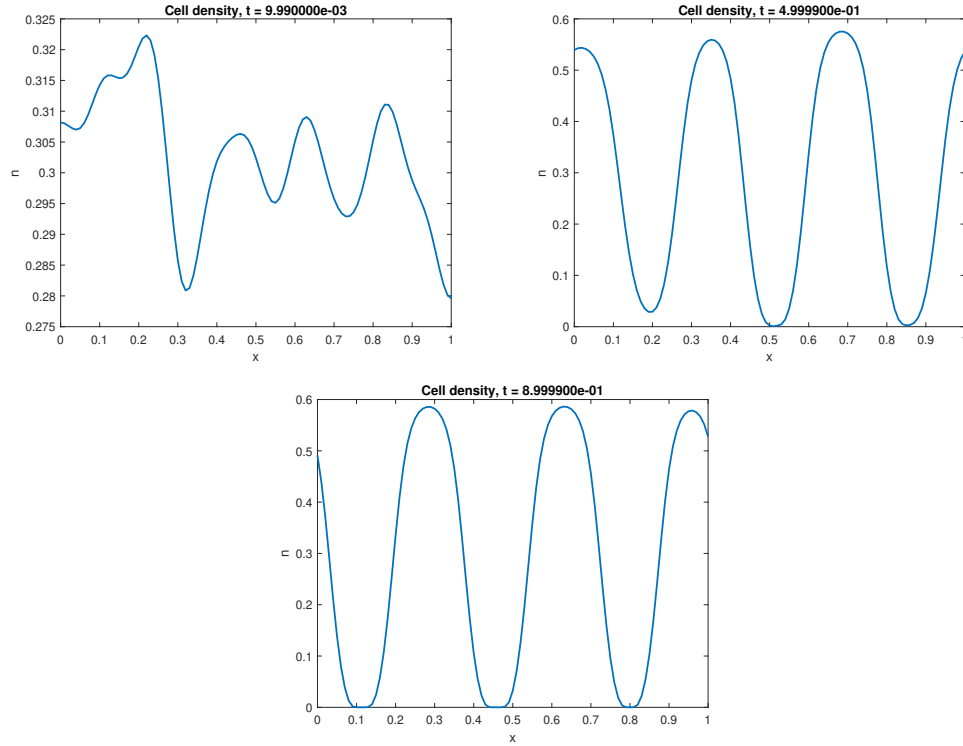
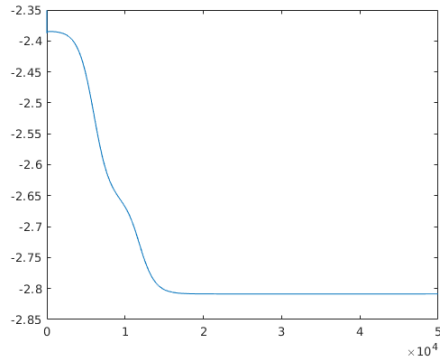
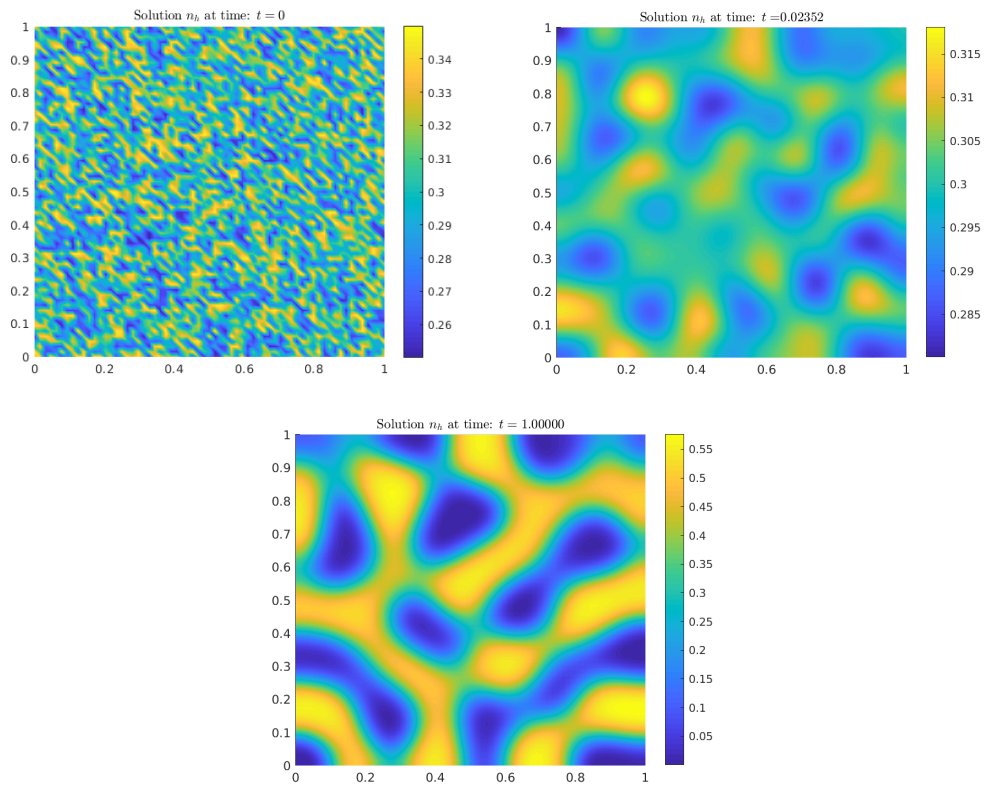
FIGURE 2. Solution n_h at 3 different times.

FIGURE 3. Evolution of discrete energy through time

proposed in [15] enables to overcome the resolution of the original fourth-order equation thanks to a spatial regularisation that can be solve using standard finite element methods.

TABLE 2. Parameters of the test case

	Parameters
γ	0.014^2
Δt	0.1γ
Δx	$1/64$
n^0	0.3
n^*	0.6
T	2
σ	10^{-5}


 FIGURE 4. Solution n_h at 3 different times.

We showed that the scheme preserves the physical properties of the solutions of the continuous model, in particular their nonnegativity. We proved that the scheme is well-posed, energy stable and convergent. We presented two test cases to validate our numerical method in one and two dimensions; the numerical simulations confirm the positivity-preserving and energy decaying properties of our scheme. We point out that thanks to the spatial

relaxation, our numerical scheme can be easily implemented and simulations of the relaxed degenerate Cahn-Hilliard model can be computed efficiently using standard softwares.

APPENDIX A. PROOF OF M-MATRIX PROPERTIES IN THE 1D AND 2D CASES

For both 1 and 2 dimensional cases, the matrix $(\frac{M}{\Delta t} + D)$ is an M-matrix. If the mass matrix is lumped, the all matrix is a Z-matrix due to the fact that the non-diagonal terms of D are negative. Therefore the sum of the lumped mass matrix M and D is a Z-matrix. Furthermore, we can write

$$\frac{M}{\Delta t} + D = cI - B,$$

where I is the identity matrix, c is a constant and B is a matrix with $b_{ij} \geq 0$, $1 \leq i, j \leq N$. Let us choose $c = \max(\frac{M_{ii}}{\Delta t} + D_{ii})$ and consequently the matrix B can be deduced and contains only positive terms. Therefore, we have proved that $(\frac{M}{\Delta t} + D)$ is a M-matrix.

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