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FULLY DISCRETE APPROXIMATION OF A THREE COMPONENT CAHN-HILLIARD MODEL.

FRANCK BOYER* AND SEBASTIAN MINJEAUD†

Abstract. In this paper, we investigate numerical schemes for solving a three component Cahn-Hilliard model. The space discretization is performed by using a Galerkin formulation and the finite element method. For the time discretization, the main difficulty is to write a scheme ensuring, at the discrete level, the decrease of the energy. We study three different schemes and propose existence and convergence theorems. Theoretical results are illustrated by the simulations of a spreading lens between two stratified phases.

Key words. Finite element, Cahn-Hilliard model, Numerical scheme, Energy estimate

AMS subject classifications. 35K55, 65M60, 65M12, 76T30

1. Introduction. Multiphase flows are involved in many industrial applications. For instance, in nuclear safety [11], during a hypothetical major accident in a reactor, the degradation of the core may produce multicomponent flows where interfaces undergo extreme topological changes, e.g. break-up and coalescence. Because of their ability to capture interfaces implicitly, diffuse interface models are attractive for the numerical simulation of such phenomena. They consist in assuming that the interfaces between phases in the system have a small but positive thickness. Each phase i is represented by a smooth function c_i called the order parameter. The evolution of the system is then driven by the gradient of the total free energy, which is a sum of two terms: the bulk free energy term with a "multiple-well" shape and the capillary term depending on the gradients of the order parameters and accounting for the energy of the interfaces, that is the surface tension. For two phase flows, there are many studies in the literature but generalizations of diffuse interface models to any number of components were only recently introduced and studied [1, 2, 3, 4, 7, 8, 9].

In this paper we investigate numerical schemes for solving the three component Cahn-Hilliard model fully derived and studied in [4]. We simply recall its main properties in Section 2. Thanks to the relevant choice of the free energy, one of the key features of this model is its exact coincidence with the diphasic Cahn-Hilliard model when only two phases are present in the mixture. Furthermore, it is able to account for some total spreading situations (see Section 5.1).

The space discretization is performed by using the finite element method. For the time discretization, the main difficulty is to write a scheme ensuring, at the discrete level, the decrease of the energy which is crucial to establish the existence and the convergence of the approximate solution. In some physical situations, the implicit Euler time discretization does not satisfy an energy inequality and the corresponding numerical solvers do not converge. To tackle this issue, semi-implicit schemes are proposed and studied in Section 3.

In Section 4, we state a convergence theorem. This result enables to get a proof

*Université Paul Cézanne, LATP (UMR CNRS 6632), FST Saint-Jérôme, Case Cour A, Avenue escadrille Normandie-Niemen, 13397 Marseille Cedex 20, France (fboyer@latp.univ-mrs.fr).
†Institut de Radioprotection et de Sûreté Nucléaire (IRSN), DPAM/SEMIC/LIMSI, BP-3, 13115 Saint-Paul-lez-Durance, France (sebastian.minjeaud@irsn.fr).

(different from [4]) of the existence of a weak solution of the Cahn-Hilliard model, thanks to numerical schemes. Note that more general boundary conditions are considered since the proof is here available for Dirichlet boundary conditions on the order parameters. Finally, in Section 5, the three schemes are numerically compared on the spreading of a lens between two stratified phases.

2. Ternary Cahn-Hilliard model. We consider the following ternary Cahn-Hilliard model:

$$\begin{cases} \dfrac{\partial c_i}{\partial t} = \nabla \cdot \left(\dfrac{M_0(\mathbf{c})}{\Sigma_i} \nabla \mu_i \right), & \text{for } i = 1,2,3, \\ \mu_i = f_i^F(\mathbf{c}) - \dfrac{3}{4}\varepsilon \Sigma_i \Delta c_i \,, & \text{for } i = 1,2,3, \end{cases} \tag{2.1}$$

on $\mathbb{R}_+ \times \Omega$, where Ω is a regular bounded domain of $\mathbb{R}^d$ with $d = 2$ or 3. The unknowns are the three pairs of order parameters and chemical potentials (c_i, μ_i), $i = 1,2,3$. The function f_i^F is defined by

$$f_i^F(\mathbf{c}) = \frac{4\Sigma_T}{\varepsilon} \sum_{j \neq i} \left(\frac{1}{\Sigma_j} \left(\partial_i F(\mathbf{c}) - \partial_j F(\mathbf{c}) \right) \right),$$

where $\dfrac{3}{\Sigma_T} = \dfrac{1}{\Sigma_1} + \dfrac{1}{\Sigma_2} + \dfrac{1}{\Sigma_3}$. Note that the model (2.1) ensures that, at any time $t \in \mathbb{R}_+$, and for almost every $x \in \Omega$, the vector $\mathbf{c}(t,x) = (c_1(t,x), c_2(t,x), c_3(t,x))$ belongs to the hyperplane $\mathcal{S}$ of $\mathbb{R}^3$ defined by

$$\mathcal{S} = \left\{ (c_1, c_2, c_3) \in \mathbb{R}^3 ; c_1 + c_2 + c_3 = 1 \right\},$$

provided that the initial condition (at time $t = 0$) lies in $\mathcal{S}$ for almost every points of Ω. Hence, one of the pairs of unknowns can be arbitrarily eliminated from the system. The parameter $\varepsilon > 0$ accounts for the interface thickness. The coefficient $M_0(\mathbf{c})$ is a diffusion coefficient called *mobility* which may depend on $\mathbf{c} = (c_1, c_2, c_3)$. We assume that:

$$M_0 \text{ is a Lipschitz continuous bounded function such that } \inf_{\mathbf{c} \in \mathcal{S}} M_0 > 0. \tag{$\mathcal{H}_M$}$$

The triple of constant parameters $\mathbf{\Sigma} = (\Sigma_1, \Sigma_2, \Sigma_3)$ is defined by $\Sigma_i = \sigma_{ij} + \sigma_{ik} - \sigma_{jk}$, for all $i \in \{1,2,3\}$ where σ_{12}, σ_{13} and σ_{23} are the prescribed surface tensions between the different phases. Following [4], the bulk energy F is chosen in the following form:

$$F(\mathbf{c}) = \underbrace{\sigma_{12} c_1^2 c_2^2 + \sigma_{13} c_1^2 c_3^2 + \sigma_{23} c_2^2 c_3^2 + c_1 c_2 c_3 (\Sigma_1 c_1 + \Sigma_2 c_2 + \Sigma_3 c_3)}_{F_0(\mathbf{c})} + \underbrace{3\Lambda c_1^2 c_2^2 c_3^2}_{P(\mathbf{c})}, \tag{2.2}$$

where Λ is a positive constant. It is proved in [4] that the term P is mandatory for the system to be well-posed in total spreading situations. Note that the bulk energy F satisfies the following general assumptions which will be useful in existence and convergence theorems:

$$\begin{aligned} &F \text{ is non negative, of } \mathrm{C}^2 \text{ class and there exist a constant } B > 0 \text{ and a real } p \\ &\text{such that } 2 \leqslant p < +\infty \text{ if } d = 2, \text{ or } 2 \leqslant p \leqslant 6 \text{ if } d = 3, \text{ and, for all } \mathbf{c} \in \mathcal{S}, \\ &|F(\mathbf{c})| \leqslant B(1 + |\mathbf{c}|^p), \; |DF(\mathbf{c})| \leqslant B(1 + |\mathbf{c}|^{p-1}), \; \left|D^2 F(\mathbf{c})\right| \leqslant B(1 + |\mathbf{c}|^{p-2}). \end{aligned} \tag{$\mathcal{H}_F$}$$

This model was fully derived and studied in [4]. The evolution of the order parameters c_i is driven by the minimisation of the following free energy:

$$\mathcal{F}_{\mathbf{\Sigma},\varepsilon}^{\text{triph}}(c_1, c_2, c_3) = \int_\Omega \frac{12}{\varepsilon} F(c_1, c_2, c_3) + \frac{3}{8}\varepsilon \sum_{i=1}^{3} \Sigma_i |\nabla c_i|^2 \, dx.$$

An important feature is that the coefficient Σ_i, whose opposite $S_i = -\Sigma_i$ is well known in the physical literature [10] as *the spreading coefficient* of the phase i, is not assumed to be positive. Therefore, the model (2.1) let us cope with some total spreading situations (Section 5.1). However, as shown in [4], in order to have a well-posed system, we need to assume that the following condition holds:

$$\Sigma_1\Sigma_2 + \Sigma_1\Sigma_3 + \Sigma_2\Sigma_3 > 0. \qquad (\mathcal{H}_{\boldsymbol{\Sigma}})$$

We supplement the system (2.1) with mixed Dirichlet-Neumann boundary conditions for each order parameter c_i and with Neumann boundary conditions for each chemical potential μ_i. That is, for $i = 1, 2, 3$,

$$c_i = c_{iD},\ M_0\nabla\mu_i \cdot \mathbf{n} = 0,\ \text{on } \Gamma_D^c \ \text{ and } \nabla c_i \cdot \mathbf{n} = M_0\nabla\mu_i \cdot \mathbf{n} = 0,\ \text{on } \Gamma_N^c\ , \qquad (2.3)$$

where the boundary Γ of the domain Ω is divided into two distinct parts $\Gamma = \Gamma_D^c \cup \Gamma_N^c$ and $\mathbf{c}_D = (c_{1D}, c_{2D}, c_{3D}) \in \left(\mathrm{H}^{\frac{1}{2}}(\Gamma)\right)^3$ is given s.t. $\mathbf{c}_D(x) \in \mathcal{S}$ for a.e. $x \in \Gamma$.

REMARK 2.1. *The Neumann boundary conditions for μ_i ensure in particular the conservation of the volume of the phase i. The Dirichlet boundary conditions for c_i, less classical, are used to simulate bubble-train flows (when the Cahn-Hilliard model is coupled to the Navier-Stokes equations [4]).*

Finally, we assume that, at the initial time, we have

$$c_i(0,\cdot) = c_i^0, \qquad (2.4)$$

where $\mathbf{c}^0 = (c_1^0, c_2^0, c_3^0) \in \left(\mathrm{H}^1(\Omega)\right)^3$ is given s.t. $\mathbf{c}^0(x) \in \mathcal{S}$ for a.e. $x \in \Omega$.

3. Numerical schemes and energy estimates. For time discretization, we use a semi-implicit discretization with a special care for nonlinear terms. Let $N \in \mathbb{N}^*$ and $t_f \in]0, +\infty[$. The temporal interval $[0, t_f]$ is uniformly discretized with a fixed time step $\Delta t = \dfrac{t_f}{N}$. For $n \in \{0, \dots, N\}$, we define $t_n = n\Delta t$.

For the space discretization, we use a Galerkin approximation and the finite element method. Let $\mathcal{V}_h^c$ and $\mathcal{V}_h^\mu$, $h > 0$, be two sequences of finite element approximation subspaces of $\mathrm{H}^1(\Omega)$. We assume that they contain constants:

$$1 \in \mathcal{V}_h^c \quad \text{and} \quad 1 \in \mathcal{V}_h^\mu, \quad \forall h > 0. \qquad (\mathcal{H}^1_{\mathcal{V}_h})$$

Since order parameters satisfy non-homogeneous Dirichlet boundary conditions on Γ_D^c, we use c_i^0 as a lifting of c_{iD} in $\mathcal{V}^c$, and we assume that functions $c_{ih}^0 \in \mathcal{V}_h^c$ are given for all $i \in \{1, 2, 3\}$, for all $h > 0$ such that

$$\mathbf{c}_h^0(x) \in \mathcal{S},\ \forall h > 0,\ \text{a.e. } x \in \Omega \text{ and } \left|\mathbf{c}_h^0 - \mathbf{c}^0\right|_{(\mathrm{H}^1(\Omega))^3} \underset{h\to 0}{\longrightarrow} 0.$$

These functions c_{ih}^0 can be obtained from c_i^0 by $\mathrm{H}^1(\Omega)$-projection or, as this is the case in practice, by finite element interpolation provided that c_i^0 is smooth enough. Note that the above property is then satisfied thanks to $(\mathcal{H}^1_{\mathcal{V}_h})$. We define the following spaces:

$$\mathcal{V}_{Dh,0}^c = \{\nu_h^c \in \mathcal{V}_h^c; \nu_h^c = 0 \text{ on } \Gamma_D^c\}, \qquad \mathcal{V}_{Dh}^{c_i} = c_{ih}^0 + \mathcal{V}_{Dh,0}^c,$$
$$\mathcal{V}_{Dh,\mathcal{S}}^{\mathbf{c}} = \{\mathbf{c}_h = (c_{1h}, c_{2h}, c_{3h}) \in \mathcal{V}_{Dh}^{c_1} \times \mathcal{V}_{Dh}^{c_2} \times \mathcal{V}_{Dh}^{c_3}; \mathbf{c}_h(x) \in \mathcal{S} \text{ for a.e. } x \in \Omega\}.$$

Required approximation properties can be expressed as follows:

$$\begin{cases} \inf_{\nu_h^\mu \in \mathcal{V}_h^\mu} |\nu^\mu - \nu_h^\mu|_{\mathrm{H}^1(\Omega)} \underset{h\to 0}{\longrightarrow} 0, \ \forall \nu^\mu \in \mathcal{V}^\mu, \\ \inf_{\nu_h^c \in \mathcal{V}_{Dh,0}^c} |\nu^c - \nu_h^c|_{\mathrm{H}^1(\Omega)} \underset{h\to 0}{\longrightarrow} 0, \ \forall \nu^c \in \mathcal{V}_{D,0}^c. \end{cases} \tag{$\mathcal{H}^2_{\mathcal{V}_h}$}$$

We assume that $\mathbf{c}_h^n \in \mathcal{V}_{Dh,\mathcal{S}}^{\mathbf{c}}$ is given and the scheme is then written as follows:

PROBLEM 3.1. *Find* $(\mathbf{c}_h^{n+1}, \boldsymbol{\mu}_h^{n+1}) \in \mathcal{V}_{Dh,\mathcal{S}}^{\mathbf{c}} \times (\mathcal{V}_h^\mu)^3$ *such that* $\forall \nu_h^c \in \mathcal{V}_{Dh,0}^c$, $\forall \nu_h^\mu \in \mathcal{V}_h^\mu$, *we have, for* $i = 1, 2, 3$,

$$\begin{cases} \displaystyle\int_\Omega \frac{c_{ih}^{n+1} - c_{ih}^n}{\Delta t} \nu_h^\mu \, dx = -\int_\Omega \frac{M_0(\mathbf{c}_h^{n+1})}{\Sigma_i} \nabla \mu_{ih}^{n+1} \cdot \nabla \nu_h^\mu \, dx, \\ \displaystyle\int_\Omega \mu_{ih}^{n+1} \nu_h^c \, dx = \int_\Omega D_i^F(\mathbf{c}_h^n, \mathbf{c}_h^{n+1}) \nu_h^c \, dx + \int_\Omega \frac{3}{4} \Sigma_i \varepsilon \nabla c_{ih}^{n+\beta} \cdot \nabla \nu_h^c \, dx, \end{cases} \tag{3.1}$$

where $D_i^F(\mathbf{a}, \mathbf{b}) = \dfrac{4\Sigma_T}{\varepsilon} \displaystyle\sum_{j\neq i} \left(\frac{1}{\Sigma_j} \left(d_i^F(\mathbf{a}, \mathbf{b}) - d_j^F(\mathbf{a}, \mathbf{b}) \right) \right), \ \forall (\mathbf{a}, \mathbf{b}) \in \mathcal{S}^2.$

The functions d_i^F represent a semi-implicit discretization of $\partial_{c_i} F$. In order to ensure consistency we assume that

$$d_i^F(\mathbf{c}, \mathbf{c}) = \frac{\partial F}{\partial c_i}(\mathbf{c}), \quad \forall \mathbf{c} \in \mathcal{S}. \tag{$\mathcal{H}^1_{\mathbf{d}^F}$}$$

Since we have a natural splitting of F: $F = F_0 + P$ in (2.2), we choose a discretization of the form $d_i^F = d_i^{F_0} + d_i^P$ where $d_i^{F_0}$ and d_i^P are discretizations of $\partial_{c_i} F_0$ and $\partial_{c_i} P$ respectively. The different choices of $d_i^{F_0}$ and d_i^P are given and discussed in Sections 3.2 to 3.5.

REMARK 3.2. *Assumption* $(\mathcal{H}^1_{\mathcal{V}_h})$ *allows to take* $\nu_h^\mu \equiv 1$ *in the first equation of* (3.1). *This yields the phase volume conservation property at the discrete level.*

3.1. Energy estimate. In this section, we give the energy estimate, at the discrete level, which is obtained from (3.1) by using $\nu_h^\mu = \mu_{ih}^{n+1}$ and $\nu_h^c = \dfrac{c_{ih}^{n+1} - c_{ih}^n}{\Delta t}$ as test functions.

PROPOSITION 3.3 (General energy estimate). *Let* $\mathbf{c}_h^n \in \mathcal{V}_{Dh,\mathcal{S}}^{\mathbf{c}}$. *We assume that there exists a solution* $(\mathbf{c}_h^{n+1}, \boldsymbol{\mu}_h^{n+1})$ *of Problem* (3.1). *Then, the following equality holds:*

$$\begin{aligned} \mathcal{F}^{triph}_{\boldsymbol{\Sigma},\varepsilon}(\mathbf{c}_h^{n+1}) - \mathcal{F}^{triph}_{\boldsymbol{\Sigma},\varepsilon}(\mathbf{c}_h^n) + \Delta t \sum_{i=1}^3 \int_\Omega \frac{M_0(\mathbf{c}_h^{n+1})}{\Sigma_i} \left| \nabla \mu_{ih}^{n+1} \right|^2 dx \\ + \frac{3}{8} \varepsilon \int_\Omega \sum_{i=1}^3 \Sigma_i \left| \nabla c_{ih}^{n+1} - \nabla c_{ih}^n \right|^2 dx = \\ \frac{12}{\varepsilon} \int_\Omega \left[F(\mathbf{c}_h^{n+1}) - F(\mathbf{c}_h^n) - \mathbf{d}^F(\mathbf{c}_h^n, \mathbf{c}_h^{n+1}) \cdot \left(\mathbf{c}_h^{n+1} - \mathbf{c}_h^n \right) \right] dx \end{aligned} \tag{3.2}$$

where $\mathbf{d}^F(\cdot,\cdot)$ *is the vector* $(d_i^F(\cdot,\cdot))_{i=1,2,3}$.

The three first terms on the left hand side are exactly the discrete counterpart of the terms involved in the continuous energy estimate. The last term on the left hand side is a term of numerical diffusion which is very useful in the proof of the convergence theorem to obtain a suitable bound for the discrete time derivative of $\mathbf{c}$. Notice that the condition $(\mathcal{H}_{\mathbf{\Sigma}})$ implies that the last two terms on the left hand side are non negative [4, Prop. 2.1]. The right hand side explicitly depends on the choice of the discretization $\mathbf{d}^F(\cdot,\cdot)$ of the nonlinear terms. To obtain a useable energy estimate and then prove existence and convergence results, we have to control this term.

3.2. Implicit scheme. The implicit discretization corresponds to $\mathbf{d}^{F_0}(\mathbf{a},\mathbf{b}) = \nabla F_0(\mathbf{b})$. We do not have $F_0(\mathbf{b}) - F_0(\mathbf{a}) - \mathbf{d}^{F_0}(\mathbf{a},\mathbf{b})\cdot(\mathbf{b}-\mathbf{a}) \leqslant 0$, since this inequality would mean that F_0 is convex. Nevertheless, in the case where all Σ_i are positive, the following proposition gives a bound independent of $\mathbf{c}^{n+1}$ and μ^{n+1}. Note that this bound holds for all $\Delta t > 0$ and will be useful to prove the existence of discrete solutions.

PROPOSITION 3.4. *Let* $\mathbf{c}_h^n \in \mathcal{V}^{\mathbf{c}}_{Dh,\mathcal{S}}$. *We assume that* $\Sigma_i > 0,\ \forall i \in \{1,2,3\}$ *and that there exists a solution* $(\mathbf{c}_h^{n+1}, \boldsymbol{\mu}_h^{n+1})$ *of Problem 3.1. Then, there exists a positive constant* $K_1^{\mathbf{\Sigma},\mathbf{c}_h^n}$ *depending only on* $\mathbf{\Sigma}$ *and* $\mathbf{c}_h^n$ *such that:*

$$\int_\Omega \left[F_0(\mathbf{c}_h^{n+1}) - F_0(\mathbf{c}_h^n) - \nabla F_0(\mathbf{c}_h^{n+1})\cdot\left(\mathbf{c}_h^{n+1}-\mathbf{c}_h^n\right)\right] dx \leqslant K_1^{\mathbf{\Sigma},\mathbf{c}_h^n}.$$

Unfortunately, this bound is not sufficient to prove convergence results. In the following proposition, we give an energy estimate obtained by controlling the right hand side of (3.2) by a term of the form $\int_\Omega \sum_{i=1}^3 \Sigma_i \left|c_{ih}^{n+1} - c_{ih}^n\right|^2 dx$. Then, this term can be bounded for Δt small enough and under the following assumption:

$$\mathcal{V}_h^c \subset \mathcal{V}_h^\mu. \qquad (\mathcal{H}^3_{\mathcal{V}_h})$$

PROPOSITION 3.5. *Let* $\mathbf{c}_h^n \in \mathcal{V}^{\mathbf{c}}_{Dh,\mathcal{S}}$. *We assume that* $\Sigma_i > 0,\ \forall i \in \{1,2,3\}$, *that the conditions* $(\mathcal{H}_M)$ *and* $(\mathcal{H}^3_{\mathcal{V}_h})$ *hold and that there exists a solution* $(\mathbf{c}_h^{n+1}, \boldsymbol{\mu}_h^{n+1})$ *of Problem* (3.1). *Then, as soon as* $\Delta t \leqslant \dfrac{\varepsilon^3}{24|M_0|_\infty}$, *we get, for* $\Lambda = 0$,

$$\mathcal{F}^{triph}_{\mathbf{\Sigma},\varepsilon}(\mathbf{c}_h^{n+1}) - \mathcal{F}^{triph}_{\mathbf{\Sigma},\varepsilon}(\mathbf{c}_h^n) + \frac{\Delta t}{2}\sum_{i=1}^3 \int_\Omega \frac{M_0(\mathbf{c}_h^{n+1})}{\Sigma_i}\left|\nabla \mu_{ih}^{n+1}\right|^2 dx + \frac{3}{16}\varepsilon \int_\Omega \sum_{i=1}^3 \Sigma_i \left|\nabla c_{ih}^{n+1} - \nabla c_{ih}^n\right|^2 dx \leqslant 0.$$

3.3. Convex-Concave scheme. The polynomial approximation of the diphasic Cahn-Hilliard potential $f(c) = c^2(1-c)^2$ can naturally be decomposed into two parts, a convex one and a concave one, as follows: $f(x) = \underbrace{\left(x-\frac{1}{2}\right)^4}_{f^+(x)} + \underbrace{\frac{1}{16}\left(1-2(2x-1)^2\right)}_{f^-(x)}$.

Since $F_0(\mathbf{c}) = \sum_{i=1}^3 \Sigma_i f(c_i)$, for all $\mathbf{c} \in \mathcal{S}$, the above decomposition of f leads to a natural decomposition of F_0. However, this is a convex-concave decomposition only in the case where all Σ_i are positive. This leads to the choice

$$\mathbf{d}^{F_0}(\mathbf{a},\mathbf{b}) = \nabla F_0^+(\mathbf{b}) + \nabla F_0^-(\mathbf{a}),$$

with $F_0^+(\mathbf{c}) = \displaystyle\sum_{i=1}^3 \frac{\Sigma_i}{2} f^+(c_i)$ and $F_0^-(\mathbf{c}) = \displaystyle\sum_{i=1}^3 \frac{\Sigma_i}{2} f^-(c_i)$. We get $F(\mathbf{b}) - F(\mathbf{a}) - \mathbf{d}^{F_0}(\mathbf{a},\mathbf{b})\cdot(\mathbf{b}-\mathbf{a}) \leqslant 0$, for all Δt but only when all Σ_i are positive.

3.4. Semi implicit scheme. The convex-concave discretization and the implicit discretization presented in the previous subsections do not ensure an energy estimate when one of the Σ_i is negative, that is in the case of total spreading (Section 5.1). Hence, we propose a semi-implicit discretization built in order to obtain, for all $(\mathbf{a},\mathbf{b}) \in \mathcal{S}^2$, $F_0(\mathbf{b}) - F_0(\mathbf{a}) - \sum_{i=1}^3 d_i^{F_0}(\mathbf{a},\mathbf{b})(b_i - a_i) = 0$.

For $i = 1,2,3$, we define $\delta_i = b_i - a_i$ and we try to write $F_0(\mathbf{b}) - F_0(\mathbf{a})$ as a sum of terms containing δ_1, δ_2 or δ_3 in factor. Since $F_0(c_1,c_2,c_3) = \sigma_{12}c_1^2c_2^2 + \sigma_{13}c_1^2c_3^2 + \sigma_{23}c_2^2c_3^2 + c_1c_2c_3\,(\Sigma_1c_1 + \Sigma_2c_2 + \Sigma_3c_3)$, it is sufficient to separately consider terms of the form $b_i^2b_jb_k - a_i^2a_ja_k$ with $(i,j,k) \in \{1,2,3\}^3$. We use the identities $a_i^2 = b_i^2 - (a_i+b_i)\delta_i$ and $a_j = b_j - \delta_j$ in order to introduce δ_i, δ_j and δ_k in the formula, we obtain:

$$b_i^2b_jb_k - a_i^2a_ja_k = (a_i+b_i)a_ja_k\delta_i + b_i^2a_k\delta_j + b_i^2b_j\delta_k.$$

Hence, we define the following consistent approximation of the non linear terms for each $i \in \{1,2,3\}$:

$$\begin{aligned} d_i^{F_0}(\mathbf{a},\mathbf{b}) =& \frac{\Sigma_i}{4}\,[b_i + a_i]\left[(b_j+b_k)^2 + (a_j+a_k)^2\right] \\ &+ \frac{\Sigma_j}{4}(b_j^2 + a_j^2)(b_i + b_k + a_i + a_k) + \frac{\Sigma_k}{4}(b_k^2 + a_k^2)(b_i + b_j + a_i + a_j). \end{aligned}$$

Thanks to Proposition 3.3, we can conclude that an energy estimate holds for all Δt and even if one of the Σ_i is negative, provided that condition $(\mathcal{H}_{\boldsymbol{\Sigma}})$ holds.

3.5. Discretization of P. We do not have a natural convex-concave decomposition for this term. Hence, we use the same kind of calculation as in the previous subsection. We define

$$d_i^P(\mathbf{a},\mathbf{b}) = 2\Lambda b_i\left[a_j^2a_k^2 + \frac{1}{2}b_j^2a_k^2 + \frac{1}{2}a_j^2b_k^2 + b_j^2b_k^2\right].$$

Thus, we get a consistent approximation satisfying for any $(\mathbf{a},\mathbf{b}) \in \mathcal{S}^2$,

$$P(\mathbf{b}) - P(\mathbf{a}) - d_1^P(\mathbf{a},\mathbf{b})\delta_1 - d_2^P(\mathbf{a},\mathbf{b})\delta_2 - d_3^P(\mathbf{a},\mathbf{b})\delta_3 \leqslant 0.$$

4. Existence and convergence. This section is devoted to presenting existence and convergence theorems for the discrete solution.

4.1. Existence. Now we state general assumptions on the discretization of non linear terms $\mathbf{d}^F : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$:

$\mathbf{d}^F$ is of C^1class and there exist a constant $B \geqslant 0$ and a real p such that

$$\begin{aligned} &2 \leq p < +\infty \text{ if } d = 2, \text{ or } p = 6 \text{ if } d = 3, \text{ and for all } i \in \{1,2,3\}, \\ &\left|d_i^F(\mathbf{a},\mathbf{b})\right| \leqslant B\left(1 + |\mathbf{a}|^{p-1} + |\mathbf{b}|^{p-1}\right), \quad \forall(\mathbf{a},\mathbf{b}) \in \mathcal{S}^2, \\ &\left|D\left(d_i^F(\mathbf{a},\cdot)\right)(\mathbf{b})\right| \leqslant B\left(1 + |\mathbf{a}|^{p-2} + |\mathbf{b}|^{p-2}\right), \quad \forall(\mathbf{a},\mathbf{b}) \in \mathcal{S}^2. \end{aligned} \qquad (\mathcal{H}^2_{\mathbf{d}^F})$$

Note that these conditions are satisfied by all the schemes presented in the previous section. The existence of the solution of discrete Problem (3.1) is based on the topological degree lemma using the discrete energy estimate (3.2).

THEOREM 4.1 (Existence of a discrete solution). *Let* $\mathbf{c}_h^n \in \mathcal{V}_{Dh}^{\mathbf{c}}$ *be given. Assume that properties* $(\mathcal{H}_{\mathbf{\Sigma}})$, $(\mathcal{H}_M)$, $(\mathcal{H}_F)$, $(\mathcal{H}^2_{\mathbf{d}^F})$, $(\mathcal{H}^1_{\mathcal{V}_h})$ *hold and that there exists a constant* $K_1^{\mathbf{\Sigma},\mathbf{c}_h^n}$ *(depending possibly on* $\mathbf{c}_h^n$*) such that, for all* $\mathbf{c}_h \in \mathcal{V}_{Dh}^{\mathbf{c}}$,

$$\int_\Omega \left[F(\mathbf{c}_h) - F(\mathbf{c}_h^n) - \mathbf{d}^F(\mathbf{c}_h^n, \mathbf{c}_h)\cdot(\mathbf{c}_h - \mathbf{c}_h^n)\right] dx \leqslant K_1^{\mathbf{\Sigma},\mathbf{c}_h^n}. \tag{4.1}$$

Then, there exists at least one solution $(\mathbf{c}_h^{n+1}, \boldsymbol{\mu}_h^{n+1}) \in \mathcal{V}_{Dh}^{\mathbf{c}} \times (\mathcal{V}_h^\mu)^3$ *of Problem* (3.1).

4.2. Convergence. For each $N \in \mathbb{N}$, we introduce piecewise linear functions defined on $[0, t_f]$, as follows:

$$c_{ih}^N(t,\cdot) = \frac{t_{n+1}-t}{\Delta t} c_{ih}^n(\cdot) + \frac{t-t_n}{\Delta t} c_{ih}^{n+1}(\cdot), \quad \mu_{ih}^N(t,\cdot) = \mu_{ih}^{n+1}(\cdot), \quad \text{if } t \in]t_n, t_{n+1}[.$$

For the proof of the convergence Theorem, we need to assume that the finite element approximation spaces satisfy:

There exists a positive constant C independent of h such that :

$$\forall \nu^\mu \in \mathcal{V}^\mu, \ \left|\Pi_0^{\mathcal{V}_h^\mu}(\nu^\mu)\right|_{\mathrm{H}^1(\Omega)} \leqslant C|\nu^\mu|_{\mathrm{H}^1(\Omega)}, \tag{$\mathcal{H}^4_{\mathcal{V}_h}$}$$

where $\Pi_0^{\mathcal{V}_h^\mu}$ denote the $\mathrm{L}^2(\Omega)$-projection on $\mathcal{V}_h^\mu$.

This property is satisfied e.g. by Lagrange finite element approximation spaces obtained from quasi-uniform meshes.

THEOREM 4.2. *Assume that properties* $(\mathcal{H}_{\mathbf{\Sigma}})$, $(\mathcal{H}_M)$, $(\mathcal{H}_F)$, $(\mathcal{H}^2_{\mathbf{d}^F})$, $(\mathcal{H}^1_{\mathcal{V}_h})$, $(\mathcal{H}^4_{\mathcal{V}_h})$, (4.1) *hold and that there exists a constant* $C > 0$ *such that, for all* $n \in \mathbb{N}$,

$$\mathcal{F}^{triph}_{\mathbf{\Sigma},\varepsilon}(\mathbf{c}_h^{n+1}) - \mathcal{F}^{triph}_{\mathbf{\Sigma},\varepsilon}(\mathbf{c}_h^n) + C\Bigg[\Delta t \sum_{i=1}^3 \int_\Omega \frac{M_0(\mathbf{c}_h^{n+1})}{\Sigma_i}\left|\nabla \mu_{ih}^{n+1}\right|^2 dx + \frac{3}{8}\varepsilon \int_\Omega \sum_{i=1}^3 \Sigma_i \left|\nabla c_{ih}^{n+1} - \nabla c_{ih}^n\right|^2 dx\Bigg] \leqslant 0. \tag{4.2}$$

Then, there exists $h_0 > 0$ *and positive constants* K_1^ε, K_2^ε, *independent of* Δt *and* h *such that, for all* $h \leqslant h_0$, *we have*

$$\sup_{n\leqslant N} |\mathbf{c}_h^n|_{(\mathrm{H}^1(\Omega))^3} + \sum_{n=0}^{N-1} \Delta t \sum_{i=1}^3 \left|\mu_{ih}^{n+1}\right|^2_{\mathrm{H}^1(\Omega)} \leqslant K_1^\varepsilon,$$

$$\Delta t \sum_{n=0}^{N-1} \Delta t \sum_{i=1}^3 \left|\frac{c_{ih}^{n+1} - c_{ih}^n}{\Delta t}\right|^2_{\mathrm{H}^1(\Omega)} + \sum_{n=0}^{N-1} \Delta t \sum_{i=1}^3 \left|\frac{c_{ih}^{n+1} - c_{ih}^n}{\Delta t}\right|^2_{(\mathrm{H}^1(\Omega))'} \leqslant K_2^\varepsilon.$$

The bounds given in theorem 4.2 enable to prove the following convergence result by using compactness properties.

THEOREM 4.3. *Assume that conditions* $(\mathcal{H}_{\mathbf{\Sigma}})$, $(\mathcal{H}_M)$, $(\mathcal{H}_F)$, $(\mathcal{H}^1_{\mathbf{d}^F})$, $(\mathcal{H}^2_{\mathbf{d}^F})$, $(\mathcal{H}^1_{\mathcal{V}_h})$, $(\mathcal{H}^2_{\mathcal{V}_h})$, $(\mathcal{H}^4_{\mathcal{V}_h})$, (4.1) *and* (4.2) *hold. Consider Problem* (2.1) *together with the initial condition* (2.4) *and boundary conditions* (2.3). *Then, there exists a weak solution* $(\mathbf{c}, \boldsymbol{\mu})$ *on* $[0, t_f[$ *such that*

$$\mathbf{c} \in \mathrm{L}^\infty(0, t_f; (\mathrm{H}^1(\Omega))^3) \cap \mathrm{C}^0([0, t_f[; (\mathrm{L}^q(\Omega))^3), \ \textit{for all } q < 6,$$
$$\boldsymbol{\mu} \in \mathrm{L}^2(0, t_f; (\mathrm{H}^1(\Omega))^3),$$
$$\mathbf{c}(t,x) \in \mathcal{S}, \ \textit{for } \text{a.e. } (t,x) \in [0, t_f[\times\Omega.$$

Furthermore, for all sequences $(h_K)_{K\in\mathbb{N}^*}$ *such that* $h_K \xrightarrow[K\to+\infty]{} 0$*, the sequences* $(\mathbf{c}^N_{h_K})_{(N,K)\in(\mathbb{N}^*)^2}$ *and* $(\boldsymbol{\mu}^N_{h_K})_{(N,K)\in(\mathbb{N}^*)^2}$*, defined by* (3.1)*, satisfy, up to a subsequence, the following convergence properties as* $\min(N,K) \longrightarrow +\infty$ *:*

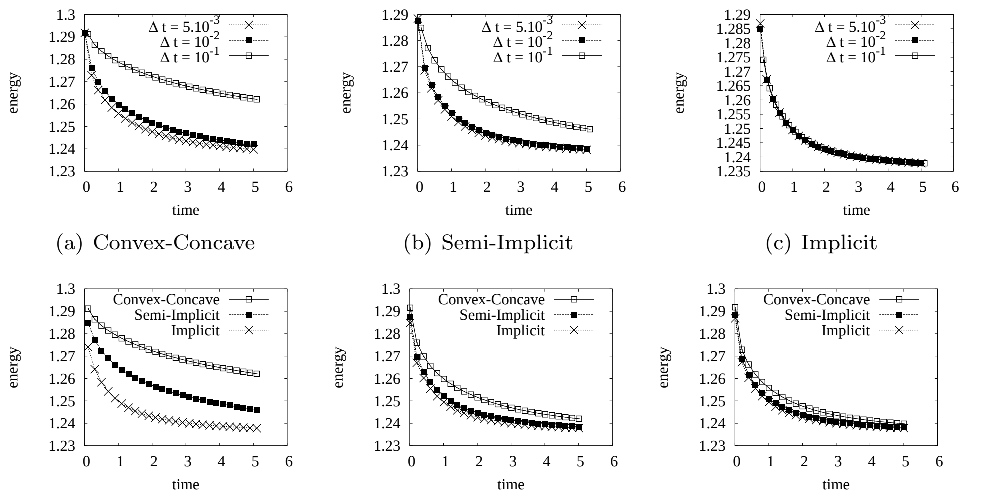
$$\mathbf{c}^N_{h_K} \to \mathbf{c} \quad \text{in } \mathrm{C}^0(0,t_f,(\mathrm{L}^q)^3) \text{ strong }, \quad \text{for all } q<6,$$
$$\boldsymbol{\mu}^N_{h_K} \rightharpoonup \boldsymbol{\mu} \quad \text{in } \mathrm{L}^2(0,t_f,(\mathrm{H}^1)^3) \text{ weak }.$$

REMARK 4.4. *Under an additional assumption on the Hessian of the Cahn-Hilliard potential F, it is shown in [4] that the model* (2.1) *has a unique weak solution. In this case, we can conclude that the convergence in the above theorem holds for the entire sequences* $(\mathbf{c}^N_{h_K}, \boldsymbol{\mu}^N_{h_K})$.

REMARK 4.5. *Assumptions* (4.1) *and* (4.2) *are always satisfied for the semi-implicit scheme provided that* $(\mathcal{H}_{\boldsymbol{\Sigma}})$ *holds. Furthermore, these assumptions hold for the convex-concave and implicit schemes when all the* Σ_i*,* $i=1,2,3$*, are positive.*

5. Numerical experiments. In this section, we illustrate the properties of the three schemes with the spreading of a liquid lens between two stratified phases in two dimensions. We use the following values for the parameters: $\Omega = [-0.4, 0.4] \times [-0.3, 0.3]$, $t_f = 5$, $\varepsilon = 10^{-2}$ and a constant mobility $M_0 = 10^{-4}$. The initial data $\mathbf{c}^0$ is given by $c_1^0(\boldsymbol{x}) = \frac{1}{2}[1+\tanh(\frac{2}{\varepsilon}\min(|\boldsymbol{x}|, x_2))]$, $c_2^0(\boldsymbol{x}) = \frac{1}{2}[1-\tanh(\frac{2}{\varepsilon}\max(-|\boldsymbol{x}|, x_2))]$ and $c_3^0(\boldsymbol{x}) = 1 - c_1(\boldsymbol{x}) - c_2(\boldsymbol{x})$ where $\boldsymbol{x} = (x_1, x_2) \in \Omega$. This corresponds to an initial spherical captive bubble of phase 3 between the two stratified phases 1 and 2. We use the same space discretization for all the simulations: $\mathbb{Q}_1$ Lagrange finite element on square local adaptive refined meshes [5] (four cells in the interfaces).

5.1. Partial spreading. In this subsection, we take $\sigma_{12} = 1$, $\sigma_{13} = 0.8$ and $\sigma_{23} = 0.4$. In this case, all the Σ_i, $i = 1, 2, 3$, are positive. We take $\Lambda = 0$, so that the Cahn-Hilliard potential is $F = F_0$.



(a) Convex-Concave (b) Semi-Implicit (c) Implicit

(d) $\Delta t = 10^{-1}$ (e) $\Delta t = 10^{-2}$ (f) $\Delta t = 5.10^{-3}$

FIG. 5.1. *Time evolution of energy in a partial spreading situation*

In Figure 5.1, we show the discrete energy $\mathcal{F}^{\text{triph}}_{\boldsymbol{\Sigma},\varepsilon}(\mathbf{c}^n_h)$ as a function of time $t_n \in [0, t_f]$. For each of the three schemes, we performed three simulations with

$\Delta t = 10^{-1}$, 10^{-2} and 5.10^{-3}. The nine results are presented in two ways: Figures 5.1(a), 5.1(b) and 5.1(c) compare the decrease of the discrete energy for the different time steps, using the same scheme, whereas Figures 5.1(d), 5.1(e) and 5.1(f) show a comparison between the three schemes, using the same time step. Since no analytic solution of the system (2.1) is available, the exact profile of the energy decrease is not known. However, in each of the three figures 5.1(a), 5.1(b) and 5.1(c), the sequence of curves tends to a limit shape when the time step decreases. For the impicit scheme (Fig. 5.1(c)), the decrease of the energy is the same for the three considered time steps. This is the reason why we consider the discrete solution obtained with the implicit scheme as a reference solution. Thus, Figures 5.1(d), 5.1(e) and 5.1(f) show that semi-implicit scheme gives significantly sharper result than the convex-concave one.

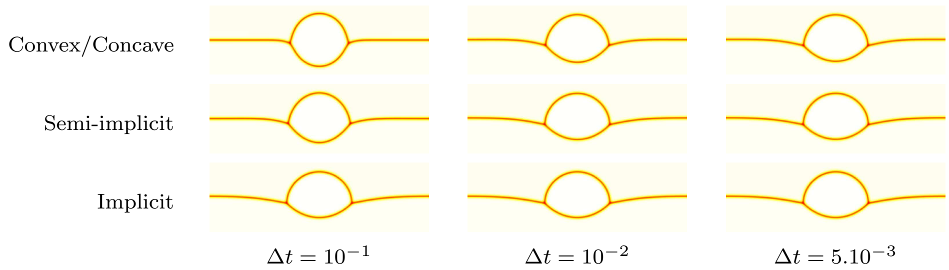


FIG. 5.2. *Interfaces position at time $t_f = 5$, partial spreading situation*

Figure 5.2 shows the influence of the truncation error on the bubble form at the simulation final time t_f. With the implicit scheme, the same form is obtained for the three time steps. For large time step, the convex-concave scheme do not give the bubble form which is expected. This phenomenon is reduced by the use of the semi-implicit scheme.

5.2. Total spreading. In this subsection, we take $\sigma_{12} = 1$, $\sigma_{13} = 1$ and $\sigma_{23} = 3$. In this case, Σ_1 is negative but the condition $(\mathcal{H}_{\boldsymbol{\Sigma}})$ holds. It corresponds to the case of the extraction of the bubble (Figure 5.4): at the steady state the bubble is entirely within one of the other phases. We take $\Lambda = 7$. In Figures 5.3 and 5.4, we present

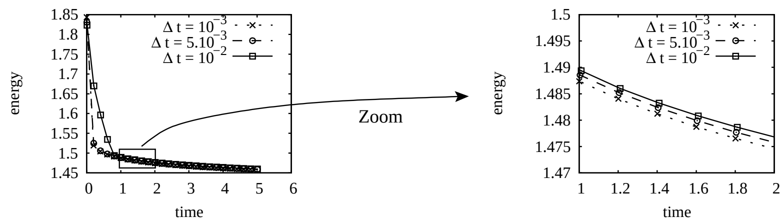
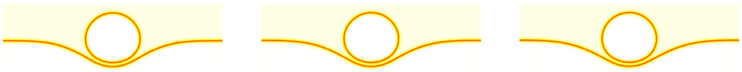


FIG. 5.3. *Time evolution of energy for the semi-implicit scheme in a total spreading situation*

the results obtained thanks to the semi-implicit scheme for $\Delta t = 10^{-2}$, 5.10^{-3} and 10^{-3}. For theses time steps, the Newton iteration at the first time step does not converge if we use the convex-concave or the implicit scheme. Implicit scheme enables to perform simulations only for $\Delta t \leqslant 10^{-4}$. For the semi-implicit scheme, such time step are not required since the limit profile of the energy decrease is achieved from $\Delta t = 5.10^{-3}$ (Figure 5.3) and the final bubble shapes (Figure 5.4) are similar for the

Semi-implicit



$\Delta t = 10^{-2}$ $\Delta t = 5.10^{-3}$ $\Delta t = 10^{-3}$

FIG. 5.4. *Interfaces position at time $t_f = 5$, total spreading situation*

three considered time step. Hence, the semi-implicit scheme can be used to perform simulations with $\Delta t = 5.10^{-3}$ avoiding the further computational cost due to smaller time steps.

6. Conclusion. We propose here a full discretization of the ternary Cahn-Hilliard model taken from [4]. Three time schemes are compared. At the theoretical level, for the implicit scheme and the convex-concave one, we are able to show the convergence of the discrete solution only in the case of partial spreading (all $\Sigma_i > 0$). The semi-implicit scheme enables to show the convergence even in the case of total spreading (provided that the condition $(\mathcal{H}_{\boldsymbol{\Sigma}})$ holds). In practice, for partial spreading situation, the implicit scheme is the more accurate and the semi-implicit one enables to reduce the truncation error compared with the convex-concave one. For total spreading situations, we observe in some numerical computations that the implicit scheme can be ill-posed if the time step is not small enough whereas we can prove that the semi-implicit scheme is well-posed. Using the implicit scheme requires smaller time step, thus leading to a further computational cost. The complete proofs of all the results in this paper and further numerical experiments are presented in [6].

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