A CONVERGENT CONVEX SPLITTING SCHEME FOR A NONLOCAL CAHN-HILLIARD-OONO TYPE EQUATION WITH A TRANSPORT TERM

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ABSTRACT. We devise a first-order in time convex splitting scheme for a nonlocal Cahn—Hilliard—Oono type equation with a transport term and subject to homogeneous Neumann boundary conditions. The presence of the transport term is not a minor modification, since, for instance, we lose the unconditional unique solvability and stability. However, we prove the stability of our scheme when the time step is sufficiently small. Furthermore, we prove the consistency of this scheme and the convergence to the exact solution. Finally, we give some numerical simulations which confirm our theoretical results and demonstrate the performance of our scheme not only for phase separation, but also for crystal nucleation, for several choices of the interaction kernel.

1. Introduction

The authors in [8] proposed the following Ginzburg-Landau type free energy:

(1.1)
$$\mathcal{E}_{CH}(\varphi) = \int_{\Omega} \left(\frac{\varepsilon^2}{2} |\nabla \varphi|^2 + F(\varphi) \right) dx$$

in order to describe the phase separation of a binary mixture, and, more precisely, the so-called spinodal decomposition. Here, $\Omega \subset \mathbb{R}^N$, $N \leq 3$, is the domain occupied by the mixture components A and B, with respective mass fractions φ_A and φ_B , and the order parameter is defined by $\varphi = \frac{\varphi_A - \varphi_B}{\varphi_A + \varphi_B}$. Furthermore, ε is the diffuse interface thickness and $\frac{\varepsilon^2}{2} |\nabla \varphi|^2$ is a surface tension term which ensures a smooth transition between the two pure states. Finally, F is a double-well potential which favors phase separation.

Once the free energy is defined, the phase separation can be described as a gradient flow (see, for instance, [25]),

$$\frac{\partial \varphi}{\partial t} = \Delta \mu, \qquad \mu := \frac{\partial \mathcal{E}_{CH}}{\partial \varphi} = f(\varphi) - \varepsilon^2 \Delta \varphi,$$

where μ is the chemical potential and $f(\varphi) = F'(\varphi)$.

This corresponds to the well-known Cahn-Hilliard equation which plays an important role in Materials Science. In particular, phase separation phenomena play an essential

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²⁰¹⁰ Mathematics Subject Classification, 34K28, 35R09, 65M12, 65M60, 82C26,

Key words and phrases. Cahn-Hilliard-Oono equation, transport term, nonlocal term, convex splitting scheme, stability, convergence, numerical simulations.

role in the mechanical properties of an alloy (for instance, its strength). We refer the reader to, e.g., [7], [8], [14], [20], [41], [42], [44], [45], [50], [51], and [52] for more details.

It is worth recalling that Cahn-Hilliard type equations are also relevant in other contexts, namely, the ones in which phase separation and coarsening/clustering processes can be observed or come into play. We can mention, for instance, population dynamics [16], bacterial films [40], wound healing and tumor growth [15], [23], [24], [39], [48], and [49], thin films [54] and [57], image processing and inpainting [6], [9], [10], [11], [12], [13], [19], and [56], and even the rings of Saturn [58] and the clustering of mussels [43].

However, the purely phenomenological derivation of the Cahn-Hilliard equation is somehow unsatisfactory from a physical point of view. This led G. Giacomin and J.L. Lebowitz to consider the problem of phase separation from a microscopic point of view, using a statistical mechanics approach (see [28] and also [29] and [30]). Performing the hydrodynamic limit, they deduced a continuum model which is a nonlocal version of the Cahn-Hilliard equation. This model is characterized by the following Helmholtz free energy functional

(1.2)
$$\mathcal{E}_{nCH1}(\varphi) = -\frac{1}{2} \int_{\Omega} \int_{\Omega} J(x - y) \varphi(x) \varphi(y) dx dy + \int_{\Omega} F(\varphi(x)) dx,$$

where $J: \mathbb{R}^N \to \mathbb{R}$ is a smooth convolution kernel such that J(x) = J(-x). Furthermore, the convex potential F here is defined as follows:

$$F(s) = s \ln(s) + (1 - s) \ln(1 - s), \quad 0 < s < 1.$$

This potential can be approximated by a convex polynomial. In that case, the nonlocal version of the Cahn–Hilliard system reads

(1.3)
$$\frac{\partial \varphi}{\partial t} = \Delta \mu, \qquad \mu := \frac{\partial \mathcal{E}_{nCH1}}{\partial \varphi} = f(\varphi) - J \star \varphi.$$

We refer the reader to the recent paper by [26] (see addition in the references) for a rather complete theoretical picture.

On the other hand, P.W. Bates and J. Han in [4] and [5] proposed the following nonlocal version of the Cahn-Hilliard energy

(1.4)
$$\mathcal{E}_{nCH2}(\varphi) = \frac{1}{4} \int_{\Omega} \int_{\Omega} J(x - y) (\varphi(x) - \varphi(y))^2 dx dy + \int_{\Omega} F(\varphi(x)) dx,$$

where F is the double-well potential as in the classical Cahn-Hilliard model. On account of (1.2) and (1.4), we introduce the following energy, for $\alpha \ge 0$,

(1.5)
$$\mathcal{E}_{nCH}(\varphi) = \frac{1}{4} \int_{\Omega} \int_{\Omega} J(x - y) (\varphi(x) - \varphi(y))^2 dx dy + \frac{\alpha - 1}{2} \int_{\Omega} \int_{\Omega} J(x - y) (\varphi(x))^2 dx dy + \int_{\Omega} F(\varphi(x)) dx,$$

where, for $\alpha = 0$, we recover the Giacomin–Lebowitz model (1.2) while for $\alpha = 1$, we recover the Bates–Han model (1.4). Therefore, we consider

(1.6)
$$\frac{\partial \varphi}{\partial t} = \Delta \mu, \qquad \mu := \frac{\partial \mathcal{E}_{nCH}}{\partial \varphi} = \alpha (J \star 1) \varphi + f(\varphi) - J \star \varphi$$

which can be rewritten as the following convective nonlocal and nonlinear diffusion equation:

(1.7)
$$\frac{\partial \varphi}{\partial t} = \nabla \cdot ((f'(\varphi) + \alpha(J \star 1))\nabla \varphi) + \alpha \nabla \cdot ((\nabla J \star 1)\varphi) - \nabla \cdot (\nabla J \star \varphi).$$

The term $[f'(\varphi) + \alpha J \star 1]$ is referred to as the diffusive mobility, or just the diffusivity. We assume that (1.6) is strictly non-degenerate,

(1.8)
$$f'(\varphi) + \alpha(J \star 1)(x) \geqslant \beta > 0, \quad \text{a.a. } x \in \Omega, \ \alpha \in \mathbb{R}^+.$$

Note that, when $\alpha = 0$, we do not need assumption (1.8) owing to the fact that F is already strictly convex in that case.

A further example of a nonlocal Cahn-Hilliard equation is obtained by considering the following Ohta-Kawasaki free energy

(1.9)
$$\mathcal{E}_{CHO}(\varphi) = \frac{\varepsilon^2}{2} \int_{\Omega} |\nabla \varphi|^2 dx + \int_{\Omega} F(\varphi) dx + \frac{\sigma}{2} \int_{\Omega} \int_{\Omega} G(x - y) (\varphi(x) - \langle \varphi \rangle) (\varphi(y) - \langle \varphi \rangle) dx dy,$$

where G describes the long-range interactions and $\sigma > 0$. In particular, in Oono's model (see [53], cf. also [59]), G is the Green function associated with the Laplace operator (up to a multiplicative constant). If $\langle \varphi \rangle$ is equal to the spatial average of φ , that is,

$$\langle \varphi \rangle = \frac{1}{meas(\Omega)} \int_{\Omega} \varphi dx,$$

and no-flux boundary conditions are considered, the gradient flow for this energy can be derived exactly as for the Cahn-Hilliard equation, namely,

$$\frac{\partial \varphi}{\partial t} = \Delta \frac{\partial \mathcal{E}_{CHO}}{\partial \varphi},$$

which is equivalent to

$$\frac{\partial \varphi}{\partial t} + \sigma(\varphi - m) = \Delta \mu, \qquad \mu = -\varepsilon^2 \Delta \varphi + f(\varphi).$$

In that case, $m = \langle \varphi \rangle$ so the mass is still conserved. However, more generally, m can be a constant which is not necessarily equal to the spatial average of the initial datum. This is the so-called off-critical case and the total mass is conserved only asymptotically. Indeed, in that case we have, for all $t \in [0, T]$,

$$\langle \varphi \rangle = m + e^{-\sigma t} (\langle \varphi_0 \rangle - m).$$

This equation is known as the Cahn-Hilliard-Oono equation and was introduced to model long-range (nonlocal) interactions; actually, this equation was also proposed in order to simplify numerical simulations (see [53]). Short-range interactions tend to homogenize

the system, whereas long-range ones forbid the formation of too large structures; the competition between these two effects translates into the formation of a micro-separated state (also called super-crystal) with a spatially modulated order parameter, defining structures with a uniform size (see [59] for more details and references). Note that the long-range interactions are repulsive when $\varphi(x)$ and $\varphi(y)$ have opposite signs and thus favor the formation of interfaces (see [59] and the references therein). For theoretical results see [31], [47] and the references therein (see also [2] for numerical results in the conserved case).

In this article, on account of the previous considerations, we consider a Cahn-Hilliard-Oono type equation which accounts for both the nonlocal effects. More precisely we want to analyse numerically the following initial and boundary value problem:

(1.10)
$$\begin{cases} \frac{\partial \varphi}{\partial t} + \nabla \cdot (u\varphi) + \sigma(\varphi - m) = \Delta \mu + g, & \text{in } \Omega \times (0, T), \\ \mu = \alpha(J \star 1)\varphi - J \star \varphi + f(\varphi), & \text{in } \Omega \times (0, T), \\ \frac{\partial \mu}{\partial n} = 0, & \text{on } \partial \Omega \times (0, T), \\ \varphi(0) = \varphi_0, & \text{in } \Omega. \end{cases}$$

More precisely, here we shall analyze the case $\alpha = 1$ while the case $\alpha = 0$ will be studied elsewhere. Therefore our initial and boundary value problem can be written as follows

(1.11)
$$\begin{cases} \frac{\partial \varphi}{\partial t} + \nabla \cdot (u\varphi) + \sigma(\langle \varphi \rangle - m) = \Delta \mu + g, & \text{in } \Omega \times (0, T), \\ \mu = (J \star 1)\varphi - J \star \varphi + f(\varphi) + \sigma G \star (\varphi - \langle \varphi \rangle), & \text{in } \Omega \times (0, T), \\ \frac{\partial \mu}{\partial n} = 0, & \text{on } \partial \Omega \times (0, T), \\ \varphi(0) = \varphi_0, & \text{in } \Omega, \end{cases}$$

where G is the Green function defined in (1.9). This equation is the fully nonlocal version of the Cahn-Hilliard-Oono equation with a transport term which accounts for a possible flow of the mixture at a certain given velocity field u and an external source g. Furthermore, m is a real constant, that is the off-critical case is included. This equation was studied in [17] (see also its references). In particular, well-posedness and the existence of the global attractor were established. Furthermore, well-posedness results for (1.10) with singular potential and a degenerate mobility were obtained in [46].

As far as the classical nonlocal Cahn-Hilliard equation is concerned (i.e. u = 0, g = 0 and $\sigma = 0$), very few results dedicated to numerical simulations, or numerical methods, are available. The authors in [1] consider an implicit-explicit time stepping framework for a nonlocal system modeling turbulence, where, as in the present article, the nonlocal term is treated explicitly. Furthermore, the finite element approximation (in space) of nonlocal peridynamic equations with various boundary conditions is addressed in [62] (cf. [18] for a review). In addition, a finite difference method for the nonlocal Allen-Cahn equation with non-periodic boundary conditions is applied and analyzed in [3]. The work

in [36] uses a spectral-Galerkin method to solve a nonlocal Allen-Cahn equation, but with a stochastic noise term and an equation modeling heat flow. For other articles dealing with approximating solutions to the nonlocal Cahn-Hilliard equation, see [1], [27], [38], and [55]. Finally, the authors in [33] and [34] study the nonlocal Cahn-Hilliard equation with periodic boundary conditions and finite difference discretizations in space. Recently, stronger convergence results of convex splitting schemes for the periodic nonlocal Allen-Cahn and Cahn-Hilliard equations have been obtained in [35].

Here we study the finite element discretization in space for homogenous Neumann boundary conditions. In that case, contrary to periodic boundary conditions, we lose the symmetry property on the convolution kernel, i.e., the convolution product between the interaction kernel and a constant is not a constant.

Our main aim is to propose a numerical approach for the continuous problem (1.10) with a stable finite element scheme. We use the convex splitting method proposed by Eyre in [21] and [22] for gradient flow-derived equations which results in an unconditionally gradient stable time discretization scheme. In particular, the scheme is stable for any arbitrarily large time step. The idea consists in dividing the energy functional into two parts, a convex one and a concave one. Then, the convex part is treated implicitly, while the concave one is treated explicitly. Unfortunately, in our scheme, we lose the unconditionally gradient stable time discretization, due of the presence of the transport term. Using the a priori stability, we then prove the time convergence of our scheme to the exact solution.

We are also able, based on the structure of our implicit-explicit method and owing to the fact that we can separate the nonlinear and nonlocal terms, to implement an efficient nonlinear solver (see Section 4).

It should be noted here that the numerical computations of the nonlocal terms are particularly heavy: computing the nonlocal terms at every iteration thus becomes very difficult when the mesh discretization is small. To overcome this, we consider, in the numerical simulations, a periodic domain Ω (e.g., Ω has a rectangular form in \mathbb{R}^2) and we use the DFFT (Discrete Fast Fourier Transformation) function to compute the nonlocal terms.

In particular, we give numerical simulations which confirm our theoretical results and demonstrate the efficiency of our scheme.

2. Preliminaries

2.1. **Notation.** We denote by $((\cdot, \cdot))$ the usual L^2 -scalar product, with associated norm $\|\cdot\|$. We further set $\|\cdot\|_* = \|(-\Delta)^{-\frac{1}{2}}\cdot\|$, where $(-\Delta)^{-1}$ denotes the inverse minus Laplace operator associated with Neumann boundary conditions and acting on functions with null spatial average. More generally, $\|\cdot\|_X$ denotes the norm of the real Banach space X.

We further denote by $\langle v \rangle$ the spatial average of a function $u \in L^1(\Omega)$,

$$\langle v \rangle = \frac{1}{meas(\Omega)} \langle v, 1 \rangle_{(H^1(\Omega))^*, H^1(\Omega)}.$$

Therefore, the norm

$$\left(\|v - \langle v \rangle\|_*^2 + \langle v \rangle^2\right)^{\frac{1}{2}}$$

is equivalent to the usual norm of $(H^1(\Omega))^*$.

- 2.2. **Assumptions.** We make the following assumptions:
- (A1) $\Omega \subset \mathbb{R}^N$, $N \leq 3$, is a bounded domain with a smooth boundary.
- (A2) $J: \mathbb{R}^N \to \mathbb{R}$ satisfies $J = J_1 J_2$, where J_1 , J_2 are nonnegative functions in $\mathcal{W}^{1,1}(\mathbb{R}^N)$.
- (A3) J_1 and J_2 are even, i.e., $J_i(-x) = J_i(x), \ \forall x \in \mathbb{R}^N, \ i = 1, 2.$
- (A4) $f'(\varphi) + (J \star 1)(x) \geqslant \beta > 0$, a.a. $x \in \Omega$.
- (A5) $F(s) = \frac{1}{4}s^4 + \frac{\gamma_1 \gamma_2}{2}s^2$, where γ_i , i = 1, 2, are nonnegative constants.
- (A6) $G: \mathbb{R}^N \to \mathbb{R}$ is the Green function (cf. (1.9)).
- (A7) σ is a nonnegative constant.
- (A8) m is a given constant.
- (A9) $u \in (L^{\infty}(\Omega) \cap H_0^1(\Omega))^N$.
- (A10) $g \in (H^1(\Omega))^*$.

We now state the existence and uniqueness of a weak solution (see [17]).

Proposition 2.1. Let $\varphi_0 \in L^2(\Omega)$ be such that $F(\varphi_0) \in L^1(\Omega)$ and assume that (A1)-(A10) are satisfied. Then, for every T > 0, there exists a unique weak solution φ to problem (1.10) on [0,T] such that

$$\varphi \in L^{\infty}(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)).$$

Remark 2.2. In the sequel for some results, we will require a higher regularity of the solution. To achieve that, the initial datum should be more regular as well as the interaction kernel J. For details the reader is referred to [4] where the existence of a classical solution is established (see also [26] for the singular potential case). The presence of an additional linear reaction term does not affect the regularity results.

2.3. Convex energy splitting. We consider the following nonlocal energy:

(2.1)
$$\mathcal{E}(\varphi) = \frac{1}{4} \int_{\Omega} \int_{\Omega} J(x - y) ((\varphi(x) - \varphi(y))^{2} dx dy + \int_{\Omega} F(\varphi) dx + \frac{\sigma}{2} \int_{\Omega} \int_{\Omega} G(x - y) (\varphi(x) - \langle \varphi \rangle) (\varphi(y) - \langle \varphi \rangle) dx dy.$$

For $\sigma = 0$ in (2.1), we obtain energy (1.5) which can be related to the (local) Ginzburg–Landau energy (1.1). This relationship between the local and nonlocal energies can formally be obtained by using a Taylor expansion. In particular, noting that $(\varphi(x) - \varphi(y)) \approx (x - y) \cdot \nabla \varphi(x)$, we find, for $J_2 = 0$ $(J = J_1)$,

$$\frac{1}{4} \int_{\Omega} \int_{\Omega} J(x-y)((\varphi(x)-\varphi(y))^2 dx dy \approx \frac{1}{4} \int_{\Omega} \int_{\Omega} J(x-y)|x-y|^2 |\nabla \varphi|^2 dx dy$$

$$= \frac{\varepsilon^2}{2} \int_{\Omega} |\nabla \varphi|^2 dx,$$

for a suitable choice of J. Furthermore, the energy (1.5) can also be related to the phase field crystal (PFC) energy (see, e.g. [32] and references therein)

(2.2)
$$\mathcal{E}_{PFC}(\varphi) = \int_{\Omega} \left[\frac{1}{2} (\Delta \varphi)^2 - |\nabla \varphi|^2 + \frac{1}{4} \varphi^4 + \frac{1 - \varepsilon}{2} \varphi^2 \right] dx.$$

To obtain this relationship, we use once more the Taylor expansion. In particular, since

$$(\varphi(x) - \varphi(y)) \approx (x - y) \cdot \nabla \varphi(x) + \frac{|x - y|^2}{2} \Delta \varphi,$$

we get

$$\frac{1}{4} \int_{\Omega} \int_{\Omega} J(x-y)((\varphi(x)-\varphi(y))^{2} dx dy$$

$$= \frac{1}{4} \int_{\Omega} \int_{\Omega} J_{1}(x-y)((\varphi(x)-\varphi(y))^{2} dx dy - \frac{1}{4} \int_{\Omega} \int_{\Omega} J_{2}(x-y)((\varphi(x)-\varphi(y))^{2} dx dy$$

$$\approx \frac{1}{4} \int_{\Omega} \int_{\Omega} J_{1}(x-y) \Big((x-y) \cdot \nabla \varphi(x) + \frac{|x-y|^{2}}{2} \Delta \varphi\Big)^{2} dx dy$$

$$-\frac{1}{4} \int_{\Omega} \int_{\Omega} J_{2}(x-y) \Big((x-y) \cdot \nabla \varphi(x)\Big)^{2} dx dy$$

$$= \frac{1}{2} \int_{\Omega} (\Delta \varphi)^{2} - |\nabla \varphi|^{2} dx,$$

for suitable choices of J_1 and J_2 and for $\gamma_1 = 1$ and $\gamma_2 = \varepsilon$. Thus we recover energy (2.2). From assumptions (A3) and (A6), we can rewrite (2.1) in the following form:

(2.3)
$$\mathcal{E}(\varphi) = \frac{1}{2}(((J \star 1)\varphi, \varphi)) + ((F(\varphi), 1)) - \frac{1}{2}((J \star \varphi, \varphi)) + \frac{\sigma}{2}((G \star (\varphi - \langle \varphi \rangle), (\varphi - \langle \varphi \rangle))).$$

We further have, also owing to assumptions (A3) and (A6),

$$\begin{split} \frac{1}{4} \int_{\Omega} \int_{\Omega} J(x-y) (\varphi(x)-\varphi(y))^2 dx dy + \frac{\sigma}{2} \int_{\Omega} \int_{\Omega} G(x-y) (\varphi(x)-\langle \varphi \rangle) (\varphi(y)-\langle \varphi \rangle) dx dy \\ &= \frac{1}{2} \int_{\Omega} \int_{\Omega} J_1(x-y) (\varphi(x))^2 dx dy - \frac{1}{2} \int_{\Omega} \int_{\Omega} J_1(x-y) \varphi(x) \varphi(y) dx dy \\ &- \frac{1}{4} \int_{\Omega} \int_{\Omega} J_2(x-y) (\varphi(x)-\varphi(y))^2 dx dy - \frac{\sigma}{4} \int_{\Omega} \int_{\Omega} G(x-y) (\varphi(x)-\varphi(y))^2 dx dy \\ &+ \frac{\sigma}{2} \int_{\Omega} \int_{\Omega} G(x-y) (\varphi(x)-\langle \varphi \rangle)^2 dx dy = -\frac{1}{4} \int_{\Omega} \int_{\Omega} J_1(x-y) (\varphi(x)+\varphi(y))^2 dx dy \\ &- \frac{1}{4} \int_{\Omega} \int_{\Omega} J_2(x-y) (\varphi(x)-\varphi(y))^2 dx dy + \int_{\Omega} \int_{\Omega} J_1(x-y) (\varphi(x))^2 dx dy \\ &- \frac{\sigma}{4} \int_{\Omega} \int_{\Omega} G(x-y) (\varphi(x)-\varphi(y))^2 dx dy + \frac{\sigma}{2} \int_{\Omega} \int_{\Omega} G(x-y) (\varphi(x)-\langle \varphi \rangle)^2 dx dy \end{split}$$

$$= -\frac{1}{4} \int_{\Omega} \int_{\Omega} \left[J_1(x-y)(\varphi(x) + \varphi(y))^2 + (J_2(x-y) + \sigma G(x-y))(\varphi(x) - \varphi(y))^2 \right] dxdy$$
$$+ \int_{\Omega} \int_{\Omega} J_1(x-y)(\varphi(x))^2 dxdy + \frac{\sigma}{2} \int_{\Omega} \int_{\Omega} G(x-y)(\varphi(x) - \langle \varphi \rangle)^2 dxdy.$$

Consequently, the convex splitting of \mathcal{E} is given by

$$\mathcal{E}(\varphi) = \mathcal{E}_1(\varphi) - \mathcal{E}_2(\varphi)$$
, where

(2.4)
$$\mathcal{E}_{1}(\varphi) = \int_{\Omega} \int_{\Omega} J_{1}(x-y)(\varphi(x))^{2} dx dy + \frac{\sigma}{2} \int_{\Omega} \int_{\Omega} G(x-y)(\varphi(x) - \langle \varphi \rangle)^{2} dx dy + \frac{c_{1}}{2} \int_{\Omega} (\varphi(x))^{2} dx$$

and

(2.5)
$$\mathcal{E}_{2}(\varphi) = \frac{1}{4} \int_{\Omega} \int_{\Omega} \left[J_{1}(x-y)(\varphi(x) + \varphi(y))^{2} + (J_{2}(x-y) + \sigma G(x-y))(\varphi(x) - \varphi(y))^{2} \right] dx dy + \frac{c_{1}}{2} \int_{\Omega} (\varphi(x))^{2} dx - \int_{\Omega} F(\varphi(x)) dx.$$

Remark 2.3. If c_1 is large enough, it is easy to show that \mathcal{E}_1 and \mathcal{E}_2 are convex (for more details, see [63]).

3. Numerical scheme: definitions and properties

As far as the Euler time discretization for this problem is concerned, the time step $\delta t > 0$ is fixed. The resulting time-stepping scheme reads

$$\frac{\varphi^{n+1} - \varphi^n}{\delta t} = \Delta \mu^{n+1}, \qquad \mu^{n+1} := \frac{\partial \mathcal{E}_1}{\partial \varphi}(\varphi^{n+1}) - \frac{\partial \mathcal{E}_2}{\partial \varphi}(\varphi^n).$$

This translates into a numerical scheme of the form $((1.11)_1-(1.11)_2)$

$$\frac{1}{\delta t}(\varphi^{n+1} - \varphi^n) = \Delta \mu^{n+1},$$

$$\mu^{n+1} = 2(J_1 \star 1)\varphi^{n+1} + c_1(\varphi^{n+1} - \varphi^n) + f(\varphi^n)$$

$$-(J_1 \star 1 + J_2 \star 1)\varphi^n + \sigma(G \star 1)(\varphi^{n+1} - \varphi^n) + \sigma G \star (\varphi^n - \langle \varphi^n \rangle) - J \star \varphi^n.$$

where $f(\varphi^n) = F'(\varphi^n)$. Using the properties of the Green function G when the problem is endowed with no-flux boundary conditions, the scheme can be rewritten as follows

$$\frac{1}{\delta t}(\varphi^{n+1} - \varphi^n) + \sigma(\varphi^n - \langle \varphi^n \rangle) = \Delta \mu^{n+1},$$

$$\mu^{n+1} = 2(J_1 \star 1)\varphi^{n+1} + c_1(\varphi^{n+1} - \varphi^n) + f(\varphi^n) - (J_1 \star 1 + J_2 \star 1)\varphi^n + \sigma(G \star 1)(\varphi^{n+1} - \varphi^n) - J \star \varphi^n.$$

More generally, we replace $\langle \varphi \rangle$ by a real constant m which is not necessarily equal to the spatial average of the initial datum since we are interested to take the off-critical case into account. So we have the following numerical scheme:

$$\frac{1}{\delta t}(\varphi^{n+1} - \varphi^n) + \sigma(\varphi^n - m) = \Delta \mu^{n+1},$$

$$\mu^{n+1} = 2(J_1 \star 1)\varphi^{n+1} + c_1(\varphi^{n+1} - \varphi^n) + f(\varphi^n)$$

$$-(J_1 \star 1 + J_2 \star 1)\varphi^n + \sigma(G \star 1)(\varphi^{n+1} - \varphi^n) - J \star \varphi^n.$$

where we have used that

$$-\Delta G(x,y) = \delta(x-y),$$

and δ is the Dirac mass at 0.

Finally, we add a transport term which models a possible flow of the mixture at a certain given velocity field u, that is, the scheme reads

(3.1)
$$\frac{1}{\delta t}(\varphi^{n+1} - \varphi^n) + \sigma(\varphi^n - m) + \nabla \cdot (u\varphi^{n+1}) = \Delta \mu^{n+1} + g,$$

(3.2)
$$\mu^{n+1} = 2(J_1 \star 1)\varphi^{n+1} + c_1(\varphi^{n+1} - \varphi^n) + f(\varphi^n) - (J_1 \star 1 + J_2 \star 1)\varphi^n + \sigma(G \star 1)(\varphi^{n+1} - \varphi^n) - J \star \varphi^n.$$

for a given external source q.

3.1. Consistency of the scheme. Let $\varphi_n = \varphi(x, n\delta t)$ be the exact solution of (1.10) at time $n\delta t$, where φ is the exact solution. Then we have the following.

Proposition 3.1. Let $\varphi(x,0) \in H^3(\Omega)$ be an initial datum for (1.10) which satisfies the compatibility condition $\frac{\partial \mu}{\partial \nu} = 0$ a.e. on $\partial \Omega$. We assume that $\|\frac{\partial^2 \varphi}{\partial t^2}(\cdot)\|$ and $\|\frac{\partial \varphi}{\partial t}(\cdot)\|_{H^1(\Omega)}$ are continuous with respect to time. Then, the numerical scheme (3.1)–(3.2) is consistent with the continuous equation (1.10) and is of order one in time. This yields that the local truncation error of the scheme, defined as (see [56] for instance):

(3.3)
$$\tau_n(\delta t) = \frac{1}{\delta t} (\varphi_{n+1} - \varphi_n) - c_1 \Delta(\varphi_{n+1} - \varphi_n) - 2\Delta((J_1 \star 1)\varphi_{n+1}) \\ - \sigma \Delta((G \star 1)(\varphi_{n+1} - \varphi_n)) - \Delta(f(\varphi_n)) + \sigma(\varphi_n - m) \\ + \Delta((J_1 \star 1 + J_2 \star 1)\varphi_n) + \Delta(J \star \varphi_n) + \nabla \cdot (u\varphi_{n+1}) - g,$$

satisfies

$$\|\tau_n\|_{(H^1(\Omega))^*} = O(\delta t), \quad as \ \delta t \to 0.$$

Furthermore, the global truncation error of the scheme satisfies

$$\tau(\delta t) = \max_{n} \|\tau_n\|_{(H^1(\Omega))^*} = O(\delta t), \quad as \ \delta t \to 0.$$

Proof. First, observe (from (1.10), $\alpha = 1$) that

$$-\frac{\partial \varphi}{\partial t}(n\delta t) + 2\Delta((J_1 \star 1)\varphi_n) - \nabla \cdot (u\varphi_n)$$

$$= \sigma(\varphi_n - m) - \Delta((J \star 1)\varphi_n) + \Delta(J \star \varphi_n) - \Delta f(\varphi_n) + 2\Delta((J_1 \star 1)\varphi_n) - g$$

$$= \sigma(\varphi_n - m) + \Delta(J \star \varphi_n) + \Delta((J_1 \star 1 + J_2 \star 1)\varphi_n) - \Delta f(\varphi_n) - g.$$

Therefore, the local truncation error $\tau_n(\delta t)$ is given by

(3.4)
$$\tau_n(\delta t) = \frac{1}{\delta t} (\varphi_{n+1} - \varphi_n) - c_1 \Delta (\varphi_{n+1} - \varphi_n) - 2\Delta ((J_1 \star 1)(\varphi_{n+1} - \varphi_n)) - \sigma \Delta ((G \star 1)(\varphi_{n+1} - \varphi_n)) + \nabla \cdot (u(\varphi_{n+1} - \varphi_n)) - \frac{\partial \varphi}{\partial t} (n\delta t).$$

Integrating (3.4) over Ω , we obtain

$$\langle \tau_n(\delta t) \rangle = \left\langle \frac{1}{\delta t} (\varphi_{n+1} - \varphi_n) - \frac{\partial \varphi}{\partial t} (n \delta t) \right\rangle$$

and by using standard Taylor expansion arguments and the boundedness of $\langle \frac{\partial^2 \varphi}{\partial t^2}(\cdot) \rangle$, it is easy to show that

(3.5)
$$\langle \tau_n(\delta t) \rangle = O(\delta t).$$

On the other hand, we can rewrite the local truncation error $\tau_n(\delta t)$ as follows:

$$\tau_n = \tau_n^1(\delta t) + \tau_n^2(\delta t), \quad \text{where}$$

$$\tau_n^1(\delta t) = \frac{1}{\delta t}(\varphi_{n+1} - \varphi_n) - \frac{\partial \varphi}{\partial t}(n\delta t)$$

and

$$\tau_n^2(\delta t) = -2\Delta((J_1 \star 1)(\varphi_{n+1} - \varphi_n)) + \nabla \cdot (u(\varphi_{n+1} - \varphi_n)) - c_1\Delta(\varphi_{n+1} - \varphi_n) - \sigma\Delta((G \star 1)(\varphi_{n+1} - \varphi_n)).$$

By using standard Taylor expansion arguments and the boundedness of $\|\frac{\partial^2 \varphi}{\partial t^2}(\cdot)\|$, it is easy to show that

$$\|\tau_n^1\| = O(\delta t).$$

Owing to the last equality, (3.5), and the continuous embedding from $(H^1(\Omega))^*$ to $L^2(\Omega)$, we then have

$$\|\tau_n^1\|_{(H^1(\Omega))^*} = O(\delta t).$$

Moreover, writing

$$\varphi_{n+1} = \varphi_n + \delta t \frac{\partial \varphi}{\partial t}(t^*), \quad t^* \in (n\delta t, (n+1)\delta t),$$

we have

$$\tau_n^2 = -\delta t \left[\Delta \left(2(J_1 \star 1) \frac{\partial \varphi}{\partial t}(t^*) \right) + \sigma \Delta \left((G \star 1) \frac{\partial \varphi}{\partial t}(t^*) \right) \right]$$
$$+ \delta t \nabla \cdot \left(u \frac{\partial \varphi}{\partial t}(t^*) \right) - c_1 \delta t \Delta \frac{\partial \varphi}{\partial t}(t^*)$$

and

$$(-\Delta)^{-\frac{1}{2}}\tau_n^2 = -\delta t(-\Delta)^{\frac{1}{2}} \left[2(J_1 \star 1) \frac{\partial \varphi}{\partial t}(t^*) + \sigma(G \star 1) \frac{\partial \varphi}{\partial t}(t^*) \right] -\delta t \left(u \frac{\partial \varphi}{\partial t}(t^*) \right) - c_1 \delta t (-\Delta)^{\frac{1}{2}} \frac{\partial \varphi}{\partial t}(t^*).$$

Thus, we get

$$\|\tau_n^2\|_* \leqslant c \,\delta t \Big[\|\nabla \big((J_1 \star 1) \frac{\partial \varphi}{\partial t}(t^*) \big) \| + \|\nabla \big((G \star 1) \frac{\partial \varphi}{\partial t}(t^*) \big) \|$$
$$+ \|u \frac{\partial \varphi}{\partial t}(t^*) \| + c_1 \|\nabla \frac{\partial \varphi}{\partial t}(t^*) \| \Big].$$

Hence we have

$$\|\tau_n^2(\delta t)\|_* \leqslant c \,\delta t \Big(\|\frac{\partial \varphi}{\partial t}(t^*)\|^2 + \|\nabla \frac{\partial \varphi}{\partial t}(t^*)\|^2 + \|\frac{\partial \varphi}{\partial t}(t^*)\|_{H^1(\Omega)}^2 \Big),$$

which yields, owing to (3.5),

$$\|\tau_n^2(\delta t)\|_{(H^1(\Omega))^*} = O(\delta t), \text{ as } \delta t \to 0,$$

and

$$\tau = \max_{n} \|\tau_n\|_{(H^1(\Omega))^*} = O(\delta t), \quad \text{as } \delta t \to 0.$$

3.2. Solvability and stability of the scheme. Assume that $u \equiv g \equiv 0$ and $\sigma = 0$. Then, it can be shown that the convex splitting framework automatically confers unconditional solvability and stability properties to our scheme (see [21] and [22]). We now assume that $u, g \not\equiv 0$ and $\sigma > 0$. The solvability follows immediately from the fact that \mathcal{E}_2 is convex, see [2], [21], [22], [60], and [61].

Stability is given by the following

Theorem 3.2. Let φ^n be the n-th iterate of (3.1)–(3.2). We assume that there exists a constant β such that

$$(3.6) 0 < \beta < J \star 1, \quad a.e. \ in \ \Omega,$$

and

$$(3.7) |f'(\varphi^k)| \leq \beta, for all \ k \leq l-1, \ \forall l \in \mathbb{N}.$$

Then, provided that δt is sufficiently small, for all positive integers l, the sequence φ^l is bounded in $L^2(\Omega)$ on a finite interval [0,T], for $l\delta t \leqslant T$, T>0 fixed, i.e.,

$$\|\varphi^l\|^2 + \delta t \|\nabla \varphi^l\|^2 \leqslant C,$$

where C is a nonnegative constant.

Proof. We have, owing to Young's inequality and multiplying (3.1) by $\psi = 2\delta t \varphi^{n+1}$,

(3.8)
$$\|\varphi^{n+1}\|^2 - \|\varphi^n\|^2 + 2\delta t((\nabla \mu^{n+1}, \nabla \varphi^{n+1}))$$

$$\leq 2\delta t((u\varphi^{n+1}, \nabla \varphi^{n+1})) + 2\delta t((g, \varphi^{n+1})) - 2\sigma \delta t((\varphi^n - m, \varphi^{n+1})).$$

Now, multiply (3.2) by $-2\delta t \Delta \varphi^{n+1}$ to obtain

$$(3.9) 2\delta t((\nabla \mu^{n+1}, \nabla \varphi^{n+1})) = 4\delta t((\nabla [(J_1 \star 1)\varphi^{n+1}], \nabla \varphi^{n+1})) + 2\sigma \delta t((\nabla [(G \star 1)(\varphi^{n+1} - \varphi^n)], \nabla \varphi^{n+1})) + 2c_1\delta t((\nabla \varphi^{n+1} - \nabla \varphi^n, \nabla \varphi^{n+1})) + 2\delta t((f'(\varphi^n)\nabla \varphi^n, \nabla \varphi^{n+1})) - 2\delta t((\nabla [(J_1 \star 1 + J_2 \star 1)\varphi^n], \nabla \varphi^{n+1})) - 2\delta t((\nabla (J \star \varphi^n), \nabla \varphi^{n+1})).$$

Collecting (3.9), on account of (3.8), we infer

(3.10)
$$\|\varphi^{n+1}\|^{2} - \|\varphi^{n}\|^{2} \leqslant -2c_{1}\delta t((\nabla\varphi^{n+1} - \nabla\varphi^{n}, \nabla\varphi^{n+1}))$$

$$-4\delta t((\nabla[(J_{1} \star 1)\varphi^{n+1}], \nabla\varphi^{n+1})) - 2\sigma\delta t((\nabla[(G \star 1)(\varphi^{n+1} - \varphi^{n})], \nabla\varphi^{n+1}))$$

$$-2\delta t((f'(\varphi^{n})\nabla\varphi^{n}, \nabla\varphi^{n+1})) + 2\delta t((\nabla[(J_{1} \star 1 + J_{2} \star 1)\varphi^{n}], \nabla\varphi^{n+1}))$$

$$-2\sigma\delta t(((\varphi^{n} - m), \varphi^{n+1})) + 2\delta t((\nabla(J \star \varphi^{n}), \nabla\varphi^{n+1}))$$

$$+2\delta t(((u\varphi^{n+1}, \nabla\varphi^{n+1})) + 2\delta t((g, \varphi^{n+1})))$$

$$= I + II + III + IV + V + VI + VII + VIII + IX.$$

Applying Young's inequality, we have

$$(3.11) I \leqslant -c_1 \delta t \|\nabla \varphi^{n+1}\|^2 + c_1 \delta t \|\nabla \varphi^n\|^2,$$

(3.12)
$$II = -4\delta t(((J_1 \star 1)\nabla \varphi^{n+1}, \nabla \varphi^{n+1}))$$

$$-4\delta t((\nabla (J_1 \star 1)\varphi^{n+1}, \nabla \varphi^{n+1}))$$

$$\leq -4\delta t \int_{\Omega} (J_1 \star 1)|\nabla \varphi^{n+1}|^2 dx$$

$$+ \frac{4}{\kappa} \delta t ||J_1||_{W^{1,1}}^2 ||\varphi^{n+1}||^2 + \kappa \delta t ||\nabla \varphi^{n+1}||^2,$$

and

(3.13)
$$III \leqslant -\sigma \delta t \int_{\Omega} (G \star 1) |\nabla \varphi^{n+1}|^2 dx + \sigma \delta t \int_{\Omega} (G \star 1) |\nabla \varphi^{n}|^2 dx$$

$$+ \frac{2\sigma^2}{\kappa} \delta t ||G||_{W^{1,1}}^2 (||\varphi^{n+1}||^2 + ||\varphi^{n}||^2) + \kappa \delta t ||\nabla \varphi^{n+1}||^2,$$

for all $\kappa > 0$. Furthermore, owing to assumption (3.7),

(3.14)
$$IV \leqslant \beta \delta t (\|\nabla \varphi^{n+1}\|^2 + \|\nabla \varphi^n\|^2).$$

Observe now that

(3.15)
$$V \leq \delta t \int_{\Omega} (J_1 \star 1 + J_2 \star 1) |\nabla \varphi^{n+1}|^2 dx$$
$$+ \delta t \int_{\Omega} (J_1 \star 1 + J_2 \star 1) |\nabla \varphi^n|^2 dx$$
$$+ \frac{c}{\kappa} \delta t (\|J_1\|_{W^{1,1}}^2 + \|J_2\|_{W^{1,1}}^2) \|\varphi^n\|^2 + \kappa \delta t \|\nabla \varphi^{n+1}\|^2,$$

for all $\kappa > 0$. Besides, we further have

(3.16)
$$VI \leq \sigma \delta t \|\varphi^n\|^2 + 2\sigma \delta t \|\varphi^{n+1}\|^2 + \sigma m^2 |\Omega| \delta t$$

and

(3.17)
$$\operatorname{VII} \leqslant \kappa \delta t \|\nabla \varphi^{n+1}\|^2 + \frac{\|J\|_{W^{1,1}}^2}{\kappa} \delta t \|\varphi^n\|^2,$$

for all $\kappa > 0$. Finally, using assumptions (A9) and (A10), we find

(3.18)
$$\operatorname{VIII} \leqslant \kappa \delta t \|\nabla \varphi^{n+1}\|^2 + \frac{\|u\|_{L^{\infty}}^2}{\kappa} \delta t \|\varphi^{n+1}\|^2$$

and

for all $\kappa > 0$. Collecting (3.11)–(3.19), on account of (3.10), we infer

$$\|\varphi^{n+1}\|^{2} - \|\varphi^{n}\|^{2} + \delta t \int_{\Omega} \left[c_{1} + 4(J_{1} \star 1) + \sigma(G \star 1) - (J_{1} \star 1 + J_{2} \star 1) - \beta - 6\kappa \right] |\nabla \varphi^{n+1}|^{2} dx$$

$$\leq \delta t \int_{\Omega} \left[c_{1} + \sigma(G \star 1) + (J_{1} \star 1 + J_{2} \star 1) + \beta \right] |\nabla \varphi^{n}|^{2} dx$$

$$+ \delta t \left(\frac{4 \|J_{1}\|_{W^{1,1}}^{2}}{\kappa} + \frac{2\sigma^{2} \|G\|_{W^{1,1}}^{2}}{\kappa} + \frac{\|u\|_{L^{\infty}}^{2}}{\kappa} + \kappa + 2\sigma \right) \|\varphi^{n+1}\|^{2} + \delta t \left(\frac{2\sigma^{2} \|G\|_{W^{1,1}}^{2}}{\kappa} + \frac{c(\|J_{1}\|_{W^{1,1}}^{2} + \|J_{2}\|_{W^{1,1}}^{2})}{\kappa} + \frac{\|J\|_{W^{1,1}}^{2}}{\kappa} + \sigma \right) \|\varphi^{n}\|^{2} + \left(\sigma m^{2} |\Omega| + \frac{\|g\|_{(H^{1}(\Omega))^{*}}^{2}}{\kappa} \right) \delta t.$$

Summing over n from n = 0 to n = l - 1, we have

with $\zeta(x) := (J \star 1)(x) - \beta > 0$ for almost any $x \in \Omega$ according to (3.6). Hence, taking $3\kappa < \zeta(x)$ for almost any $x \in \Omega$, we obtain

$$(3.22) 2\zeta(x) - 6\kappa > 0, \text{ for a.a. } x \in \Omega,$$

and

$$\eta(x) := c_1 + 4(J \star 1) + \sigma(G \star 1) - (J_1 \star 1 + J_2 \star 1) - \beta - 6\kappa
= \zeta(x) + 2(J_1 \star 1) + \sigma(G \star 1) + c_1 - 6\kappa
= 2\zeta(x) - 6\kappa + (J_1 \star 1) + (J_2 \star 1) + \sigma(G \star 1) + c_1 + \beta \geqslant 1, \text{ for a.a. } x \in \Omega.$$

Setting

$$C_{1} = \frac{4\|J_{1}\|_{W^{1,1}}^{2}}{\kappa} + \frac{2\sigma^{2}\|G\|_{W^{1,1}}^{2}}{\kappa} + \frac{\|u\|_{L^{\infty}}^{2}}{\kappa} + \kappa + 2\sigma,$$

$$C_{2} = \frac{2\sigma^{2}\|G\|_{W^{1,1}}^{2}}{\kappa} + c\left(\frac{\|J_{1}\|_{W^{1,1}}^{2}}{\kappa} + \frac{\|J_{2}\|_{W^{1,1}}^{2}}{\kappa}\right) + \frac{\|J\|_{W^{1,1}}^{2}}{\kappa} + \sigma,$$

and

$$C_3 = \sigma m^2 |\Omega| + \frac{\|g\|_{(H^1(\Omega))^*}^2}{\kappa} + \int_{\Omega} \left(c_1 + \sigma(G \star 1) + (J_1 \star 1 + J_2 \star 1) + \beta \right) |\nabla \varphi^0|^2 dx,$$

it thus follows from (3.21)-(3.23) that

(3.24)
$$\|\varphi^{l}\|^{2} + \delta t \|\nabla \varphi^{l}\|^{2}$$

$$\leq C_{1} \delta t \sum_{l=1}^{l-1} \|\varphi^{n+1}\|^{2} + C_{2} \delta t \sum_{l=1}^{l-1} \|\varphi^{n}\|^{2} + C_{3} l \delta t + \|\varphi^{0}\|^{2},$$

whence, after some simplifications,

(3.25)
$$\|\varphi^{l}\|^{2} + \delta t \|\nabla\varphi^{l}\|^{2} \leqslant C_{1}\delta t \|\varphi^{l}\|^{2}$$

$$+ (C_{1} + C_{2})\delta t \sum_{n=1}^{l-1} \|\varphi^{n}\|^{2} + (C_{3} + C_{2}\|\varphi^{0}\|^{2})l\delta t + \|\varphi^{0}\|^{2}.$$

Assuming that $\delta t < \frac{1}{2C_1}$ and $l\delta t \leqslant T$, we arrive at

(3.26)
$$\|\varphi^{l}\|^{2} + \frac{1}{1 - C_{1}\delta t} \delta t \|\nabla\varphi^{l}\|^{2}$$

$$\leq \frac{C_{1} + C_{2}}{1 - C_{1}\delta t} \delta t \sum_{n=1}^{l-1} \|\varphi^{n}\|^{2} + T \frac{C_{3} + C_{2} \|\varphi^{0}\|^{2}}{1 - C_{1}\delta t} + \frac{1}{1 - C_{1}\delta t} \|\varphi^{0}\|^{2}.$$

An application of the discrete Gronwall's inequality yields the desired result and the proof is complete. \Box

3.3. Convergence to the exact solution. In this section, we establish the convergence of the discrete solution to the continuous one as the time step $\delta t \to 0$.

Taking Remark 2.2 into account, we have

Theorem 3.3. Let $\varphi(x,0) \in H^3(\Omega)$ be an initial datum for (1.10) which satisfies the compatibility condition $\frac{\partial \mu}{\partial \nu} = 0$ a.e. on $\partial \Omega$. Then define the discretization error $e_n = \varphi_n - \varphi^n$, where $\varphi_n = \varphi(n\delta t)$. Assume that the assumptions of Proposition 3.1 and Theorem 3.2 hold. Then, provided that δt is sufficiently small, for all positive integers l such that $l\delta t \leqslant T$, we have

$$||e_l||^2 + |\delta t||\nabla e_l||^2 \le C(\delta t)^2$$

where C > 0 is independent of l and δt .

Proof. It follows from (3.1), (3.2), (3.3) that

$$\frac{e_{n+1} - e_n}{\delta t} - c_1 \Delta e_{n+1} - 2\Delta ((J_1 \star 1)e_{n+1}) - \sigma \Delta ((G \star 1)e_{n+1}) + \nabla \cdot (ue_{n+1})$$

$$= \frac{1}{\delta t} (\varphi_{n+1} - \varphi_n) - \frac{1}{\delta t} (\varphi^{n+1} - \varphi^n) - c_1 \Delta \varphi_{n+1} + c_1 \Delta \varphi^{n+1} + \nabla \cdot (u\varphi_{n+1}) - \nabla \cdot (u\varphi^{n+1})$$

$$-2\Delta ((J_1 \star 1)\varphi_{n+1}) + 2\Delta ((J_1 \star 1)\varphi^{n+1}) - \sigma \Delta ((G \star 1)\varphi_{n+1}) + \sigma \Delta ((G \star 1)\varphi^{n+1})$$

$$= \left(\Delta (f(\varphi_n)) - c_1 \Delta \varphi_n - \Delta ((J_1 \star 1 + J_2 \star 1)\varphi_n) - \Delta (J \star \varphi_n) - \sigma \Delta ((G \star 1)\varphi_n) - \sigma \varphi_n\right) + \tau_n$$

$$-\left(\Delta (f(\varphi^n)) - c_1 \Delta \varphi^n - \Delta ((J_1 \star 1 + J_2 \star 1)\varphi^n) - \Delta (J \star \varphi^n) - \sigma \Delta ((G \star 1)\varphi^n) - \sigma \varphi^n\right)$$

$$= -\left(\Delta (f(\varphi^n) - f(\varphi_n)) - c_1 \Delta (\varphi^n - \varphi_n) - \Delta ((J_1 \star 1 + J_2 \star 1)(\varphi^n - \varphi_n)) - \sigma \Delta ((J_1 \star 1 + J_2 \star 1)(\varphi^n - \varphi_n))\right)$$

$$-\Delta (J \star (\varphi^n - \varphi_n)) - \sigma \Delta ((G \star 1)(\varphi^n - \varphi_n)) - \sigma (\varphi^n - \varphi_n)\right) + \tau_n.$$

Therefore, we find

$$(3.27) e_{n+1} - e_n = c_1 \delta t \Delta(e_{n+1} - e_n) + 2 \delta t \Delta((J_1 \star 1)e_{n+1})$$

$$+ \sigma \delta t \Delta((G \star 1)(e_{n+1} - e_n)) - \delta t \nabla \cdot (ue_{n+1}) + \delta t \Delta(f(\varphi_n) - f(\varphi^n))$$

$$- \delta t \Delta((J_1 \star 1 + J_2 \star 1)e_n) - \delta t \Delta(J \star e_n) - \sigma \delta t e_n + \delta t \tau_n.$$

Integrating (3.27) over Ω , we get

(3.28)
$$\frac{1}{\delta t} \langle e_{n+1} - e_n \rangle + \sigma \langle e_n \rangle = \langle \tau_n \rangle.$$

Using the fact that $e_0 \equiv 0$, we have

$$\langle e_0 \rangle = 0$$

and, owing to (3.5), we obtain

$$\frac{1}{\delta t} \langle e_1 \rangle = O(\delta t).$$

So by mathematical induction, assuming that the assertion is true for n = k, i.e.

$$\frac{1}{\delta t} \langle e_k \rangle = O(\delta t),$$

we find, thanks to (3.28) and (3.5),

$$\frac{1}{\delta t} \langle e_{k+1} - e_k \rangle + \sigma \langle e_k \rangle = \langle \tau_k \rangle.$$

Hence, we have that

$$\frac{1}{\delta t} \langle e_{k+1} \rangle + (\sigma \delta t - 1) O(\delta t) = O(\delta t),$$

which yields

$$\langle e_{k+1} \rangle = O((\delta t)^2)$$

and

$$\langle e_n \rangle = O((\delta t)^2), \qquad \forall n \geqslant 1.$$

We multiply (3.27) by $2e_{n+1}$. This gives

$$(3.30) \begin{aligned} \|e_{n+1}\|^2 - \|e_n\|^2 + \|e_{n+1} - e_n\|^2 &= -2\delta t((\nabla(f(\varphi_n) - f(\varphi^n)), \nabla e_{n+1})) \\ - 4\delta t((\nabla((J_1 \star 1)e_{n+1}), \nabla e_{n+1})) - 2c_1\delta t((\nabla(e_{n+1} - e_n), \nabla e_{n+1})) \\ - 2\sigma\delta t((\nabla((G \star 1)(e_{n+1} - e_n)), \nabla e_{n+1})) + 2\delta t((ue_{n+1}, \nabla e_{n+1})) \\ + 2\delta t((\nabla((J_1 \star 1 + J_2 \star 1)e_n), \nabla e_{n+1})) + 2\delta t((\nabla(J \star e_n), \nabla e_{n+1})) \\ - 2\sigma\delta t((e_n, e_{n+1})) + 2\delta t((\tau_n, e_{n+1})) \\ &= I + II + III + IV + V + VI + VII + VIII + IX. \end{aligned}$$

Note that, since f' is locally Lipschitz continuous, then

$$I = +2\delta t((-f'(\varphi^n)\nabla e_n + \nabla \varphi_n(f'(\varphi^n) - f'(\varphi_n)), \nabla e_{n+1}))$$

$$\leq 2\beta \delta t \|\nabla e_n\| \|\nabla e_{n+1}\| + 2c\delta t \|\nabla \varphi_n\|_{L^{\infty}(\Omega)} \|e_n\| \|\nabla e_{n+1}\|$$

$$\leq \beta \delta t \|\nabla e_n\|^2 + \frac{c^2 \|\nabla \varphi_n\|_{L^{\infty}(\Omega)}^2}{\kappa} \delta t \|e_n\|^2 + (\beta + \kappa)\delta t \|\nabla e_{n+1}\|^2,$$
(3.31)

for all $\kappa > 0$. Arguing as for the estimates obtained above ((3.11)–(3.13) and (3.15)–(3.19)) we find

(3.32)
$$II \leqslant -4\delta t \int_{\Omega} (J_1 \star 1) |\nabla e_{n+1}|^2 dx$$

$$+ \frac{4}{\kappa} \delta t ||J_1||_{W^{1,1}}^2 ||e_{n+1}||^2 + \kappa \delta t ||\nabla e_{n+1}||^2,$$

(3.33)
$$III \leqslant -c_1 \delta t \|\nabla e_{n+1}\|^2 + c_1 \delta t \|\nabla e_n\|^2,$$

(3.34)
$$IV \leqslant -\sigma \delta t \int_{\Omega} (G \star 1) |\nabla e_{n+1}|^2 dx + \sigma \delta t \int_{\Omega} (G \star 1) |\nabla e_n|^2 dx + \frac{2\sigma^2}{\kappa} \delta t ||G||_{W^{1,1}}^2 (||e_{n+1}||^2 + ||e_n||^2) + \kappa \delta t ||\nabla e_{n+1}||^2,$$

(3.35)
$$V \leq \kappa \delta t \|\nabla e_{n+1}\|^2 + \frac{\|u\|_{L^{\infty}(\Omega)}^2}{\kappa} \delta t \|e_{n+1}\|^2,$$

(3.36)
$$VI \leq \delta t \int_{\Omega} (J_1 \star 1 + J_2 \star 1) |\nabla e_{n+1}|^2 dx + \delta t \int_{\Omega} (J_1 \star 1 + J_2 \star 1) |\nabla e_n|^2 dx$$

$$+ \frac{c}{\kappa} \delta t (\|J_1\|_{W^{1,1}}^2 + \|J_2\|_{W^{1,1}}^2) \|e_n\|^2 + \kappa \delta t \|\nabla e_{n+1}\|^2,$$

(3.37)
$$VII \leqslant \frac{\|J\|_{W^{1,1}}^2}{\kappa} \delta t \|e_n\|^2 + \kappa \delta t \|\nabla e_{n+1}\|^2,$$

(3.38)
$$VIII \leqslant \sigma \delta t ||e_n||^2 + \sigma \delta t ||e_{n+1}||^2,$$

for all $\kappa > 0$. From Proposition 3.1 and (3.29), we further have

(3.39)
$$||X| \leq 2c \, \delta t ||\tau_{n}||_{(H^{1}(\Omega))^{*}} ||e_{n+1}||_{H^{1}(\Omega)}$$

$$\leq \kappa \delta t ||e_{n+1}||_{H^{1}(\Omega)}^{2} + C(\delta t)^{2} \delta t$$

$$\leq \kappa \delta t (||\nabla e_{n+1}||^{2} + \langle e_{n+1} \rangle^{2}) + C(\delta t)^{2} \delta t$$

$$\leq \kappa \delta t ||\nabla e_{n+1}||^{2} + C(\delta t)^{3},$$

where C > 0. Combining the above results, we infer

with C independent of δt and l. Summing over n from n = 0 to n = l - 1 and using the fact that $e_0 \equiv 0$, we obtain

where we have used the fact that $\zeta(x) = (J \star 1)(x) - \beta > 0$, for almost any $x \in \Omega$. Since (3.6) holds and taking $4\kappa < \zeta(x)$, for almost any $x \in \Omega$, we obtain

(3.42)
$$2\zeta(x) - 8\kappa > 0$$
, for a.a. $x \in \Omega$,

and

(3.43)
$$\zeta(x) + 2(J_1 \star 1) + \sigma(G \star 1) + c_1 - 8\kappa \ge 1$$
, for a.a. $x \in \Omega$.

Proceeding as in the proof of Theorem 3.2, we introduce the constants

$$C_1' = \frac{4\|J_1\|_{W^{1,1}}^2}{\kappa} + \frac{2\sigma^2\|G\|_{W^{1,1}}^2}{\kappa} + \frac{\|u\|_{L^{\infty}(\Omega)}^2}{\kappa} + \sigma$$

and

$$C_2' = \frac{2\sigma^2 \|G\|_{W^{1,1}}^2}{\kappa} + \frac{c(\|J_1\|_{W^{1,1}}^2 + \|J_2\|_{W^{1,1}}^2)}{\kappa} + \frac{\|J\|_{W^{1,1}}^2}{\kappa} + \frac{c^2 \|\nabla \varphi_n\|_{L^{\infty}(\Omega)}^2}{\kappa} + \sigma$$

and obtain

$$||e_l||^2 (1 - \delta t C_1') + \delta t ||\nabla e_l||^2 \le \delta t (C_1' + C_2') \sum_{n=1}^{l-1} ||e_n||^2 + C l(\delta t)^3.$$

Then, dividing the last inequality by $(1 - \delta t C_1')$ and choosing $\delta t < \frac{1}{2C_1'}$ and $l\delta t \leqslant T$ yields

$$||e_l||^2 + \delta t ||\nabla e_l||^2 \le 2\delta t (C_1' + C_2') \sum_{n=1}^{l-1} ||e_n||^2 + 2Cl(\delta t)^3.$$

An application of the discrete Gronwall Lemma entails

$$||e_l||^2 + \delta t ||\nabla e_l||^2 \le C(\delta t)^2$$

with C independent of δt and l.

4. Numerical simulations

In the time-stepping scheme (3.1)–(3.2), we use a P1-finite element for the space discretization. The numerical simulations are performed with the software Freefem++ (see [37]).

In the numerical results presented below, Ω is a $(0, 10) \times (0, 10)$ -square, so that we can use the DFFT function to compute the nonlocal terms.

The numerical simulations presented below show the efficiency of the model not only for phase separation phenomena, but also for crystal nucleation. In particular, when $\sigma=0$, and $u\equiv g\equiv 0$, the results can be compared with the ones presented in [33] and [34]. The simulations presented below illustrate, from the numerical point of view, the modified nonlocal model proposed by Bates and Han with different value of σ (which allows to change the convolution kernel), with different value of m (which characterizes of the loss of mass in the model) and different value of u (corresponding to a transport term that accounts for a possible flow of the mixture at a certain given velocity field u). Note that the numerical results show that the solution seems to converge to a homogeneous state when σ and m are sufficiently large.

4.1. Phase separation and coarsening: dynamics of the solutions of the non-local Cahn-Hilliard-Oono equation with positive Gaussian kernel. Here, the triangulation of Ω is obtained by dividing Ω into 128×128 rectangles and by dividing each rectangle along the same diagonal.

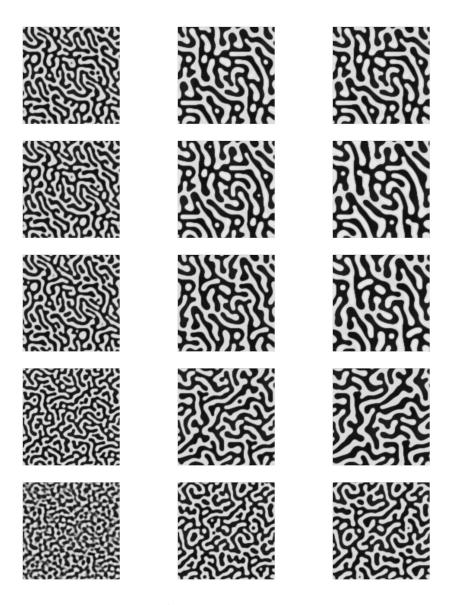


FIGURE 1. $u \equiv 0$, $f(s) = s^3 - s$, $m = \langle \varphi_0 \rangle \approx 0$. First row to fifth row: solutions at T = 0.4, T = 1.2, and T = 2. First row: $\sigma = 0$, second row: $\sigma = 0.005$, third row: $\sigma = 0.05$, fourth row: $\sigma = 0.5$, fifth row: $\sigma = 2$.

Dynamics of the solutions with a null transport term. In Figure 1, we consider a random initial datum between -0.05 and 0.05, which leads to a spatial average close to 0. In that case, the interaction kernel J is given by a positive Gaussian function defined as follows

(4.1)
$$J(x,y) = \frac{1}{\varepsilon_1^2} e^{-\frac{(x-5)^2 + (y-5)^2}{\varepsilon_1^2}}$$

and the long-ranged interaction kernel G in two space dimensions is the Green-like function defined as

(4.2)
$$G(x,y) = \ln(\sqrt{(x-y)^2 + \lambda^2}),$$

where $\varepsilon_1=0.05$ and $\lambda=10^{-2}$ (here, we have used the usual regularization $|x-y|\approx \sqrt{(x-y)^2+\lambda^2}$). Furthermore, we consider the typical choice of the nonlinear term $f(s)=s^3-s$ and take $m=\langle \varphi_0\rangle\approx 0$. The parameters of the numerical simulations are $h=\frac{10}{128}$, $\delta t=2.10^{-4},\ u\equiv (0,0),\ {\rm and}\ g=0.$ The final time for the simulation is T=2.

For $\sigma=0$, we present the dynamics of the solution to the nonlocal Cahn-Hilliard equation at T=0.4, T=1.2, and T=2, respectively. Next, for $\sigma=0.005$, we show that the results obtained in [47] for the Cahn-Hilliard-Oono equation are also satisfied for the nonlocal Cahn-Hilliard-Oono equation. This means that, when σ is close to zero, the dynamics of the nonlocal Cahn-Hilliard-Oono equation is close to that of the nonlocal Cahn-Hilliard equation. Finally, we show the effects of the long-range interaction kernel G on the nonlocal Cahn-Hilliard equation with $\sigma=0.05$, $\sigma=0.5$, and $\sigma=2$ respectively.

Effects of the transport term. We present in Figures 2 and 3 the evolution of the nonlocal Cahn–Hilliard–Oono equation again, with the same parameters and functions as in Figure 1 and a nonlinear term $f(s) = s^3 - s$, but we now take a non-vanishing transport term. First, in Figure 2, we take a transport term u = (10,0) and then, in Figure 3, we take $u = (-2\cos^2(\frac{\pi(x-5)}{10})\cos(\frac{\pi(y-5)}{10}), 2\cos^2(\frac{\pi(y-5)}{10})\cos(\frac{\pi(x-5)}{10}))$.

Off critical case (i.e., $m \neq \langle \varphi_0 \rangle$). We present in Figures 4 and 5 the evolution of the nonlocal Cahn-Hilliard-Oono equation, with the same parameters and functions as in Figure 1 and a nonlinear term $f(s) = s^3 - s$, but we now assume loss of mass (i.e., $m \neq \langle \varphi_0 \rangle$), where $\langle \varphi_0 \rangle \approx 0$ in Figure 4 and $\langle \varphi_0 \rangle \approx 0.02$ (φ_0 randomly distributed between -003 and 0.007) in Figure 5. First, in Figure 4 we take m = 1 and then in Figure 5 we take m = -1.

4.2. Crystal nucleation. Here, the triangulation of Ω is obtained by dividing Ω into 300×300 rectangles and by dividing each rectangle along the same diagonal.

Six-fold anisotropic shape. In Figures 6, we consider a random initial datum between -0.3 and 0.7, which leads to a spatial average close to 0.2. In that case, the interaction kernel J_s (in view of [34]) is given by the difference of two positive Gaussian functions defined as

we consider the interaction kernel J_a (in view of [34]) given by

$$(4.3) J_a(x,y) = \frac{0.1}{3\varepsilon_1^2} e^{\left(-\frac{(x-5)^2}{\varepsilon_1^2} - \frac{4(y-5)^2}{\varepsilon_1^2}\right)} + \frac{0.1}{3\varepsilon_1^2} e^{\left(-\frac{(\frac{(x-5)}{2} - \frac{\sqrt{3}(y-5)}{2})^2}{\varepsilon_1^2} - \frac{4(\frac{\sqrt{3}(x-5)}{2} + \frac{(y-5)}{2})^2}{\varepsilon_1^2}\right)}$$

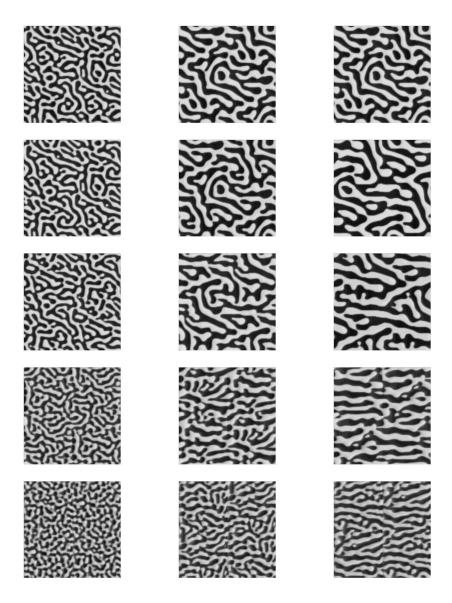


FIGURE 2. $J,\ u=(10,0),\ f(s)=s^3-s,\ m=\langle\varphi_0\rangle\approx 0.$ First row to fifth row: solutions at $T=0.4,\ T=1.2,$ and T=2. First row: $\sigma=0,$ second row: $\sigma=0.005,$ third row: $\sigma=0.05,$ fourth row: $\sigma=0.5,$ fifth row: $\sigma=2.$

$$+\frac{0.1}{3\varepsilon_{1}^{2}}e^{\left(-\frac{(\frac{(x-5)}{2}-\frac{\sqrt{3}(y-5)}{2})^{2}}{\varepsilon_{1}^{2}}-\frac{4(\frac{\sqrt{3}(x-5)}{2}-\frac{(y-5)}{2})^{2}}{\varepsilon_{1}^{2}}\right)}-\frac{0.08}{3\varepsilon_{2}^{2}}e^{\left(-\frac{(x-5)^{2}}{\varepsilon_{2}^{2}}-\frac{4(y-5)^{2}}{\varepsilon_{2}^{2}}\right)}\\ -\frac{0.08}{3\varepsilon_{2}^{2}}e^{\left(-\frac{(\frac{(x-5)}{2}-\frac{\sqrt{3}(y-5)}{2})^{2}}{\varepsilon_{2}^{2}}-\frac{4(\frac{\sqrt{3}(x-5)}{2}+\frac{(y-5)}{2})^{2}}{\varepsilon_{2}^{2}}\right)}-\frac{0.08}{3\varepsilon_{2}^{2}}e^{\left(-\frac{(\frac{(x-5)}{2}-\frac{\sqrt{3}(y-5)}{2})^{2}}{\varepsilon_{2}^{2}}-\frac{4(\frac{\sqrt{3}(x-5)}{2}-\frac{(y-5)}{2})^{2}}{\varepsilon_{2}^{2}}\right)}\\ -\frac{0.08}{3\varepsilon_{2}^{2}}e^{\left(-\frac{(\frac{(x-5)}{2}-\frac{\sqrt{3}(y-5)}{2})^{2}}{\varepsilon_{2}^{2}}-\frac{4(\frac{\sqrt{3}(x-5)}{2}-\frac{(y-5)}{2})^{2}}{\varepsilon_{2}^{2}}\right)}$$

where $\varepsilon_1 = 0.08$, $\varepsilon_2 = 0.2$. The long-ranged interaction kernel G is defined by (4.2) with $\lambda = 10^{-6}$.

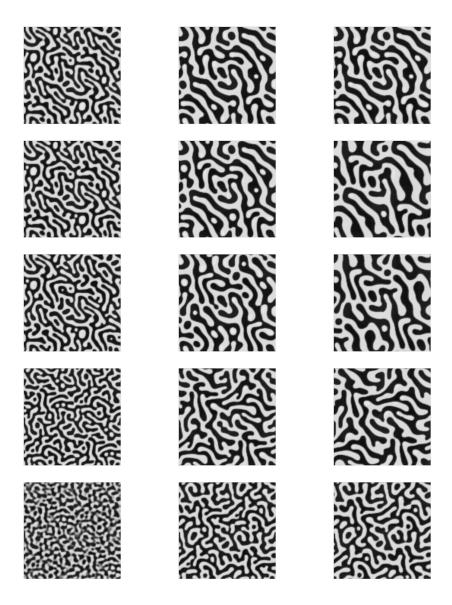


FIGURE 3. $J, u = (-2\cos^2(\frac{\pi(x-5)}{10})\cos(\frac{\pi(y-5)}{10}), 2\cos^2(\frac{\pi(y-5)}{10})\cos(\frac{\pi(x-5)}{10})), f(s) = s^3 - s, m = \langle \varphi_0 \rangle \approx 0$. First row to fifth row : solutions at T = 0.4, T = 1.2, and T = 2. First row : $\sigma = 0$, second row : $\sigma = 0.005$, third row : $\sigma = 0.05$, fourth row : $\sigma = 0.5$, fifth row : $\sigma = 0.05$.

Furthermore, we take $f(s)=s^3-s$. The parameters of the numerical simulations are $h=\frac{10}{300},\,\delta t=10^{-2},\,m=\langle\varphi_0\rangle,\,u=(0,0),\,{\rm and}\,\,g=0$. The final time for the simulations is T=5. We present the results for the nonlocal Cahn–Hilliard equation $(\sigma=0)$ and the nonlocal Cahn–Hilliard–Oono equation for $\sigma=0.05$ at $T=0.5,\,T=1$, and T=5.

Acknowledgments. The third author thanks the Laboratoire de Mathématiques et Applications de L'Université de Poitiers for its kind hospitality which allowed all the authors to exchange their ideas on this research subject. The third author is a member

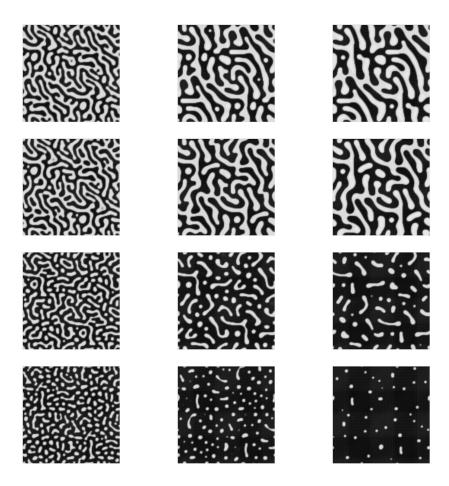


FIGURE 4. $u \equiv 0$, $f(s) = s^3 - s$, $\langle \varphi_0 \rangle \approx 0$, m = 1. First row to fourth row : solutions at T = 0.4, T = 1.2, and T = 2. First row : $\sigma = 0.005$, second row : $\sigma = 0.05$, third row : $\sigma = 0.5$, and fourth row : $\sigma = 1$.

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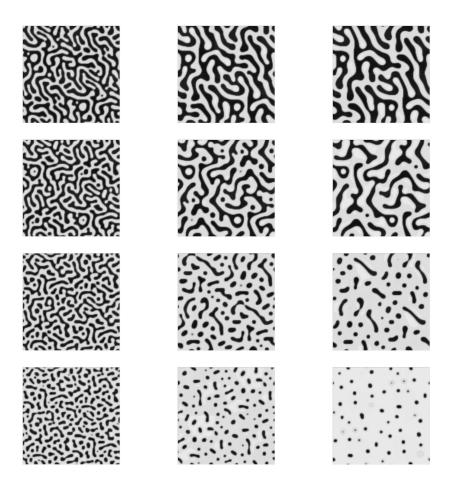


FIGURE 5. $u \equiv 0$, $f(s) = s^3 - s$, $\langle \varphi_0 \rangle \approx 0.02$, m = -1. First row to fourth row: solutions at T = 0.4, T = 1.2, and T = 2. First row: $\sigma = 0.05$, second row: $\sigma = 0.2$, third row: $\sigma = 0.5$, and fourth row: $\sigma = 1$.

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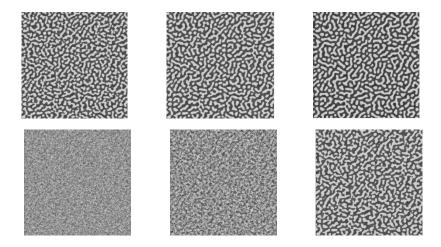


FIGURE 6. J_a , $u \equiv 0$, $f(s) = s^3 - s$, $m = \langle \varphi_0 \rangle \approx 0.2$. First row and second row: T = 0.5, T = 1, and T = 5. First row: $\sigma = 0$ and second row: $\sigma = 0.05$.

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