Phase field method for mean curvature flow with boundary constraints

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Abstract

This paper is concerned with the numerical approximation of mean curvature flow $t \to \Omega(t)$ satisfying an additional inclusion-exclusion constraint $\Omega_1 \subset \Omega(t) \subset \Omega_2$. Classical phase field model to approximate these evolving interfaces consists to solve the Allen-Cahn equation with Dirichlet boundary conditions. In this work, we introduce a new phase field model, which can be viewed as an Allen Cahn equation with penalized double well potential. We first justify this method by a Γ-convergence result and then we give some numerical comparisons of these two different models.

Contents

1 Introduction

In the last decades, a lot of work has been devoted to the motion of interfaces, and particularly to motion by mean curvature. Applications concern image processing (denoising, segmentation), material sciences (motion of grain boundaries in alloys, crystal growth), biology (modelling of vesicles and blood cells), image denoising, image segmentation and motion of grain boundaries.

Let $\Omega(t) \subset \mathbb{R}^d$, $0 \leq t \leq T$, denotes the evolution by mean curvature of a smooth bounded domain Ω_0 : the outward normal velocity V_n at a point $x \in \partial\Omega(t)$ is given by

$$V_n = \kappa, \tag{1}$$

where κ denotes the mean curvature at x, with the convention that κ is negative if the set is convex. We will consider only smooth motions, which are well-defined if T is sufficiently small [3]. Singularities may develop in finite time, however, one may need to consider evolutions in the sense of viscosity solutions [4, 11].

The evolution of $\Omega(t)$ is closely related to the minimization of the following energy:

$$J(\Omega) = \int_{\partial\Omega} 1 \, d\sigma.$$

Indeed, (1) can be viewed as a L^2-gradiant flow of this energy.

The functional J can be approximated by a Ginzburg–Landau functional [14, 13]:

$$J_\epsilon(u) = \int_{\mathbb{R}^d} \left(\frac{\epsilon}{2} |\nabla u|^2 + \frac{1}{\epsilon} W(u) \right) \, dx.$$

where $\epsilon > 0$ is a small parameter, and W is a double well potential with wells located at 0 and 1 (for example $W(s) = \frac{1}{2} s^2 (1-s)^2$).

Modica and Mortola [14, 13] have shown the Γ-convergence of J_ϵ to $c_W J$ in $L^1(\mathbb{R}^d)$ (see also [5]), where

$$c_W = \int_0^1 \sqrt{2W(s)} ds.$$

The corresponding Allen–Cahn equation [2], obtained as the L^2-gradient flow of J_ϵ, reads

$$\frac{\partial u}{\partial t} = \Delta u - \frac{1}{\epsilon^2} W'(u). \tag{2}$$

Existence, uniqueness, and a comparison principle have been established for this equation (see for example chapters 14 and 15 in [3]). To this equation, one usually associates the profile

$$q = \arg\min \left\{ \int_{\mathbb{R}} \left(\frac{1}{2} \gamma'^2 + W(\gamma) \right) \; ; \; \gamma \in H^1_{loc}(\mathbb{R}), \; \gamma(-\infty) = +1, \; \gamma(+\infty) = 0, \; \gamma(0) = \frac{1}{2} \right\} \tag{3}$$

The motion $\Omega(t)$ can be approximated by

$$\Omega_\epsilon(t) = \left\{ x \in \mathbb{R}^d \; ; \; u_\epsilon(x,t) \geq \frac{1}{2} \right\},$$

where u_ϵ is the solution of the Allen Cahn equation with the initial condition

$$u_\epsilon(x,0) = q\Big(\frac{d(x, \Omega(0))}{\epsilon} \Big).$$

Here $d(x, \Omega)$ denotes the signed distance of a point x to the set Ω.

The convergence of $\partial\Omega_\epsilon(t)$ to $\partial\Omega(t)$ has been proved for smooth motions [10, 6] and in the general case without fattening [4, 11]. The convergence rate has been proved to be $O(\epsilon^2 |\log \epsilon|^2)$.

Note also that this equation is usually solved in a box Q, with periodic boundary conditions and solutions can be computed via a semi-implicit Fourier-spectral method as in the paper [9].

Our investigations concern here the approximation of interfaces evolving in a restricted area, which is classically the case in several physical applications. More precisely, we considere mean curvature flow $t \to \Omega(t)$ which evolves as the L^2 gradiant flow of the following energy

$$J_{\Omega_1,\Omega_2}(\Omega) = \begin{cases} \int_{\partial\Omega} 1 \, d\sigma & \text{if } \Omega_1 \subset \Omega \subset \Omega_2 \\ +\infty & \text{otherwise} \end{cases}$$

where Ω_1 and Ω_2 are two given smooth subsets of $\mathbb{R}^d$ such that $dist(\partial\Omega_1, \partial\Omega_2) > 0$. These evolving interfaces clearly satisfy the following constraint $\Omega_1 \subset \Omega(t) \subset \Omega_2$.

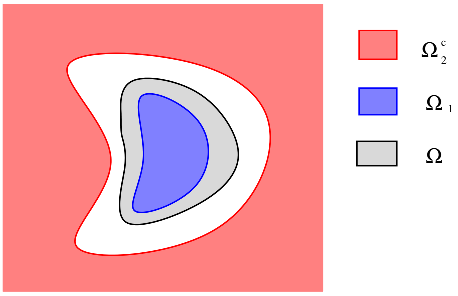

Figure 1: Mean curvature flow constrained

One classical phase field model to approximate these evolving interfaces considers the Allen Cahn equation in $\Omega_2 \setminus \Omega_1$ with Dirichlet boundary condition on $\partial\Omega_1$ and $\partial\Omega_2$ [15]. Yet, some limitations appear in this model :

- The Dirichlet boundary conditions prevent interfaces to touch boundaries $\partial\Omega_1$ and $\partial\Omega_2$. This can be seen as a consequence of thickness of the interface layer which is about $O(\epsilon \ln(\epsilon))$. This highlights the fact that the rate of convergence of this model can not be better than $O(\epsilon \ln(\epsilon))$.

- From a numerical point of view, resolution of the Allen Cahn equation with Dirichlet boundary condition can be done by a finite element method, which appears less efficient and more difficult to implement in dimensions greater than 2 than a semi-implicit Fourier-spectral method.

To compensate these limitations, we introduce in this paper a new phase field model. This idea is to consider the Allen-Cahn in the whole domaine with a penalization technique to take into account boundary constraint.

The paper is organised as follow:

- In section 2, we present the two phase field models describe previously

- In section 3, we justify the penalized approach by a Γ-convergence result.

- In section 4, the two phase field models are compared in numerical illustrations. This will clarify the numerical convergence rate of each model.

2 Phase field model for boundary constraints

We now introduce the two Allen Cahn models for the approximation of mean curvature flow $t \to \Omega(t)$ evolving as the L^2 gradiant flow of the following energy

$$J_{\Omega_1,\Omega_2}(\Omega) = \begin{cases} \int_{\partial\Omega} 1\, d\sigma & \text{if } \Omega_1 \subset \Omega \subset \Omega_2 \\ +\infty & \text{otherwise} \end{cases}$$

where Ω_1 and Ω_2 are two given smooth subsets of $\mathbb{R}^d$ satisfying $dist(\partial\Omega_1, \partial\Omega_2) > 0$.

2.1 Model with Dirichlet boundary conditions

One classical strategy, see for instance [7], consists in introducing the function space

$$X_{\Omega_1,\Omega_2} = \left\{ u \in H^1(\Omega_2 \setminus \Omega_1) \; ; \; u_{|\partial\Omega_1} = 1 \quad , u_{|\partial\Omega_2} = 0 \right\},$$

and a penalized Ginzburg-Landau energy of the form

$$\tilde{J}_{\epsilon,\Omega_1,\Omega_2}(u) = \begin{cases} \int_{\Omega_2\setminus\Omega_1} \left(\frac{\epsilon}{2}|\nabla u|^2 + \frac{1}{\epsilon}W(u) \right) dx & \text{if } u \in X_{\Omega_1,\Omega_2} \\ +\infty & \text{otherwise.} \end{cases}$$

Indeed, Chambolle and Bourdin [7] have shown the Γ-convergence of $\tilde{J}_{\epsilon,\Omega_2,\Omega_1}$ to $c_W J_{\Omega_2,\Omega_1}$ in $L^1(\mathbb{R}^d)$. This approximation conduces to following Allen-Cahn equation

$$\begin{cases} u_t = \triangle u - \frac{1}{\epsilon^2} W'(u), & \text{on} \quad \Omega_2 \setminus \Omega_1 \\ u_{|\partial\Omega_1} = 1, \quad u_{|\partial\Omega_2} = 0 \\ u(0,x) = u_0 \in X_{\Omega_1,\Omega_2}. \end{cases}$$

More general Γ-convergence result for the Allen-equation with Dirichlet boundary conditions can be found in [15].

2.2 An approach with a penalized double well potential

Now, we describe an alternative approach to force the boundary constraints, based on a penalized double well potential. Let us introduce two continuous and positive potentials W_1 and W_2 satisfying the following assumption :

$$(H1) \begin{cases} W_1(s) = W(s) & \text{for } s \geq 1/2 \\ W_1(s) \geq \max(W(s), \lambda) & \text{for } s \leq 1/2 \end{cases} \quad \text{and} \quad \begin{cases} W_2(s) = W(s) & \text{for } s \leq 1/2 \\ W_2(s) \geq \max(W(s), \lambda) & \text{for } s \geq 1/2, \end{cases}.$$

where $\lambda > 0$.

Let us introduce also a penalized double well potential $W_{\epsilon,\Omega_1,\Omega_2,\alpha}$ defined by

$$\begin{aligned} W_{\epsilon,\Omega_1,\Omega_2,\alpha}(s,x) &= W_1(s) q\left(\frac{dist(x,\Omega_1)}{\epsilon^\alpha}\right) + W_2(s) q\left(\frac{dist(x,\Omega_2^c)}{\epsilon^\alpha}\right) \\ &\quad + W(s)\left(1 - q\left(\frac{dist(x,\Omega_1)}{\epsilon^\alpha}\right) - q\left(\frac{dist(x,\Omega_2^c)}{\epsilon^\alpha}\right)\right), \end{aligned}$$

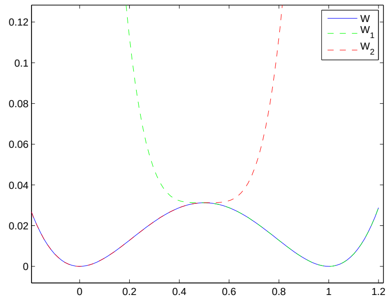

Figure 2: Example of potential W, W_1 and W_2

where $\alpha > 1$, $dist(x, \Omega_1)$ and $dist(x, \Omega_2^c)$ are respectively the signed distance function to the set Ω_1 and Ω_2^c, and q is the profil function associate to W defined at (3).

Our modified Ginzburg-Landau energy $J_{\epsilon,\Omega_1,\Omega_2,\alpha}$ reads

$$J_{\epsilon,\Omega_1,\Omega_2,\alpha}(u) = \int_{\mathbb{R}^d} \left(\frac{\epsilon}{2} |\nabla u|^2 dx + \frac{1}{\epsilon} W_{\epsilon,\Omega_1,\Omega_2,\alpha}(u,x) \right) dx.$$

We prove in the next section that this energy Γ-converge to $c_W J_{\Omega_1,\Omega_2}$. The associated Allen-Cahn equation reads now

$$\begin{cases} u_t = \triangle u - \frac{1}{\epsilon^2} \partial_s W_{\epsilon,\Omega_1,\Omega_2,\alpha}(u,x), & \text{on } \mathbb{R}^d \\ u(0,x) = u_0. \end{cases}$$

3 Approximation result of the penalized Ginzburg-Landau energy

Now we prove the convergence of the Ginzburg-Landau energy $J_{\epsilon,\Omega_1,\Omega_2,\alpha}$ to the following penalized perimeter

$$J_{\Omega_1,\Omega_2}(u) = \begin{cases} |Du|(\mathbb{R}^d) & \text{if } u = \mathbb{1}_\Omega \text{ and } \Omega_1 \subset \Omega \subset \Omega_2 \\ +\infty & \text{otherwise} \end{cases}.$$

Remark 1. *Given $u \in L^1(\mathbb{R}^d)$, $|Du|(\mathbb{R}^d)$ is defined by*

$$|Du|(\mathbb{R}^d) = \sup \left\{ \int_{\mathbb{R}^d} u \ \operatorname{div}(g) dx \ ; \ g \in C_c^1(\mathbb{R}^d, \mathbb{R}^d) \right\},$$

where $C_c^1(\mathbb{R}^d; \mathbb{R}^d)$ is the set of C^1 vector functions from $\mathbb{R}^d$ to $\mathbb{R}^d$ with compact support on $\mathbb{R}^d$. If $u \in W^{1,1}(\mathbb{R}^d)$, $|Du|$ coincides with the L^1-norm of ∇u and if $u = \mathbb{1}_\Omega$ where Ω has a smooth boundary, $|Du|$ coincides with the perimeter of Ω. Moreover, $u \to |Du|(\mathbb{R}^d)$ is lower semi-continuous in $L^1(\mathbb{R}^d)$ topology.

Recall that

$$J_{\epsilon,\Omega_1,\Omega_2,\alpha}(u) = \int_{\mathbb{R}^d} \left[\frac{\epsilon |\nabla u|^2}{2} + \frac{1}{\epsilon} W_{\epsilon,\Omega_1,\Omega_2,\alpha}(u,x) \right] dx,$$

where $W_{\epsilon,\Omega_1,\Omega_2,\alpha}(s,x)$ is defined by

$$\begin{aligned} W_{\epsilon,\Omega_1,\Omega_2,\alpha}(s,x) &= W_1(s) q\left(\frac{dist(x,\Omega_1)}{\epsilon^\alpha}\right) + W_2(s) q\left(\frac{dist(x,\Omega_2^c)}{\epsilon^\alpha}\right) \\ &\quad + W(s)\left(1 - q\left(\frac{dist(x,\Omega_1)}{\epsilon^\alpha}\right) - q\left(\frac{dist(x,\Omega_2^c)}{\epsilon^\alpha}\right)\right), \end{aligned}$$

with $\alpha > 1$.

We assume in this section that Ω_1 and Ω_2 are two given smooth subsets of $\mathbb{R}^d$ satisfying $dist(\partial\Omega_1, \partial\Omega_2) > 0$, and that ϵ is sufficiently small such as

$$1 - q\left(\frac{dist(x,\Omega_1)}{\epsilon^\alpha}\right) - q\left(\frac{dist(x,\Omega_2^c)}{\epsilon^\alpha}\right) > 1/2,$$

for all x in $\Omega_2 \setminus \Omega_1$.

Theorem 1. *Assume that W is a positive double-well potential with wells located at 0 and 1, continuous on $\mathbb{R}$ and such that $W(s) = 0$ if and only if $s \in \{0,1\}$. Assume also that W_1 and W_2 are two continuous potentials satisfying assumption $(H1)$. Then, for any $u \in L^1(\mathbb{R}^d)$, it holds*

$$\Gamma - \lim_{\epsilon \to 0} J_{\epsilon,\Omega_1,\Omega_2,\eta}(u) = c_W J_{\Omega_1,\Omega_2}(u),$$

where $c_W = \int_0^1 \sqrt{2W(s)}ds$.

Proof. We first prove the liminf inequality.
i) *Liminf inequality :*
Let (u_ϵ) converges to u in $L^1(\mathbb{R}^d)$. As $J_{\epsilon,\Omega_1,\Omega_2} \geq 0$, it is not restrictive to assume that the lim inf of $J_{\epsilon,\Omega_1,\Omega_2}(u_\epsilon)$ is finite. So we can extract a subsequence $u_h = u_{\epsilon_h}$ such that

$$\lim_{h \to +\infty} J_{\epsilon_h,\Omega_1,\Omega_2,\alpha}(u_h) = \liminf_{\epsilon \to 0} J_{\epsilon,\Omega_1,\Omega_2,\alpha}(u_\epsilon) \in \mathbb{R}^+.$$

Remark that for ϵ sufficiently small, it holds

$$\begin{cases} q\left(\frac{dist(x,\Omega_1)}{\epsilon^\alpha}\right) \geq 1/2 & \text{for } x \in \Omega_1, \\ q\left(\frac{dist(x,\Omega_2^c)}{\epsilon^\alpha}\right) \geq 1/2 & \text{for } x \in \Omega_2^c, \\ 1 - q\left(\frac{dist(x,\Omega_1)}{\epsilon^\alpha}\right) - q\left(\frac{dist(x,\Omega_2^c)}{\epsilon^\alpha}\right) \geq 1/2 & \text{for } x \in \Omega_2 \setminus \Omega_1, \\ 1 - q\left(\frac{dist(x,\Omega_1)}{\epsilon^\alpha}\right) - q\left(\frac{dist(x,\Omega_2^c)}{\epsilon^\alpha}\right) \geq 0 & \text{for } x \in \mathbb{R}^d. \end{cases}$$

This implies that

$$\begin{aligned} \int_{\Omega_1} W_1(u_h)dx &\leq \int_{\Omega_1} 2q\left(\frac{dist(x,\Omega_1)}{\epsilon^\alpha}\right) W_1(u_h)dx \\ &\leq 2\int_{\mathbb{R}^d} W_{\epsilon,\Omega_1,\Omega_2,\alpha}(s,x)dx \\ &\leq 2\epsilon_h J_{\epsilon_h,\Omega_1,\Omega_2,\alpha}(u_h), \end{aligned}$$

$$\int_{\mathbb{R}^d \setminus \Omega_2} W_2(u_h)dx \leq 2\epsilon_h J_{\epsilon_h,\Omega_1,\Omega_2,\alpha}(u_h) \quad \text{and} \quad \int_{\Omega_2 \setminus \Omega_1} W(u_h)dx \leq 2\epsilon_h J_{\epsilon_h,\Omega_1,\Omega_2,\alpha}(u_h).$$

The Fatou's Lemma and the continuity of W, W_1 and W_2 imply that $\int_{\Omega_1} W_1(u)dx = 0$, $\int_{\mathbb{R}^d \setminus \Omega_2} W_2(u)dx = 0$ and $\int_{\Omega_2 \setminus \Omega_1} W(u)dx = 0$. By our assumptions on W, W_1 and W_2, this means that

$$u(x) \in \begin{cases} \{1\} & \text{a.e in } \Omega_1 \\ \{0\} & \text{a.e in } \mathbb{R}^d \setminus \Omega_2 \\ \{0,1\} & \text{a.e in } \Omega^2 \setminus \Omega_1, \end{cases}$$

almost everywhere. Hence, we can represent u by $\mathbb{1}_\Omega$ for some Borel set $\Omega \in \mathbb{R}^d$ satisfying $\Omega_1 \subset \Omega \subset \Omega_2$. Using the Cauchy inequality, we can estimate

$$\begin{aligned}
J_{\epsilon_h,\Omega_1,\Omega_2,\alpha}(u_h) &\geq \int_{\mathbb{R}^d} \left[\frac{\epsilon_h |\nabla u_h|^2}{2} + \frac{1}{\epsilon_h} W(u_h) \right] dx \quad (\text{ because } W_1 \geq W \text{ and } W_2 \geq W) \\
&\geq \int_{\mathbb{R}^d} \left[\frac{\epsilon_h |\nabla u_h|^2}{2} + \frac{1}{\epsilon_h} \tilde{W}(u_h) \right] dx \quad (\text{ where } \tilde{W}(s) = \min \left\{ W(s) \ ; \ \sup_{s\in[0,1]} W(s) \right\}) \\
&\geq \int_{\mathbb{R}^d} \sqrt{2\tilde{W}(u_h)} |\nabla u_h| dx = \int_{\mathbb{R}^d} |\nabla[\phi(u_h)]| dx = |D[\phi(u_h)]|(\mathbb{R}^d),
\end{aligned}$$

where $\phi(s) = \int_0^s \sqrt{2\tilde{W}(t)}dt$. Since ϕ is a Lipschitz function (because $\tilde{W}$ is bounded), $\phi(u_\epsilon)$ converges in $L^1(\mathbb{R}^d)$ to $\phi(u)$. Using the lower semicontinuity of $v \to |Dv|(\mathbb{R}^d)$, we obtain

$$\lim_{h\to+\infty} J_{\epsilon_h,\Omega_1,\Omega_2}(u_h) \geq \liminf_{h\to+\infty} |D\phi(u_h)|(\mathbb{R}^d) \geq |D\phi(u)|(\mathbb{R}^d).$$

The lim inf inequality is finally obtained remarking that $\phi(u) = \phi(\mathbb{1}_\Omega) = c_W \mathbb{1}_\Omega = c_W u$.

Let us now prove the limsup inequality.
i) *Limsup inequality :*
We first assume that $u = \mathbb{1}_\Omega$ for some bounded open set Ω satisfying $\Omega_1 \subset \Omega \subset \Omega_2$ with smooth boundaries; Introduce the sequence

$$u_\epsilon(x) = q\left(\frac{dist(x,\Omega)}{\epsilon} \right).$$

Let us introduce the two constants c_1 and c_2 defined by

$$c_1 = \sup_{s\in[0,1]} \{W_1(s) - W(s)\}, \quad \text{and} \quad c_2 = \sup_{s\in[0,1]} \{W_1(s) - W(s)\}.$$

Note that

$$\begin{aligned}
J_{\epsilon,\Omega_1,\Omega_2,\alpha}(u^\epsilon) &= \int_{\mathbb{R}^d} \left[\frac{\epsilon |\nabla u^\epsilon|^2}{2} + \frac{1}{\epsilon} W(u^\epsilon) \right] dx + \int_{\mathbb{R}^d} \frac{1}{\epsilon} q\left(\frac{dist(x,\Omega_1)}{\epsilon^\alpha} \right) (W_1(u^\epsilon) - W(u^\epsilon))\, dx \\
&\quad + \int_{\mathbb{R}^d} \frac{1}{\epsilon} q\left(\frac{dist(x,\Omega_2^c)}{\epsilon^\alpha} \right) (W_2(u^\epsilon) - W(u^\epsilon))\, dx
\end{aligned}$$

Each of these 3 terms above is now analyzed.

(1) By co-area formula, we estimate

$$\begin{aligned}
\int_{\mathbb{R}^d} \left[\frac{\epsilon |\nabla u^\epsilon|^2}{2} + \frac{1}{\epsilon} W(u^\epsilon) \right] dx &= \frac{1}{\epsilon} \int_{\mathbb{R}^d} \left[\frac{q'(d(x,\Omega)/\epsilon)^2}{2} + W(q(d(x,\Omega)/\epsilon)) \right] dx \\
&= \frac{1}{\epsilon} \int_{\mathbb{R}} g(s) \left[\frac{q'(s/\epsilon)^2}{2} + W(q(s/\epsilon)) \right] ds \\
&= \int_{\mathbb{R}} g(\epsilon t) \left[\frac{q'(t)^2}{2} + W(q(t)) \right] dt
\end{aligned}$$

where $g(s) = |D\mathbb{1}_{\{d\leq s\}}|(\mathbb{R}^d)$.
By the smoothness of $\partial\Omega$, $g(\epsilon t)$ converges to $|D\mathbb{1}_{dist(x,\Omega)\leq t}|(R^d)$ as $\epsilon \to 0$; moreover, by the definition of the profil q, u_ϵ converges to $\mathbb{1}_\Omega$ and

$$\limsup_{\epsilon\to 0} J_{\epsilon,\Omega_1,\Omega_2}(u_\epsilon) \leq |D\mathbb{1}_\Omega|(\mathbb{R}^d) \int_{-\infty}^{+\infty} \left[\frac{1}{2}|q'(s)|^2 + W(q(s)) ds \right].$$

Remark 2. *The profil q (when W is continuous) can also be obtained [1] as the global decreasing solution of the following Cauchy problem*

$$\begin{cases} q'(s) = -\sqrt{W(s)}, & s \in \mathbb{R} \\ q(0) = \frac{1}{2}, \end{cases}$$

and satisfies

$$\int_{\mathbb{R}} \left(\frac{1}{2} q'(s)^2 + W(q(s)) \right) = \int_0^1 \sqrt{2W(s)} ds.$$

By the previsous remark, it follows that

$$\int_{-\infty}^{+\infty} \left[\frac{1}{2} |q'(s)|^2 + W(q(s)) \right] ds = \int_0^1 \sqrt{2W(s)} ds = c_W,$$

which implies that

$$\limsup_{\epsilon \to 0} \int_{\mathbb{R}^d} \left[\frac{\epsilon |\nabla u^\epsilon|^2}{2} + \frac{1}{\epsilon} W(u^\epsilon) \right] dx \leq c_W |D\mathbb{1}_\Omega|(\mathbb{R}^d).$$

(2) The function $dist(x, \Omega)$ is negative on Ω_1, thus $u_\epsilon(x) \geq \frac{1}{2}$ on Ω_1 and $W_1(u_\epsilon(x)) = W(u_\epsilon(x))$ for all $x \in \Omega_1$. This means that

$$\begin{aligned} \int_{\mathbb{R}^d} \frac{1}{\epsilon} q \left(\frac{dist(x, \Omega_1)}{\epsilon^\alpha} \right) (W_1(u^\epsilon) - W(u^\epsilon)) \, dx &= \int_{\mathbb{R}^d \setminus \Omega_1} \frac{1}{\epsilon} q \left(\frac{dist(x, \Omega_1)}{\epsilon^\alpha} \right) (W_1(u^\epsilon) - W(u^\epsilon)) \, dx \\ &\leq c_1 \int_{\mathbb{R}^d \setminus \Omega_1} \frac{1}{\epsilon} q \left(\frac{dist(x, \Omega_1)}{\epsilon^\alpha} \right) dx, \end{aligned}$$

where $c_1 = \sup_{s \in [0,1]} \{W_1(s) - W(s)\}$.
Using co-area formula, we estimate

$$\int_{\mathbb{R}^d \setminus \Omega_1} \frac{1}{\epsilon} q \left(\frac{dist(x, \Omega_1)}{\epsilon^\alpha} \right) dx = \int_0^\infty \frac{1}{\epsilon} g_1(s) q \left(\frac{s}{\epsilon^\alpha} \right) ds = \epsilon^{\alpha - 1} \int_0^\infty g_1(\epsilon^\alpha s) q(s) ds,$$

where $g_1(s) = |D\mathbb{1}_{\{dist(x, \Omega_1) \leq s\}}|(\mathbb{R}^d)$.
By the smoothness of Ω_1, $g(\epsilon^\alpha t)$ converges to $|D\mathbb{1}_{dist(x, \Omega_1) \leq 0}|(R^d)$ as $\epsilon \to 0$. We then deduce that

$$\limsup_{\epsilon \to 0} \int_{\mathbb{R}^d \setminus \Omega_1} \frac{1}{\epsilon} q \left(\frac{dist(x, \Omega_1)}{\epsilon^\alpha} \right) dx = 0,$$

as $\alpha > 1$ and $\int_0^\infty q(s) ds$ is bounded.

(3) The last term is similar to the second one. The function $dist(x, \Omega)$ is positive on $\mathbb{R}^d \setminus \Omega_2$, this means $u_\epsilon(x) \leq \frac{1}{2}$ on $\mathbb{R}^d \setminus \Omega_2$ and $W_2(u_\epsilon(x)) = W(u_\epsilon(x))$ for all $x \in \mathbb{R}^d \setminus \Omega_2$. Then, we have

$$\begin{aligned} \int_{\mathbb{R}^d} \frac{1}{\epsilon} q \left(\frac{dist(x, \Omega_2^c)}{\epsilon^\alpha} \right) (W_2(u^\epsilon) - W(u^\epsilon)) \, dx &= \int_{\Omega_2} \frac{1}{\epsilon} q \left(\frac{dist(x, \Omega_2^c)}{\epsilon^\alpha} \right) (W_2(u^\epsilon) - W(u^\epsilon)) \, dx \\ &\leq c_2 \int_{\Omega_2} \frac{1}{\epsilon} q \left(\frac{dist(x, \Omega_2^c)}{\epsilon^\alpha} \right) dx, \end{aligned}$$

and using co-area formula, it holds

$$\int_{\Omega_2} \frac{1}{\epsilon} q \left(\frac{dist(x, \Omega_2^c)}{\epsilon^\alpha} \right) dx = \int_0^\infty \frac{1}{\epsilon} g_2(s) q \left(\frac{s}{\epsilon^\alpha} \right) ds = \epsilon^{\alpha - 1} \int_0^\infty g_2(\epsilon^\alpha s) q(s) ds,$$

where $g_2(s) = |D\mathbb{1}_{\{dist(x,\Omega_2)\leq -s\}}|(\mathbb{R}^d)$. We deduce as previously that

$$\limsup_{\epsilon\to 0} \int_{\Omega_2} \frac{1}{\epsilon} q\left(\frac{dist(x,\Omega_2^c)}{\epsilon^\alpha}\right) dx = 0.$$

Finally, we conclude that

$$\limsup_{\epsilon\to 0} J_{\epsilon,\Omega_1,\Omega_2,\alpha}(u_\epsilon) \leq c_W |D\mathbb{1}_\Omega|(\mathbb{R}^d).$$

□

Remark 3. *This theorem is still true in the limiting case $\alpha \to \infty$, where $J_{\epsilon,\Omega_1,\Omega_2,\alpha=\infty}(u)$ reads*

$$\begin{aligned} J_{\epsilon,\Omega_1,\Omega_2,\infty}(u) &= \int_{\Omega_1} \left[\frac{\epsilon|\nabla u|^2}{2} + \frac{1}{\epsilon} W_1(u)\right] dx + \int_{\Omega_2\setminus\Omega_1} \left[\frac{\epsilon|\nabla u|^2}{2} + \frac{1}{\epsilon} W(u)\right] dx \\ &+ \int_{\mathbb{R}^d\setminus\Omega_2} \left[\frac{\epsilon|\nabla u|^2}{2} + \frac{1}{\epsilon} W_2(u)\right]. \end{aligned}$$

4 Algorithms and numerical simulations

We now compare numerically the two phase field models describes previously. The first model is integrated by a semi-implicite finite element method whereas our penalized Allen Cahn equation is solved by semi-implicite Fourier spectral algorithm. In particular, we will observe that these two approaches give similar solutions but,

- the algorithm used for the penalized Allen Cahn is more efficient and more simple than the semi-implicite finite element used for the Allen Cahn equation with Dirichlet boundary conditions
- the convervenge rate of the phase field approximation appears about $O(\epsilon \ln(\epsilon))$ for the Allen Cahn equation with Dirichlet boundary condition and about $O(\epsilon^2 \ln(\epsilon)^2)$ for our penalized version of Allen Cahn equation.

4.1 A semi-implicite finite element method for the Allen Cahn equation with Dirichlet boundary condition

Let us give more precision about the classic semi-implicite finite element method used for the equation

$$u_t(x,t) = \Delta u(x,t) - \frac{1}{\epsilon^2} W'(u)(x,t), \quad \text{on} \quad \Omega_2 \setminus \Omega_1 \times [0,T], \tag{4}$$

where $u_{|\partial\Omega_1} = 1$, $u_{|\partial\Omega_2} = 0$ and $W(s) = \frac{1}{2}s^2(1-s)^2$.

Note that when the initial condition u_0 is chosen on the form $u_0 = q\left(dist(\Omega_0, x)/\epsilon\right)$ with Ω_0 satisfying the constraint $\Omega_1 \subset \Omega_0 \subset \Omega_2$, then we expect that the set Ω^ϵ defined by

$$\Omega^\epsilon = \Omega_1 \cup \{x \in \Omega_2 \setminus \Omega_1 \ ; \ u(x,t) \geq 1/2\},$$

should be a good approximation to the contraint mean curvature flow $t \to \Omega(t)$.

Let us introduce a triangulation mesh $\mathcal{T}_h$ on the set $\Omega_2 \setminus \Omega_1$ and the discretization time step δ_t. Then, we consider the approximations spaces $X_{h,0}$ and X_h defined by

$$\begin{cases} X_h & = \left\{ v \in H^1(\overline{\Omega_2 \setminus \Omega_1}) \cup C^0(\overline{\Omega_2 \setminus \Omega_1}) \ ; \ v_{|K \in \mathcal{T}_h} \in P_k(K), \quad v_{|\Omega_1} = 1 \text{ and } v_{|\Omega_2} = 0 \right\} \\ X_{h,0} & = \left\{ v \in H^1_0(\Omega_2 \setminus \Omega_1) \cup C^1(\Omega_2 \setminus \Omega_1) \ ; \ v_{|K \in \mathcal{T}_h} \in P_2(K) \right\} \end{cases}$$

where P_k denotes the polynomial space of degree k. We take $k = 2$ in the future numerical illustrations. Then, the solution $u(x, t_n)$ at time $t_n = n\delta t$ is approximated by $U^{h,n}$, defined for $n > 1$ as the solution on X_h of

$$\int_{\Omega_2 \setminus \Omega_1} U^{h,n} \varphi \, dx + \delta_t \int_{\Omega_2 \setminus \Omega_1} \nabla U^{h,n} \nabla \varphi \, dx = \int_{\Omega_2 \setminus \Omega_1} \left(U^{h,n-1} - \frac{\delta_t}{\epsilon^2} W'(U^{h,n-1}) \right) \varphi \, dx, \quad \forall \varphi \in X_{h,0},$$

and for $n = 0$ by

$$U^{h,0} = \underset{v \in X_h}{\arg\min} \, \|v - u_0\|_{L^2(\Omega_2 \setminus \Omega_1)}.$$

This algorithm is known to be stable under the condition

$$\delta_t \quad \leq \quad c_W \epsilon^2,$$

where $c_W = \left[\sup_{t \in [0,1]} \{W''(s)\} \right]^{-1}$. More results about stability and convergence of this algorithm can be found in [12].

4.2 A semi-implicite Fourier spectral algorithm for the penalized Allen-Cahn equation

We also consider the seconde model

$$u_t(x,t) = \triangle u(x,t) - \frac{1}{\epsilon^2} \partial_s W_{\epsilon, \Omega_1, \Omega_2, \alpha}(u)(x,t), \quad \text{on} \quad Q \times [0,T], \tag{5}$$

with peridic boundary conditions on a given box Q, chosen suffiently large to contain Ω_2. In future numerical tests, we use $\alpha = 2$, $W(s) = \frac{1}{2}s^2(1-s)^2$ and the potentials W_1, W_2 are defined by

$$W_1(s) = \begin{cases} \frac{1}{2}s^2(1-s)^2 & \text{if } s \geq \frac{1}{2} \\ 10(s-0.5)^4 + 1/32 & \text{otherwise} \end{cases} \quad \text{and} \quad W_2(s) = \begin{cases} \frac{1}{2}s^2(1-s)^2 & \text{if } s \leq \frac{1}{2} \\ 10(s-0.5)^4 + 1/32 & \text{otherwise} \end{cases},$$

which clearly satisfy the assumption $(H1)$ (see figure (2)).

The initial condition u_0 satisfies $u_0 = q\left(dist(\Omega_0, x)/\epsilon\right)$ and we expect that the set

$$\Omega^\epsilon = \left\{ x \in Q \ ; \ u(x,t) \geq 1/2 \right\},$$

is a good approximation of $\Omega(t)$ as ϵ tends to zero.

About numerical scheme, equation (5) is numerically approximated via a splitting method between the diffusion and reaction terms. We take advantage of the periodicity of u by integrating exactly the diffusion term in the Fourier space. More precisely, the solution $u(x, t_n)$ at time $t_n = t_0 + n\delta t$ is approximated by

$$u_P^n(x) \quad = \quad \sum_{|p|_\infty = P} c_p^n e^{2i\pi p \cdot x},$$

where $|p|_\infty = \max_{1 \leq i \leq d} |p_i|$ and P represents the number of Fourier modes in each direction. In step n :

- $u_P^{n+1/2}(x) = \sum c_p^{n+1/2} \, e^{2i\pi p \cdot x}, \quad$ with $\quad c_p^{n+1/2} = c_p^n \, e^{-4\pi^2 \delta t \, |p|^2}$.
- $u_P^{n+1} = u_P^{n+1/2} - \frac{\delta t}{\epsilon^2} \partial_s W_{\epsilon,\Omega_2,\Omega_1 \alpha}(u_P^{n+1/2})$.

In practice, the first step is performed via a fast Fourier transform, with a computational cost $O(P^d \ln(P))$.

The corresponding numerical scheme turns out to be stable under the condition

$$\delta t \quad \leq \quad c_W \epsilon^2.$$

Some basic tests on the convergence of this algorithm can be found in [8].

4.3 Simulations and numerical convergence

We now compare some numerical solutions obtained with these two algorithms. For each test, we take $\epsilon = 2^{-8}$ and $\delta_t = \epsilon^2$. The P_2 finite element algorithm is implemented in Freefem++. The mesh $\mathcal{T}_h$ used in these simulations are ploted in figure (3). The penalization method is implemented in MATLAB where we take $P = 2^8$.

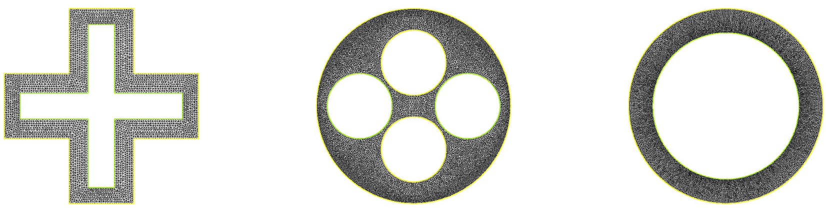

Figure 3: Mesh $\mathcal{T}_h$ generated by Freefem++, and used in simulations ploted on figures (4) and (5). In both case, $\partial\Omega_1$ and $\partial\Omega_2$ are respectively identified as the green and the yellow boundaries.

We plot first two situations on figures (4) and (5). The solutions obtained by the different methods seem to be very similar.

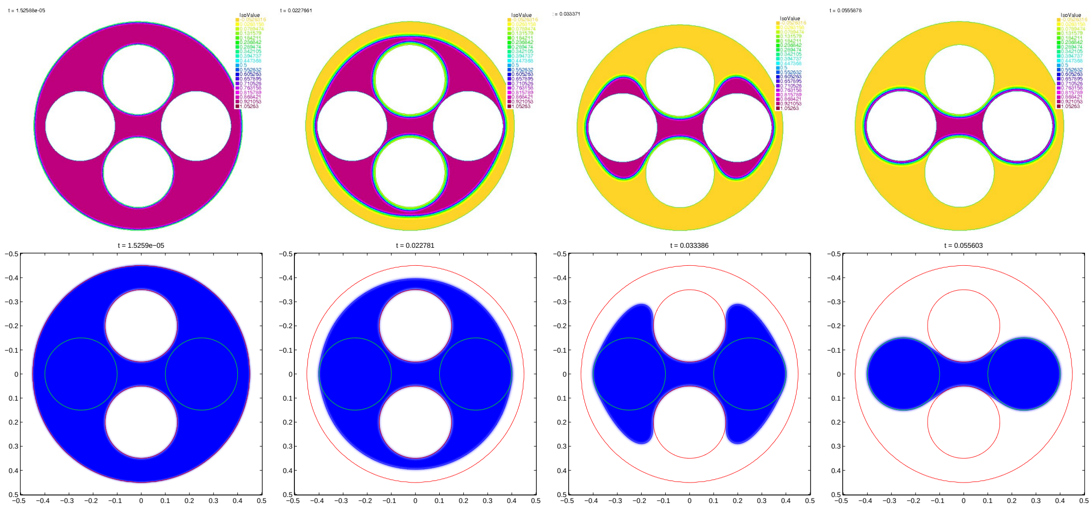

Figure 4: Numerical solutions obtained at different times t. The first line corresponds to the Dirichlet method and the second line to the penalization approach.

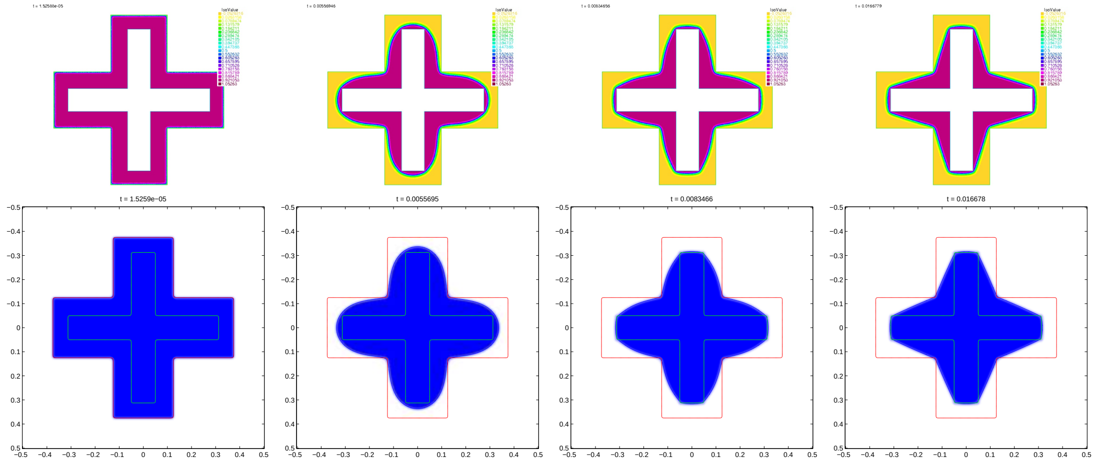

Figure 5: Numerical solutions obtained at different time t. The first line corresponds to the Dirichlet method and the second line to the penalization approach.

In order to estimate the convergence rate of both models, we consider the case where Ω_1 and Ω_2 are two circles of radii equal to $R_1 = 0.3$ and $R_2 = 0.4$. Then, the sitution is very simple when the initial set Ω_0 is also a circle with radius R_0 satisfying $R_1 < R_0 < R_2$. Indeed, the penalized mean curvature motion $\Omega(t)$ evolves as a circle, with radius satisfying

$$R(t) = \max\left(\sqrt{R_0^2 - 2t}, R_1\right),$$

that decreases until $R(t) = R_1$.

The solutions of the two different models are computed for different values of ϵ with $P = 2^8$, $\delta_t = 1/P^2$ and $R_0 = 0.35$. In both cases, the set $\Omega^\epsilon(t)$ appears as a circle of radius R^ϵ. We then estimate the numerical error between $R^\epsilon(t)$ and $R(t)$.

The results obtained for the first method are ploted on figure (6) : the first figure corresponds to the evolution $t \to \mathbb{R}^\epsilon(t)$ for 4 different values of ϵ and the second figure shows the error

$$\epsilon \to \sup_{t\in[0,T]} \{|R(t) - R^\epsilon(t)|\},$$

in logarithmic scale. It clearly appears an error of $O(\epsilon \ln(\epsilon))$.
The same test is done for the penalisation algorithm : the results are ploted on figure (7) and we now clearly observed a convergence rate of $O(\epsilon^2 \ln(\epsilon^2))$.

Moreover, we present in figure (8) a simulation in dimension 3 obtained by our approach : the solution of the Allen Cahn equation is ploted for different time t.

4.4 Some extensions

Another advantage of our penalisation approach is that it can be easily extended for more general situation of evolving interfaces. For example, we can consider a mean curvature flow with an additional forcing term g and a conservation of the volume. Following our recent work [8], this approach leads to the following pertubed Allen-Cahn equation

$$u_t = \Delta u - \frac{1}{\epsilon^2} F(u),$$

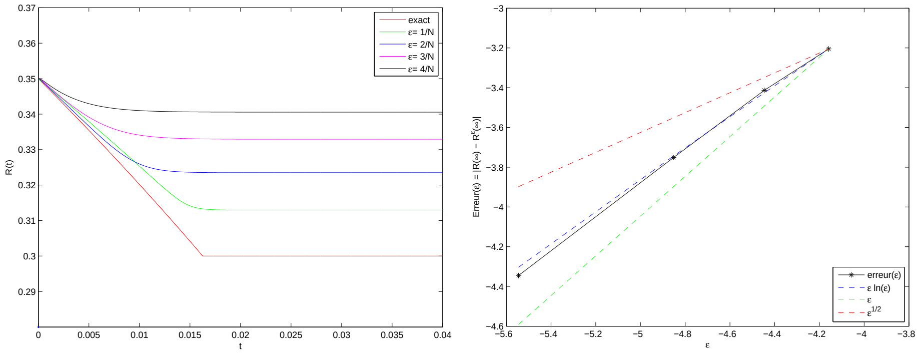

Figure 6: Dirichlet algorithm : numerical error $|R^{\epsilon} - R(t)|$; Left: $t \to R^{\epsilon}$ for different values of ϵ; Right: $\epsilon \to \sup_{t\in[0,T]} \{|R(t) - R^{\epsilon}(t)|\}$ in logarithmic scale

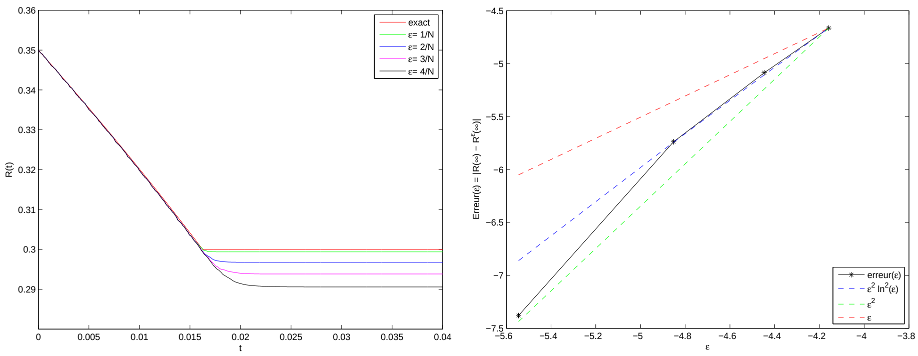

Figure 7: Penalisation algorithm : numerical error $|R^{\epsilon} - R(t)|$; Left: $t \to R^{\epsilon}$ for different values of ϵ; Right: $\epsilon \to \sup_{t\in[0,T]} \{|R(t) - R^{\epsilon}(t)|\}$ in logarithmic scale

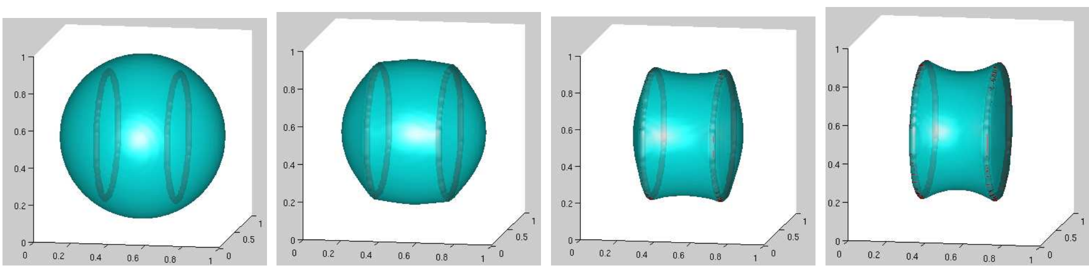

Figure 8: Minimal surface estimation : solution of the Allen Cahn equation at different time t. The set Ω_1 is the union of the two red circles.

where

$$F(u) = W'_{\Omega_1,\Omega_2}(u) - \epsilon g \sqrt{2W_{\Omega_1,\Omega_2}(u)} - \frac{\int_Q W'_{\Omega_1,\Omega_2}(u) - \epsilon g \sqrt{2W_{\Omega_1,\Omega_2}(u)} dx}{\int_Q \sqrt{2W_{\Omega_1,\Omega_2}(u)} dx} \sqrt{2W_{\Omega_1,\Omega_2}(u)}.$$

Two simulations obtained from this model are ploted in figure (9).

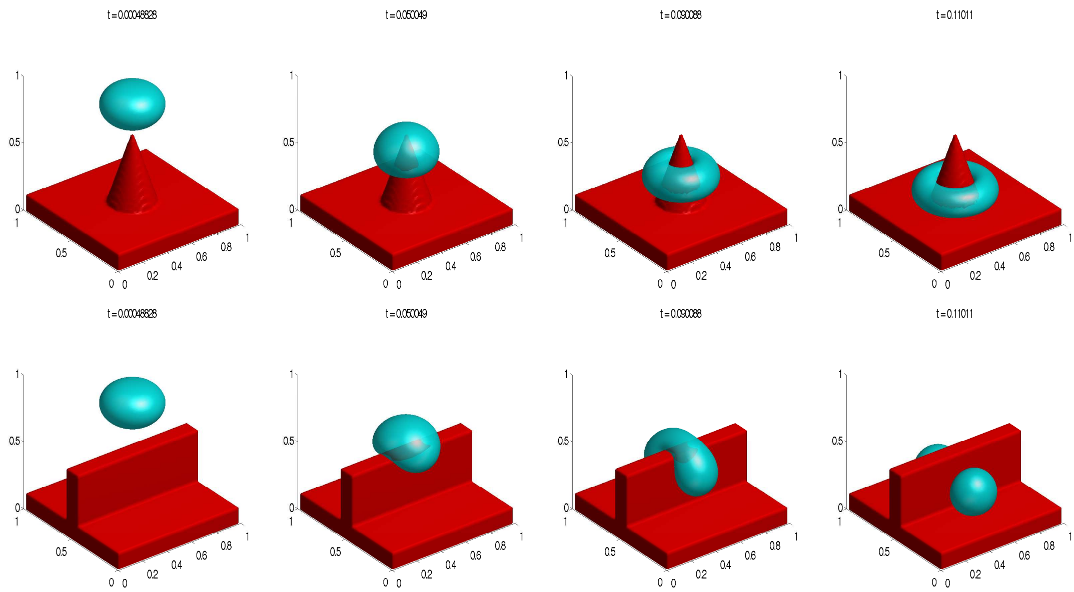

Figure 9: Two simulations with an additional forcing term (gravity force) and volume conservation.

5 Conclusion

This paper deals with phase field models for the approximation of mean curvature flow with inclusion-exclusion constraints. Classical method consists to solve Allen-Cahn equation with Dirichlet boundary conditions. Unfortunately, this method is not optimal in the sense that its convergence is observed with a rate about $O(\epsilon \ln(\epsilon))$ only. We have introduced a new approach based on a penalized double well potential. This method is motivated by a Γ-convergence result and some numerical tests suggest that its convergence rate is now about $O(\epsilon^2 \ln(\epsilon)^2)$. We finally explained how to generalize this strategy in the case of mean curvature flow with forcing term and conservation of volume.

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