A new phase field model for inhomogeneous minimal partitions, and applications to droplets dynamics

Elie Bretin
Univ Lyon, INSA de Lyon, CNRS UMR 5208, Institut Camille Jordan
20 avenue Albert Einstein, F-69621 Villeurbanne Cedex, France
elie.bretin@insa-lyon.fr

Simon Masnou
Univ Lyon, Université Claude Bernard Lyon 1, CNRS UMR 5208, Institut Camille Jordan
43 blvd. du 11 novembre 1918, F-69622 Villeurbanne cedex, France
masnou@math.univ-lyon1.fr

Abstract

We propose and analyze in this paper a new derivation of a phase-field model to approximate inhomogeneous multiphase perimeters. It is based on suitable decompositions of perimeters under some embeddability condition which allows not only an explicit derivation of the model from the surface tensions, but also gives rise to a Γ-convergence result. Moreover, thanks to the nice form of the approximating energy, we can use a simple and robust scheme to simulate its gradient flow. We illustrate the efficiency of our approach with a series of numerical simulations in 2D and 3D, and we address in particular the dynamics of droplets evolving on a fixed solid.

2010 Mathematics Subject Classification: 49Q05, 49Q20, 49M25.
Keywords: phase field model; multiphase perimeter; Γ-convergence; droplets; material sciences; image processing.

1 Introduction

This paper is devoted to the approximation with a phase field model of a N-phase perimeter of the form

$$P(\Omega_1, \dots, \Omega_N) = \frac{1}{2} \sum_{i,j=1}^{N} \sigma_{i,j} \operatorname{area}(\Gamma_{i,j}), \tag{1.1}$$

where $\Omega_1, \dots, \Omega_N$ are relatively closed subsets of an open domain $\Omega \subset \mathbb{R}^d$ which form a partition of Ω, i.e. $\Omega = \bigcup_{i=1}^N \Omega_i$ and $\Gamma_{i,j} = \Omega_i \cap \Omega_j = \partial\Omega_i \cap \partial\Omega_j \cap \Omega$ for $i \neq j$ (with the additional convention $\Gamma_{i,i} = \emptyset$), and $\sigma_{i,j}$ is the surface tension associated with $\Gamma_{i,j}$ for $i, j = 1, \cdots, N$. It is physically sound to assume that the surface tensions satisfy $\sigma_{i,j} = \sigma_{j,i} > 0$ whenever $i \neq j$ and $\sigma_{i,i} = 0$. We will denote in the sequel

$$S_N = \{\sigma = (\sigma_{i,j}) \in \mathbb{R}^{N\times N},\ \sigma_{i,j} = \sigma_{j,i} > 0 \text{ if } i \neq j \text{ and } \sigma_{i,i} = 0\}.$$

In order to guarantee the lower semicontinuity of the N-phase perimeter, it is necessary and sufficient to assume that the surface tensions satisfy the triangle inequality [37, 13, 33], i.e.

$$\sigma_{i,k} \leq \sigma_{i,j} + \sigma_{j,k} \quad \forall i,j,k \in \{1,\ldots,N\}. \tag{1.2}$$

Although mathematically sound, this property is however not fulfilled by all physical systems, so that the approximation issue needs also to be addressed in the non triangle case.

From the mathematical viewpoint, the study of the lower semicontinuity of the above energy requires to rephrase it in a suitable setting, namely the space of sets of finite perimeter [2, 33]. In this setting, the perimeter can be written as

$$P(\Omega_1,\ldots,\Omega_N) = \frac{1}{2}\sum_{i,j=1}^{N} \sigma_{i,j}\mathcal{H}^{d-1}(\partial^*\Omega_i \cap \partial^*\Omega_j),$$

where $\Omega_1,\cdots,\Omega_N$ are now assumed to be sets of finite perimeter in Ω such that $\Omega = \bigcup_{i=1}^N \Omega_i$ up to a Lebesgue negligible set, $|\Omega_i \cap \Omega_j| = 0$ for all $i \neq j$ (denoting as $|\cdot|$ the Lebesgue measure), $\Gamma_{i,j} = \partial^*\Omega_i \cap \partial^*\Omega_j$ for all i,j, with $\partial^*\Omega_i$ the reduced boundary of Ω_i in Ω, i.e. the sets of boundary points of Ω_i in Ω where an approximate normal exists (remark in particular that $\partial^*\Omega_i \subset \Omega$, i.e. $\partial\Omega$ does not play any role here), and $\mathcal{H}^{d-1}$ is the $(d-1)$-dimensional Hausdorff measure – see [2, 33] for details on functions of bounded variation (BV) and sets of finite perimeter. We shall denote as P the BV perimeter, i.e., if $A \subset \Omega$ has finite perimeter in Ω we denote $P(A) = \mathcal{H}^{d-1}(\partial^* A)$. In the BV context, the lower semicontinuity of the perimeter holds with respect to the strong convergence in L^1 of characteristic functions of sets.

There are many applications where the multiphase perimeter plays a role. It is for instance the natural energy associated with a polycrystalline material, i.e. a material which is an aggregation of tiny grains with different crystalline orientations, like most metals and ceramics. As such material is heated, the grains configuration evolves in order to decrease the multiphase perimeter (considering each grain as a phase), see [25] for more details and references on connexions of the model with material science. Such energetic dependence is actually common to many multiphase situations, either with uniform surface tensions (soap foams, honeycombs, etc) or with nonuniform surface tensions as in material synthesis, nanowires growth, etc. We focus in this paper on possibly nonuniform but isotropic surface tensions, which is coherent with many physical situations, but notice that many other physical situations (e.g. nanowire growth) involve anisotropic surface tensions (this is the topic of another paper in preparation). Only applications to material science have been mentioned so far but image processing is another field where multiphase perimeters are very useful, in particular in the context of image segmentation, image restoration, optical flow estimation or stereo reconstruction [38, 15, 45].

A multiphase system which energetically depends on the multiphase perimeter rearranges so as to decrease the perimeter, and the rearrangement consists in the evolution of the interfaces between phases [36]. The classical physical theory states [31] that this evolution must follow at least two rules :

1. at every interfacial point which is not a junction point between three or more interfaces, the normal velocity $V_{i,j}$ of the interface $\Gamma_{i,j}$ is proportional to the product of its mean curvature $\kappa_{i,j}$ with its surface tension $\sigma_{i,j}$:

$$V_{i,j}(x) = \sigma_{i,j}\mu_{i,j}\kappa_{i,j}(x), \quad \text{a.e. } x \in \Gamma_{i,j}, \tag{1.3}$$

   where $\mu_{i,j}$ is the interface mobility coefficient.

2. the Herring's angle condition holds at every triple junction, e.g. if x is a junction between phases i, j and k then

$$\sigma_{i,j}n_{i,j} + \sigma_{j,k}n_{j,k} + \sigma_{k,i}n_{k,i} = 0,$$

   where $n_{i,j}$ denotes the unit normal at x to $\Gamma_{i,j}$, pointing from Ω_i to Ω_j. An equivalent formulation using conormals is also used in the literature, emphasizing the fact that Herring's condition is actually a force balance condition.

Notice however that these two rules are not sufficient in general to characterize fully the L^2 gradient flow of the multiphase perimeter, since they do not constrain the evolution of the multiple points with multiplicity at least 4 (they do not even guarantee that the evolution of such multiple points is well-posed).

It is natural for numerical purposes to try to approximate the multiphase perimeter but there are several difficulties: the high singularity of the perimeter, the necessity of a good notion of convergence of the approximating energies, and the necessity to guarantee that, at each scale of approximation, the L^2-gradient flow with respect to the approximating energy is coherent (at least asymptotically) with both evolution rules mentioned above.

The most simple instance of a multiphase system is the binary system with constant surface tension whose perimeter's gradient flow is the celebrated mean curvature flow. There is a vast literature on numerical methods for the approximation of mean curvature flows. The methods can be roughly classified into five categories (some of them are exhaustively reviewed and compared in [20]):

1. parametric methods [22, 23, 5] where typically the interface is approximated by a point cloud, a triangulated surface or more complex discrete patched surfaces;

2. level set methods [41, 39, 40, 26, 18], where the problem is rewritten in terms of a suitable function of which the interface of interest is an isolevel; this lifting turns the flow into an

equation which is easier to handle both theoretically and numerically, in particular regarding topology changes.

3. convolution/thresholding type algorithms [8, 32, 43], where the mean curvature flow is the asymptotic limit of a time-discrete scheme alternating the convolution of the characteristic function of the set at time t delimited by the interface, followed by a thresholding step in order to define the set at time $t + dt$.

4. convexification methods [14] where it is observed first that minimizing the perimeter of a set is equivalent to minimizing the total variation of the set's characteristic function on the non convex class of functions with values in $\{0, 1\}$. Then it turns out that the mean curvature flow can be numerically approximated by convexifying the constraint and using a nice and simple projection algorithm.

5. phase field approaches [35, 17], where the sharp transition between the two phases at the interface is approximated by a smooth transition, the perimeter is approximated by a smooth energy depending on the smooth transition, and the gradient flow turns into a relatively simple reaction-diffusion system. Phase field approaches have a long history in physics that dates back to the Van der Waals' model for liquid-vapor transition (1893), and later with the supraconduction model of Landau & Ginzbug (1950), and the binary alloy model of Cahn & Hilliard (1958).

The literature on the approximation of multiphase perimeters is more reduced, but there have been contributions in the same five categories of methods. For instance, a parametric approach for anisotropic surface tensions is introduced in [4], various level set methods have been proposed in [34, 51, 44] (the latter reference proposes a method to encode a large variety of evolution laws at the interfaces). Convexifications approaches are much more involved for multiphase perimeters than for the binary perimeter. A simple convexification of the constraint is not enough as shown in [15] where a general method is proposed first for the homogeneous case $\sigma_{i,k} = 1$, then for more general surface tensions of the form $\sigma_{i,j} = \sigma(|i - j|)$ where σ is a concave, positive, and nondecreasing function.

As for convolution/thresholding type methods, [24] addresses the case of uniform surface tension $\sigma_{i,j} = 1$ and in [46], some constraints on the volume of each phases are added. More recently, an important step forward has been achieved by Esedoḡlu and Otto in [25]. For a large category of tensions matrices Esedoḡlu and Otto proposed a scheme which is able to decrease the multiphase perimeter in a way which yields asymptotically the correct evolution laws at simple and triple points. The major difficulty of a convolution/thresholding strategy in a multiphase setting is to handle correctly the variety of interfacial speeds yielded by different surface tensions. The key contribution of Esedoḡlu and Otto is precisely a consistent way of doing this using a smart combination of delay functions which manage consistently the communications between the various interfaces. The surface tensions matrices that the method can handle are negative forms on $(1, 1, \cdots, 1)^\perp$, i.e. the matrices $\sigma = (\sigma_{i,j}) \in S_N$ such that

$$\sum_{i,j=1}^{N} \sigma_{i,j} u_i u_j \leq 0 \quad \text{for all } (u_i) \in \mathbb{R}^N \text{ such that } \sum_{i=1}^{N} u_i = 0. \tag{1.4}$$

There is an interesting discussion in [25] about the properties of such matrices which are called conditionally semi-definite matrices.

The method that we propose in this paper belongs to the fifth category of approaches for the approximation and the minimization of multiphase perimeters, that is the category of phase field methods. Both theoretical and numerical contributions are related to this topic, see for instance [3, 42, 29, 28, 27, 30, 50, 9] and the numerous references therein. Before entering into more details, let us sketch the main properties of the model that will be derived in the paper:

(P1) it is a phase-field model with a potential term that can be derived consistently and explicitly from a given matrix $\sigma \in S_N$ of surface tensions, as soon as σ can be associated with ℓ^1 distances between vectors in $\mathbb{R}^M$ for a suitable dimension M (such σ is called ℓ^1-embeddable, see more details below). As will be discussed later, the consistent derivation of the potential is a major difference with the derivations that can be found in the literature;

(P2) in the strict ℓ^1-embeddability case (see below), the Γ-convergence of our approximating model to the multiphase perimeter can be proven. In view of the previous item, it is to the best of our knowledge the first contribution where one can derive the model from the surface tensions and recover them back from the Γ-convergence;

(P3) our approximating perimeter falls in a large category of phase field models studied with great accuracy by Garcke, Nestler, and Stoth in [28] where it is shown using the matched asymptotic expansion method that the correct evolution laws for simple and triple points are recovered asymptotically;

(P4) the model we propose is well suited for numerical approximation: the L^2-gradient flow yields an Allen-Cahn system with a linear diffusive part, which allows simple and robust numerical schemes with a very good spatial accuracy;

(P5) various interesting constraints can be easily added to the model, e.g. volume constraints or stationarity constraint on a phase, which can be very useful for simulating wetting phenomena.

2 Phase fields models for multiphase perimeters

Let us first examine the standard and simple case where all surface tensions are constant, i.e. $\sigma_{i,j} = 1$ therefore

$$P(\Omega_1, ...\Omega_N) = \frac{1}{2}\sum_{i,j=1}^{N} \mathcal{H}^{d-1}(\Gamma_{i,j}) = \frac{1}{2}\sum_{i=1}^{N} \mathcal{H}^{d-1}(\partial^*\Omega_i).$$

(recall from the introduction that all boundaries are considered in Ω i.e. $\partial^*\Omega_i = \partial^*\Omega_i \cap \Omega$). An interesting property of the latter formulation is the dependence of the energy on *full* interface boundaries $\partial^*\Omega_i$ (full with respect to Ω), and not partial interface boundaries $\Gamma_{i,j} = \partial^*\Omega_i \cap \partial^*\Omega_j$. Indeed, the dependence on full boundaries is well-suited for phase-field approximations: denoting

$$\Sigma = \left\{ \mathbf{u} : \Omega \to \mathbb{R}^N, \ \mathbf{u} = (u_1, \dots, u_N) \text{ measurable }, \ \sum_{i=1}^{N} u_i(x) = 1 \ \text{ for a.e. } x \in \Omega \right\},$$

P can be easily approximated in $(\mathrm{BV}(\Omega, \mathbb{R}))^N$ – in the sense of Γ–convergence – by

$$P_\epsilon(\mathbf{u}) = \begin{cases} \frac{1}{2}\sum_{i=1}^{N} \int_\Omega \left(\frac{\epsilon}{2}|\nabla u_i|^2 + \frac{1}{\epsilon}F(u_i) \right) dx & \text{if } \mathbf{u} \in \Sigma \cap (\mathrm{W}^{1,2}(\Omega))^N, \\ +\infty & \text{otherwise,} \end{cases}$$

where ϵ is a small parameter that characterizes the width of the diffuse interface, and $F(s) = \frac{s^2(1-s)^2}{2}$ is a double-well potential. This follows from Modica-Mortola's theorem [35] which states that the family of functionals J_ϵ defined by

$$J_\epsilon(u) = \int_\Omega \left(\frac{\epsilon}{2}|\nabla u|^2 + \frac{1}{\epsilon}F(u) \right) dx,$$

approximates (in the sense of Γ- convergence) $c_F P$ with $c_F = \int_0^1 \sqrt{2F(s)}ds$ and

$$P(u) = \begin{cases} |Du|(\Omega) & \text{when } u \in \mathrm{BV}(\Omega, \{0,1\}), \\ +\infty & \text{otherwise,} \end{cases}$$

where the total variation $|Du|(\Omega)$ of a function $u \in \mathrm{BV}(\Omega)$ (see [2]) is defined by

$$|Du|(\Omega) = \int_\Omega |Du| = \sup \left\{ \int_\Omega u \operatorname{div} g dx; \quad g \in C_0^1(\Omega, \mathbb{R}^n), \quad |g| \le 1 \right\}.$$

Using this approximation for every phase u_i yields P_ϵ, of which the Γ-convergence to $c_W P$ can be obtained as in [3, 42].

Moreover, the L^2-gradient flow of P_ϵ reads

$$\partial_t u_i = \frac{1}{2}\left(\Delta u_i - \frac{1}{\epsilon^2}F'(u_i) \right) + \lambda(t), \quad \text{for all } i \in \{1, \dots, N\},$$

where $\lambda(t)$ is a Lagrange multiplier associated to the constraint $\mathbf{u} \in \Sigma$ that can be explicitly computed as $\lambda(t) = \frac{1}{N\epsilon^2}\sum_{i=1}^N F'(u_i)$. The flow is an Allen-Cahn system that can be easily approximated numerically, for instance using a splitting method with an implicit resolution of the diffusion term in Fourier space coupled with an explicit treatment of the reaction term [16].

The case of a general surface tension $\sigma \in S_N$ is more involved. In [29, 28], Garcke et al studied phase-field approximations of the general form

$$P_\epsilon(\mathbf{u}) = \begin{cases} \int \epsilon f(\mathbf{u}, \nabla \mathbf{u}) + \frac{1}{\epsilon}\mathbf{W}(\mathbf{u})dx & \text{if } \mathbf{u} \in \Sigma \cap (\mathrm{W}^{1,2}(\Omega,\mathbb{R}))^N, \\ +\infty & \text{otherwise.} \end{cases}$$

The category of functions f and $\mathbf{W}$ for which the results obtained in the paper apply is quite general, but the authors have a preference for

$$f(\mathbf{u}, \nabla \mathbf{u}) = \sum_{i,j=1}^N \frac{\alpha_{i,j}}{2}\left|u_i \nabla u_j - u_j \nabla u_i\right|^2, \quad \text{with } (\alpha_{i,j})_{i,j} \in S_N, \tag{2.1}$$

and $\mathbf{W}$ a positive multi-well potential defined on Σ and vanishing only at each standard unit vector of the canonical basis $(e_1, \ldots, e_N)$ of $\mathbb{R}^N$. Each vector $\mathbf{e}_i$ corresponds to a phase, and a N-phase system is given by $\mathbf{u} = \sum_{i=1}^N u_i \mathbf{e}_i$ with $\sum u_i = 1$. The authors of [29] propose a multi-well potential of the form

$$\mathbf{W}(\mathbf{u}) = \sum_{i,j=1}^N \frac{1}{2}\alpha_{i,j}u_i^2u_j^2 + \sum_{i<j<k}\alpha_{i,j,k}u_i^2u_j^2u_k^2. \tag{2.2}$$

It is explained in [28] that to expect the Γ-convergence of P_ϵ to P the following equality *must* be true

$$\sigma_{i,j}(n) = 2\inf_p \int_{-1}^1 \sqrt{\mathbf{W}(p)f(p, p' \otimes n)}ds, \quad \text{for all } n \in S(\mathbb{R}^d), \tag{2.3}$$

where p ranges over all Lipschitz continuous functions $p : [-1,1] \to \Sigma$, connecting the vectors $\mathbf{e}_i$ to $\mathbf{e}_j$. This condition raises a central issue in all phase-field models for the approximation of multiphase perimeters: given a set of surface tensions $(\sigma_{i,j})$, how to define $\mathbf{W}$ so that the previous equality holds and the Γ-convergence is guaranteed? It is really not a purely formal question: Γ-convergence does not only allow to approximate the energy of local minimizers, it also guarantees that minimizers of P_ϵ do converge, up to a subsequence, to a minimizer of P [19, 10].

So far, the only results in this direction are due to Haas, who proved in [30] that, if $\mathbf{W}$ is a polynomial of order at most four, then only polynomials of the form

$$\sum_{i,j=1}^N \alpha_{i,j}u_i^2u_j^2 + \sum_{i,j,k}\alpha_{i,j,k}u_iu_ju_k^2 + \sum_{i,j,k,l}\alpha_{i,j,k,l}u_iu_ju_ku_l$$

prevent from the creation of ghost phases in the limit, i.e. a geodesic defined as in the right term of (2.3) and connecting two phases $\mathbf{e}_i$ and $\mathbf{e}_j$ passes only through the points $t\mathbf{e}_i + (1-t)\mathbf{e}_j$. However, no way is provided in [30] of consistently deriving the parameters $\alpha_{i,j}$, $\alpha_{i,j,k}$, and $\alpha_{i,j,k,l}$ from the $\sigma_{i,j}$'s so that (2.3) holds.

We will show in this paper that, assuming a ℓ^1-embeddability condition for σ (see below), there is a consistent and explicit way to construct a polynomial $\mathbf{W}$. As for the gradient term, the choice (2.1) yields a gradient flow corresponding to a reaction-diffusion system where the diffusion terms are nonlinear and ill-conditioned, which raises numerical issues. Another choice will be shown to be more convenient. More precisely, we propose an energy of the form

$$P_\epsilon(\mathbf{u}) = \begin{cases} \int_\Omega -\frac{\epsilon}{4}\sigma\nabla\mathbf{u}\cdot\nabla\mathbf{u} + \frac{1}{\epsilon}\mathbf{W}_\sigma(\mathbf{u})dx & \text{if } \mathbf{u}\in\Sigma\cap(\mathrm{W}^{1,2}(\Omega,\mathbb{R}))^N, \\ +\infty & \text{otherwise,} \end{cases}$$

where the diffusion term reads $\sigma\nabla\mathbf{u}\cdot\nabla\mathbf{u} = \sum_{i,j=1}^N \sigma_{i,j}\nabla u_i\cdot\nabla u_j$ and $\mathbf{W}_\sigma(\mathbf{u})$ is defined from the $\sigma_{i,j}$'s as

$$\mathbf{W}_\sigma(\mathbf{u}) = \frac{1}{4}\sum_{i,j=1}^N \sigma_{i,j}u_i^2u_j^2 + \frac{1}{2}\sum_{i<j,k\neq i,k\neq j}\sigma_{i,k,j}u_iu_ju_k^2 + \sum_{i<j<k<l}\sigma_{i,j,k,l}u_iu_ju_ku_l,$$

with

$$\sigma_{i,j,k} = (\sigma_{i,k}+\sigma_{j,k}-\sigma_{i,j}) \quad \text{and} \quad \sigma_{i,j,k,l} = 6\sigma^*_{i,j,k,l} - \sum_{(i',j')\subset\{i,j,k,l\},\ i'<j'}\sigma_{i',j'},$$

where $\sigma^*_{i,j,k,l}$ is chosen in the following interval (see the beginning of Section 4 for more details):

$$I_{i,j,k,l} = \left[\max_{\substack{i',j',k',l'\in\{i,j,k,l\}\\ i'\neq j'\neq k'\neq l'}}\left\{\frac{\sigma_{i',j'}+\sigma_{k',l'}}{2}\right\},\ \min_{\substack{i',j',k',l'\in\{i,j,k,l\}\\ i'\neq j'\neq k'\neq l'}}\left\{\frac{\sigma_{i',j'}+\sigma_{i',k'}+\sigma_{i',l'}}{2}\right\}\right].$$

We will prove that this model fulfills properties (P1)-(P5) mentioned above.

The next section is devoted to the derivation of our phase field energy P_ϵ. In Section 4, we give a proof of the Γ-convergence of P_ϵ to $c_F P$. Section 5 addresses the L^2-gradient flow of P_ϵ, and some extensions to incorporate additional constraints of volume and partial phase stationarity, in particular for the evolution of multi-droplets. Finally, we present n Section 6 some numerical experiments which highlight the good behavior of our model.

3 Derivation of the phase field model

We first consider the particular case of additive surface tensions, and then the more general ℓ^1-embeddable surface tensions, for which it turns out that the perimeter P can be expressed as the sum of perimeters associated with union of different phases. This particular form of perimeter is the key for deriving our Γ-convergent phase-field model.

3.1 Additive surface tensions

The simplest case of inhomogeneous surface tensions $\sigma_{i,j}$ is the case of additive surface tensions, i.e. surface tensions $(\sigma_{i,j})$ for which there exist some positive coefficients $(\sigma_1, \sigma_2, \dots, \sigma_N) \in (\mathbb{R}^+)^N$ such that

$$\sigma_{i,j} = \sigma_i + \sigma_j, \quad \text{with } \sigma_i > 0, \quad \text{for all} \quad i, j = 1, \dots, N.$$

In this situation we have

$$P(\Omega_1, ...\Omega_N) = \frac{1}{2}\sum_{i,j=1}^{N} \sigma_{i,j}\mathcal{H}^{d-1}(\Gamma_{i,j}) = \sum_{i=1}^{N} \sigma_i \mathcal{H}^{d-1}(\partial^*\Omega_i),$$

which is, once again, a rewriting of the multiphase perimeter as a linear combination of simple perimeters. It leads to the following natural approximating candidate (denoting as before, and in the sequel as well, $F(s) = \frac{s^2(1-s)^2}{2}$):

$$P_\epsilon(\mathbf{u}) = \begin{cases} \displaystyle\sum_{i=1}^{N} \sigma_i (\int_\Omega \frac{\epsilon}{2}|\nabla u_i|^2 + \frac{1}{\epsilon}F(u_i))dx, & \text{if } \mathbf{u} \in \Sigma \cap (\mathrm{W}^{1,2}(\Omega, \mathbb{R}))^N, \\ +\infty & \text{otherwise.} \end{cases}$$

An easy adaptation of the homogeneous case to this inhomogeneous setting yields the Γ-convergence of P_ϵ to $c_F P$ as ϵ goes to 0. Remark also that, as $\nabla \sum_{j=1}^N u_j = \nabla 1 = 0$, one has

$$\begin{aligned} -\frac{1}{4}\sigma\nabla\mathbf{u}\cdot\nabla\mathbf{u} &= -\frac{1}{4}\sum_{i,j=1}^{N}(\sigma_{i,j})\nabla u_i \cdot \nabla u_j = -\frac{1}{4}\sum_{i,j=1, i\neq j}^{N}(\sigma_i + \sigma_j)\nabla u_i \cdot \nabla u_j \\ &= -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\sigma_i \nabla u_i \cdot \nabla u_j + \frac{1}{2}\sum_{i=1}^{N}\sigma_i|\nabla u_i|^2 \\ &= \frac{1}{2}\sum_{i=1}^{N}\sigma_i|\nabla u_i|^2. \end{aligned}$$

This implies that P_ϵ can be expressed as:

$$P_\epsilon(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega (-\frac{\epsilon}{4}\sigma\nabla\mathbf{u}\cdot\nabla\mathbf{u} + \frac{1}{\epsilon}\mathbf{W}_\sigma(\mathbf{u}))dx & \text{if } \mathbf{u} \in \Sigma \cap (\mathrm{W}^{1,2}(\Omega, \mathbb{R}))^N, \\ +\infty & \text{otherwise,} \end{cases}$$

where the multi-well potential $\mathbf{W}_\sigma$ is defined as:

$$\mathbf{W}_\sigma(\mathbf{u}) = \sum_{i=1}^{N}\sigma_i F(u_i).$$

3.1.1 Potential for triphasic systems ($N = 3$) with triangle inequality

It is easily seen that all surface tension matrix $\sigma \in S_3$ satisfying the triangle inequality (1.2) is actually additive. Indeed, we have

$$\sigma_1 = \frac{\sigma_{1,2} + \sigma_{1,3} - \sigma_{2,3}}{2}, \quad \sigma_2 = \frac{\sigma_{2,1} + \sigma_{2,3} - \sigma_{1,3}}{2}, \text{ and } \sigma_3 = \frac{\sigma_{3,1} + \sigma_{3,2} - \sigma_{1,2}}{2},$$

We deduce from the previous section the form of the potential term:

$$\begin{aligned} \mathbf{W}_\sigma(\mathbf{u}) &= \sigma_1 F(u_1) + \sigma_2 F(u_2) + \sigma_3 F(u_3) \\ &= \frac{\sigma_{1,2}}{2}\left(F(u_1) + F(u_2) - F(u_3)\right) + \frac{\sigma_{1,3}}{2}\left(F(u_1) + F(u_3) - F(u_2)\right) + \frac{\sigma_{2,3}}{2}\left(F(u_2) + F(u_3) - F(u_1)\right). \end{aligned}$$

More precisely, remark that for all $\mathbf{u} \in \Sigma$,

$$\begin{aligned} F(u_1) + F(u_2) - F(u_3) &= \frac{1}{2}u_1^2(1-u_1)^2 + \frac{1}{2}u_2^2(1-u_2)^2 - \frac{1}{2}u_3^2(1-u_3)^2 \\ &= \frac{1}{2}u_1^2(u_2+u_3)^2 + \frac{1}{2}u_2^2(u_1+u_3)^2 - \frac{1}{2}u_3^2(u_1+u_2)^2 \\ &= u_1^2u_2^2 + u_1^2u_2u_3 + u_2^2u_1u_3 - u_3^2u_1u_2. \end{aligned}$$

In particular, this shows that

$$\begin{aligned} \mathbf{W}_\sigma(\mathbf{u}) &= \frac{1}{2}\sigma_{1,2}u_1^2u_2^2 + \frac{1}{2}\sigma_{1,3}u_1^2u_3^2 + \frac{1}{2}\sigma_{2,3}u_2^2u_3^2 \\ &+ \frac{1}{2}(\sigma_{1,2} + \sigma_{1,3} - \sigma_{2,3})u_2u_3u_1^2 + \frac{1}{2}(\sigma_{1,3} + \sigma_{2,3} - \sigma_{1,2})u_1u_2u_3^2 + \frac{1}{2}(\sigma_{1,2} + \sigma_{2,3} - \sigma_{1,3})u_1u_3u_2^2 \\ &= \frac{1}{4}\sum_{i,j=1}^{N} \sigma_{i,j}u_i^2u_j^2 + \frac{1}{2}\sum_{i<j,k\neq i,k\neq j} \sigma_{i,j,k}u_iu_ju_k^2, \end{aligned}$$

where

$$\sigma_{i,j,k} = \sigma_{i,k} + \sigma_{k,j} - \sigma_{i,j}.$$

3.1.2 Potential for additive surface tensions when $N > 3$

The additive case $N > 3$ follows from the computation above. Let us assume the existence of some positive coefficients $(\sigma_1, \sigma_2, \dots, \sigma_N) \in (\mathbb{R}^+)^N$ such that

$$\sigma_{i,j} = \sigma_i + \sigma_j, \quad \text{with } \sigma_i > 0, \quad \text{for all} \quad i = 1, \dots, N.$$

Then, for all $u \in \Sigma$, the multi-well potential $\mathbf{W}$ is as before :

$$\begin{aligned} \mathbf{W}_\sigma(\mathbf{u}) &= \sum_{i=1}^{N} \sigma_i F(u_i) = \frac{1}{2}\sum_{i=1}^{N} \sigma_i u_i^2(1-u_i)^2 = \frac{1}{2}\sum_{i=1}^{N} \sigma_i u_i^2 (\sum_{j=1,j\neq i}^{N} u_j)^2 \\ &= \frac{1}{2}\sum_{i,j=1,i\neq j}^{N} \sigma_i u_i^2u_j^2 + \sum_{j<k,i\neq j,i\neq k}^{N} \sigma_i u_ju_ku_i^2 \\ &= \frac{1}{4}\sum_{i,j=1}^{N} \sigma_{i,j}u_i^2u_j^2 + \frac{1}{2}\sum_{i<j,i\neq k,j\neq k}^{N} \sigma_{i,j,k}u_iu_ju_k^2, \end{aligned}$$

where

$$\sigma_{i,j} = \sigma_i + \sigma_j, \quad \text{and} \quad \sigma_{i,j,k} = \sigma_{i,k} + \sigma_{k,j} - \sigma_{i,j} = 2\sigma_k.$$

We now synthesize the results of this section on additive surface tensions:

Proposition 3.1. Let $(\sigma_1, \sigma_2, \ldots, \sigma_N) \in (\mathbb{R}^+)^N$ such that $\sigma_{i,j} = \sigma_i + \sigma_j$ with $\sigma_i > 0$ for all $i = 1, \ldots, N$. Then the phase-field perimeter

$$P_\epsilon(\mathbf{u}) = \begin{cases} \int_\Omega (-\frac{\epsilon}{4}\sigma \nabla \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\epsilon}\mathbf{W}_\sigma(\mathbf{u}))dx & \text{if } \mathbf{u} \in \Sigma \cap (\mathrm{W}^{1,2}(\Omega, \mathbb{R}))^N, \\ +\infty & \text{otherwise,} \end{cases}$$

$$\text{where} \quad \mathbf{W}_\sigma(\mathbf{u}) = \frac{1}{4}\sum_{i,j=1}^{N} (\sigma_i + \sigma_j) u_i^2 u_j^2 + \sum_{i<j, i\neq k, j\neq k}^{N} \sigma_k u_i u_j u_k^2,$$

Γ-converges to $c_F P$ as $\epsilon \to 0^+$.

We conclude this section observing that the Γ-convergence follows from a rewriting of the multiphase perimeter in terms of full boundaries. Let us now describe how the same idea can be applied as well for a much more general class of surface tensions, namely the ℓ^1-embeddable surface tensions whose definition is given in the next section.

3.2 ℓ^1-embeddable surface tensions

Definition 3.2. A matrix $\sigma = (\sigma_{i,j}) \in S_N$ is called ℓ^1-embeddable if there exist some integer M and N points $p_i \in \mathbb{R}^M$ such that $\sigma_{i,j} = \|p_i - p_j\|_1$ where $\|\cdot\|_1$ is the ℓ^1 metric in $\mathbb{R}^M$.

The notion of embeddability in metric spaces plays an important role in graph theory, see the remarkable survey [21]. Interestingly, it has connections with conditionally semi-definite matrices (i.e. matrices satisfying condition 1.4) for which the minimizing scheme proposed in [25] applies. More precisely, the following properties hold [25, 21]:

1. All ℓ^1-embeddable matrices satisfy the triangle inequality (1.2). The converse is true if and only if $N \leq 4$. Every ℓ^1-embeddable matrix is conditionally negative semi-definite, but the converse is false according to the next item.

2. Being conditionally negative semi-definite is neither a necessary nor a sufficient condition for a matrix to satisfy the triangle inequality; as an important consequence, Esedoḡlu-Otto's scheme [25] is also valid for many matrices which violate the triangle inequality, which is useful for the consistent simulation of wetting and nucleation phenomena.

3. Given a set of N points $\mathcal{P} = \{p_1, \ldots, p_N\} \subset \mathbb{R}^M$, a metric d on $\mathcal{P}$ is a cut-metric if there exists $S \subset \mathcal{P}$ such that

$$d(p_i, p_j) = d_S(p_i, p_j) = \begin{cases} 1 & \text{if } \delta_S(p_i) \neq \delta_S(p_j), \\ 0 & \text{otherwise,} \end{cases}$$

where $\delta_S(p_i) = 1$ if $p_i \in S$ and 0 otherwise. A fundamental property of ℓ^1-embeddable matrices is that they can be expressed in terms of cut-metrics [21]. We will refer to it as the Cut Cone Property in the sequel:

(**Cut Cone Property**)

Let $\sigma = (\sigma_{ij})_{i,j\in\{1,\dots,N\}}$ be a ℓ^1-embeddable surface tension matrix. Then there exists $M \in \mathbb{N}^*$, a collection of N points $\{p_1,\dots,p_N\} \subset \mathbb{R}^M$ and a collection of coefficients $\sigma_S \geq 0$, $S \subset \{1,\dots,N\}$, such that

$$\sigma_{i,j} = \|p_i - p_j\|_1 = \sum_{S\subset\{1,\dots,N\}} \sigma_S d_S(p_i,p_j), \qquad i,j \in \{1,\dots,N\}. \tag{3.1}$$

It is important to notice that this decomposition involves *all* subsets of $\{1,\dots,N\}$, and that it needs not be unique.

This latter property has a very interesting consequence for multiphase perimeters [25, 21] which is stated below, and which plays a key role for exhibiting Γ-converging approximation perimeters in the general context of ℓ^1-embeddable surface tensions (see the next section).

Lemma 3.3. If $\sigma = (\sigma_{i,j}) \in S_N$ is ℓ^1-embeddable then there exists a collection of nonnegative coefficients σ_S defined for all $S \subset \{1,\dots,N\}$ such that:

$$P(\Omega_1,\Omega_2,\dots,\Omega_N) = \frac{1}{2}\sum_{i,j=1}^N \sigma_{i,j}\mathcal{H}^{d-1}(\Gamma_{i,j}) = \sum_{S\subset\{1,\dots,N\}} \sigma_S P(\cup_{i\in S}\Omega_i),$$

where P denotes the perimeter.

PROOF The result follows directly from the Cut Cone Property decomposition $\sigma_{i,j} = \|p_i - p_j\|_1 = \sum_{S\subset\{1,\dots,N\}} \sigma_S d_S(p_i,p_j)$. Indeed,

$$P(\Omega_1,\Omega_2,\dots,\Omega_N) = \frac{1}{2}\sum_{i,j=1}^N \sum_{S\subset\{1,\dots,N\}} \sigma_S d_S(p_i,p_j)\mathcal{H}^{d-1}(\Gamma_{i,j}) = \frac{1}{2}\sum_{S\subset\{1,\dots,N\}} \sigma_S \sum_{i,j=1}^N d_S(p_i,p_j)\mathcal{H}^{d-1}(\Gamma_{i,j}).$$

However, $d_S(p_i,p_j)\mathcal{H}^{d-1}(\Gamma_{i,j})$ vanishes when i,j are either both in S or both outside, therefore the only remaining interfaces $\Gamma_{i,j}$ are those between a phase in S and a phase outside S. Therefore, given $S \subset \{1,\dots,N\}$,

$$\frac{1}{2}\sum_{i,j=1}^N d_S(p_i,p_j)\mathcal{H}^{d-1}(\Gamma_{i,j}) = \mathcal{H}^{d-1}(\partial^*(\cup_{i\in S}\Omega_i)) = P(\cup_{i\in S}\Omega_i),$$

and the lemma ensues. □

Example 3.4. Let $N = 4$ and consider $\sigma_{1,2} = \sigma_{1,3} = \sigma_{2,4} = \sigma_{3,4} = 2$, and $\sigma_{2,3} = \sigma_{1,4} = 1$. These surface tension coefficients do not satisfy the additive property, as $\sigma_{1,2} + \sigma_{1,3} - \sigma_{2,3} \neq \sigma_{1,2} + \sigma_{1,4} - \sigma_{2,4}$. Furthermore, the perimeter can be expressed as:

$$\frac{1}{2}\sum_{i,j=1}^{4} \sigma_{i,j}\mathcal{H}^{d-1}(\Gamma_{i,j}) = \frac{1}{2}\sum_{i=1}^{4} P(\Omega_i) + P(\Omega_1 \cup \Omega_4),$$

therefore a possible choice for coefficients σ_S is:

$$\sigma_S = \begin{cases} \frac{1}{2} & \text{if } S = \{i\}, \quad i \in \{1, \dots, 4\}, \\ 1 & \text{if } S = \{1, 4\}, \\ 0 & \text{otherwise.} \end{cases}$$

The model introduced in this paper will be proved to Γ-converge whenever the surface tension matrix is *strictly* ℓ^1-embeddable, according to the following definition.

Definition 3.5. A matrix $\sigma = (\sigma_{i,j}) \in S_N$ is called strictly ℓ^1-embeddable if the Cut Cone Property (3.1) holds for a collection $\{\sigma_S \geq 0,\ S \subset \{1, \dots, N\}\}$ such that $\sigma_{\{i\}} > 0$, $\forall i \in \{1, \dots, N\}$.

Remark 3.6. A *necessary* condition for strict ℓ^1-embeddability is the strict triangle inequality, i.e.

$$\textit{(Strict triangle inequality)} \qquad \sigma_{i,k} < \sigma_{i,j} + \sigma_{j,k}, \qquad \forall (i,j,k),\ i \neq j \neq k. \tag{3.2}$$

Indeed, we have that $\sigma_{i,j} + \sigma_{j,k} = \sum \sigma_S[d_S(p_i, p_j) + d_S(p_j, p_k)]$. Then, observe that $d_S(p_i, p_j) + d_S(p_j, p_k) \geq d_S(p_i, p_k)$ since the right term is either 0 or 1, it equals 1 as soon as $\delta_S(p_i) \neq \delta_S(p_k)$ i.e. p_i and p_k are not both in S or both outside S, and in this case the left term equals at least 1 since p_k is either in S or outside S. Then, we focus on the case $S = \{j\}$: since $i, k \neq j$ and $\sigma_{i,j}, \sigma_{j,k} > 0$ (because $\sigma \in S_N$), $d_{\{j\}}(p_i, p_k) = 0$ but $d_{\{j\}}(p_i, p_j) + d_{\{j\}}(p_j, p_k) = 2$. It follows from $\sigma_{\{j\}} > 0$ that $\sigma_{i,k} < \sigma_{i,j} + \sigma_{j,k}$.

In the case $N = 4$, the strict triangle inequality is also a *sufficient* condition for strict ℓ^1-embeddability, see Remark 3.7. From the same remark, it follows when $N > 4$ that the ℓ^1-embeddability together with the strict triangle inequality imply the strict ℓ^1-embeddability.

3.3 Derivation of the approximation perimeter for ℓ^1-embeddable surface tensions

In the case of additive surface tensions, as we saw above, the multiphase perimeter can be directly written as a nonnegative combination of integrals on boundaries of sets (and not subsets of boundaries), which allows a multiphase approximation. As it follows from Lemma 3.3, a similar decomposition holds for ℓ^1-embeddable surface tensions. Thus, a multiphase approximation is again possible, and a natural candidate to approximate P is given by

$$P_\epsilon(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \left[\sum_{S \subset \{1,\dots,N\}} \sigma_S \left(\frac{\epsilon}{2} \left| \nabla (\sum_{i \in S} u_i) \right|^2 + \frac{1}{\epsilon} F(\sum_{i \in S} u_i) \right) \right] dx & \text{if } u \in \Sigma \cap (\mathrm{W}^{1,2}(\Omega, \mathbb{R}))^N, \\ +\infty & \text{otherwise,} \end{cases}$$

where the coefficients σ_S are given by the Cut Cone Property (3.1). Note that for $N \geq 4$, the decomposition is not unique.

This expression has a drawback: the σ_S's are unknown. We will now derive another expression which can be explicitly computed from the surface tension matrix $\sigma = (\sigma_{i,j})$ as soon as $\sigma_{i,j} > 0$ whenever $i \neq j$.

3.3.1 A condensed form for the approximating multiphase perimeter

Let $\alpha_i = \sum_{S\subset\{1,\dots,N\}} \sigma_S \delta_{i\in S}$ and $\alpha_{i,j} = \sum_{S\subset\{1,\dots,N\}} \sigma_S \delta_{i\in S}\delta_{j\in S}$ with $\delta_{i\in S} = 1$ if $i \in S$, 0 otherwise. Since σ is assumed to be ℓ^1-embeddable, it follows from the Cut Cone Property (3.1) that

$$\sigma_{i,j} = \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{i\in S}\delta_{j\notin S} + \delta_{i\notin S}\delta_{j\in S}\right) = \alpha_i + \alpha_j - 2\alpha_{i,j}.$$

Then we have for all $\mathbf{u} \in \Sigma \cap (\mathrm{W}^{1,2}(\Omega,\mathbb{R}))^N$:

$$\begin{aligned}
\sum_{S\subset\{1,\dots,N\}} \sigma_S \left|\nabla(\sum_{i\in S} u_i)\right|^2 &= \sum_{S\subset\{1,\dots,N\}} \sigma_S \nabla\left[\sum_{i\in S} u_i\right] \cdot \nabla\left[\sum_{j\in S} u_j\right] \\
&= \sum_{i,j=1}^{N} \left[\sum_{S\subset\{1,\dots,N\}} \sigma_S \delta_{i\in S}\delta_{j\in S}\right] \nabla u_i \cdot \nabla u_j \\
&= \sum_{i,j=1, i\neq j}^{N} \alpha_{i,j} \nabla u_i \cdot \nabla u_j + \sum_{i=1}^{N} \alpha_i |\nabla u_i|^2 \\
&= -\frac{1}{2} \sum_{i,j=1,i\neq j}^{N} \sigma_{i,j} \nabla u_i \cdot \nabla u_j + \sum_{i,j=1,i\neq j}^{N} \alpha_i \nabla u_i \cdot \nabla u_j + \sum_{i=1}^{N} \alpha_i |\nabla u_i|^2 \\
&= -\frac{1}{2}\sigma \nabla\mathbf{u} \cdot \nabla\mathbf{u} + \sum_{i=1}^{N} \alpha_i \nabla u_i \cdot \nabla\left(\sum_{j=1}^{N} u_j\right) \\
&= -\frac{1}{2}\sigma \nabla\mathbf{u} \cdot \nabla\mathbf{u}.
\end{aligned}$$

To conclude, the approximating perimeter introduced above can be rewritten as

$$P_\epsilon(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega -\frac{\epsilon}{4}\sigma\nabla\mathbf{u}\cdot\nabla\mathbf{u} + \frac{1}{\epsilon}\mathbf{W}_\sigma(\mathbf{u})dx & \text{if } \mathbf{u} \in \Sigma \cap (\mathrm{W}^{1,2}(\Omega,\mathbb{R}))^N, \\ +\infty & \text{otherwise,} \end{cases}$$

where the multi-well potential $\mathbf{W}_\sigma(\mathbf{u})$ reads

$$\mathbf{W}_\sigma(u) = \sum_{S\subset\{1,\dots,N\}} \sigma_S F(\sum_{i\in S} u_i). \tag{3.3}$$

3.3.2 Rewriting the potential when $N = 4$

When $N = 4$, any surface tension matrix satisfying the triangle inequality (1.2) is ℓ^1–embeddable [21], thus the perimeter is decomposable as:

$$P(\Omega_1, \Omega_2, \dots, \Omega_4) = \frac{1}{2}\sum_{i,j=1}^{4} \sigma_{i,j}\mathcal{H}^{d-1}(\Gamma_{i,j}) = \sum_{S\subset\{1,2,3,4\}} \sigma_S \mathcal{H}^{d-1}(\partial^*(\cup_{i\in S}\Omega_i)), \tag{3.4}$$

but no explicit formula is known for the coefficients σ_S. Let us try to reformulate the decomposition in order to make it more explicit. Considering the whole collection of sets $\cup_{i\in S}\Omega_i$, $S \subset \{1, \dots, N\}$ we define :

$$Q_1 = \Omega_1,\ Q_2 = \Omega_2,\ Q_3 = \Omega_3,\ Q_4 = \Omega_4,$$

and

$$\begin{cases} Q_5 = \Omega_1 \cup \Omega_2 = (\Omega_3 \cup \Omega_4)^c, \\ Q_6 = \Omega_1 \cup \Omega_3 = (\Omega_2 \cup \Omega_4)^c, \\ Q_7 = \Omega_2 \cup \Omega_3 = (\Omega_1 \cup \Omega_4)^c. \end{cases}$$

Remark first that for all i, j

$$2\mathcal{H}^{d-1}(\partial^*\Omega_i \cap \partial^*\Omega_j) = \mathcal{H}^{d-1}(\partial^*\Omega_i) + \mathcal{H}^{d-1}(\partial^*\Omega_j) - \mathcal{H}^{d-1}(\partial^*(\Omega_i \cup \Omega_j)).$$

Then we define

$$\begin{cases} \tilde\sigma_1 & = (\sigma_{12} + \sigma_{13} + \sigma_{14})/2, \\ \tilde\sigma_2 & = (\sigma_{12} + \sigma_{23} + \sigma_{24})/2, \\ \tilde\sigma_3 & = (\sigma_{13} + \sigma_{23} + \sigma_{34})/2, \\ \tilde\sigma_4 & = (\sigma_{14} + \sigma_{24} + \sigma_{34})/2, \end{cases} \quad \text{and} \quad \begin{cases} \tilde\sigma_5 & = -(\sigma_{12} + \sigma_{34})/2, \\ \tilde\sigma_6 & = -(\sigma_{13} + \sigma_{24})/2, \\ \tilde\sigma_7 & = -(\sigma_{14} + \sigma_{23})/2, \end{cases}$$

and we calculate from (3.4) that

$$P(\Omega_1, \Omega_2, \Omega_3, \Omega_4) = \sum_{i=1}^{7} \tilde\sigma_i \mathcal{H}^{d-1}(\partial^* Q_i).$$

This new formulation is however not convenient because $\tilde\sigma_5$, $\tilde\sigma_6$ and $\tilde\sigma_7$ are negative, which is an obstacle to the Γ-convergence. However, the fact that

$$\sum_{i=1}^{4} \mathcal{H}^{d-1}(\partial^*\Omega_i) = \mathcal{H}^{d-1}(\partial^*(\Omega_1 \cup \Omega_2)) + \mathcal{H}^{d-1}(\partial^*(\Omega_1 \cup \Omega_3)) + \mathcal{H}^{d-1}(\partial^*(\Omega_1 \cup \Omega_4)),$$

implies that

$$P(\Omega_1, \Omega_2, \Omega_3, \Omega_4) = \sum_{i=1}^{4}(\tilde\sigma_i - \sigma^*)\mathcal{H}^{d-1}(\partial^* Q_i) + \sum_{i=5}^{7}(\tilde\sigma_i + \sigma^*)\mathcal{H}^{d-1}(\partial^* Q_i),$$

for all $\sigma^* \in \mathbb{R}$. In particular, the previous equality gives one degree of freedom depending on the value of σ^*. Remark now that

$$\tilde{\sigma}_1 + \tilde{\sigma}_5 = \frac{(\sigma_{12} + \sigma_{13} + \sigma_{14})}{2} - \frac{(\sigma_{12} + \sigma_{34})}{2} = \frac{(\sigma_{13} + \sigma_{14} - \sigma_{34})}{2},$$

which is always positive as σ satisfies the triangle inequality (1.2). Therefore, for all $i \in \{1, 2, 3, 4\}$ and for all $j \in \{5, 6, 7\}$, we have $\tilde{\sigma}_i + \tilde{\sigma}_j \geq 0$. Denoting

$$\sigma_{min} = \max_{i=5,6,7} \{-\tilde{\sigma}_i\}, \quad \text{and} \quad \sigma_{max} = \min_{i=1,2,3,4} \{\tilde{\sigma}_i\},$$

we deduce that $\sigma_{min} \leq \sigma_{max}$. Let us now choose arbitrarily $\sigma^* \in [\sigma_{min}, \sigma_{max}]$ and define

$$\begin{cases} \sigma_i = \tilde{\sigma}_i - \sigma^* & \text{for } i = 1, \dots, 4, \\ \sigma_i = \tilde{\sigma}_i + \sigma^* & \text{otherwise }, \end{cases}$$

Obviously

$$P(\Omega_1, \Omega_2, \Omega_3, \Omega_4) = \sum_{i=1}^{7} \sigma_i \mathcal{H}^{d-1}(\partial^* Q_i),$$

and, from our observations above, $\sigma_i \geq 0$ for all $i \in \{1, \dots, 7\}$.

Remark 3.7. In the particular case where $(\sigma_{i,j})$ satisfies the strict triangle inequality (3.2), then $\sigma_{min} < \sigma_{max}$ thus one can choose $\sigma^* = (\sigma_{min} + \sigma_{max})/2$ so that $\sigma_i > 0$ for every $i \in \{1, \dots, 7\}$, i.e. σ is strictly ℓ^1-embeddable.

Remark 3.8. Combined with a dimensional argument, the previous construction shows that, for every decomposition of P of the form

$$P(\Omega_1, \Omega_2, \Omega_3, \Omega_4) = \sum_{i=1}^{7} \alpha_i \mathcal{H}^{d-1}(\partial^* Q_i),$$

with $\alpha_i \geq 0$, we can associate a coefficient $\sigma^* \in [\sigma_{min}, \sigma_{max}]$ such that

$$\begin{cases} \alpha_i = \tilde{\sigma}_i - \sigma^* & \text{for } i = 1, \dots, 4, \\ \alpha_i = \tilde{\sigma}_i + \sigma^* & \text{for } i = 5, \dots, 7. \end{cases}$$

The decomposition we have obtained leads to a natural potential for the phase-field approximation, i.e. $\mathbf{W}_\sigma$ can be chosen as

$$\begin{aligned} \mathbf{W}_\sigma(\mathbf{u}) &= \left(\sum_{i=1}^{4} \sigma_i F(u_i) \right) + \sigma_5 F(u_1 + u_2) + \sigma_6 F(u_1 + u_3) + \sigma_7 F(u_1 + u_4) \\ &= \frac{1}{2} \sum_{i,j=1, i<j}^{4} \sigma_{i,j} \left(F(u_i) + F(u_j) - F(u_i + u_j) \right) + \sigma^* \left(\sum_{i=2}^{4} F(u_1 + u_i) - \sum_{i=1}^{4} F(u_i) \right). \end{aligned}$$

Moreover, remark that for all $\mathbf{u} \in \Sigma$, we have

$$\begin{aligned}
\sum_{i=1}^{4} F(u_i) &= F(u_1) + F(u_2) + F(u_3) + F(u_4) \\
&= \frac{1}{2}\left[u_1^2(u_2+u_3+u_4)^2 + u_2^2(u_1+u_3+u_4)^2 + u_3^2(u_1+u_3+u_4)^2 + u_4^2(u_1+u_2+u_3)^2\right] \\
&= \sum_{i<j} u_i^2 u_j^2 + \sum_{i<j,k\neq i,k\neq j} u_i u_j u_k^2,
\end{aligned}$$

$$\begin{aligned}
\sum_{i=2}^{4} F(u_1+u_i) &= F(u_1+u_2) + F(u_1+u_3) + F(u_1+u_4) \\
&= \frac{1}{2}\left[(u_1+u_2)^2(u_3+u_4)^2 + (u_1+u_3)^2(u_2+u_4)^2 + (u_1+u_4)^2(u_2+u_3)^2\right] \\
&= \sum_{i<j} u_i^2 u_j^2 + \sum_{i<j,k\neq i,k\neq j} u_i u_j u_k^2 + 6u_1u_2u_3u_4,
\end{aligned}$$

and

$$\begin{aligned}
F(u_1) + F(u_2) - F(u_1+u_2) &= \frac{1}{2}\left(u_1^2(u_2+u_3+u_4)^2 + u_2^2(u_1+u_3+u_4)^2 - (u_1+u_2)^2(u_3+u_4)^2\right) \\
&= u_1^2u_2^2 + u_1^2u_2u_3 + u_1^2u_2u_4 + u_2^2u_1u_3 + u_2^2u_1u_4 \\
&\quad - u_3^2u_1u_2 - u_4^2u_1u_2 - 2u_1u_2u_3u_4.
\end{aligned}$$

In particular, this shows that the potential $\mathbf{W}_\sigma$ has the form

$$\mathbf{W}_\sigma(\mathbf{u}) = \frac{1}{4}\sum_{i,j=1}^{N} \sigma_{i,j} u_i^2 u_j^2 + \frac{1}{2}\sum_{i<j,k\neq i,k\neq j} \sigma_{i,j,k} u_i u_j u_k^2 + \lambda u_1u_2u_3u_4,$$

where $\lambda = (6\sigma^* - \sum_{i<j}\sigma_{i,j})$ and $\sigma_{i,j,k} = \sigma_{i,k} + \sigma_{j,k} - \sigma_{i,j}$.

Remark 3.9. Remark that, as $\sigma_{min} \geq \frac{1}{2}\max\{\sigma_{12}+\sigma_{34}, \sigma_{13}+\sigma_{24}, \sigma_{14}+\sigma_{23}\} \geq \frac{1}{6}\sum_{i<j}\sigma_{i,j}$, it follows that λ is nonnegative. In addition, if $\lambda = 0$ then $\sigma^* = \sigma_{\min} = \frac{1}{6}\sum_{i<j}\sigma_{i,j}$, thus

$$\sigma_{12} + \sigma_{34} = \sigma_{1,3} + \sigma_{2,4} = \sigma_{1,4} + \sigma_{2,3}, \tag{3.5}$$

from which follows the additivity of σ. Indeed, it holds $\sigma_{ij} = \sigma_i + \sigma_j$, $i<j$, $i,j \in \{1,\ldots,4\}$ with

$$\begin{cases}
\sigma_1 &= \frac{1}{2}(\sigma_{12}+\sigma_{13}-\sigma_{23}) = \frac{1}{2}(\sigma_{12}+\sigma_{14}-\sigma_{24}) = \frac{1}{2}(\sigma_{14}+\sigma_{13}-\sigma_{34}), \\
\sigma_2 &= \frac{1}{2}(\sigma_{12}+\sigma_{23}-\sigma_{13}) = \frac{1}{2}(\sigma_{12}+\sigma_{24}-\sigma_{14}) = \frac{1}{2}(\sigma_{23}+\sigma_{24}-\sigma_{34}), \\
\sigma_3 &= \frac{1}{2}(\sigma_{13}+\sigma_{23}-\sigma_{12}) = \frac{1}{2}(\sigma_{13}+\sigma_{34}-\sigma_{14}) = \frac{1}{2}(\sigma_{23}+\sigma_{34}-\sigma_{24}), \\
\sigma_4 &= \frac{1}{2}(\sigma_{14}+\sigma_{24}-\sigma_{12}) = \frac{1}{2}(\sigma_{24}+\sigma_{34}-\sigma_{23}) = \frac{1}{2}(\sigma_{34}+\sigma_{14}-\sigma_{13}).
\end{cases}$$

Conversely, if σ is additive then (3.5) holds, and choosing $\sigma^* = \sigma_{\min}$ yields $\lambda = 0$. This is consistent with the results of Section 3.1 and, in particular, with the expression of the potential $\mathbf{W}_\sigma$ in Proposition 3.1. Notice that since $\sigma_{\max} > \sigma_{\min}$, it is possible to choose $\sigma^* > \sigma_{\min}$ which leads to a new, but of course still admissible, potential.

3.3.3 Extension to $N \geq 5$

We deduce from (3.3) that

$$\begin{aligned}
\mathbf{W}_\sigma(u) &= \sum_{S\subset\{1,\dots,N\}} \sigma_S F(\sum_{i\in S} u_i) = \frac{1}{2}\sum_{S\subset\{1,\dots,N\}} \sigma_S (\sum_{i\in S} u_i)^2 (\sum_{j\notin S} u_j)^2 \\
&= \frac{1}{2}\sum_{i<j} \alpha_{i,j} u_i^2 u_j^2 + \sum_{i<j,k\neq i,k\neq i} \alpha_{i,j,k} u_i u_j u_k^2 + 2\sum_{i<j<k<l} \alpha_{i,j,k,l} u_i u_j u_k u_l,
\end{aligned}$$

where

$$\begin{cases}
\alpha_{i,j} &= \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{i\in S}\delta_{j\notin S} + \delta_{i\notin S}\delta_{j\in S}\right), \\
\alpha_{i,j,k} &= \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{k\in S}\delta_{i\notin S}\delta_{j\notin S} + \delta_{k\notin S}\delta_{i\in S}\delta_{j\in S}\right), \\
\alpha_{i,j,k,l} &= \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{k\in S}\delta_{l\in S}\delta_{i\notin S}\delta_{j\notin S} + \delta_{k\notin S}\delta_{l\notin S}\delta_{i\in S}\delta_{j\in S} + \delta_{k\in S}\delta_{l\notin S}\delta_{i\in S}\delta_{j\notin S}\right. \\
&\qquad \left. + \delta_{k\notin S}\delta_{l\in S}\delta_{i\notin S}\delta_{j\in S} + \delta_{k\in S}\delta_{l\notin S}\delta_{i\notin S}\delta_{j\in S} + \delta_{k\notin S}\delta_{l\in S}\delta_{i\in S}\delta_{j\notin S}\right).
\end{cases}$$

A first key observation is that **no more than four phases** are considered simultaneously in the above decomposition. Recall then that

$$P(\Omega_1, \Omega_2, \dots, \Omega_N) = \frac{1}{2}\sum_{i,j=1}^{N} \sigma_{i,j}\mathcal{H}^{d-1}(\Gamma_{i,j}) = \sum_{S\subset\{1,\dots,N\}} \sigma_S \mathcal{H}^{d-1}(\partial^*\left(\cup_{i\in S}\Omega_i\right)),$$

which yields to a second key observation: according to the Cut Cone Property (3.1), the coefficients σ_S depend only on the surface tensions $\sigma_{i,j}$, but absolutely **not** on the values $\mathcal{H}^{d-1}(\Gamma_{i,j})$. Therefore, to identify the contribution of four phases, the remaining phases can be assumed empty! Now if one assumes for instance that only $\Omega_1, \Omega_2, \Omega_3$ and Ω_4 are non-empty, then

$$\begin{aligned}
P(\Omega_1, \Omega_2, \Omega_3, \Omega_4, \emptyset, \cdots, \emptyset) &= \frac{1}{2}\sum_{i,j=1}^{4} \sigma_{i,j}\mathcal{H}^{d-1}(\Gamma_{i,j}) \\
&= \sum_{S\subset\{1,\dots,N\}} \sigma_S \mathcal{H}^{d-1}(\partial^*\left(\cup_{i\in S, i\in\{1,2,3,4\}}\Omega_i\right)) \\
&= \sum_{i=1}^{4} \beta_i \mathcal{H}^{d-1}(\partial^*\Omega_i) + \sum_{i=2}^{4} \beta_{1,i}\mathcal{H}^{d-1}(\partial^*(\Omega_1\cup\Omega_i)),
\end{aligned}$$

where

$$\begin{cases}
\beta_1 &= \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{1\in S}\delta_{2\notin S}\delta_{3\notin S}\delta_{4\notin S} + \delta_{1\notin S}\delta_{2\in S}\delta_{3\in S}\delta_{4\in S}\right), \\
\beta_2 &= \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{2\in S}\delta_{1\notin S}\delta_{3\notin S}\delta_{4\notin S} + \delta_{2\notin S}\delta_{1\in S}\delta_{3\in S}\delta_{4\in S}\right), \\
\beta_3 &= \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{3\in S}\delta_{2\notin S}\delta_{1\notin S}\delta_{4\notin S} + \delta_{3\notin S}\delta_{2\in S}\delta_{1\in S}\delta_{4\in S}\right), \\
\beta_4 &= \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{4\in S}\delta_{2\notin S}\delta_{3\notin S}\delta_{1\notin S} + \delta_{4\notin S}\delta_{2\in S}\delta_{3\in S}\delta_{1\in S}\right),
\end{cases}$$

and

$$\begin{cases}
\beta_{12} = \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{1\in S}\delta_{2\in S}\delta_{3\notin S}\delta_{4\notin S} + \delta_{1\notin S}\delta_{2\notin S}\delta_{3\in S}\delta_{4\in S}\right), \\
\beta_{13} = \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{1\in S}\delta_{2\notin S}\delta_{3\in S}\delta_{4\notin S} + \delta_{1\notin S}\delta_{2\in S}\delta_{3\notin S}\delta_{4\in S}\right), \\
\beta_{14} = \sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\delta_{1\in S}\delta_{2\notin S}\delta_{3\notin S}\delta_{4\in S} + \delta_{1\notin S}\delta_{2\in S}\delta_{3\in S}\delta_{4\notin S}\right).
\end{cases}$$

From the case $N = 4$ (see Remark 3.8), we deduce that there exists $\sigma^*_{1,2,3,4} \in I_{1,2,3,4}$, with

$$I_{i,j,k,l} = \left[\max_{\substack{i',j',k',l' \in \{i,j,k,l\} \\ i' \neq j' \neq k' \neq l'}} \left\{ \frac{\sigma_{i',j'} + \sigma_{k',l'}}{2} \right\}, \min_{\substack{i',j',k',l' \in \{i,j,k,l\} \\ i' \neq j' \neq k' \neq l'}} \left\{ \frac{\sigma_{i',j'} + \sigma_{i',k'} + \sigma_{i',l'}}{2} \right\} \right],$$

such that

$$\beta_{12} = \sigma^*_{1,2,3,4} - \left(\frac{\sigma_{12} + \sigma_{34}}{2} \right), \quad \beta_{13} = \sigma^*_{1,2,3,4} - \left(\frac{\sigma_{13} + \sigma_{24}}{2} \right), \quad \beta_{14} = \sigma^*_{1,2,3,4} - \left(\frac{\sigma_{14} + \sigma_{23}}{2} \right),$$

and

$$\beta_1 = \frac{\sigma_{12} + \sigma_{13} + \sigma_{14}}{2} - \sigma^*_{1,2,3,4}, \quad \beta_2 = \frac{\sigma_{12} + \sigma_{23} + \sigma_{24}}{2} - \sigma^*_{1,2,3,4},$$
$$\beta_3 = \frac{\sigma_{13} + \sigma_{23} + \sigma_{34}}{2} - \sigma^*_{1,2,3,4}, \quad \text{and } \beta_4 = \frac{\sigma_{14} + \sigma_{24} + \sigma_{34}}{2} - \sigma^*_{1,2,3,4}.$$

As was shown in the previous section, the triangle inequality (1.2) guarantees that $I_{i,j,k,l} \neq \emptyset$ for $i \neq j \neq k \neq l$. Furthermore, if the strict triangle inequality (3.2) is satisfied then $I_{i,j,k,l}$ is an interval of positive length. Using the same argument for any collection of four regions $\{\Omega_i, \Omega_j, \Omega_k, \Omega_l\}$, we can conclude that for all $\{i,j,k,l\} \in \{1, \dots, N\}$, $i \neq j \neq k \neq l$, there exists $\sigma^*_{i,j,k,l} \in I_{i,j,k,l}$ (we can choose it in the interior if the strict triangle inequality holds) such that

$$\mathbf{W}_\sigma(u) = \frac{1}{2} \sum_{i<j} \alpha_{i,j} u_i^2 u_j^2 + \sum_{i<j, k \neq i, k \neq i} \alpha_{i,j,k} u_i u_j u_k^2 + 2 \sum_{i<j<k<l} \alpha_{i,j,k,l} u_i u_j u_k u_l,$$

with

$$\begin{aligned}
\alpha_{i,j,k,l} &= \sum_S \sigma_S \left(\delta_{k \in S} \delta_{l \in S} \delta_{i \notin S} \delta_{j \notin S} + \delta_{k \notin S} \delta_{l \notin S} \delta_{i \in S} \delta_{j \in S} + \delta_{k \in S} \delta_{l \notin S} \delta_{i \in S} \delta_{j \notin S} \right. \\
&\qquad \left. + \delta_{k \notin S} \delta_{l \in S} \delta_{i \notin S} \delta_{j \in S} + \delta_{k \in S} \delta_{l \notin S} \delta_{i \notin S} \delta_{j \in S} + \delta_{k \notin S} \delta_{l \in S} \delta_{i \in S} \delta_{j \notin S} \right) \\
&= \beta_{i,j} + \beta_{i,k} + \beta_{i,l} \\
&= 3\sigma^*_{i,j,k,l} - \frac{1}{2} \sum_{(i',j') \subset \{i,j,k,l\},\, i'<j'} \sigma_{i',j'},
\end{aligned}$$

and

$$\begin{aligned}
\alpha_{i,j,k} &= \sum_S \sigma_S \left(\delta_{k \in S} \delta_{i \notin S} \delta_{j \notin S} + \delta_{k \notin S} \delta_{i \in S} \delta_{j \in S} \right) = \beta_k + \beta_{i,j} = \frac{\sigma_{i,k} + \sigma_{k,j} - \sigma_{i,j}}{2} = \frac{1}{2} \sigma_{i,j,k}, \\
\alpha_{i,j} &= \sum_S \sigma_S \left(\delta_{i \in S} \delta_{j \notin S} + \delta_{i \notin S} \delta_{j \in S} \right) = \beta_i + \beta_j + \beta_{i,k} + \beta_{i,l} = \sigma_{i,j}.
\end{aligned}$$

The following result is proved:

Theorem 3.10. Let $\sigma \in S_N$ be ℓ^1-embeddable and let $\{\sigma_S \geq 0,\, S \subset \{1,\dots,N\}\}$ the associated coefficients given by the Cut Cone Property (3.1). For all $i,j,k,l \in \{1,\dots,N\}$, $i \neq j \neq k \neq l$ the interval

$$I_{i,j,k,l} = \left[\max_{\substack{i',j',k',l' \in \{i,j,k,l\} \\ i' \neq j' \neq k' \neq l'}} \left\{ \frac{\sigma_{i',j'} + \sigma_{k',l'}}{2} \right\}, \min_{\substack{i',j',k',l' \in \{i,j,k,l\} \\ i' \neq j' \neq k' \neq l'}} \left\{ \frac{\sigma_{i',j'} + \sigma_{i',k'} + \sigma_{i',l'}}{2} \right\} \right]$$

is not empty. Given a potential of the form $\mathbf{W}_\sigma(u) = \sum_{S \subset \{1,\dots,N\}} \sigma_S F(\sum_{i \in S} u_i)$, there exist $\{\sigma^*_{i,j,k,l} \in I_{i,j,k,l},\ i,j,k,l \in \{1,\dots,N\},\ i \neq j \neq k \neq l\}$, such that

$$\mathbf{W}_\sigma(u) \;=\; \frac{1}{4}\sum_{i,j=1}^{N} \sigma_{i,j} u_i^2 u_j^2 + \frac{1}{2} \sum_{i<j, k\neq i, k \neq j} \sigma_{i,k,j} u_i u_j u_k^2 + \sum_{i<j<k<l} \sigma_{i,j,k,l} u_i u_j u_k u_l,$$

where $\sigma_{i,j,k} = \sigma_{i,k} + \sigma_{k,j} - \sigma_{i,j}$ and $\sigma_{i,j,k,l} = 6\sigma^*_{i,j,k,l} - \sum_{(i',j') \subset \{i,j,k,l\},\, i'<j'} \sigma_{i',j'}$ are nonnegative.

Furthermore, if σ satisfies the strict triangle inequality (3.2) then every interval $I_{i,j,k,l}$ has positive length and every coefficient $\sigma^*_{i,j,k,l}$ can be chosen in the interior of $I_{i,j,k,l}$ so that all coefficients $\sigma_{i,j}, \sigma_{i,j,k}, \sigma_{i,j,k,l}$ are positive for all $i \neq j \neq k \neq l$.

3.3.4 Remarks on geodesics in the ℓ^1 embeddable case

In the case of either additive or ℓ^1 embeddable surface tensions, we have derived a specific form of multi-well potential $\mathbf{W}_\sigma$ and we will prove in the next section the Γ-convergence of the associated approximation perimeter P_ϵ to $c_W P$. This Γ-convergence result yields an explicit formula linking the surface tensions and the interface energy:

$$c_F \sigma_{i,j} = \inf_{p \in \Sigma_{i,j}} \int_{\mathbb{R}} -\frac{\epsilon}{4} \sigma p'(s) \cdot p'(s) + \frac{1}{\epsilon} \mathbf{W}_\sigma(p(s)) ds,$$

where $\Sigma_{i,j}$ is the set of all Lipschitz continuous functions $p : \mathbb{R} \to \Sigma$, connecting the vectors $\mathbf{e}_i$ to $\mathbf{e}_j$ i.e $p(-\infty) = \mathbf{e}_i$, $p(+\infty) = \mathbf{e}_j$ and satisfying $p(0) \cdot \mathbf{e}_i = \frac{1}{2}$.

Note that the Euler-Lagrange equation of this minimization problem reads $\frac{\epsilon}{2}\sigma p'' + \frac{1}{\epsilon}\partial_u \mathbf{W}_\sigma(p) = 0$. Computing the scalar product with p' and a simple integration yields a constant, which can be identified with zero simply passing to the limit. This shows the equipartition of the energy $-\frac{\epsilon}{4}\sigma p' \cdot p' = \frac{1}{\epsilon}\mathbf{W}_\sigma(p)$, and then we have

$$c_F \sigma_{i,j} = \inf_{p \in \Sigma_{i,j}} \int_{\mathbb{R}} \sqrt{\mathbf{W}_\sigma(p(s))(-\sigma p'(s) \cdot p'(s))} ds, \quad \text{for all } (i,j) \in \{1,\dots,N\}. \tag{3.6}$$

We can also introduce the profile-geodesic $q_{i,j}$ defined as

$$q_{i,j} = \mathrm{argmin}_{p \in \Sigma_{i,j}} \inf_{p \in \Sigma_{i,j}} \int_{\mathbb{R}} -\frac{1}{4} \sigma p'(s) \cdot p'(s) + \mathbf{W}_\sigma(p(s)) ds,$$

Equation (3.6) proves that $q_{i,j} = \mathbf{e}_i q + (1-q)\mathbf{e}_j$ where the scalar profile q satisfies $q(s) = \frac{1-\tanh(s)}{2}$. Indeed, remark that if p is expressed as $\mathbf{e}_i q + (1-q)\mathbf{e}_j$, then

$$\begin{aligned}
\inf_p \int_{\mathbb{R}} \sqrt{\mathbf{W}_\sigma(p)(-\sigma p' \cdot p')} ds &= \inf_q \int_{\mathbb{R}} \sqrt{\sigma_{i,j} \frac{1}{2} q^2 (1-q)^2 2\sigma_{i,j} |q'|^2} ds \\
&= \sigma_{i,j} \inf_q \int_{\mathbb{R}} \sqrt{2F(q)} |q'| ds \\
&= \sigma_{i,j} \int_0^1 \sqrt{2F(s)} ds = c_F \sigma_{i,j},
\end{aligned}$$

where the equality on the second line line holds only for the profile function $q(s) = \frac{1-\tanh(s)}{2}$. In particular, it means that the geodesic $q_{i,j}$ which minimizes equation (3.6) does not introduce artificial phases between phases i and j.

3.3.5 Consequences for the non ℓ^1 embeddable case

What happens now in the case of a surface tension matrix σ which is not ℓ^1 embeddable? If there is Γ-convergence of P_ϵ to $c_W P$, then, again, the geodesic between two phases do not meet any other phase. But the experiments of Figure 3 show that a bad penalization of the 3-phases term in the potential does not prevent a geodesic from meeting more than two phases. Our potential is able to fix this, but does not penalize 5-phases (and more) situations. Therefore, we believe that Γ-convergence does not hold in general when σ is not ℓ^1 embeddable, and that it should be possible to design an example with at least five phases, where there would exist two phases i and j and a geodesic $p_{i,j} \in \Sigma_{i,j}$ such that

$$c_F \sigma_{i,j} > \int_{\mathbb{R}} -\frac{\epsilon}{4} \sigma p'_{i,j}(s) \cdot p'_{i,j}(s) + \frac{1}{\epsilon} \mathbf{W}_\sigma(p_{i,j}(s)) ds.$$

We claim that this geodesic would meet at least five phases, because otherwise, using a localization argument, we could reduce to a situation with at most four phases, and we know that when $N \leq 4$ every surface tension matrix which satisfies the triangle inequality (1.2) is ℓ^1-embeddable.

To force the Γ-convergence, it is necessary to modify the potential, introducing an additional term which penalizes the configurations where more than five phases coexist at the same location. For instance a suitable modified potential is

$$\mathbf{W}_\sigma(\mathbf{u}) = \frac{1}{4} \sum_{i,j=1}^N \sigma_{i,j} u_i^2 u_j^2 + \frac{1}{2} \sum_{i<j, k\neq i, k\neq j} \sigma_{i,k,j} u_i u_j u_k^2 + \sum_{i<j<k<l} \sigma_{i,j,k,l} u_i u_j u_k u_l + \mathbf{W}_{pen}(\mathbf{u}),$$

where

$$\mathbf{W}_{pen}(\mathbf{u}) = \sum_{m=5}^N \left[\sum_{1 \leq i_1 < i_2 < \cdots < i_m \leq M} \sigma_{i_1, i_2, \ldots, i_m} u_{i_1} u_{i_2} \cdots u_{i_m} \right].$$

and the coefficients $\sigma_{i_1, i_2, \cdots, i_m}$ are taken large enough.

As a consequence, we claim that there are surface tension matrices which are not ℓ^1-embeddable, and for which there is **no** fourth-order polynomial potential which guarantees the Γ-convergence of the approximating multiphase perimeter. In other words, in the non ℓ^1-embeddable case with a polynomial potential, a **necessary** condition for the Γ-convergence to be true is to use a polynomial of degree at least 5.

4 Convergence of the approximating multi-phase perimeter

Recall from the previous sections that if a surface tension σ is strictly ℓ^1-embeddable then there exists a collection of nonnegative coefficients $\{\sigma_S,\, S \subset \{1,\dots,N\}\}$, such that $\sigma_{\{i\}} > 0$ for all $i \in \{1,\dots,N\}$ and

$$P(\Omega_1,\dots,\Omega_N) = \sum_{S\subset\{1,\dots,N\}} \sigma_S \mathcal{H}^{d-1}(\partial^*\left(\cup_{i\in S}\Omega_i\right)).$$

The purpose of this section is to prove the following result:

Theorem 4.1. Let $\sigma = (\sigma_{ij})_{i,j\in\{1,\dots,N\}}$ be a strictly ℓ^1–embeddable surface tension matrix. There exists a collection of coefficients $\sigma_S > 0$ for all $S \subset \{1,\dots,N\}$ such that

$$P(\Omega_1,\dots,\Omega_N) = \sum_{S\subset\{1,\dots,N\}} \sigma_S |D(\sum_{i\in S} \mathbb{1}_{\Omega_i})|(\Omega)$$

for every partition $\{\Omega_1,\dots,\Omega_N\}$ of Ω with sets of finite perimeter. Moreover, the phase-field perimeter P_ϵ defined by

$$P_\epsilon(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega \left[\sum_{S\subset\{1,\dots,N\}} \sigma_S \left(\frac{\epsilon}{2}\left|\nabla(\sum_{i\in S} u_i)\right|^2 + \frac{1}{\epsilon}F(\sum_{i\in S} u_i)\right)\right] dx & \text{if } \mathbf{u} \in \Sigma \cap (\mathrm{W}^{1,2}(\Omega))^N \\ +\infty & \text{otherwise,} \end{cases},$$

Γ-converges in the L^1 topology to $c_F\tilde{P}$, with

$$\tilde{P}(\mathbf{u}) = \begin{cases} \displaystyle\sum_{S\subset\{1,\dots,N\}} \sigma_S |D(\sum_{i\in S} u_i)|(\Omega) & \text{if } \mathbf{u} = (\mathbb{1}_{\Omega_1},\cdots,\mathbb{1}_{\Omega_N}) \in \Sigma \cap (\mathrm{BV}(\Omega))^N, \\ +\infty & \text{otherwise.} \end{cases}.$$

Remark 4.2. Notice that if $\mathbf{u} = (\mathbb{1}_{\Omega_1},\cdots,\mathbb{1}_{\Omega_N}) \in \Sigma \cap (\mathrm{BV}(\Omega))^N$ then $\tilde{P}(\mathbf{u}) = P(\Omega_1,\dots,\Omega_N)$. Remark also that $\tilde{P}$ is a lower semicontinuous extension of P for the L^1 topology. In [3], S. Baldo used another extension which obviously coincides with ours on finite partitions.

Remark 4.3. The phase-field perimeter P_ϵ in the above theorem depends on the coefficients σ_S whose existence is guaranteed by the property of σ to be ℓ^1-embeddable. However, for a given ℓ^1-embeddable surface tensions matrix σ, there is no unique choice of the coefficients σ_S for $N \geq 4$.

Another possible formulation for P_ϵ follows from the previous section, where we proved that P_ϵ can be rewritten as:

$$P_\epsilon(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega -\frac{\epsilon}{4}\sigma\nabla\mathbf{u}\cdot\nabla\mathbf{u} + \frac{1}{\epsilon}\mathbf{W}_\sigma(\mathbf{u})dx & \text{if } \mathbf{u}\in\Sigma\cap(\mathrm{W}^{1,2}(\Omega,\mathbb{R}))^N, \\ +\infty & \text{otherwise,} \end{cases}$$

where $\sigma\nabla\mathbf{u}\cdot\nabla\mathbf{u} = \sum_{i,j=1}^N \sigma_{i,j}\nabla u_i\cdot\nabla u_j$, and the potential $\mathbf{W}_\sigma(\mathbf{u})$ is defined from the $\sigma_{i,j}$'s as

$$\mathbf{W}_\sigma(\mathbf{u}) = \frac{1}{4}\sum_{i,j=1}^N \sigma_{i,j}u_i^2u_j^2 + \frac{1}{2}\sum_{i<j,k\neq i,k\neq j}\sigma_{i,k,j}u_iu_ju_k^2 + \sum_{i<j<k<l}\sigma_{i,j,k,l}u_iu_ju_ku_l,$$

and

$$\sigma_{i,j,k} = (\sigma_{i,k}+\sigma_{j,k}-\sigma_{i,j}), \quad \sigma_{i,j,k,l} = 6\sigma^*_{i,j,k,l} - \sum_{(i',j')\subset\{i,j,k,l\},\, i'<j'}\sigma_{i',j'},$$

where

$$\sigma^*_{i,j,k,l}\in I_{i,j,k,l} = \left[\max_{\substack{i',j',k',l'\in\{i,j,k,l\}\\ i'\neq j'\neq k'\neq l'}}\left\{\frac{\sigma_{i',j'}+\sigma_{k',l'}}{2}\right\}, \min_{\substack{i',j',k',l'\in\{i,j,k,l\}\\ i'\neq j'\neq k'\neq l'}}\left\{\frac{\sigma_{i',j'}+\sigma_{i',k'}+\sigma_{i',l'}}{2}\right\}\right].$$

Now, the dependence of P_ϵ on the choice of a particular collection $\{\sigma_S\}$ lies in the choice of $\sigma^*_{i,j,k,l}$.

Remark 4.4. In practice, for a given ℓ^1-embeddable surface tensions matrix σ, we can choose with the notations of the previous remark:

$$\sigma^*_{i,j,k,l} = \max I_{i,j,k,l} = \min_{\substack{i',j',k',l'\in\{i,j,k,l\}\\ i'\neq j'\neq k'\neq l'}}\left\{\frac{\sigma_{i',j'}+\sigma_{i',k'}+\sigma_{i',l'}}{2}\right\}.$$

We claim that the Γ-convergence result proven in the next subsections still holds with such assumption. Indeed, it is easily seen that the $\Gamma-\liminf$ result remains true as the multiphase field perimeter associated with such choice of $\sigma^*_{i,j,k,l}$ is larger than the multiphase field perimeter associated with any other choice of $\sigma^*_{i,j,k,l}$ in $I_{i,j,k,l}$. As for the $\Gamma-\limsup$, the proof follows from an argument involving only two phases along each interface, except at the multiple points whose influence is shown to be negligible. Since $\sigma^*_{i,j,k,l}$ plays a role when at least four phases appear at the same point, the $\Gamma-\limsup$ argument remains true with $\sigma^*_{i,j,k,l} = \max I_{i,j,k,l}$.

4.1 Equi-coerciveness and $\liminf$ inequality

As usual in Γ-convergence theory, the convergence holds with respect to a parameter ϵ tending to 0^+, but this has to be underst1ood in the sequential sense, i.e. for any sequence of real numbers $(\epsilon_n)_{n\in\mathbb{N}}$ converging to 0 as $n\to\infty$.

Let $(\mathbf{u}^\epsilon)_{\{\epsilon>0\}}$ be a sequence in $\Sigma\cap(\mathrm{W}^{1,2}(\Omega))^N$ such that $(P_\epsilon(\mathbf{u}^\epsilon))_{\{\epsilon>0\}}$ is uniformly bounded. With our assumption that $\sigma_{\{i\}}>0$ for every $i\in\{1,\dots,N\}$, it follows that for every $i\in\{1,\dots,N\}$,

$\int_\Omega (\frac{\epsilon}{2}|\nabla u_i^\epsilon|^2 + \frac{1}{\epsilon}F(u_i^\epsilon))dx$ is uniformly bounded. We deduce from Modica-Mortola's Theorem [35], possibly extracting a subsequence, that $(u_i^\epsilon)_{\{\epsilon>0\}}$ converges in L^1 to a function $u_i \in \mathrm{BV}(\Omega,\{0,1\})$ for every $i \in \{1,\dots,N\}$, and denoting $\Omega_i = \{x \in \Omega,\ u_i = 1\}$ it holds that

$$c_F|D\mathbb{1}_{\Omega_i}|(\Omega) \le \liminf_{n\to\infty} \int_\Omega (\frac{\epsilon}{2}|\nabla u_i^\epsilon|^2 + \frac{1}{\epsilon}F(u_i^\epsilon))dx.$$

Define $\mathbf{u} = (u_1,\cdots,u_N)$ and observe that $\mathbf{u} \in (\mathrm{BV}(\Omega,\{0,1\})^N$. Since $\mathbf{u}^\epsilon \in \Sigma$, taking a subsequence which converges a.e. in Ω yields $\mathbf{u} \in \Sigma \cap (\mathrm{BV}(\Omega,\{0,1\})^N$. In particular, $\cup_i\Omega_i$ is a Caccioppoli partition of Ω [2, 33], i.e. a partition made of sets with finite perimeter which are pairwise disjoint (up to a Lebesgue negligible set).

We can now apply Modica-Mortola's Theorem to every sequence $(\sum_{i\in S} u_i^\epsilon)_{\{\epsilon>0\}}$ and we get that

$$c_F\left|D\left(\sum_{i\in S} u_i\right)\right|(\Omega) \le \liminf_{n\to\infty}\int_\Omega\left[\frac{\epsilon}{2}\left|\nabla(\sum_{i\in S}u_i^\epsilon)\right|^2 + \frac{1}{\epsilon}F(\sum_{i\in S}u_i^\epsilon)\right]dx,$$

and finally

$$c_F P(\Omega_1,\cdots,\Omega_N) = c_F\tilde{P}(\mathbf{u}) = c_F\sum_{S\subset\{1,\dots,N\}}\sigma_S\left|D\left(\sum_{i\in S}u_i\right)\right|(\Omega) \le \liminf P_\epsilon(\mathbf{u}^\epsilon).$$

4.2 $\limsup$ inequality

Let us consider $\mathbf{u} = (\mathbb{1}_{\Omega_1},\cdots,\mathbb{1}_{\Omega_N})$, with $\Omega_1,\dots,\Omega_N$ pairwise disjoint sets with finite perimeter in Ω such that $|\Omega\setminus\cup_{i=1}^N\Omega_i| = 0$.

The aim of this section is to construct a sequence $\{\mathbf{u}^\epsilon\}_{\epsilon>0}$ which converges to $\mathbf{u}$ in $L^1(\Omega)$ and such that

$$\lim_{\epsilon\to 0} P_\epsilon(\mathbf{u}^\epsilon) \le c_F\tilde{P}(\mathbf{u}).$$

4.2.1 Restriction to a polygonal partition

Note that, by density (see Lemma 3.1 in [3]), we can assume that each Ω_i is a finite union of polygonal domains. We consider the signed distance function h_i associated with each domain Ω_i, i.e.

$$h_i(x) = \begin{cases} \mathrm{dist}(x,\Omega_i) & \text{if } x\notin\Omega_i,\\ -\mathrm{dist}(x,\Omega_i) & \text{if } x\in\Omega_i.\end{cases}$$

Then, Lemma 3.3 in [3] establishes the existence of a constant $\eta > 0$ such that for all $i \in \{1,\dots,N\}$, h_i is Lipschitz-continuous on $H_{\eta,i} = \{x\in\Omega; |h_i(x)| < \eta\}$, and $|\nabla h_i| = 1$ for almost all $x \in H_{\eta,i}$.

4.2.2 ϵ-partition of Ω

Let $\delta > 3$ and assume that ϵ is sufficiently small so that

$$s_\epsilon = 2\delta|\log(\epsilon)| < \frac{\eta}{\epsilon}.$$

For all $i \in \{1, \dots, N\}$, let

$$\Omega_i^\epsilon = \{x \in \Omega; h_i(x) \leq -\epsilon s_\epsilon\},$$

and, for all $1 \leq i < j \leq N$, let us define

$$\Gamma_{i,j}^\epsilon = \{x \in \Omega; |h_i(x)| \leq \epsilon s_\epsilon, |h_j(x)| \leq \epsilon s_\epsilon, \text{ and } |h_k| > \epsilon s_\epsilon \text{ for all } k \notin \{i,j\}\}.$$

Then, with

$$B_\epsilon = \{x \in \Omega, \exists i,j,k \in \{1, 2 \cdots, N\} \text{ such that } |h_i(x)| > \epsilon s_\epsilon, |h_j(x)| > \epsilon s_\epsilon \text{ and } |h_k(x)| > \epsilon s_\epsilon\},$$

we have the following partition of Ω (see Figure 1):

$$\Omega = \{\cup_i^N \Omega_i^\epsilon\} \cup \{\cup_{1\leq i<j\leq N}\Gamma_{i,j}^\epsilon\} \cup B_\epsilon.$$

Moreover, it is not difficult to see that, since the set of triple points has codimension 2 for polygonal partitions, one has

$$|B_\epsilon| \leq O\left(\epsilon^2|\log(\epsilon)|^2\right).$$

Indeed, to be convinced, consider first the case of dimension 2. As $(\Omega_1, \Omega_2, \cdots, \Omega_N)$ is a polygonal partition of Ω, there exists a finite number M of multiple junctions $x_1, x_2, \cdots, x_M$. Let α_i denote the minimal angle between any two branches at junction x_i. Then, it is not difficult to see that $B_\epsilon \subset \cup_{i=1}^M B(x_i, \epsilon s_\epsilon/\sin(\alpha_i))$, where $B(x,r)$ is the ball centered at x with radius r. In particular, this shows that in dimension 2:

$$|B_\epsilon| \leq M\pi \frac{\epsilon^2 s_\epsilon^2}{\min_i\{\sin(\alpha_i)^2\}}.$$

In higher dimension, triple junctions still have codimension 2 and can therefore be covered by sets B_ϵ of size $O(\epsilon^2|\log(\epsilon)|^2)$.

4.2.3 Profile approximation

Recall that the Allen-Cahn profile function q is defined as

$$q = \underset{p}{\operatorname{argmin}} \left\{ \int_{\mathbb{R}} \sqrt{F(p(s)}|p'(s)|ds; p(-\infty) = 1, p(0) = 1/2, p(+\infty) = 0 \right\},$$

where p ranges over all Lipschitz continuous functions $p : \mathbb{R} \to \mathbb{R}$. It is a well-known fact that

$$q'(s) = -\sqrt{2F(q(s))} \text{ and } q''(s) = W'(q(s)), \quad \text{for all } s \in \mathbb{R},$$

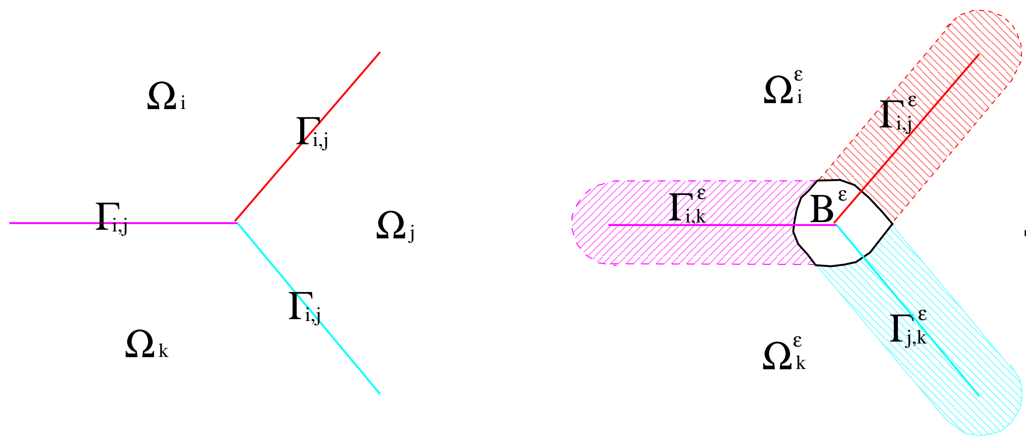

Figure 1: ϵ-partition of Ω

which implies that $q(s) = (1 - \tanh(s))/2$ in the case of the standard double well potential $F(s) = \frac{1}{2}s^2(1-s)^2$.

We will now introduce an approximation q_ϵ of q of which the support of variation is bounded. Following [6], we take

$$\begin{cases} q_\epsilon(s) = q(s), \quad \forall |s| \leq s_\epsilon/2, \\ q_\epsilon(s) = 1 \text{ if } s < -s_\epsilon, \quad \text{ and } q_\epsilon(s) = 0 \text{ if } s > s_\epsilon, \\ q_\epsilon(s) = p_-(s), \ \forall s \in I_\epsilon^- = [-s_\epsilon, -s_\epsilon/2], \text{ and } q_\epsilon(s) = p_+(s), \ \forall s \in I_\epsilon^+ = [s_\epsilon/2, s_\epsilon], \end{cases}$$

where p_- and p_+ are two polynomials of degree 3, defined in such a way that $q_\epsilon \in C^1(\mathbb{R})$. Note that these polynomials are unique (by the standard interpolation theory) and it can be proven (see [6]) that

$$q_\epsilon - q = o(\epsilon^{2\delta-1}), \quad q'_\epsilon - W'(q_\epsilon) = o(\epsilon^{2\delta-1}), \text{ and } q'_\epsilon + \sqrt{2F(q_\epsilon)} = o(\epsilon^{2\delta-1}).$$

4.2.4 Recovery sequence

We are now able to define an approximation $\mathbf{u}^\epsilon$ of $\mathbf{u} = (\mathbb{1}_{\Omega_1}, \cdots, \mathbb{1}_{\Omega_N})$ as

$$\mathbf{u}^\epsilon(x) = \mathcal{P}_\Sigma\left[\sum_{i=1}^N \mathbf{e}_i q_\epsilon\left(\frac{h_i}{\epsilon}\right)\right] = \begin{cases} \mathbf{e}_i & \text{if } x \in \Omega_i^\epsilon, \\ q_\epsilon(h_i/\epsilon)\mathbf{e}_i + (1 - q_\epsilon(h_i/\epsilon))\mathbf{e}_j & \text{if } x \in \Gamma_{i,j}^\epsilon \\ \mathcal{P}_\Sigma[\sum_i \mathbf{e}_i q_\epsilon(h_i/\epsilon)] & \text{otherwise,} \end{cases},$$

where $\mathcal{P}_\Sigma$ is the orthogonal projection onto $\Sigma = \{\mathbf{u} : \Omega \to \mathbb{R}^N, \sum_{i=1}^N u_i = 1 \text{ a.e.}\}$ defined for a.e. $x \in \Omega$ as

$$\mathcal{P}_\Sigma[\mathbf{u}](x) = \begin{cases} \mathbf{u}(\mathbf{x}) / \left(\sum_{i=1}^N u_i(x)\right) & \text{if } \sum_{i=1}^N u_i(x) \neq 0, \\ \frac{1}{N}\mathbb{1}_N & \text{otherwise,} \end{cases}$$

with $\mathbb{1}_N = (1, 1, \dots, 1) \in \mathbb{R}^N$. Here we use that for all $x \in \Gamma^\epsilon_{i,j}$, $h_i(x) = -h_j(x)$ and that q_ϵ satisfies the following symmetry principle

$$q_\epsilon(s) = 1 - q_\epsilon(-s), \text{ for all } s \in \mathbb{R}.$$

Moreover, as $s_\epsilon = \delta|\log(\epsilon)| < \frac{\eta}{2\epsilon}$, $\mathbf{u}^\epsilon$ is a Lipschitz continuous function and $\mathbf{u}^\epsilon$ clearly converges to $\mathbf{u}$ in $L^1(\Omega)$.

4.2.5 Final convergence

Recall that

$$P_\epsilon(\mathbf{u}^\epsilon) = \int_\Omega \left[-\frac{\epsilon}{4}\sigma\nabla\mathbf{u}^\epsilon \cdot \nabla\mathbf{u}^\epsilon + \frac{1}{\epsilon}\mathbf{W}_\sigma(\mathbf{u}^\epsilon) \right] dx.$$

First, remark that

$$\int_{\Omega_i^\epsilon} \left[-\frac{\epsilon}{4}\sigma\nabla\mathbf{u}^\epsilon \cdot \nabla\mathbf{u}^\epsilon + \frac{1}{\epsilon}\mathbf{W}_\sigma(\mathbf{u}^\epsilon) \right] dx = 0,$$

and that

$$\int_{B_\epsilon} \left[-\frac{\epsilon}{4}\sigma\nabla\mathbf{u}^\epsilon \cdot \nabla\mathbf{u}^\epsilon + \frac{1}{\epsilon}\mathbf{W}_\sigma(\mathbf{u}^\epsilon) \right] dx = O(\epsilon|\log(\epsilon)|^2),$$

using the fact that $|B_\epsilon| = O(\epsilon^2|\log(\epsilon)|^2)$, $|\nabla\mathbf{u}^\epsilon| = O(\frac{1}{\epsilon})$ and $\mathbf{W}_\sigma$ is locally bounded on $\mathbb{R}^N$.

It is sufficient now to evaluate for all $1 \leq i < j \leq N$ the integral

$$J^\epsilon_{i,j} = \int_{\Gamma^\epsilon_{i,j}} \left[-\frac{\epsilon}{4}\sigma\nabla\mathbf{u}^\epsilon \cdot \nabla\mathbf{u}^\epsilon + \frac{1}{\epsilon}\mathbf{W}_\sigma(\mathbf{u}^\epsilon) \right] dx.$$

Recall that for all $x \in \Gamma^\epsilon_{i,j}$, we have $\mathbf{u}^\epsilon = q_\epsilon(h_i/\epsilon)\mathbf{e}_i + (1 - q_\epsilon(h_i/\epsilon))\mathbf{e}_j$ and so

$$\begin{cases} -\sigma\nabla\mathbf{u}^\epsilon \cdot \nabla\mathbf{u}^\epsilon = 2\sigma_{i,j}|\nabla q_\epsilon(h_i/\epsilon)|^2, \\ \mathbf{W}_\sigma(\mathbf{u}^\epsilon) = \sigma_{i,j}\frac{1}{2}q_\epsilon(h_i/\epsilon)^2(1 - q_\epsilon(h_i/\epsilon))^2. \end{cases}$$

In particular, this shows that

$$J^\epsilon_{i,j} = \sigma_{i,j}\int_{\Gamma^\epsilon_{i,j}} \left[\frac{\epsilon}{2}|\nabla q_\epsilon(h_i/\epsilon)|^2 + \frac{1}{\epsilon}F(q_\epsilon(h_i/\epsilon)) \right] dx = \sigma_{i,j}\int_{\Gamma^\epsilon_{i,j}} \left[\frac{1}{2}|q_\epsilon'(h_i/\epsilon)|^2 + F(q_\epsilon(h_i/\epsilon)) \right] \frac{|\nabla h_i|}{\epsilon} dx.$$

Thus, the coarea formula proves that

$$J^\epsilon_{i,j} = \int_{-s_\epsilon}^{s_\epsilon} \mathcal{H}^{d-1}(\partial\Gamma^{\epsilon,\epsilon s}_{i,j}) \left[\frac{1}{2}|q_\epsilon'(s)|^2 + F(q_\epsilon(s)) \right] ds,$$

where the set $\Gamma^{\epsilon,s}_{i,j}$ is defined as

$$\Gamma^{\epsilon,s}_{i,j} = \{x \in \Gamma^\epsilon_{i,j}; h_i(x) \leq s\}, \quad \forall s \in \mathbb{R}.$$

Finally, taking the limit as ϵ goes to zero, the regularity of both $\Gamma_{i,j}$ and the distance function h_i, and an application of the Dominated Convergence Theorem, lead to

$$\lim_{\epsilon\to 0} J^{\epsilon}_{i,j} = \sigma_{i,j}\mathcal{H}^{d-1}(\Gamma_{i,j}) \left[\int_{\mathbb{R}} \frac{1}{2}|q'(s)|^2 + F(q(s)ds\right] = c_F\sigma_{i,j}\mathcal{H}^{d-1}(\Gamma_{i,j}),$$

thus

$$\lim_{\epsilon\to 0} P_\epsilon(\mathbf{u}^\epsilon) = \frac{c_F}{2}\sum_{i,j=1}^{N} \mathcal{H}^{d-1}(\Gamma_{i,j}) = c_F P(\mathbf{u}).$$

This concludes the proof of Theorem 4.1.

5 L^2-gradient flow and some extensions

We now derive the L^2-gradient flow of

$$P_\epsilon(\mathbf{u}) = \begin{cases} \displaystyle\int_\Omega -\frac{\epsilon}{4}\sigma\nabla\mathbf{u}\cdot\nabla\mathbf{u} + \frac{1}{\epsilon}\mathbf{W}_\sigma(\mathbf{u})dx & \text{if } \mathbf{u}\in\Sigma\cap(\mathrm{W}^{1,2}(\Omega,\mathbb{R}))^N, \\ +\infty & \text{otherwise.}\end{cases}$$

The gradient of P_ϵ is

$$\nabla P_\epsilon(\mathbf{u}) = \frac{\epsilon}{2}\sigma\Delta\mathbf{u} + \frac{1}{\epsilon}\partial_u\mathbf{W}_\sigma(\mathbf{u}),$$

thus, considering that multiphase fields are now time-dependent, we get the following Allen-Cahn system, up to time rescaling:

$$\begin{cases} \mathbf{u}:\Omega\times[0,+\infty)\to\mathbb{R}^N, \\ \partial_t\mathbf{u} = -T_\Sigma\left[\frac{1}{2}\sigma\Delta\mathbf{u}\right] - \frac{1}{\epsilon^2}T_\Sigma\left[\partial_u\mathbf{W}_\sigma(\mathbf{u})\right], \\ \mathbf{u}(\cdot,0) = u_0,\end{cases}$$

where T_Σ is the orthogonal projection onto the tangent space $\{\mathbf{u}:\Omega\times[0,+\infty)\to\mathbb{R}^N:\ \sum u_i = 0\}$, defined as

$$T_\Sigma[\mathbf{u}(\cdot,t)] = \mathbf{u}(\cdot,t) - \frac{1}{N}\left(\sum_{i=1}^N u_i(\cdot,t)\right)\mathbb{1}_N, \qquad \text{with } \mathbb{1}_N = (1,\dots,1)\in\mathbb{R}^N.$$

Moreover, we have

$$T_\Sigma[\sigma\Delta\mathbf{u}] = \Delta T_\Sigma[\sigma\mathbf{u}] = \Delta T_\Sigma[\sigma]\mathbf{u} = T_\Sigma[\sigma]\Delta\mathbf{u} \quad \text{where} \quad T_\Sigma[\sigma]_{i,j} = T_\Sigma[\sigma_{\cdot,j}]_i,$$

and the Allen-Cahn system can be written as

$$\partial_t\mathbf{u} = -\frac{1}{2}T_\Sigma[\sigma]\Delta\mathbf{u} - \frac{1}{\epsilon^2}T_\Sigma\left[\partial_u\mathbf{W}_\sigma(\mathbf{u})\right].$$

Since $\sum_{i=1}^N u_i = 1$, one has $\sum_{i=1}^N \Delta u_i = 0$, thus the system

$$\partial_t\mathbf{u} = -\frac{1}{2}\left(T_\Sigma[\sigma] - \lambda\mathbb{1}_N\otimes\mathbb{1}_N\right)\Delta\mathbf{u} - \frac{1}{\epsilon^2}T_\Sigma\left[\partial_u\mathbf{W}_\sigma(\mathbf{u})\right], \tag{5.1}$$

is equivalent to the previous one. The existence and uniqueness of solutions to this system follow easily from standard results on semi-linear systems of reaction-diffusion. Furthermore, this new form is easier to handle numerically. In particular, λ is a parameter which can be chosen large enough to force the matrix $(T_\Sigma[\sigma] - \lambda \mathbb{1}_N \otimes \mathbb{1}_N)$ to be negative definite. This is of course a requirement for the scheme to be stable. Note that it is always possible to find such a $\lambda \in \mathbb{R}$ as soon as σ defines a negative form on $(1, 1, \cdots, 1)^\perp \subset \mathbb{R}^N$ (which is the case of all ℓ^1-embeddable matrices). This assumption also appears in the convergence of the algorithm introduced in [25], and simple examples show that it is necessary. For instance, if $N = 3$ and $\sigma_{i,j} = 1$ whenever $i \neq j$, then

$$\sigma = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad T_\Sigma[\sigma] = \begin{pmatrix} -2/3 & 1/3 & 1/3 \\ 1/3 & -2/3 & 1/3 \\ 1/3 & 1/3 & -2/3 \end{pmatrix} \text{ and } T_\Sigma[\sigma] - \frac{1}{3}\mathbb{1}_3 \otimes \mathbb{1}_3 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

and it is easily seen that $T_\Sigma[\sigma]$ is not invertible whereas $T_\Sigma[\sigma] - \frac{1}{3}\mathbb{1}_3 \otimes \mathbb{1}_3$ is negative definite.

5.1 Sharp interface limits

As mentioned earlier, Garcke et al studied in [28] the flow associated with energies of the general form

$$P_\epsilon(\mathbf{u}) = \int \epsilon f(\mathbf{u}, \nabla \mathbf{u}) + \frac{1}{\epsilon} \mathbf{W}(\mathbf{u}) dx,$$

where $f : \mathbb{R}^N \times \mathbb{R}^{N \times n} \to \mathbb{R}^+$ is such that:

- $f(\mathbf{u}, \lambda X) = \lambda^2 f(\mathbf{u}, X)$ for all $\lambda \in \mathbb{R}$,
- $f(\mathbf{u}, X) > 0$, whenever $u \in \Sigma$, $X \neq 0$,
- $f(\mathbf{u}, .)$ is convex for all $\mathbf{u} \in \Sigma$,

and where the potential $\mathbf{W}$ is assumed to have exactly N local minima on the hypersurface Σ.

The new model that we introduced in the previous sections is based on ℓ^1-embeddable surface tension matrices σ, a potential $\mathbf{W} = \mathbf{W}_\sigma$ (see Theorem 3.10), and a regularity term

$$f(\mathbf{u}, \nabla \mathbf{u}) = -\frac{1}{4} (\sigma \nabla \mathbf{u} \cdot \nabla \mathbf{u}),$$

which is nonnegative since σ is conditionally semi-definite negative. Therefore, our model falls in the general category studied in [28], provided that one replaces the second condition with the following one:

- $f(\mathbf{u}, X) > 0$, whenever $u \in \Sigma$, $X \in (T\Sigma)^N$, $X \neq 0$,

which is not more restrictive since, in practice, $X = \nabla u \in (T\Sigma)^N$ as soon as $u \in \Sigma$.

The Allen-Cahn system corresponding to the gradient flow of the general energy is, up to time rescaling,

$$\partial_t \mathbf{u} = \operatorname{div} \left(T_\Sigma[\partial_X f(\mathbf{u}, \nabla \mathbf{u}) - \partial_{\mathbf{u}} f(\mathbf{u}, \nabla \mathbf{u})] \right) - \frac{1}{\epsilon^2} T_\Sigma[\partial_{\mathbf{u}} \mathbf{W}(\mathbf{u})].$$

Using the formal asymptotic expansion method, Garcke et al showed that the sharp interface limit of the solution to this system is an anisotropic multiphase mean curvature flow which satisfies

$$\mu_{i,j}(n_{i,j})V_{i,j} = \left(\tilde{\sigma}_{i,j}(n_{i,j}) + \tilde{\sigma}''_{i,j}(n_{i,j})\right)\kappa_{i,j},$$

where

- $n_{i,j}$ denotes the normal at the interface $\Gamma_{i,j}$ pointing from Ω_i to Ω_j;
- $V_{i,j}$ is the normal velocity of the flow at the interface $\Gamma_{i,j}$;
- $\kappa_{i,j}$ is the mean curvature at the interface;
- $\tilde{\sigma}_{i,j}(n) = \inf_{p\in\Sigma_{i,j}} \int_{\mathbb{R}} 2\sqrt{\mathbf{W}(p)f(p,p'\otimes n)}ds$ is the anisotropic surface energy;
- $\mu_{i,j}(n) = \int_{\mathbb{R}} |\partial_s q_{i,j}(s,n)|^2 ds$ is the anisotropic mobility, denoting

  $$q_{i,j}(.,n) = \mathrm{argmin}_{p\in\Sigma_{i,j}} \int_{\mathbb{R}} 2\sqrt{\mathbf{W}(p)f(p,p'\otimes n)}ds$$

  the anisotropic geodesic;

In addition, it is shown also in [28] that Herring's angle condition is satisfied at every triple junction.

Let us now focus on the gradient term used in our model, i.e. $f(\mathbf{u},X) = -\frac{1}{4}\sigma X\cdot X$. Then the multiphase mean curvature flow is isotropic as

$$f(p,p'\otimes n) = -\frac{1}{4}(\sigma p'\cdot p')(n\cdot n) = -\frac{1}{4}\sigma p'\cdot p'.$$

Moreover as written earlier,

$$\tilde{\sigma}_{i,j} = \inf_{p\in\Sigma_{i,j}} \int_{\mathbb{R}} \sqrt{\mathbf{W}_\sigma(p(s))(-\sigma p'(s)\cdot p'(s))}ds = c_W\sigma_{i,j}.$$

The geodesics $q_{i,j}(.,n)$ satisfy

$$q_{i,j}(s,n) = q_{i,j}(s) = q(s)\mathbf{e}_i + (1-q(s))\mathbf{e}_j,$$

where q is the classical Allen-Cahn profile $q(s) = \frac{1-\tanh(s)}{2}$ which satisfies the equation $q' = -\sqrt{2F(q)}$. In particular, it follows that the mobility equals

$$\mu_{i,j}(n) = \int_{\mathbb{R}} |\partial_s q_{i,j}(s,n)|^2 ds = \int_{\mathbb{R}} 2|q'(s)|^2 ds = 2c_F.$$

In conclusion, it follows from the results of [28] that the sharp interface limit of our phase field model follows a mean curvature motion with speed

$$V_{i,j} = \frac{1}{2}\sigma_{i,j}\kappa_{i,j},$$

which corresponds to the multiphase mean curvature flow (1.3) with interface mobility $\mu_{i,j} = 1/2$.

5.2 Additional volume constraints

In view of applications to droplets, we also consider the L^2-gradient flow of P_ϵ with additional constraints on the volume of each phase u_i:

$$\partial_t \left(\int u_i dx \right) = 0.$$

Plugging this constraint into the problem yields the following mass conservation Allen-Cahn system:

$$\partial_t \mathbf{u} = -\frac{1}{2} T_\Sigma[\sigma]\Delta \mathbf{u} - \frac{1}{\epsilon^2} T_\Sigma \left[\partial_u \mathbf{W}_\sigma(\mathbf{u}) - \mathbf{\Lambda} \right],$$

where $\mathbf{\Lambda}$ is a local Lagrange multiplier [11, 1] associated to the constraint $\partial_t \left(\int u_i dx \right) = 0$, which can be calculated as

$$\mathbf{\Lambda}_i = \frac{\int (\partial_u \mathbf{W}_\sigma(\mathbf{u}))_i dx}{\int \sqrt{2F(u_i)} dx} \sqrt{2F(u_i)}, \quad i \in \{1, \dots, N\}.$$

5.3 Application to the wetting of multiphase droplets on solid surfaces

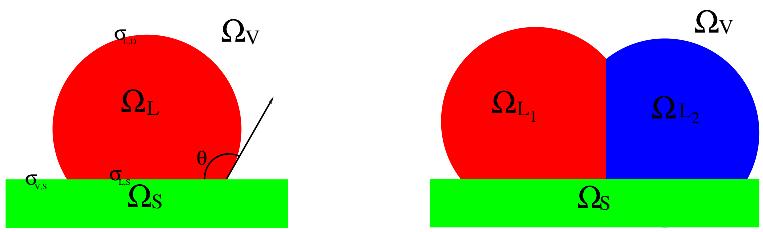

Figure 2: Wetting of droplets on a solid surface. The contact angle θ satisfies Young's law.

The behavior of liquids on solid surfaces has been of interest to academic and engineering communities for many decades. Capillarity theory is a well established theory, and two centuries ago, Young [48] determined the optimal shape of a drop in equilibrium on a solid surface. More precisely, the drop shape can be seen as the solution to the minimization of the following energy:

$$P(\Omega_L) = \sigma_{L,S}\mathcal{H}^{d-1}(\Gamma_{L,S}) + \sigma_{L,V}\mathcal{H}^{d-1}(\Gamma_{L,V}) + \sigma_{S,V}\mathcal{H}^{d-1}(\Gamma_{L,V}),$$

under a constraint on the volume of the set Ω_L which represents the droplet. Here, $\sigma_{L,S}$, $\sigma_{L,V}$, and $\sigma_{L,V}$ are the surface tensions between liquid (L), solid (S), and vapor (S) phases. In particular, minimizers of this energy satisfy Young's law for the contact angle θ of the droplet on the solid, see Figure 2 :

$$\cos(\theta) = \frac{\sigma_{S,V} - \sigma_{S,L}}{\sigma_{L,V}}.$$

The wetting phenomenon was modeled by Cahn in [12] in a phase-field setting. Cahn proposed to extend the Cahn-Hilliard energy by adding a surface energy term which describes the interaction between liquid and solid. This approach has been recently used in [47] for numerical simulations of one droplet but can not be used in the case of angle $\theta \geq \frac{\pi}{2}$. Another approach [49], using the smoothed boundary method, proposes to compute the Allen-Cahn equation using generalized Neumann boundary conditions to force the correct contact angle condition. Note that an extension of these approaches to many droplets can be found in [7].

Our approach in this paper is slightly different and the novelty is to formulate the optimal drop shape problem as the minimization of the multiphase perimeter

$$P(\Omega_V, \Omega_L, \Omega_S) = \int_{\Gamma_{L,S}} \sigma_{L,S} d\mathcal{H}^{d-1} + \int_{\Gamma_{L,V}} \sigma_{L,V} d\mathcal{H}^{d-1} + \int_{\Gamma_{L,V}} \sigma_{S,V} d\mathcal{H}^{d-1},$$

under a volume constraint on the set Ω_L and an additional constraint on Ω_S, which is given and **assumed to be fixed**. The advantage of this approach is that the contact angle condition is implicitly incorporated in the phase field approximation of P. The case of many droplets is a natural extension of the single droplet case. Let us introduce for instance $N-2$ droplets, denoted by Ω_{L_1}, Ω_{L_2} ... $\Omega_{L_{N-2}}$, and take by convention

$$\Omega_N = \Omega_S, \quad \Omega_{N-1} = \Omega_V, \quad \text{and} \quad \Omega_i = \Omega_{L_i} \text{ for all } i \in \{1, \dots, N-2\}.$$

Then, the optimal shapes of the droplets can be viewed as regions of a minimizer of the multiphase perimeter

$$P(\Omega_1, ...\Omega_N) = \frac{1}{2} \sum_{i,j=1}^{N} \int_{\Gamma_{i,j}} \sigma_{i,j} d\sigma,$$

under a volume constraint on the droplets Ω_{L_i} and a constancy constraint of Ω_N. Here the coefficients $\sigma_{i,N-1}$ and $\sigma_{i,N}$ represent the surface tensions at the interfaces between droplets on one hand and, respectively, vapor and solid phases.

Our phase field approximation to this model is

$$P_\epsilon(\mathbf{u}) = \begin{cases} \int_\Omega -\frac{\epsilon}{4} \sigma \nabla \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\epsilon} \mathbf{W}_\sigma(u) dx & \text{if } \mathbf{u} \in \Sigma, \\ +\infty & \text{otherwise,} \end{cases}$$

under volume constraints and the additional **solid constancy constraint**

$$\partial_t u_N = 0.$$

Denoting $\tilde{\mathbf{u}} = (u_1, u_2, \cdots, u_{N-1})$, let us consider the projection $\tilde{T}_\Sigma : \mathbb{R}^N \to \mathbb{R}^{N-1}$ onto

$$\left\{ \tilde{\mathbf{u}}, \sum_{i=1}^{N-1} u_i = \text{constant in time} = 1 - u_N \right\},$$

defined as

$$\tilde{T}_\Sigma[\mathbf{u}(\cdot,t)] = \tilde{\mathbf{u}}(\cdot,t) - \frac{1}{N-1}\left(\sum_{i=1}^{N-1} u_i(\cdot,t)\right)\mathbb{1}_{N-1}, \qquad \text{with } \mathbb{1}_{N-1} = (1,1,\dots,1) \in \mathbb{R}^{N-1}.$$

The L^2-gradient flow of the above problem is the following Allen-Cahn system:

$$\partial_t \tilde{\mathbf{u}} = -\frac{1}{2}\tilde{T}_\Sigma\left[\sigma\Delta\mathbf{u}\right] - \frac{1}{\epsilon^2}\tilde{T}_\Sigma\left[\partial_u \mathbf{W}_\sigma(\mathbf{u}) - \mathbf{\Lambda}\right].$$

where $\mathbf{\Lambda} = (\Lambda_1, \cdots, \Lambda_N)$ are Lagrange multipliers associated to the volume constraints:

$$\Lambda_i = \frac{\int (\partial_u \mathbf{W}(\mathbf{u}))_i dx}{\int \sqrt{2F(u_i)}dx}\sqrt{2F(u_i)}, \quad i \in \{1,\dots,N\}.$$

Note also that as

$$\tilde{T}_\Sigma\left[\sigma\Delta\mathbf{u}\right] = \tilde{T}[\sigma]\Delta\mathbf{u}, \quad \text{where} \quad \tilde{T}[\sigma]_{i,j} = \tilde{T}[\sigma_{\cdot,j}]_i,$$

we can consider the following variant equation

$$\partial_t \tilde{\mathbf{u}} = -\frac{1}{2}\left(\tilde{T}_\Sigma\left[\sigma\right] - \lambda\mathbb{1}_{N-1}\otimes\mathbb{1}_{N-1}\right)\Delta\mathbf{u} - \frac{1}{\epsilon^2}\tilde{T}\left[\partial_u \mathbf{W}_\sigma(\mathbf{u}) - \mathbf{\Lambda}\right].$$

where, as before, λ is assumed to be sufficiently large so that $\tilde{\sigma} = \tilde{T}\left[\sigma\right] - \lambda\mathbb{1}_{N-1}\otimes\mathbb{1}_{N-1}$ is a negative definite matrix.

6 Numerical experiments

We use a Fourier spectral splitting scheme [16] to compute numerically the solution to the Allen-Cahn system

$$\partial_t \mathbf{u} = -\frac{1}{2}\tilde{\sigma}\Delta\mathbf{u} - \frac{1}{\epsilon^2}T_\Sigma\left[\partial_u \mathbf{W}_\sigma(\mathbf{u})\right],$$

where $\tilde{\sigma} = T_\Sigma[\sigma] - \lambda\mathbb{1}_N\otimes\mathbb{1}_N$ with λ sufficiently large so that $\tilde{\sigma}$ is negative definite. We compute the solution for any time $t \in [0,T]$ in a box $\Omega = [0,1]^d$ with periodic boundary conditions. Then, the splitting scheme consists in handling:

- the diffusion term exactly in Fourier space

$$\mathbf{u}^{n+1/2} = \exp\left(\frac{1}{2}\delta_t\tilde{\sigma}\Delta\right)\mathbf{u}_n,$$

- the reaction term explicitly in the space domain

$$\mathbf{u}^{n+1} = \mathbf{u}^{n+1/2} - \frac{\delta_t}{\epsilon^2}T\left(\partial_u \mathbf{W}(\mathbf{u}^{n+1/2})\right).$$

Note that the space discretization is built with Fourier series. It has the advantage of preserving a high order approximation in space while allowing a fast and simple processing of the homogeneous operator $(I_d + \delta_t T(\sigma)\Delta)^{-1}$. In practice, the solutions $u(x, t_n)$ at time $t_n = n\delta_t$ are approximated by the truncated Fourier series :

$$\mathbf{u}^n_{\mathcal{P}}(x) = \sum_{\|p\|_\infty \le \mathcal{P}} \mathbf{u}^n_p e^{2i\pi x\cdot p},$$

where $\|p\|_\infty = \max_{1\le i\le d} |p_i|$ and $\mathcal{P}$ is the maximal number of Fourier modes in each direction. Then, the implicit treatment of the diffusion term in Fourier space can be written as

$$\mathbf{u}^{n+1/2} = \sum_{\|p\|_\infty \le \mathcal{P}} \mathbf{u}^{n+1/2}_p e^{2i\pi x\cdot p} \quad \text{with} \quad \mathbf{u}^{n+1/2}_p = \exp\left(2\pi^2 |p|^2 \delta_t \tilde{\sigma}\right) \mathbf{u}^n_p.$$

Here, $\exp\left(2\pi^2 |p|^2 \delta_t \tilde{\sigma}\right)$ is the exponential of the matrix $(2\pi^2 |p|^2 \delta_t \tilde{\sigma})$, which can be computed numerically with the function `exp` in *Matlab*.

Note that this scheme (as for the classical Allen-Cahn equation) appears to be stable under a condition of the form

$$\delta_t \le \frac{c_{\mathbf{W}}}{\epsilon^2},$$

where $c_{\mathbf{W}}$ is a constant which depends only on the multi-potential $\mathbf{W}$ (and not on ϵ, δ_t or $\mathcal{P}$).

The experiments presented in the remainder of the paper have been realized using Matlab. The isolevel sets $\Omega_i(t) = \{x \,:\, u_i(x,t) = \frac{1}{2}\}$ are computed and drawn using the Matlab functions `contour` in 2D and `isosurface` in 3D. We use the double-well potential $F(s) = \frac{1}{2}s^2(1-s)^2$ in the expression of the Lagrange multiplier associated to the volume constraint, and we consider the PDE system

$$\begin{cases} \partial_t \mathbf{u}(x,t) & = -\frac{1}{2}\tilde{\sigma}\Delta \mathbf{u}(x,t) - \frac{1}{\epsilon^2} T_\Sigma \left[\partial_u \mathbf{W}_\sigma(\mathbf{u}(x,t))\right], \\ \mathbf{u}(x,0) & = \mathbf{u}_0(x), \end{cases}$$

where the initial condition $\mathbf{u}_0(x)$ is given by

$$(\mathbf{u}_0)_i(x) = \frac{(\tilde{\mathbf{u}}_0)_i(x)}{\sum_{j=1}^N (\tilde{\mathbf{u}}_0)_j(x)} \quad \text{and} \quad (\tilde{\mathbf{u}}_0)_i(x) = q\left(\frac{\operatorname{dist}(x,\Omega_i)}{\epsilon}\right).$$

Here, Ω_i is the i^{th} set of the given initial partition, $\operatorname{dist}(x,\Omega_i)$ is the signed distance function to Ω_i and q is the profile function associated to $F(s) = \frac{1}{2}s^2(1-s)^2$. Note that $\mathbf{u}_0 \in \Sigma$.

6.1 Experimental consistency

The aim of this section is to compare numerically the behavior of our scheme associated to three different multi-well potentials $\mathbf{W}$:

$$\begin{cases} \mathbf{W}_1(\mathbf{u}) & = \frac{1}{4}\sum_{i,j} \sigma_{i,j} u_i^2 u_j^2, \\ \mathbf{W}_2(\mathbf{u}) & = \frac{1}{4}\sum_{i,j} \sigma_{i,j} u_i^2 u_j^2 + \frac{1}{2}\sum_{i<j<k} 50\, u_i^2 u_j^2 u_k^2, \\ \mathbf{W}_\sigma(\mathbf{u}) & = \sum_{i,j=1}^N \frac{1}{4}\sigma_{i,j} u_i^2 u_j^2 + \frac{1}{2}\sum_{i<j,k\neq i,k\neq j} \sigma_{i,k,j} u_i u_j u_k^2 + \sum_{i<j<k<l} \sigma_{i,j,k,l} u_i u_j u_k u_l. \end{cases}$$

Remark that potentials $\mathbf{W}_1$ and $\mathbf{W}_2$ are currently used in the literature [29]. It is only for potential $\mathbf{W}_\sigma$ that our results (see Theorem 4.1) guarantee the Γ-convergence of the associated approximating perimeter. This is partially illustrated in the following experiment, which shows also that using either $\mathbf{W}_1$ or $\mathbf{W}_2$ leads in contrast to undesirable effects, and implies in particular that Γ-convergence cannot be expected for the energies associated with these potentials.

More precisely, we compute numerically the geodesics $p_{i,j}$ and the numerical values of the surface tension coefficients $\delta_{i,j}$:

$$\delta_{i,j} = \frac{1}{c_F} \inf_p \int_{-1}^{1} \sqrt{\mathbf{W}(p(s))(-\sigma p'(s) \cdot p'(s))} ds.$$

The geodesics are obtained by resolution of the phase field system in dimension one with a "good" initial condition for $\mathbf{u}$. We consider the case $N = 3$ associated with the following surface tension coefficients: $\sigma_{12} = 1$, $\sigma_{13} = 0.6$ and $\sigma_{23} = 0.8$. We also take the numerical parameters equal to $\mathcal{P} = 2^{11}$, $\epsilon = 16/\mathcal{P}$, and $\delta_t = \epsilon^2/10$. The geodesics between every pair among $\{\mathbf{e_1}, \mathbf{e_2}, \mathbf{e_3}\}$ are represented in black on the first line of Figure 3 for each potential. A focus on the values of $\mathbf{u}$ along the geodesic g_{12} is shown in the second line. We observe that only the potential $\mathbf{W}_\sigma$ ensures that only two phases are visited along the geodesic. Moreover, the numerical estimations of the surface tensions $\delta_{i,j}$ (shown on the top of each figure) show a good approximation of $\sigma_{i,j}$ only in the case of the potentials $\mathbf{W}_2$ and $\mathbf{W}_\sigma$. To conclude, the potential $\mathbf{W}_1$ is unusable here, whereas $\mathbf{W}_2$ approximates correctly the multiphase perimeter P, and $\mathbf{W}_\sigma$ does even better.

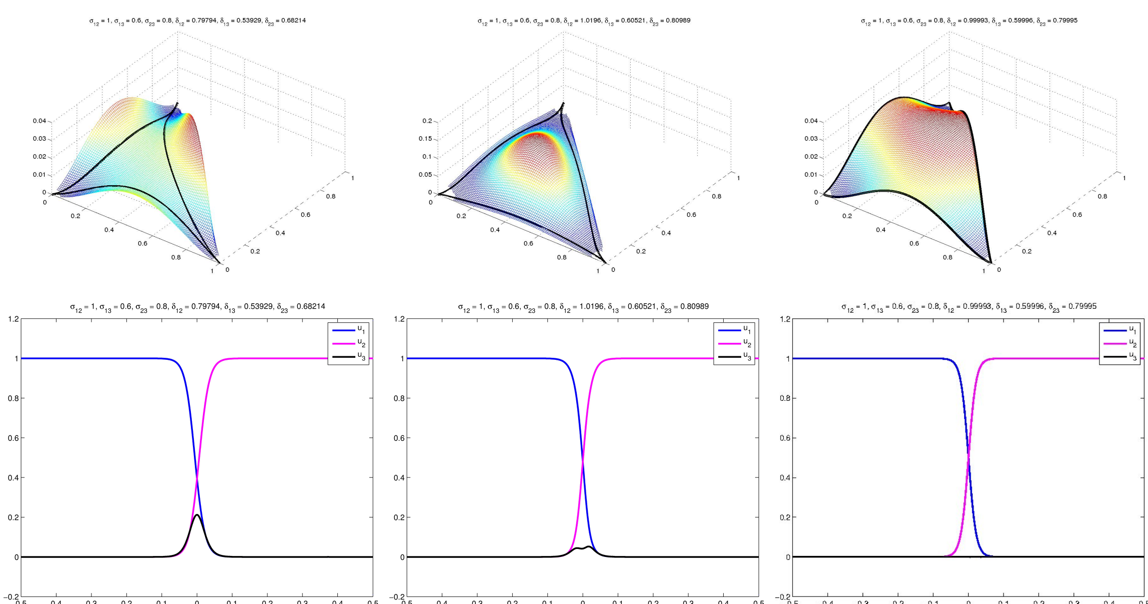

Figure 3: First line: Geodesics p_{ij} between phases e_i and e_j, $i, j \in \{1, 2, 3\}$, Second line: values of u_1, u_2, u_3 along geodesic p_{12} (from left to right: with potentials $\mathbf{W}_1$, $\mathbf{W}_2$ and $\mathbf{W}_\sigma$)

The second test concerns the evolution of an initial partition defined by :

- Ω_1 is a circle of radius $R_0 = 0.25$,
- $\Omega_2 = \Omega \setminus \Omega_1$,
- Ω_3 is empty.

Then, the L^2-gradient flow of P is explicit and satisfies

- $\Omega_1(t)$ is a circle of radius $R(t) = \sqrt{R_0^2 - 2\,t}$,
- $\Omega_2(t) = \Omega \setminus \Omega_1(t)$,
- Ω_3 remains empty.

The first line on Figure 4 shows the error between the numerical radius $R_\epsilon(t)$ and the theoretical radius $R(t)$, at different times t and for three different values of ϵ. The other numerical parameters are equal to $\mathcal{P} = 2^7$ and $\delta_t = 1/(10\mathcal{P}^2)$. It is reasonable to believe that this experiment illustrates the convergence of R_ϵ to R as ϵ goes to zero only in the case of the potentials $\mathbf{W}_2$ and $\mathbf{W}_\sigma$. More precisely, the second line of (4) presents a zoom on each figure which shows a convergence order $O(\epsilon)$ in the case of the potential $\mathbf{W}_2$ and $O(\epsilon^2)$ for the potential $\mathbf{W}_\sigma$. Note that the bad convergence order for the potential $\mathbf{W}_2$ is certainly the consequence of the presence of a third phase along the geodesics.

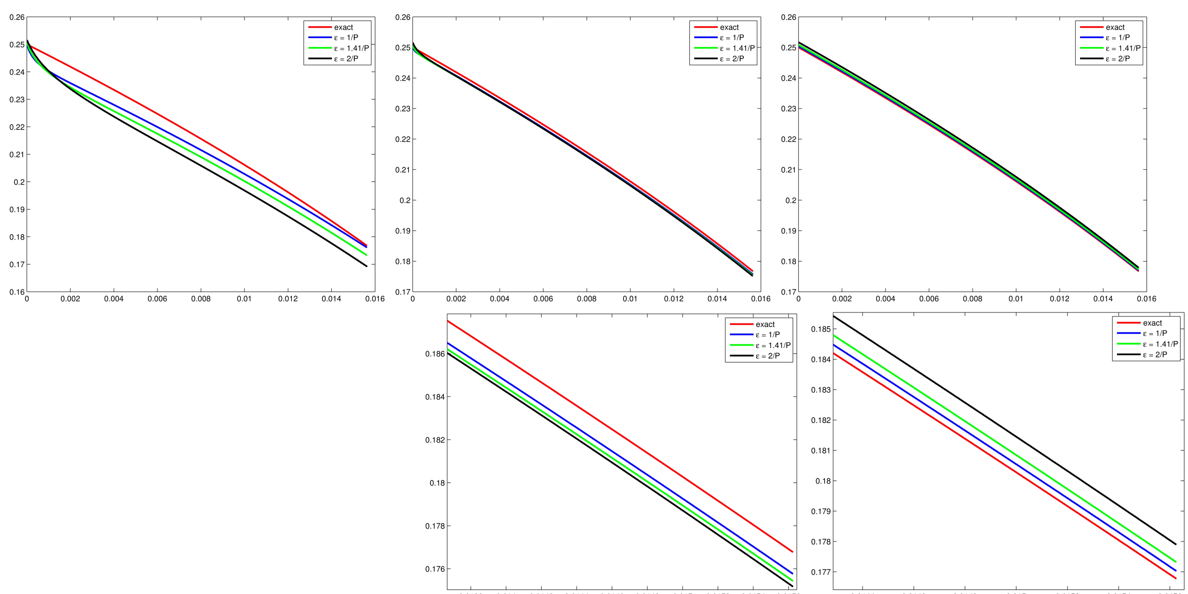

Figure 4: The graphs of $t \to R_\epsilon(t)$ for $\epsilon = 1/\mathcal{P}$, $\epsilon = \sqrt{2}/\mathcal{P}$ and $\epsilon = 2/\mathcal{P}$, compared with the exact solution. Left to right: with potentials $\mathbf{W}_1$, $\mathbf{W}_2$, and $\mathbf{W}_\sigma$. Second line: Zoom on the first line.

6.2 Evolution of partitions

We present now some experiments obtained with the following numerical parameters: $\mathcal{P} = 2^8$, $\epsilon = 1/\mathcal{P}$ and $\delta_t = \epsilon^2/4$. In all examples, $N = 4$, and Ω_1, Ω_2, Ω_3 and Ω_4 are plotted in blue, red, light blue and green, respectively.

Figure 5 shows two evolutions of three bubbles obtained with the following set of surface tensions

$$\sigma_1 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \qquad \text{and} \qquad \sigma_2 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1/2 & 1 \\ 1 & 1/2 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}.$$

In particular, we observe a slightly different evolution of the same initial partition, and the triple junctions between phases $1, 2, 3$ and $2, 3, 4$ are clearly different .

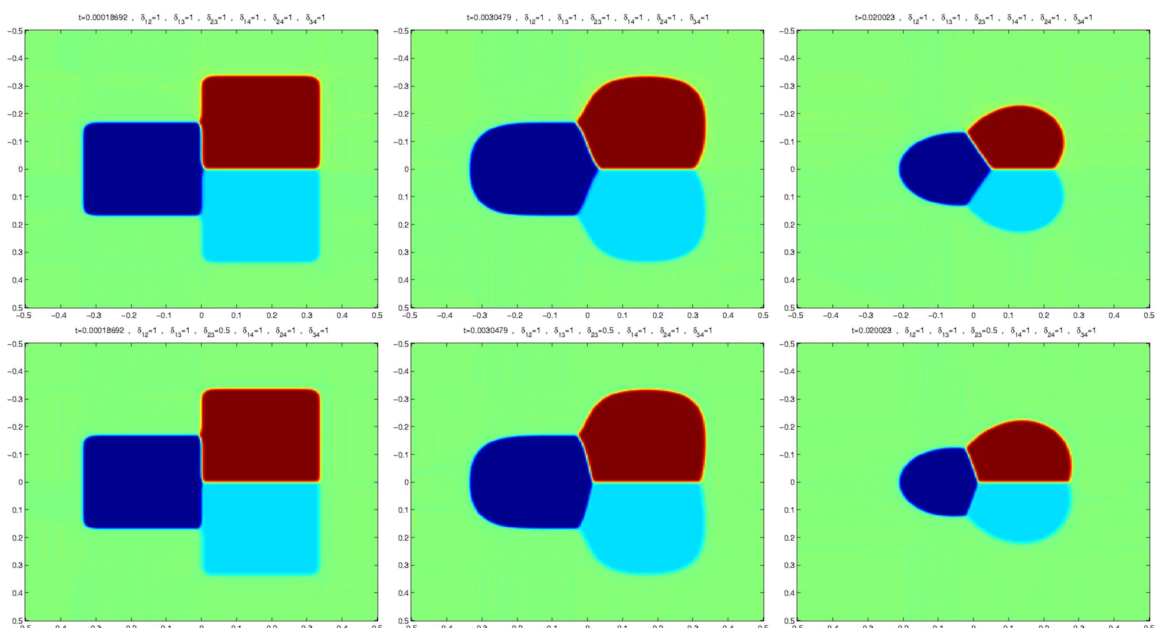

Figure 5: Evolution of a 4-partition; first line: $\sigma_{i,j} = 1$; second line: $\sigma_{1,2} = 1$, $\sigma_{1,3} = 1$, $\sigma_{2,3} = 0.5$, $\sigma_{1,4} = 1$, $\sigma_{2,4} = 1$, $\sigma_{3,4} = 1$.

The second test is inspired by a similar experiment in [25], and shows an example of wetting phenomenon when the triangle inequality (1.2) does not hold. Let us consider the two sets of surface tension coefficients

$$\sigma_3 = \begin{pmatrix} 0 & 3/2 & 1 & 1 \\ 3/2 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \qquad \text{and} \qquad \sigma_4 = \begin{pmatrix} 0 & 3/2 & 1 & 1/2 \\ 3/2 & 0 & 1 & 1/2 \\ 1 & 1 & 0 & 1 \\ 1/2 & 1/2 & 1 & 0 \end{pmatrix}.$$

Note that σ_3 satisfies the triangle inequality (1.2), but not σ_4 as

$$(\sigma_2)_{1,4} + (\sigma_2)_{2,4} < (\sigma_2)_{1,2}.$$

We consider an initial partition with an empty fourth phase. The first and second lines of Figure 6 show the evolution of this initial partition at different times t with σ_3 and σ_4, respectively. We can observe a nucleation phenomenon with the spontaneous growth of the fourth phase when σ_4 is used.

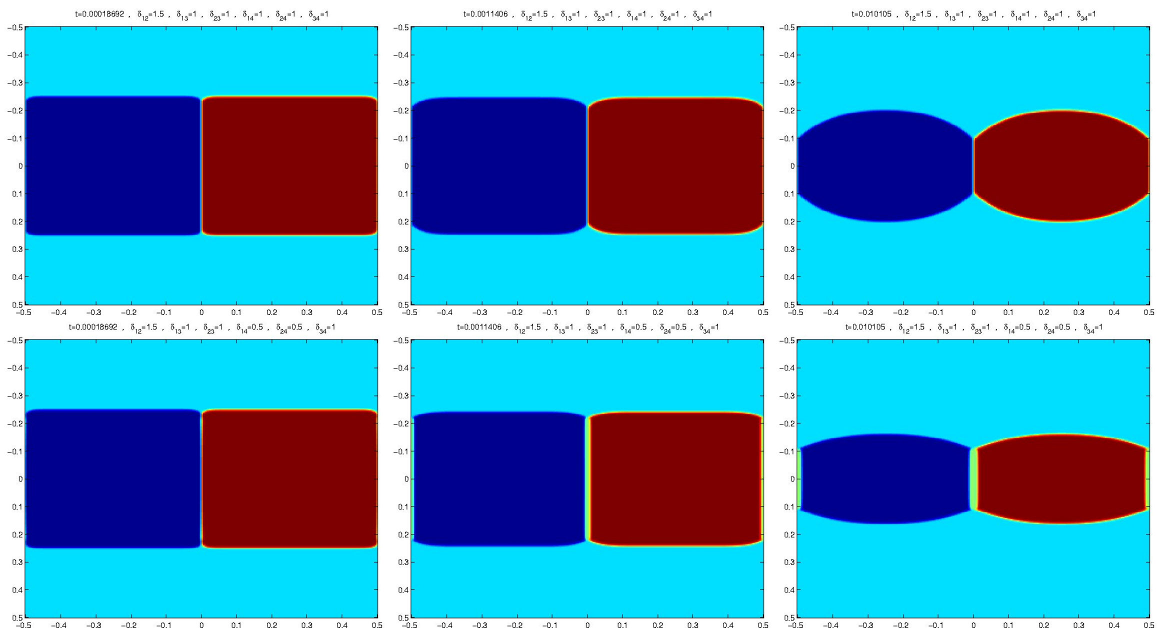

Figure 6: Starting from 3 phases out of 4, a nucleation may occur when the triangle inequality is not satisfied. First line: $\sigma_{1,2} = 1.5$, $\sigma_{1,3} = 1$ $\sigma_{2,3} = 1$ $\sigma_{1,4} = 1$, $\sigma_{2,4} = 1$ $\sigma_{3,4} = 1$ (no nucleation, triangle inequality holds); Second line with $\sigma_{1,2} = 1.5$, $\sigma_{1,3} = 1$ $\sigma_{2,3} = 1$ $\sigma_{1,4} = 0.5$, $\sigma_{2,4} = 0.5$ $\sigma_{3,4} = 1$ (nucleation occurs, $\sigma_{1,2} > \sigma_{1,4} + \sigma_{2,4}$).

The last example shows that nucleation phenomena can occur even for a matrix σ satisfying the triangle inequality (1.2), as observed also in [25]. Let

$$\sigma_5 = \begin{pmatrix} 0 & 1 & 1 & 1/2+\varepsilon \\ 1 & 0 & 1 & 1/2+\varepsilon \\ 1 & 1 & 0 & 1/2+\varepsilon \\ 1/2+\varepsilon & 1/2+\varepsilon & 1/2+\varepsilon & 0 \end{pmatrix},$$

where $\varepsilon \in [0, 3/2]$ to ensure the triangle inequality. For $\varepsilon \in [0, \frac{2-\sqrt{3}}{2\sqrt{3}}]$ a triple point between phases 1,2, and 3 cannot be stable, for it has larger energy than a triangle containing only phase 4. This can be easily seen on an optimal triple point configuration with all angles equal to $2\pi/3$: the energy of the triple point in a unit ball of which it is the center is 3; instead, the maximal equilateral triangle with same center and full of phase 4 has energy $3\sqrt{3}(\frac{1}{2}+\varepsilon)$. Therefore the choice $0 \leq \epsilon < \frac{2-\sqrt{3}}{2\sqrt{3}}$ guarantees that $3\sqrt{3}(\frac{1}{2}+\varepsilon) < 3$, i.e. a triangle full of phase 4 is more favorable. We plot in Figure 7 an evolution of a partition with $\varepsilon = \frac{0.9(2-\sqrt{3})}{2\sqrt{3}}$ and with $\varepsilon = \frac{1.1(2-\sqrt{3})}{2\sqrt{3}}$, and we observe the nucleation of phase 4 at each unstable triple junction only in the first case.

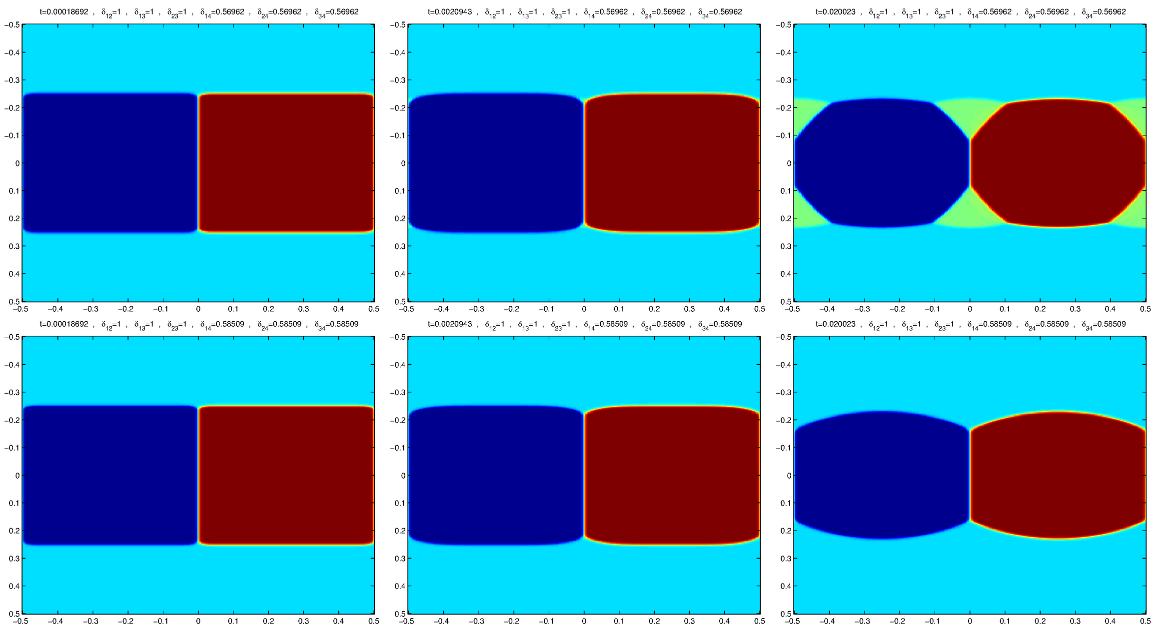

Figure 7: A nucleation example in the case $\sigma_{1,2} = 1$, $\sigma_{1,3} = 1$, $\sigma_{2,3} = 1$, $\sigma_{1,4} = 1/2 + \varepsilon$, $\sigma_{2,4} = 1/2+\varepsilon$, $\sigma_{3,4} = 1/2+\varepsilon$. First line with $\varepsilon = \frac{0.9(2-\sqrt{3})}{2\sqrt{3}}$ (triple points are unstable, the triangle inequality holds but the configuration with a triple point between phases 1,2,3 has larger energy than a triangle containing only phase 4 ; second line with $\varepsilon = \frac{1.1(2-\sqrt{3})}{2\sqrt{3}}$ (triple points are stable).

6.3 Wetting of multiphase droplets on solid surfaces

We now consider the system

$$\begin{cases} \partial_t \tilde{\mathbf{u}} & = \tilde{T}_\Sigma[\sigma \Delta \mathbf{u}] - \frac{1}{\epsilon^2} \tilde{T}_\Sigma \left[\partial_u \mathbf{W}(\mathbf{u}) - \mathbf{\Lambda} \right], \\ \mathbf{u}(x,0) & = \mathbf{u}_0(x). \end{cases}$$

As before $\tilde{\mathbf{u}} = (u_1, u_2, \cdots, u_{N-1})^T$ and $\tilde{T} : \mathbb{R}^N \to \mathbb{R}^{N-1}$ denotes the projection defined by

$$\tilde{T}[\mathbf{u}(\cdot,t)] = \tilde{\mathbf{u}}(\cdot,t) - \frac{1}{N-1} \left(\sum_{i=1}^{N-1} u_i(\cdot,t) \right) \mathbb{1}_{N-1}, \quad \text{where } \mathbb{1}_{N-1} = (1,1,\ldots,1) \in \mathbb{R}^{N-1},$$

and $\mathbf{\Lambda} = (\Lambda_i)$ are the Lagrange multipliers associated to droplets volume constraints:

$$\mathbf{\Lambda}_i = \frac{\int (\partial_u \mathbf{W}_\sigma(\mathbf{u}))_i dx}{\int \sqrt{2F(u_i)} dx} \sqrt{2F(u_i)}, \quad \text{for} \quad i \in \{1,\ldots,N\}.$$

In practice, we use the double-well potential $F(s) = \frac{1}{2} s^2 (1-s)^2$ in the expression of Λ.

Moreover, for a given initial partition $\{\Omega_i\}_{i=1^N}$, recall that the boundary of the N^{th} phase Ω_N is assumed to be the solid surface, and we take as initial condition $\mathbf{u}_0$ such that

$$\begin{cases} (\mathbf{u}_0)_N(x) & = q\left(\frac{\text{dist}(x,\Omega_N)}{\epsilon}\right), \\ (\tilde{\mathbf{u}}_0)_i(x) & = q\left(\frac{\text{dist}(x,\Omega_i)}{\epsilon}\right) \quad \text{for} \quad i \in \{1,\ldots,N-1\}, \\ (\mathbf{u}_0)_i(x) & = \frac{(\tilde{\mathbf{u}}_0)_i(x)}{\sum_{j=1}^{N-1} (\tilde{\mathbf{u}}_0)_i(x) + (\mathbf{u}_0)_N(x)} \quad \text{for} \quad i \in \{1,\ldots,N-1\}. \end{cases}$$

As before, the numerical scheme is a Fourier spectral splitting scheme with implicit resolution of the diffusion term in Fourier space and explicit resolution of the reaction term in spatial space.

The first experiment highlights the good behavior of our approach. We compute the optimal shape of a single droplet (Ω_2 in red) localized on a solid line (Ω_3 in green) with numerical parameters $\mathcal{P} = 2^8, \epsilon = 1/\mathcal{P}$, and $\delta_t = \epsilon^2/4$. We show in Figure 8 the different approximated optimal shapes obtained with our approach for the following surface tension matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 & 1/2 \\ 1 & 0 & 1 \\ 1/2 & 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1/2 \\ 1 & 1/2 & 0 \end{pmatrix}.$$

We also plot in each figure the optimal shape given by Young's law

$$\cos(\theta) = \frac{\sigma_{1,3} - \sigma_{2,3}}{\sigma_{1,2}},$$

and we can observe a quasi-perfect reconstruction of the optimal shape by the phase-field method. We emphasize that the angle condition is **not** prescribed, it follows naturally from the minimization of the multiphase perimeter.

Both final tests are inspired by the experiments in [7]. We now approximate the evolution of two droplets on a solid line with two different sets of surface tensions:

$$\sigma_4 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \quad \text{and} \quad \sigma_5 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0.9 & 0.7 \\ 1 & 0.9 & 0 & 1.3 \\ 0 & 0.7 & 1.3 & 0 \end{pmatrix}.$$

We plot in Figure 9 the evolution of both droplets in $2D$ at different times t with $\mathcal{P} = 2^8, \epsilon = 1/\mathcal{P}$ and $\delta_t = \epsilon^2/4$. The same experiment is done in 3D in Figure 10.

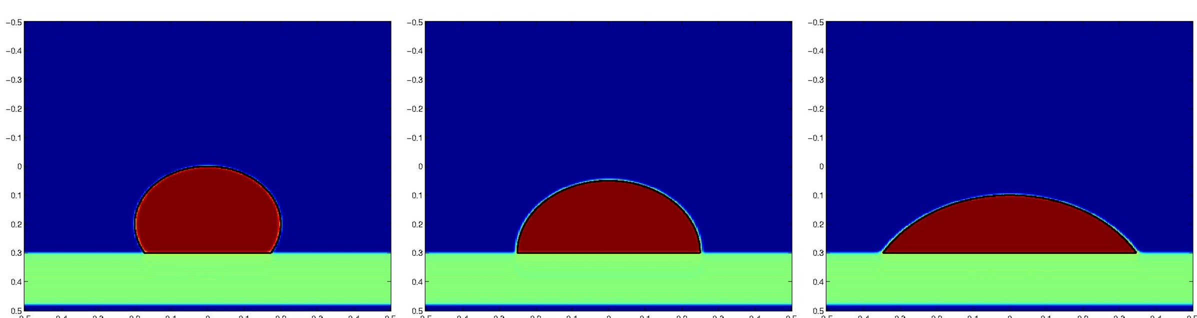

Figure 8: Optimal shape of a droplet. Left: $\sigma_{1,2} = 1$, $\sigma_{1,3} = 0.5$, $\sigma_{2,3} = 1$; middle : $\sigma_{1,2} = 1$, $\sigma_{1,3} = 1$, $\sigma_{2,3} = 1$; right: $\sigma_{1,2} = 1$, $\sigma_{1,3} = 1$, $\sigma_{2,3} = 0.5$

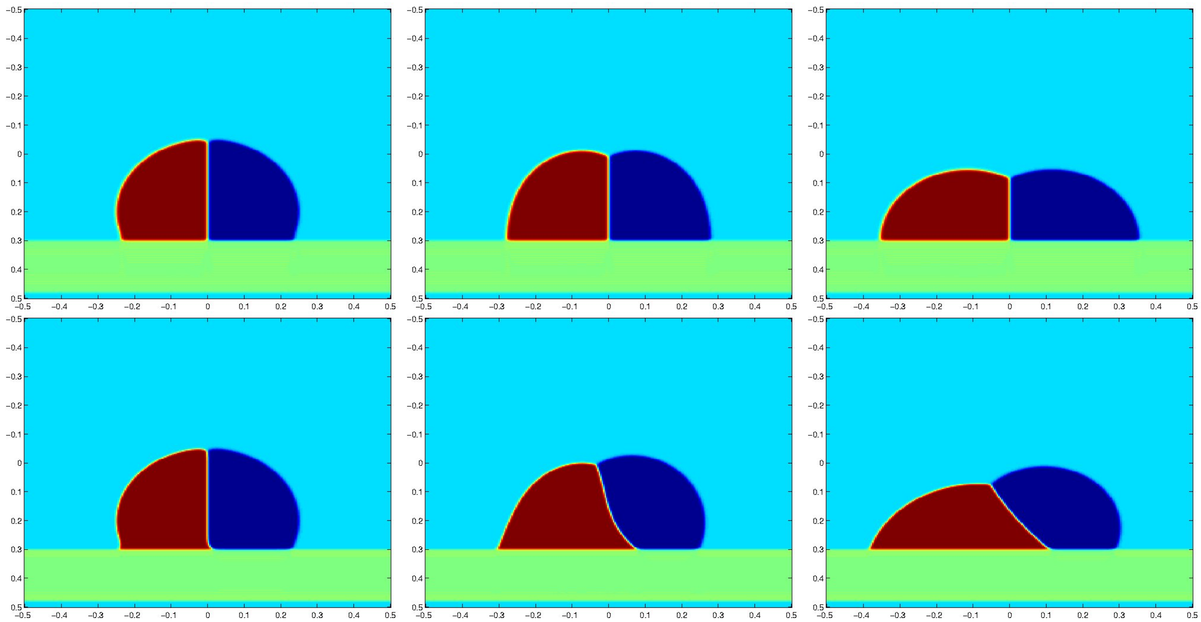

Figure 9: Dynamics of two droplets. First line: $\sigma_{i,j} = 1$; second line: $\sigma_{1,2} = 1$, $\sigma_{1,3} = 1$, $\sigma_{2,3} = 0.9$, $\sigma_{1,4} = 1$, $\sigma_{2,4} = 0.7$, and $\sigma_{3,4} = 1.3$

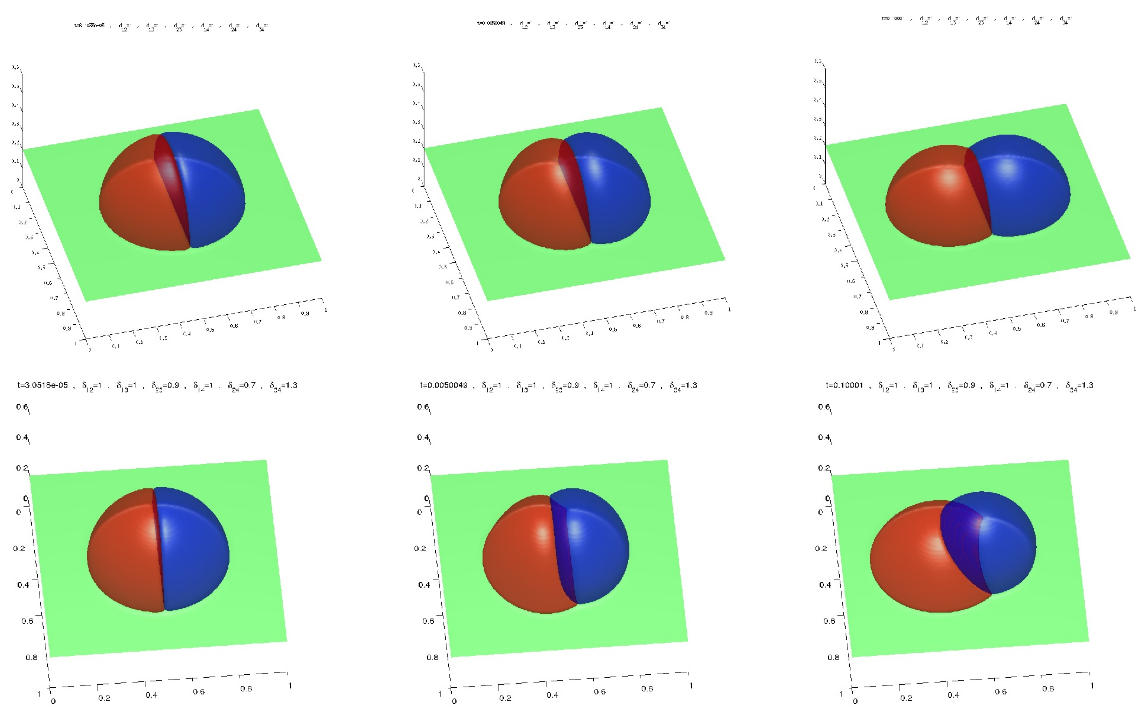

Figure 10: Dynamics of two droplets in 3D. First line: $\sigma_{i,j} = 1$; Second line: $\sigma_{1,2} = 1$, $\sigma_{1,3} = 1$, $\sigma_{2,3} = 0.9$, $\sigma_{1,4} = 1$, $\sigma_{2,4} = 0.7$, and $\sigma_{3,4} = 1.3$

Acknowledgments

The authors warmly thank Dorin Bucur and Edouard Oudet for fruitful discussions, and acknowledge the support of the French National Research Agency (ANR) under grant ANR-12-BS01-0014-01 (project GEOMETRYA). This work was also supported by the LABEX MILYON (ANR-10-LABX-0070) of Université de Lyon, within the program "Investissements d'Avenir" (ANR-11-IDEX-0007) operated by the French National Research Agency (ANR).

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