ALGORITHMS FOR MOTION OF NETWORKS BY WEIGHTED MEAN CURVATURE

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Abstract
I will report on recent developments in a class of algorithms, known as threshold dynamics, for computing the motion of interfaces by mean curvature. These algorithms try to generate the desired interfacial motion just by alternating two very simple operations: Convolution, and thresholding. They can be extended to the multi-phase setting of networks of surfaces, and to motion by weighted (anisotropic) mean curvature, while maintaining the simplicity of the original version. These extensions are relevant in applications such as materials science, where they allow large scale simulation of models for microstructure evolution in polycrystals.

1 Introduction
We will discuss algorithms for simulating the motion of a network of intersecting interfaces in $\mathbb{R}^d$, with focus on $d = 2$ or 3. Mathematically, we describe such a network as the union of boundaries $\bigcup_{i=1}^{N} \partial \Sigma_i$ of sets $\Sigma = (\Sigma_1, \ldots, \Sigma_N)$ (also called phases) that partition a domain $D \subset \mathbb{R}^3$ (typically a periodic box) without overlaps or vacuum:

$$D = \bigcup_{j=1}^{N} \Sigma_j, \text{ and } \Sigma_i \cap \Sigma_j = (\partial \Sigma_i) \cap (\partial \Sigma_j) \text{ for } i \neq j.$$
Many applications in science and engineering, ranging from models of microstructural evolution in polycrystalline materials to segmentation of images in computer vision, entail variational models with cost functions of the form

\[ E(\Sigma) = \sum_{i,j=1 \atop i \neq j}^{N} \int_{(\partial \Sigma_i) \cap (\partial \Sigma_j)} \sigma_{i,j} \left( n_{i,j}(x) \right) dS(x) \]

Here, \( dS \) is the length element in \( d = 2 \) or surface area element in \( d = 3 \), \( n_{i,j}(x) \) for \( x \in (\partial \Sigma_i) \cap (\partial \Sigma_j) \) denotes the unit normal from \( \Sigma_i \) to \( \Sigma_j \), and the continuous, even functions \( \sigma_{i,j} : \mathbb{S}^{d-1} \to \mathbb{R}^+ \) are the surface tensions associated with the interfaces.

In materials science, energy (2) and its \( L^2 \) gradient descent dynamics we recall below, was proposed by Mullins [1956] as a continuum model for grain boundary motion in polycrystalline materials – a class that includes most metals and ceramics. In this context, the sets \( \Sigma_i \) in (1) represent the space occupied by single crystal pieces (grains) in the material that differ from one another only in their crystallographic orientations. When the material is heated, atoms may detach from one grain and attach to a neighbor, leading to the motion of the boundaries: Some grains grow at the expense of others, leading to many topological changes in the network as it coarsens; see Figures 1 and 2. There are models that describe how the surface tensions \( \sigma_{i,j} \) are to be determined from the orientations of any two grains \( \Sigma_i \) and \( \Sigma_j \). The orientations may be chosen e.g. at random at the beginning of a simulation and are typically assumed to remain constant in time. The \( \sigma_{i,j} \) turn out to also depend on the normal to the interface between the two neighboring grains. For this application, it is therefore important to have numerical algorithms capable of treating the full generality of model (2).

When \( \sigma_{i,j}(x) = 1 \) for all \( x \) and \( i \neq j \), energy (2) becomes simply the sum of Euclidean surface areas of the interfaces in the network. In this form, it appears often as part of variational models in image segmentation, such as the Mumford-Shah model Mumford and Shah [1989] and its piecewise constant variants Chan and Vese [2001] and Vese and Chan [2002], where the sets \( \Sigma_i \) represent the space occupied by distinct objects in a scene. The goal of image segmentation is then to automatically discover these regions, which variational models such as Mumford and Shah [1989] exhibit as the minimizer of a cost function. Perimeter of the unknown sets is penalized in the cost function to control the level of detail in the segmentation obtained. While gradient flow for suitable approximations of (2) is certainly often employed to minimize the cost function, in this application the minimizer rather than the precise evolution required to reach it is of main interest, and there may be more effective ways than gradient flow to do so.
It is convenient to extend \( \sigma_{i,j} \) as one-homogeneous, continuous functions to all of \( \mathbb{R}^d \)

\[
\sigma(x) = |x| \sigma \left( \frac{x}{|x|} \right) \text{ for } x \neq 0
\]

in which case well-posedness of model \((2)\) requires them to be also convex. We will in fact assume that all \( \sigma_{i,j} \) have strongly convex and smooth unit balls in this discussion, in particular staying away from crystalline cases where the unit ball is a polytope.

For \( d = 2 \) or \( 3 \), we will study approximations for \( L^2 \) gradient flow of energy \((2)\), which is known as multiphase weighted mean curvature flow. In three dimensions, for an \( x \in (\partial \Sigma_i) \cap (\partial \Sigma_j) \) away from junctions (where three or more phases meet), normal speed under this flow is given by

\[
v_\perp(x) = \mu_{i,j}(n_{i,j}(x)) \left( (\partial^2_{s_1} \sigma_{i,j}(n_{i,j}(x)) + \sigma_{i,j}(n_{i,j}(x))) \kappa_1(x) \right. \\
\left. + (\partial^2_{s_2} \sigma_{i,j}(n_{i,j}(x)) + \sigma_{i,j}(n_{i,j}(x))) \kappa_2(x) \right)
\]

where \( \kappa_1 \) and \( \kappa_2 \) are the two principal curvatures, and \( \partial_{s_i} \) denotes differentiation along the great circle on \( S^2 \) that passes through \( n(x) \) and has as its tangent the \( i \)-th principal curvature direction. The additional factor \( \mu_{i,j} \) is known as the \textit{mobility} associated with the interface \( (\partial \Sigma_i) \cap (\partial \Sigma_j) \), and may be an anisotropic: \( \mu_{i,j} : S^2 \to \mathbb{R}^+ \). We will assume that it is smooth and has a one-homogeneous extension to \( \mathbb{R}^3 \) that is a norm. In two dimensions, \((4)\) simplifies to

\[
v_\perp(x) = \mu_{i,j}(n_{i,j}(x)) \left( \sigma''_{i,j}(n_{i,j}(x)) + \sigma_{i,j}(n_{i,j}(x)) \right) \kappa(x).
\]

In addition to \((4)\), a condition known as the \textit{Herring angle condition} Herring [1951] holds along triple junctions: In three dimensions, at a junction formed by the meeting of the three phases \( \Sigma_i, \Sigma_j, \) and \( \Sigma_k \), this condition reads

\[
(\ell \times n_{i,j}) \sigma_{i,j}(n_{i,j}) + (\ell \times n_{j,k}) \sigma_{j,k}(n_{j,k}) + (\ell \times n_{k,i}) \sigma_{k,i}(n_{k,i}) \\
+ n_{j,i} \sigma'_{i,j}(n_{i,j}) + n_{k,j} \sigma'_{j,k}(n_{j,k}) + n_{i,k} \sigma'_{k,i}(n_{k,i}) = 0
\]

where \( \ell = n_{j,k} \times n_{i,j} \) is a unit vector tangent to the triple junction, and \( \sigma'_{i,j}(n_{i,j}) \) denotes derivative of \( \sigma_{i,j} \) taken on \( S^2 \) in the direction of the vector \( \ell \times n_{i,j} \). In the isotropic setting, \((6)\) simplifies to the following more familiar form, known as Young’s law:

\[
\sigma_{i,j} n_{i,j} + \sigma_{j,k} n_{j,k} + \sigma_{k,i} n_{k,i} = 0.
\]

which can be rearranged to determine the angles between interfaces at a triple junction in terms of their surface tensions. For example, in the simplest case \( \sigma_{i,j} = 1 \) for all \( i \neq j \), \((7)\) implies all three angles at a triple junction are 120°.
Finally, we note that well-posedness of the multiphase energy (2) in its full generality is complicated Ambrosio and Braides [1990]. At the very least, in addition to convexity, the $\sigma_{i,j}$ need to satisfy a pointwise triangle inequality

$$\sigma_{i,j}(n) + \sigma_{j,k}(n) \geq \sigma_{i,k}(n)$$

for all distinct $i$, $j$, and $k$, and all $n \in \mathbb{S}^{d-1}$. In case the $\sigma_{i,j}$ are positive constants, (8) is known to be also sufficient for well-posedness of model (2).

## 2 Isotropic and Equal Surface Tensions

In Merriman, Bence, and Osher [1992, 1994], the authors proposed a remarkably elegant algorithm for dynamics (Equations (4) and (7)) in the special case that all surface tensions and mobilities satisfy $\sigma_{i,j}(x) = \mu_{i,j}(x) = 1$ for all $x$ and $i \neq j$. Called threshold dynamics (also diffusion generated motion), it generates a discrete in time approximation to the flow from an initial partition $\Sigma^0 = (\Sigma^0_1, \ldots, \Sigma^0_N)$ as follows:

**Algorithm:** (from Merriman, Bence, and Osher [1994]): Given a time step size $\delta t > 0$, alternate the following steps:

1. Convolution:

   $$(9) \quad \psi_i^k = K\sqrt{\delta t} \ast 1_{\Sigma_i^k}.$$  

2. Redistribution:

   $$(10) \quad \Sigma_i^{k+1} = \left\{ x : \psi_i^k(x) \geq \max_{j \neq i} \psi_j^k(x) \right\}.$$  

where $K$ is a convolution kernel that has the properties

$$K(x) \in L^1(\mathbb{R}^d), \ xK(x) \in L^1(\mathbb{R}^d), \text{ and } K(x) = K(-x)$$

and the notation $K_\varepsilon(x) = \varepsilon^{-d} K(x/\varepsilon)$ denotes its rescaled version. In the original papers Merriman, Bence, and Osher [1992, 1994], the convolution kernel $K$ is chosen to be the Gaussian

$$G(x) = \frac{1}{(4\pi)^{d/2}} \exp \left(-\frac{|x|^2}{4}\right)$$

but the intriguing possibility of replacing it with other kernels that may not be radially symmetric is also suggested.

Benefits of the algorithm include
Figure 1: A large scale simulation in two dimensions at an earlier (left) and later (right) time using a variant of threshold dynamics (Equations (9) and (10)). This is the isotropic, equal surface tension and mobility case.

1. Unconditional stability: Time step size is restricted only by accuracy considerations.

2. Low per time step cost: Step (9) can be implemented on uniform grids via the fast Fourier transform at $O(M \log M)$ cost, where $M$ is the number of grid points. Step (10) is pointwise and costs even less.

3. All points $x \in D$, whether they are in the interior of a phase, on an interface $(\partial \Sigma_i) \cap (\partial \Sigma_j)$, or at a junction, are treated equally: No need to track or even detect surfaces or junctions. The correct Herring angle condition (all $120^\circ$) is attained automatically at triple junctions.

4. As in phase field, level set, and other implicit interface methods, topological changes in the network occur with no need for intervention.

These benefits have made it possible to carry out very large scale simulations (hundreds of thousands of phases) of dynamics (Equations (4) and (6)) in both two and three dimensions – a capability desired by e.g. materials scientists interested in the statistics of shapes and sizes of grains during microstructural evolution. See Figures 1 and 2 for sample computations from Elsey, Esedoğlu, and Smereka [2009, 2011] that used a variant of Equations (9) and (10), and Barmak et al. [2006] for examples of grain statistics of interest for materials scientists.
In the two-phase setting, writing $\Sigma = \Sigma_1$ so that $\Sigma_2 = D \setminus \Sigma$ and taking $K = G$, steps (Equations (9) and (10)) can be combined to succinctly read

$$
\Sigma^{k+1} = \left\{ x \in D : G \sqrt{\delta_t} * 1_{\Sigma^k}(x) \geq \frac{1}{2} \right\}
$$

in the original form given in Merriman, Bence, and Osher [1992]. The motivation behind Equation (13) is an older idea known as the phase field, or diffuse interface method: To approximate the motion by mean curvature of the boundary $\partial \Sigma$ of a set $\Sigma$, one carries out gradient descent

$$
u_t = \Delta u - \frac{1}{\varepsilon^2} W'(u)
$$

for the energy

$$\int \frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} W(u) \, dx
$$

starting with the initial condition $u(x, 0) = 1_\Sigma$. Here, $W$ is a double well potential with equal depth wells at 0 and 1, e.g. $W(\xi) = \xi^2(1 - \xi)^2$. The second term in (15) is thus a penalty term that forces $u$ to approximate the characteristic function of a set as $\varepsilon \to 0^+$, while the Dirichlet energy term exacts a penalty on the rapid transition across the boundary.
of the set. Following Merriman, Bence, and Osher [ibid.], time splitting Equation (14) leads to

\begin{equation}
\text{Step 1: } u_t = \Delta u, \text{ followed by Step 2: } u_t = -\frac{1}{\varepsilon^2} W'(u).
\end{equation}

Step 1 explains the convolution with the Gaussian in (13), whereas Step 2 turns to thresholding in the limit \( \varepsilon \to 0 \): Gradient descent for the pointwise energy \( W(u) \), represented by Step 2, ends in either one of the wells 0 or 1 of \( W \), depending on whose basin of attraction \( u \) starts in. For \( W(\xi) = \xi^2(1-\xi)^2 \), the basins of attraction are separated by \( \xi = \frac{1}{2} \), which explains the threshold value of \( \frac{1}{2} \) in (13).

Unfortunately, this original motivation, based on time splitting the evolutionary PDE (14), turns out to be an inadequate explanation for even the consistency of threshold dynamics. Indeed, (15) \( \Gamma \)-converges to perimeter of sets Modica and Mortola [1977], and (14) approximates motion by mean curvature Rubinstein, Sternberg, and Keller [1989] and Evans, Soner, and Souganidis [1992], for e.g. \( W(\xi) = \xi^4(1-\xi)^2 \) also, the basins of attraction of which are separated by \( \frac{2}{3} \). The naive time splitting idea then suggests (13) with threshold value \( \frac{1}{2} \) replaced by \( \frac{2}{3} \) as an algorithm for motion by mean curvature. However, a simple truncation error analysis (as in Ruuth [1996]) shows that in the limit \( \varepsilon \to 0^+ \), the resulting dynamics is not motion by mean curvature. We were lucky above in choosing a \( W \) that is symmetric about its local maximum. This also means that, in general, one cannot find extensions of threshold dynamics (Equation (13)) to more general flows simply by time splitting corresponding phase field models and sending \( \varepsilon \to 0^+ \).

However, consistency of the two-phase scheme (13) on smooth interfaces can be verified easily with a simple Taylor expansion. For example, in \( \mathbb{R}^2 \) with \( K = G \), take a point \( p \in \partial \Sigma \). We may assume that \( p = 0 \) and \( \partial \Sigma \) is given as the graph of a function \( f \) near 0 and is tangent to the \( x \)-axis there, as shown in Figure 3. Then, according to Mascarenhas [1992] and Ruuth [1996, 1998b], Taylor expanding \( f \) at 0 in the convolution integral of (13) gives

\begin{equation}
\left( G_{\sqrt{\delta t}} * 1_\Sigma \right)(0, y) = \frac{1}{2} - \frac{1}{\sqrt{4\pi \delta t}} y + \sqrt{\frac{t}{4\pi}} f''(0) + O(t)
\end{equation}

as \( t \to 0 \), provided that \( y = O(t) \). Setting (17) to \( \frac{1}{2} \) as scheme (13) prescribes, and solving for \( y \) (the new position of the interface along the normal direction at present) exhibits the curvature of the curve as the leading order contribution to normal speed.

The analogue of Taylor expansion (17) for general kernels \( K \) (that need not be radially symmetric) was given in Ishii, Pires, and Souganidis [1999] in any dimension \( d \). When \( K \geq 0 \), the two-phase scheme (13) enjoys the following monotonicity property: If two different evolutions \( \Sigma^k \) and \( \Omega^k \) are generated by Equation (13) from the two different initial conditions \( \Sigma^0 \) and \( \Omega^0 \), respectively, satisfying the ordering \( \Sigma^0 \subseteq \Omega^0 \), the same
order is preserved at later times by the algorithm: $\Sigma^k \subseteq \Omega^k$ for all $k$. Combined with the consistency implied by (17), this comparison principle can be used to prove the convergence of scheme (13) to the viscosity solution of the level-set formulation of motion by mean curvature; see e.g. Evans [1993], Barles and Georgelin [1995], and Ishii, Pires, and Souganidis [1999] for the earliest rigorous convergence results for two-phase thresholding schemes. More recently, Swartz and Yip [2017] does not require the maximum principle and establishes convergence to the classical solution of two-phase mean curvature motion, with a rate.

In the multi-phase ($N > 2$) setting, Ruuth [1996, 1998a] present a truncation error analysis similar to (17) in the vicinity of a triple junction in order to verify that Equations (9) and (10) imposes the correct (in this case symmetric, $120^\circ$) Herring angle condition (7). This analysis also suggests an extension of Equations (9) and (10) to constant (isotropic) but unequal surface tensions. However, the resulting algorithm is considerably more complicated than the original, and contains some heuristic steps to handle multiple junctions. A natural, systematic extension of multi-phase threshold dynamics even to constant but unequal surface tensions (let alone anisotropic ones) was thus unavailable until recently.

### 3 New Algorithms: Arbitrary Surface Tensions

We will discuss the following questions:

1. What is the analogue of Equations (9) and (10) for:
   - Constant but possibly unequal surface tensions $\sigma_{i,j} \in \mathbb{R}^+$, and then
• The full generality of model (2), where \( n \) possibly distinct surface tension and mobility functions are specified?

2. Can we find a convolution kernel \( K \) for any given \( \sigma, \mu : S^{d-1} \rightarrow \mathbb{R}^+ \) pair? If so, can we ensure \( K \geq 0 \) (hence two-phase monotonicity) or \( \hat{K} \geq 0 \)?

Our starting point is a variational interpretation that was given in joint work Esedoğlu and Otto [2015] with Felix Otto for the original threshold dynamics Equations (9) and (10). It turns out that there is a systematic way to derive elegant algorithms in the style of Equations (9) and (10) from certain non-local approximations to perimeter of sets. In the simplest two-phase setting of (13), consider the energy

\[
E_\varepsilon(\Sigma) = \frac{1}{\varepsilon} \int_{\Sigma^c} K_\varepsilon \ast 1_\Sigma \, dx
\]

Energies of this type and their limit as \( \varepsilon \to 0 \) had been studied previously, e.g. in Alberti and Bellettini [1998], and with \( K \) the Gaussian in Miranda, Pallara, Paronetto, and Preunkert [2007]. Called the “heat content” of the set \( \Sigma \) in Miranda, Pallara, Paronetto, and Preunkert [ibid.], energies \( E_\varepsilon \) converge to a multiple of the Euclidean perimeter of sets in the sense of \( \Gamma \)-convergence Dal Maso [1993].

As explained in Esedoğlu and Otto [2015], Equation (13) can be recognized as the solution of the following optimization problem:

\[
\Sigma^{k+1} = \arg \min_{\Sigma \in D} E_{\sqrt{\delta t}}(\Sigma) + \frac{1}{\sqrt{\delta t}} \int (1_\Sigma - 1_{\Sigma^k}) K_{\sqrt{\delta t}} \ast (1_\Sigma - 1_{\Sigma^k}) \, dx
\]

revealing a previously unknown connection between heat content and threshold dynamics. For any kernel \( K \) with positive Fourier transform \( \hat{K} \geq 0 \) (such as the Gaussian), the second term in (19) is easily seen to be positive; it also vanishes at \( \Sigma = \Sigma^k \). It follows that

\[
E_{\sqrt{\delta t}}(\Sigma^{k+1}) \leq E_{\sqrt{\delta t}}(\Sigma^k),
\]

identifying (18) as a Lyapunov functional for scheme (13).

Moreover, (19) is reminiscent of the minimizing movements De Giorgi [1993] formulation of motion by mean curvature, due to Almgren, Taylor, and Wang [1993] and Luckhaus and Sturzenhecker [1995], the second term in (19) playing the role of the movement limiter. Indeed, it is easily verified on smooth interfaces that it measures (as \( \delta t \to 0 \)) the squared \( L^2 \) norm of the normal vector field that is needed to perturb \( \Sigma^k \) to \( \Sigma \). Along with the previously known \( \Gamma \)-convergence of energies (18), formulation (19) thus suggests very strongly that threshold dynamics (13) carries out gradient flow for approximately the right energy with respect to approximately the right metric.
One point is worth repeating: If all we want is a computational method to approximate the perimeter of a set, energy (18) would be a rather indirect and complicated way of doing it; certainly there are more practical and accurate methods. The reason for our interest is, as indicated above, these non-local approximations to perimeter turn out to offer a systematic way of deriving fast and elegant algorithms for curvature motion, such as (13).

3.1 Arbitrary Isotropic Surface Tensions. The following non-local energy is a natural candidate for approximating the surface area of \((\partial \Sigma_i) \cap (\partial \Sigma_j)\) in the multiphase setting of (2), in the same nonlocal style as (18):

\[
\frac{1}{\varepsilon} \int_{\Sigma_j} K_\varepsilon \ast 1_{\Sigma_i} \, dx
\]

With \(K\) the Gaussian, for example, it measures the amount of heat that escapes from \(\Sigma_i\) to \(\Sigma_j\), starting from the initial binary temperature distribution \(1_{\Sigma_i}\), which ought to be related to the size of the boundary between the two phases. This simple intuition leads us to the following non-local approximation for the multiphase model (2) in the isotropic case that all surface tensions \(\sigma_{i,j}\) are (possibly different) constants:

\[
E_\varepsilon(\Sigma) = \frac{1}{\varepsilon} \sum_{i,j=1}^{N} \sigma_{i,j} \int_{\Sigma_j} K_\varepsilon \ast 1_{\Sigma_i} \, dx.
\]

The analogue for (21) of the minimizing movements step (19) is

\[
\Sigma^k = \arg\min_{\Sigma} E^{\sqrt{\delta t}}(\Sigma) - \frac{1}{\sqrt{\delta t}} \sum_{i,j=1}^{N} \sigma_{i,j} (1_{\Sigma_j} - 1_{\Sigma^k_j}) K^{\sqrt{\delta t}} \ast (1_{\Sigma_i} - 1_{\Sigma^k_i}) \, dx
\]

the solution of which is given by the following algorithm from Esedoğlu and Otto [2015] which is the natural extension of the original threshold dynamics Equations (9) and (10) to isotropic, unequal surface tensions:
Algorithm: (from Esedoḡlu and Otto [ibid.]): Given a time step size $\delta t > 0$, alternate the following steps:

1. Convolution:

$$\psi_i^k = K \sqrt{\delta t} * \sum_{j \neq i} \sigma_{i,j} 1_{\Sigma_j^k}.$$  

2. Redistribution:

$$\Sigma_i^{k+1} = \left\{ x : \psi_i^k(x) \leq \min_{j \neq i} \psi_j^k(x) \right\}.$$  

Equations (23) and (24) reduces to Equations (9) and (10) if $\sigma_{i,j} = 1$ ($i \neq j$). Two immediate questions concerning the new algorithm are:

1. Do the non-local energies $E_\varepsilon$ in (21) approximate (2)?

2. Does Equations (23) and (24) decrease $E_\varepsilon$?

Theorem 1. (from Esedoḡlu and Otto [ibid.]) Let $K$ be the Gaussian, and let the surface tensions $\sigma_{i,j}$ satisfy the triangle inequality (8). Then, as $\varepsilon \to 0^+$, $E_\varepsilon$ $\Gamma$-converge to the appropriate formulation of (2) in terms of sets of finite perimeter.

Whether $E_{\sqrt{\delta t}}(\Sigma)$ is a Lyapunov functional for scheme (Equations (23) and (24)) appears to depend (even when $\tilde{K} \geq 0$) on whether the surface tension matrix $\sigma_{i,j}$ is conditionally negative semi-definite, which is known Schoenberg [1938], Avis and Deza [1991], and Deza and Laurent [1997] to be related to isometric embedding of finite metric spaces in Euclidean spaces. Based on these references, we conclude Equations (23) and (24) dissipates energy Equation (21) if

1. There exist $p_1, \ldots, p_N \in \mathbb{R}^k$ for some $k$ such that $\sigma_{i,j} = |p_i - p_j|_1$, or

2. There exist $p_1, \ldots, p_N \in \mathbb{R}^k$ for some $k$ such that $\sigma_{i,j} = |p_i - p_j|_2^2$.

The latter is also necessary for the movement limiter in (22) to be positive.

As a more immediately applicable example of allowed surface tensions, let us consider models of grain boundary motion from materials science. In Read and Shockley [1950], Read and Shockley describe a well known surface tension model for a two dimensional material with a square lattice structure. Subsequently, extensions of this model to three dimensional crystallography were given, see e.g. Holm, Hassold, and Miodownik [2001]. Let the orientations of the grains in the network be $g_1, \ldots, g_N \in SO(3)$, describing the
rotations needed to map a reference cubic lattice to those of the grains. Then, the surface
tension of the interface between grains $\Sigma_i$ and $\Sigma_j$ is given by

\[
\sigma_{i,j} = \begin{cases} 
\frac{\theta}{\theta^*} \left( 1 - \log \left( \frac{\theta}{\theta^*} \right) \right) & \text{if } \theta < \theta^* \\
\frac{\theta^*}{\theta^*} & \text{if } \theta \geq \theta^*.
\end{cases}
\]

with $\theta = \min_{r \in \mathcal{O}} \arccos \left( \frac{\text{tr} (rg_j g_i^{-1}) - 1}{2} \right)$

where $\mathcal{O}$ is the octahedral group of symmetries of the cube in $d = 3$, and $\theta^*$ is a cut-off
value. The angle $\theta$ represents the minimum angle needed to rotate the lattice of grain $\Sigma_i$
to that of grain $\Sigma_j$; Read and Shockley tell us that $\sigma_{i,j}$ is the specific function shown of
this angle. We have

**Theorem 2.** *from Esedoğlu and Otto [2015]*** Let the surface tensions $\sigma_{i,j}$ be determined
from orientations $g_i \in SO(3)$ of the grains by the Read and Shockley model (25). Then,
movement limiter in (22) is positive, so that energy (21) is a Lyapunov function for Equations (23) and (24).

Theorems 1 and 2 do not establish convergence of the evolution generated by Equations (9) and (10) or (23) and (24) to their intended limits. This was recently achieved by Laux and Otto in Laux and Otto [2016] and Laux and Otto [2017]. In a culmination of the minimizing movements formulation (22) of threshold dynamics, they obtain the first
convergence result for the multi-phase dynamics generated by thresholding algorithms (Equations (9) and (10)) and Equations (23) and (24). Roughly speaking, their result says

**Theorem 3.** *from Laux and Otto [2016]*** Given a sequence of $\delta t \to 0$, the piecewise constant in time extensions of the discrete in time approximations generated by Equations (23) and (24) have a subsequence that converges. If the time integral of their energies converge to that of the limit, then the limit solves the multi-phase version of the weak formulation of mean curvature motion given in Luckhaus and Sturzenhecker [1995].

More recently, Laux and Otto [2017] establishes that this limit is a solution of motion
by mean curvature also in Brakke’s sense Brakke [1978]. These are the first rigorous
convergence results on practical numerical algorithms for multi-phase motion by mean
curvature, persisting through possible topological changes.

### 3.2 Anisotropic Surface Tensions and Mobilities

Generalizations of Merriman, Bence, and Osher’s Equations (9) and (10) to anisotropic surface energies had been considered in
a number of works previously, though always in the two-phase setting.

One of the first contributions to the study of Equation (13) with general convolution
kernels $K$ (replacing $G$) is by Ishii, Pires, and Souganidis [1999], who establish the convergence of the algorithm to the viscosity solution of the equation $u_t = F(D^2u, Du)$
where

\[ F(M, p) = \left( \int_{p} K(x) dS(x) \right)^{-1} \left( \frac{1}{2} \int_{p} \langle Mx, x \rangle K(x) dS(x) \right) \]

for \( p \in \mathbb{R}^d \) and \( M \) a \( d \times d \) symmetric matrix, provided that \( K \) is a \textit{positive} convolution kernel with certain additional decay and continuity properties. Positivity of the kernel is required for the scheme to preserve the comparison principle that applies to the underlying interfacial motion, and is essential for the viscosity solutions approach taken in Ishii, Pires, and Souganidis [ibid.] (but the consistency calculation given in the paper applies to more general – i.e. sign changing – kernels).

Yet Ishii, Pires, and Souganidis [ibid.] does not address the inverse problem of constructing a convolution kernel for a given surface tension – mobility pair, which is perhaps the more practical question. The first contribution in this direction is by Ruuth and Merriman [2000], who propose a construction in \( \mathbb{R}^2 \). They show how to construct a kernel (characteristic function of a judiciously chosen star shaped domain) that, when used in (13), would generate a normal speed of the form

\[ v_\perp(x) = \left( f''(\theta(x)) + f(\theta(x)) \right) \kappa(x) \]

for a desired \( f : [0, 2\pi] \to \mathbb{R}^+ \), where \( \theta(x) \) is the angle that the normal at \( x \in \partial \Sigma \) makes with the positive \( x \)-axis. However, there are infinitely many surface tension and mobility pairs \((\sigma, \mu)\) that correspond to the same \( f \) and hence the same normal speed in (27); the discussion in Ruuth and Merriman [ibid.] does not elucidate what the two factors \( \sigma \) and \( \mu \) are for their kernel construction. This is particularly important in the multi-phase setting, since surface tensions determine the angles (6) at junctions.

More recently, Bonnetier et. al. Bonnetier, Bretin, and A. Chambolle [2012] have proposed a construction that works in both \( \mathbb{R}^2 \) and \( \mathbb{R}^3 \). The Fourier transform of their kernels is explicit in terms of the surface tension:

\[ \hat{K}(\xi) = \exp(-\sigma^2(\xi)). \]

It turns out that the corresponding mobility satisfies \( \mu = \sigma \), an important but very special case. This construction often yields sign changing kernels, even in two dimensions, preventing the authors from giving a rigorous proof of convergence. Moreover, as soon as the anisotropy \( \sigma \) does not have an ellipsoid as its unit ball, (28) has a singularity at the origin, leading to slow decay of \( K \).

The variational formulation (19) of threshold dynamics and its multiphase extension (22) prove particularly helpful with questions of anisotropy. For example, simply by evaluating the limit as \( \varepsilon \to 0^+ \) of energy (18) on a set \( \Sigma \) with smooth boundary, we are led to
the following natural candidate for the surface tension associated with a given kernel $K$:

$$\sigma_K(n) := \frac{1}{2} \int_{\mathbb{R}^d} |n \cdot x| K(x) \, dx. \tag{29}$$

Likewise, evaluating the movement limiter in the minimizing movements formulation (19) on smooth interfaces yields the following natural candidate for the mobility associated with $K$:

$$\frac{1}{\mu_K(n)} := \int_{n^\perp} K(x) \, dS(x). \tag{30}$$

It can be verified Elsey and Esedoğlu [2017] on smooth interfaces that threshold dynamics (13) is consistent with the normal speed (4) where $\sigma$ and $\mu$ in (4) are given by (29) and (30). Formula (29) can be expressed in terms of the cosine transform $\mathcal{T}$ for even functions on $S^d$:

$$\sigma_K(n) = \mathcal{T} \omega_K := \int_{S^d} \omega_K(x) |n \cdot x| \, dS(x) \tag{31}$$

where, according to (29), $\omega_K$ is given by

$$\omega_K(x) = \frac{1}{2} \int_0^\infty K(rn) r^d \, dr \tag{32}$$

$\omega_K$ is known as the generating function of the anisotropy $\sigma_K$. Formula (30) can alternatively be written using the spherical Radon transform $\mathcal{R}_s$:

$$\frac{1}{\mu_K} = \mathcal{R}_s \int_0^\infty K(rn) r^{d-2} \, dr. \tag{33}$$

Also helpful are the following expressions of (29) and (30) in terms of the Fourier transform of the kernel $K$:

$$\sigma_K(n) = -\frac{1}{2\pi} \text{F. P.} \int_{\mathbb{R}} \hat{K}(n\xi) \frac{d\xi}{\xi^2}, \text{ and} \tag{34}$$

$$\mu_K(n) = 2\pi \left( \int_{\mathbb{R}} \hat{K}(n\xi) \, d\xi \right)^{-1}.$$

These formulas allow us to draw upon existing results concerning the positivity of inverse cosine and inverse spherical Radon transforms in the convex geometry literature. For example, it is known that the generating function $\mathcal{T}^{-1} \sigma$ of an anisotropy $\sigma$ is always positive in $\mathbb{R}^2$, but may be negative for certain anisotropies in $\mathbb{R}^3$ Goodey and Weil [1992] and
Bolker [1969]. Those \( \sigma \) for which \( T^{-1} \sigma \) is positive have a nice geometric characterization: The unit ball of the dual norm, known as the Wulff shape \( W_\sigma \) of the anisotropy \( \sigma \), is a **zonoid**. Zonoids are convex bodies that are the limits with respect to the Hausdorff distance of centrally symmetric polytopes each face of which are also centrally symmetric Goodey and Weil [1992]. For example, in \( \mathbb{R}^3 \), there is a neighborhood of the octahedron that contains no zonoids. On the other hand, (32) tells us that the corresponding anisotropy \( \sigma_K \) of any positive convolution kernel \( K \) in threshold dynamics Equation (13) must have a positive generating function \( \omega_K \) and hence has to be zonoidal.

Moreover, it turns out there are restrictions on the attainable mobilities with positive kernels as well. Via (33), this matter is clearly related to positivity properties of the inverse spherical Radon transform \( J_s^{-1} \), which also appears prominently in the convex geometry literature, especially in the context of the Busemann-Petty problem Busemann and Petty [1956] and Gardner [1994b]. Indeed, results given in Gardner [1994a] on \( J_s^{-1} \), together with the foregoing discussion, yields the following limitation of threshold dynamics schemes (under assumptions on \( \sigma \) and \( \mu \) from the Introduction):

For certain surface tensions \( \sigma \) in \( \mathbb{R}^3 \), it is not possible to design a threshold dynamics Equation (13) that preserves the two-phase comparison principle. In particular, unless the Wulff shape of the anisotropy \( \sigma \) is the dilation of a zonoid by a sphere, there is no monotone threshold dynamics scheme for it.

It is interesting to compare with an alternative approach due to Chambolle and Novaga M. Chambolle A. N. [2006] for generating weighted motion by mean curvature that was inspired by threshold dynamics. Their idea is to replace the convolution (9) in the original Equation (13) with the solution of a nonlinear parabolic PDE:

**Threshold Dynamics**

**Nonlinear Threshold Dynamics**

**Step 1: Convolution:**

\[
\psi^k = K \sqrt{\delta t} * 1_{\Sigma^k}
\]

**Step 2: Thresholding:**

\[
\Sigma^{k+1} = \left\{ x : \psi^k(x) \geq \frac{1}{2} \int_{\mathbb{R}^d} K(x) \, dx \right\}
\]

**Step 1: Nonlinear Diffusion**

\[
\begin{align*}
\partial_t \psi^k &= \nabla \cdot \left( \sigma(\nabla \psi^k) \nabla \sigma(\nabla \psi^k) \right) \\
\psi^k(x, 0) &= 1_{\Sigma^k}(x).
\end{align*}
\]

**Step 2: Thresholding:**

\[
\Sigma^{k+1} = \left\{ x : \psi^k(x, \delta t) \geq \frac{1}{2} \right\}
\]

The Chambolle and Novaga scheme preserves the comparison principle for any anisotropy \( \sigma \), since the nonlinear diffusion equation in Step 1 of their algorithm enjoys this principle. Their Step 1, however, is more costly than the simple convolution involved in the
corresponding step of the original threshold dynamics scheme. It thus appears that the variational formulation (19) along with formulas (Equations (29) and (30)) suggest the following guideline in searching for diffusion generated motion algorithms with various desirable properties:

If we want to get away with just convolutions and avoid the costly solution of nonlinear PDE, we have to give up something: Namely, the two-phase comparison principle, for certain anisotropies in three dimensions.

Formulas (29) and (30), (32) and (33), and (34) also help explore how to construct a convolution kernel $K$ to be used in threshold dynamics Equation (13) to generate motion (4) with a given desired surface tension and mobility pair $\sigma, \mu : S^{d-1} \to \mathbb{R}^+$. For example, we can look for a kernel that in polar coordinates has the form

\begin{equation}
K(r, \theta) = \alpha(\theta, \phi)\eta(\beta(\theta, \phi)r)
\end{equation}

where $\eta : \mathbb{R} \to \mathbb{R}$ is any smooth, positive, non-zero function supported in $[1, 2]$. Substituting (35) in equations (32) and (33) yields simple, pointwise equations for $\alpha(\theta, \phi)$ and $\beta(\theta, \phi)$ in terms of $T^{-1}\sigma$ and $\mathcal{J}^{-1}(\frac{1}{\mu})$ which, in case $d = 2$, can always be solved with $\alpha \geq 0$:

**Theorem 4. (from Esedoğlu, Jacobs, and Zhang [2017])** In $\mathbb{R}^2$, for any desired surface tension $\sigma : S^1 \to \mathbb{R}^+$ and any desired mobility $\mu : S^1 \to \mathbb{R}^+$, there exists a smooth, positive, compactly supported convolution kernel $K$ such that $\sigma_K$ and $\mu_K$ given by (29) and (30) satisfy $\sigma_K = \sigma$ and $\mu_K = \mu$, so that threshold dynamics Equation (13) generates the corresponding motion by weighted curvature (4) and satisfies the comparison principle. This is also possible in $\mathbb{R}^3$, provided that the Wulff shape of $\sigma$ is the dilation of a zonoid by a sphere.

If we give up the two-phase comparison principle (as we must in general in $\mathbb{R}^3$), we can turn to (34) and look for e.g. kernels of the form

\begin{equation}
\hat{K}(\xi) = \exp(-\xi(\alpha(\xi))) + \exp(-\xi(\beta(\xi))).
\end{equation}

where $\zeta : \mathbb{R} \to \mathbb{R}^+$ is smooth, even, with $\zeta(x) = 0$ for $|x| \leq 1$ and $\zeta(x) = x^2$ for $|x| \geq 2$. Once again, one gets simple pointwise equations for $\alpha$ and $\beta$ that can always be solved Esedoğlu, Jacobs, and Zhang [ibid.], yielding a version of (28) that allows baking the mobility as well as the surface tension into a kernel with positive Fourier transform.

The immediate analogue of our non-local energies (21) in the multi-phase anisotropic setting is

\begin{equation}
E_\varepsilon(\Sigma) = \frac{1}{\varepsilon} \sum_{i,j=1} \int_{\Sigma_j} (K_{i,j})_\varepsilon * 1_{\Sigma_i} \, dx
\end{equation}
along with the following analogue of Equations (23) and (24):

**Algorithm:** (from Elsey and Esedoğlu [2017]) Alternate the following steps:

1. **Convolution:**
   \[
   \psi_i^k = \sum_{j \neq i} (K_{i,j}) \sqrt{\delta t} \star 1_{\Sigma_j^k}.
   \]  
   \(38\)

2. **Thresholding:**
   \[
   \Sigma_i^{k+1} = \left\{ x : \psi_i^k(x) \leq \min_{j \neq i} \psi_j^k(x) \right\}.
   \]  
   \(39\)

The \(n\) surface tensions and mobilities can be baked into the kernels \(K_{i,j}\) by one of the new constructions \((35)\) or \((36)\). We repeat that in \(\mathbb{R}^2\), there are infinitely many surface tension - mobility pairs \((\sigma_{i,j}, \mu_{i,j})\) corresponding to the same normal speed \((5)\) for each interface in the network. However, if kernels \(K\) are more stringently chosen by specifying their surface tensions and mobilities separately via \((29)\) and \((30)\) by e.g. the new kernel construction \((35)\), numerical experiments show that in addition to achieving the correct normal speed along interfaces, threshold dynamics attains the correct angle conditions \((6)\) at junctions, as the variational formulation \((22)\) suggests. Figure 4 shows a three-phase simulation using \((38)\) and \((39)\) from Esedoğlu, Jacobs, and Zhang [2017] where the kernels are constructed via \((35)\) corresponding to the following surface tension-mobility pairs:

\[
\sigma_{1,2}(x_1, x_2) = \sqrt{x_1^2 + x_2^2} \quad \mu_{1,2}(x_1, x_2) = 1,
\]

\(40\)

\[
\sigma_{1,3}(x_1, x_2) = \sqrt{\frac{1}{4} x_1^2 + x_2^2} + \sqrt{x_1^2 + \frac{1}{4} x_2^2} \quad \mu_{1,3}(x_1, x_2) = \frac{2x_1^2 + 3x_2^2}{4 \sqrt{x_1^2 + x_2^2}}
\]

\(41\)

\[
\sigma_{2,3}(x_1, x_2) = \sqrt{x_1^2 + \frac{25}{16} x_2^2} \quad \mu_{2,3}(x_1, x_2) = 1.
\]

\(42\)

Although Equations \((38)\) and \((39)\) thus appears to work as expected, we do not know sufficiently general conditions to be of interest on the surface tensions \(\sigma_{i,j}\) that would ensure an analogue of Theorem 2, guaranteeing dissipation of energy \((37)\). However, we can come up with slightly slower versions of Equations \((38)\) and \((39)\) for which an analogue of Theorem 2 can be easily shown to hold. The idea is to refresh convolutions more frequently during the course of a single time step. In the interest of brevity, let us consider the two-phase setting as an example. The following analogue of the original threshold dynamics scheme \((13)\) requires two convolutions per time step vs. one:
Figure 4: Kernels constructed using formulas (29) and (30) for the prescribed \((\sigma_{i,j}, \mu_{i,j})\) pairs (40), (41), (42), and a sample three-phase simulation: The black curves are the initial condition, the red curves are by Equations (38) and (39) using the kernels shown, and the blue curves are a benchmark result using front tracking Bronsard and Wetton [1995] and Kinderlehrer, Livshitz, and Taasan [2006] – a very accurate method that can have difficulties with topological changes. Being able to bake in a target surface tension and mobility of an interface into the convolution kernel of threshold dynamics is a new capability elucidated by the variational formulation (19) and (22). Taken from Esedoğlu, Jacobs, and Zhang [2017].

Algorithm: (from Esedoğlu and Jacobs [2017]) Alternate the following steps:

1. 1st Convolution:

   \[
   \psi^{k+\frac{1}{2}} = K_{\sqrt{\delta t}} \ast 1_{\Sigma^k} \tag{43}
   \]

2. 1st Thresholding:

   \[
   \Sigma^{k+\frac{1}{2}} = \Sigma^k \cup \left\{x : \psi^{k+\frac{1}{2}}(x) \geq \frac{1}{2}\right\} \tag{44}
   \]

3. 2nd Convolution:

   \[
   \psi^{k+1} = K_{\sqrt{\delta t}} \ast 1_{\Sigma^{k+\frac{1}{2}}} \tag{45}
   \]
Unlike (13), this slightly more costly version dissipates energy (18) for a much wider class of convolution kernels, e.g. any kernel $K$ of the form $K = f + g$ where $f \geq 0$ and $\hat{g} \geq 0$. This additional ease in establishing stability extends to multiple phases, so that similarly slowed down (but still unconditionally gradient stable) versions of Equations (38) and (39) are given in Esedoğlu and Otto [2015], Esedoğlu and Jacobs [2017], and Esedoğlu, Jacobs, and Zhang [2017] under a variety of assumptions on the convolution kernels that include the new constructions (35) and (36) that allow baking anisotropic surface tensions and mobilities simultaneously into convolution kernels.

References


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