A numerical level set method for the Stefan problem with a crystalline Gibbs-Thomson law

Norbert Požár
Institute of Science and Engineering
Kanazawa University

Abstract

We present a simple numerical method for the Stefan problem with the Gibbs-Thomson law based on a coupling of a total variation minimization algorithm and the finite element method for the heat equation, and discuss a few numerical results.

1 Introduction

In this note we present a simple numerical method for solving a Stefan-type problem with the Gibbs-Thomson law to model a growth of small crystals. Our goal is to explore the feasibility of coupling the algorithm due to Oberman, Osher, Takei and Tsai [OOTT] to solve the crystalline mean curvature flow problem without any regularization with a finite element method for the heat equation. Our main motivation are the recent advances in the theory of the crystalline mean curvature flow in an arbitrary dimension [CMP, CMNP, GP1, GP2].

In a dimension $n \in \mathbb{N}$, the problem is to find a relatively open set $E \subset \mathbb{R}^n \times [0, \infty)$ and a function $u : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}$ that satisfy

$$\begin{cases} u_t = \operatorname{div}(k\nabla u) & \text{in } \mathbb{R}^n \times (0,\infty) \setminus \partial E, \\ LV = (-k\nabla u)^{\text{out}} \cdot \nu - (-k\nabla u)^{\text{in}} \cdot \nu & \text{on } \partial E, \\ V = \beta(\nu)(\alpha\kappa_\sigma - u) & \text{on } \partial E, \end{cases} \tag{1.1}$$

with appropriate initial data u_0 and E_0. The set $E_t := \{x : (x,t) \in E\}$ represents the shape of an evolving crystal at the time $t \geq 0$, and V and ν are respectively the outer normal velocity and the spatial outer unit normal vector of its boundary ∂E_t. u represents the temperature, and the heat conductivity k is a given function that can depend on u as well. $(\cdot)^{\text{out}}$ and $(\cdot)^{\text{in}}$ denote the limits from the outside and the inside of E respectively. Note that a negative temperature on the crystal surface will force the crystal to grow, which will in turn release the latent heat of phase transition. The crystalline mean curvature κ_σ of the surface ∂E_t will be explained below. The function $\beta : \mathcal{S}^{n-1} \to (0, \infty)$ is a given mobility on the unit sphere, and $\alpha, L > 0$ are fixed constants.

Problem (1.1) is a model of a phase transition with the so-called kinetic undercooling represented by the Gibbs-Thomson law in the third equation. The second equation states the conservation of energy during the phase transition, where the amount of energy needed

to change the phase per unit volume is given by the specific latent heat of phase transition L, and this energy is delivered by the heat flux $-k\nabla u$. This problem appears in models of dendritic growth and solidification. For a more detailed discussion, see [CMOS, BGN] and the survey article [Ga] and the references therein.

2 Crystalline mean curvature

Following [AG, T], the crystalline mean curvature can be introduced as the first variation of the anisotropic surface energy functional defined for any sufficiently smooth set $U \subset \mathbb{R}^n$ as

$$\mathcal{F}(U) := \int_{\partial U} \sigma(\nu)\, dS,$$

where $\sigma : \mathcal{S}^{n-1} \to (0, \infty)$ is a given *anisotropy*. For the detailed overview of this topic, see the survey [B] or [Gu, GG, GP1, CMP]. In what follows we extend σ positively one-homogeneously to whole $\mathbb{R}^n$ as

$$\sigma(p) = \begin{cases} |p|\sigma(\frac{p}{|p|}), & p \neq 0, \\ 0, & p = 0. \end{cases}$$

We will assume that the extended σ is convex.

The anisotropy σ determines the optimal crystal shape (Wulff shape), that is, the shape that minimizes the anisotropic surface energy among shapes with the same volume as

$$\mathcal{W} := \{x : x \cdot p \leq \sigma(p),\ p \in \mathbb{R}^n\}, \tag{2.1}$$

see [T].

If σ is smooth on $\mathbb{R}^n \setminus \{0\}$ and $\{p : \sigma(p) \leq 1\}$ is a strictly convex set, and ∂U is smooth, the first variation of $\mathcal{F}$ with respect to a change of volume is $\operatorname{div}_{\partial U}(\nabla\sigma(\nu))$, where $\operatorname{div}_{\partial U}$ is the surface divergence, see [B]. We define

$$\kappa_\sigma := -\operatorname{div}_{\partial U}(\nabla\sigma(\nu)). \tag{2.2}$$

We are, however, specifically interested in anisotropies that are not smooth, in particular whose level set $\{\sigma \leq 1\}$ is a convex polytope and $\mathcal{W}$ above is the dual convex polytope [R]. In other words, when $\sigma : \mathbb{R}^n \to [0, \infty)$ is a convex, piece-wise linear function. We call such anisotropies *crystalline*. In this case, the definition of κ_σ becomes much more involved since $\nabla\sigma(\nu)$ is no longer defined pointwise and might be discontinuous even on a smooth surface. A natural generalization of (2.2), consistent with the general abstract theory of monotone operators due to Kōmura and Brézis [K, Br], is to replace the first variation of $\mathcal{F}$ with a subdifferential on an appropriate Hilbert space. This leads to the definition [B, CMP, GP1]

$$\kappa_\sigma := -\operatorname{div}_{\partial U} z_{\min},$$

where $z_{\min}$ is the element of the set

$$\left\{z \in L^\infty(\partial U) : z \in \partial\sigma(\nu),\ \operatorname{div} z \in L^2(\partial U)\right\} \tag{2.3}$$

that minimizes $\|\operatorname{div} z\|_{L^2(\partial U)}$, if the set is nonempty. Here $\partial\sigma$ is the subdifferential of σ,

$$\partial\sigma(p) := \{\xi \in \mathbb{R}^n : \sigma(p+h) - \sigma(p) \geq \xi \cdot h,\ h \in \mathbb{R}^n\}.$$

While $z_{\min}$ might not be unique, $\operatorname{div} z_{\min}$ is. Unfortunately, even for smooth ∂U the above set (2.3) might be empty, in which case κ_σ is not defined.

We call such κ_σ the *crystalline mean curvature of* ∂U. This quantity enjoys a number of interesting properties, including the comparison principle. Furthermore, it is a singular, nonlocal quantity on the surface ∂U. In particular, if ∂U has a flat part, called a facet, with normal ν such that σ is not differentiable at ν, κ_σ then depends on the shape of the facet. For example, in dimension $n = 2$, facets of U are line segments, and on each of them κ_σ is a constant that is inversely proportional to their length.

The well-posedness of (1.1) with a crystalline σ seems to be open. A general theory of solutions for the crystalline mean curvature flow (3.1) has been available only recently [CMP, CMNP, GP1, GP2].

3 Numerical algorithm

There have been many very successful algorithms developed to solve (1.1) with a smooth σ numerically and listing them all is beyond the scope of this note. One of the difficulties is the unstable nature of the dendritic growth and an extra care must be taken to avoid the discretization and the choice of a mesh to produce unwanted artifacts. See [CMOS, BGN, Ga] and the references therein. In this work to treat the crystalline mean curvature directly without any regularization, we instead use the algorithm proposed by [OOTT] that relies on the split Bregman iteration scheme introduced in [GO] to efficiently find minimizers of anisotropic total variation functionals. This approach builds on the level set formulation due to Chambolle [C] of the minimizing movements time semidiscretization of the anisotropic mean curvature flow

$$V = \beta(\nu)(\kappa_\sigma + f) \qquad \text{on } \partial E \tag{3.1}$$

by Almgren, Taylor and Wang [ATW].

In this algorithm, we fix a computational domain $\Omega \subset \mathbb{R}^n$ sufficiently large so that $E_t \subset \Omega$ for all $t \in [0, T]$ for some fixed $T > 0$, and choose a time step $h > 0$. Then we approximate E_{t_m}, $t_m = mh$, $m = 1, 2, \cdots$, by a sequence of sets $E_m \subset \Omega$, where $E_m := \{x : v_m(x) < 0\}$, and $v_m \in L^2(\Omega) \cap BV(\Omega)$ is the minimizer of the functional

$$J_m(v) := \frac{1}{2h}\|v - w_{m-1}\|_{L^2}^2 + \int_\Omega \sigma(\nabla v)\, dx - \langle v, f_m\rangle_{L^2}.$$

Here w_{m-1} is the signed distance function to the set E_{m-1} with respect to the anisotropy β,

$$w_{m-1}(x) = \operatorname{signdist}_\beta E_{m-1}(x) := \inf_{y \in E_{m-1}} \beta^\circ(x-y) - \inf_{y \in E_{m-1}^c} \beta^\circ(y-x),$$

where β° is the polar of β [R],

$$\beta^\circ(x) := \sup\left\{\frac{x \cdot \nu}{\beta(\nu)} : \nu \in \mathcal{S}^{n-1}\right\}.$$

The minimizer of J_m can be found efficiently by the split Bregman minimization method of [GO] as observed in [OOTT]. We proceed by introducing a new variable $d : \mathbb{R}^n \to \mathbb{R}^n$ and add a constraint $d = \nabla v$ that is then relaxed by a L^2-penalization term. In other words, we choose $\lambda > 0$ and in place of J_m we minimize

$$\tilde{J}_m(v, d) := \frac{1}{2h} \|v - w_{m-1}\|_{L^2}^2 + \int_\Omega \sigma(\nabla v)\, dx - \langle v, f_m \rangle_{L^2} + \frac{\lambda}{2} \|d - \nabla v\|_{L^2}^2 .$$

Since all the terms are convex, we can attempt to find the minimizer by alternatively minimizing with respect to v and d. This produces a sequence converging to the unique minimizer of $\tilde{J}_m$. However, this minimizer does not generally satisfy $d = \nabla v$ and therefore is not a minimizer of J_m.

This is addressed by introducing a third variable $b : \mathbb{R}^n \to \mathbb{R}^n$ that accumulates the "error" $\nabla v - d$ during the iteration. The full algorithm can be stated as follows: Set $b_{m,0} = d_{m,0} = 0$ and for $k = 0, 1, \ldots$ iterate

$$v_{m,k+1} \leftarrow \arg\min_v \frac{1}{2h} \|v - w_{m-1}\|^2 - \langle v, f_m \rangle + \frac{\lambda}{2} \|d_{m,k} - \nabla v - b_{m,k}\|^2 , \tag{3.2a}$$

$$d_{m,k+1} \leftarrow \arg\min_d \int_\Omega \sigma(d)\, dx + \frac{\lambda}{2} \|d - \nabla v_{m,k} - b_{m,k}\|^2 , \tag{3.2b}$$

$$b_{m,k+1} \leftarrow b_{m,k} + \nabla v_{m,k+1} - d_{m,k+1}, \tag{3.2c}$$

until convergence is achieved, for instance, until $\|v_{m,k+1} - v_{m,k}\|$ is sufficiently small.

This algorithm converges to a stationary point, see [GO]. When that happens, we deduce from the third step (3.2c) that the limit (v_m, d_m, b_m) satisfies $\nabla v_m = d_m$ and therefore v_m is the unique minimizer of J_m. In particular, it does not depend on the choice of λ. However, λ influences the difficulty to solve the minimization problem (3.2a) and the overall speed of convergence.

Note that solving (3.2a) is equivalent to solving a linear elliptic partial differential equation for v, while solving (3.2b) after discretization yields a completely decoupled minimization problem at each node, which only requires evaluating the projection on the optimal shape $\mathcal{W}$ in (2.1). See [GO, OOTT] for more details.

To couple this scheme with the heat equation in (1.1), we interpret the second equation in (1.1) as an energy source concentrated on the surface ∂E and add it to the heat equation:

$$u_t = \operatorname{div}(k \nabla u) + LV \mathcal{H}^{n-1} \lfloor \partial E_t.$$

After time discretization, for each $m = 1, 2, \ldots$, we

1. solve for E_m using the above algorithm with $f_m = -\alpha^{-1} u_{m-1}$ (in the TV minimization, we take $\tilde{\beta} = \alpha\beta$ with β from (1.1)), and then

2. solve for the solution u_m of

$$u_m - h \operatorname{div}(k \nabla u_m) = u_{m-1} + hLV_m \mathcal{H}^{n-1} \lfloor \partial E_m, \tag{3.3}$$

   where the normal velocity V_m is estimated using the value of the signed distance function signdist E_{m-1} with respect to the usual Euclidean metric on the set ∂E_m as

$$hV_m = \operatorname{signdist} E_{m-1}.$$

We discretize both (3.2) and (3.3) by the standard piece-wise linear finite elements on a regular triangular grid in two dimensions or a regular tetrahedral grid in three dimensions [P]. The discrete signed distance function is computed using the fast sweeping algorithm [Z] with the initialization scheme proposed in [P].

Recomputing the signed distance function necessarily moves the level set and introduces an error. However, we observe that v_m is still very close to a distance function of E_m near its boundary and therefore we usually set $w_m = v_m$. We recompute the actual signed distance function using the fast sweeping algorithm only after a prescribed number of steps.

It would be more appropriate to set the value of f_m using the extension of the value of $-u_{m-1}|_{\partial E_{m-1}}$ via a transport equation as in [AS] to increase the accuracy and reduce the need to reinitialize the distance function. This will be explored in the future.

It is natural to consider an adaptive mesh or perform the computation only near the boundary of the evolving domain. This is a subject of ongoing work.

4 Numerical results

In this section we present results of a few simple numerical experiments using the above algorithm, see Figures 1–4.

We fix the domain $\Omega = (-\frac{1}{2}, \frac{1}{2})^2$ for the total variation minimization and the fast sweeping method, and the domain $\Omega_{\text{heat}} = \left\{x \in \mathbb{R}^2 : |x| < \frac{1}{2}\right\}$ for the heat equation. The boundary data for the heat equation is set to -10^{-3}. For the mobility, we always use $\beta(p) = 100|p|_2$. The conductivity is taken to be 1 outside the crystal and 0 inside.

We discretize the domain by subdividing it uniformly into 256^2 squares and split each of those in half to produce the triangular mesh. The time step is fixed at $\tau = 2.5 \times 10^{-4}$. Larger time steps lead to instability, most likely due to the explicit nature of the coupling of the heat equation with the anisotropic mean curvature flow.

The optimal choice of the parameter λ is an interesting problem. In the original paper [GO] for total variation denoising applications, the value $\lambda = \frac{2}{h}$ was used. However, in the current computations the value $\lambda = \frac{1}{10h}$ was found using numerical experiments to provide a significant speed-up of the convergence. With this choice, only about 3–5 iterations of the algorithm (3.2) per time step are needed, and each of the presented results takes 15–30 minutes to compute on an Intel Core i7-4770K processor.

The simple numerical results show that the method can reproduce facet breaking due to the uneven cooling of the facets, and that neighboring crystals do not merge because the diffusion is limited inside the crystal. Due to the technical limitations of the current implementation, the fixed boundary for the heat equation is relatively close to the growing crystal, and this leads to a strong forcing at the exposed vertices. The facets there are therefore short and the crystal surface is not fully faceted. On the other hand, this illustrates that the method is capable of handling not fully faceted crystals, which is observed in practice in such strongly forced situations.

In summary, the initial implementation produces promising results, but more work is needed to make it competitive with other available algorithms. Adaptive meshes, a more accurate treatment of the boundary forcing term in the level set method and various other improvements are being considered. In particular, a three dimensional simulation is in preparation.

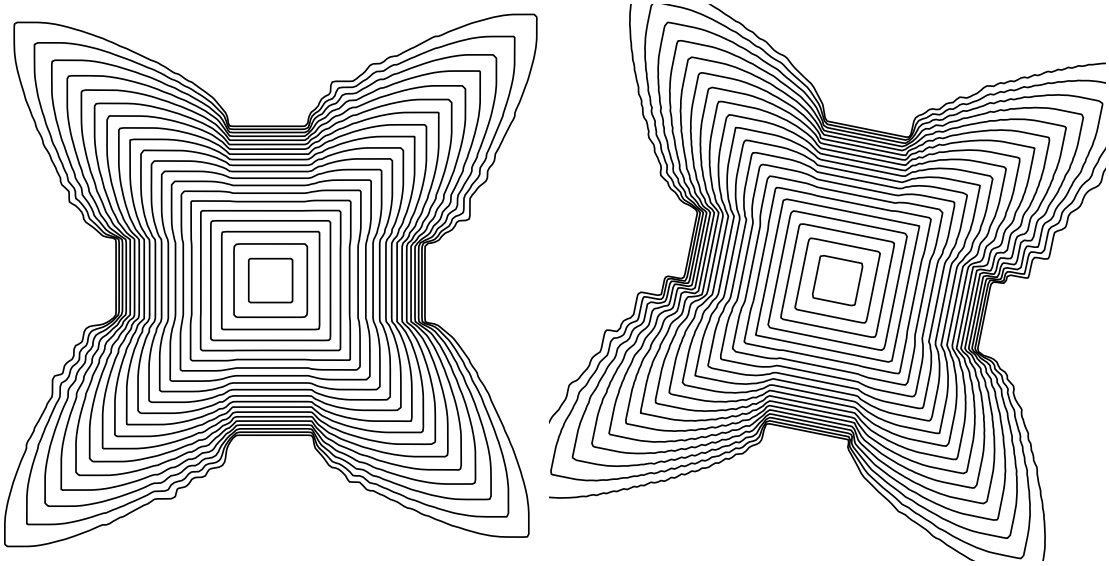

Figure 1: The evolution of a single square crystal of initial side length 0.05 growing with $\alpha = 5 \times 10^{-7}$, plotted at 2 second intervals aligned with the mesh (left) and rotated by 0.2 radians (right).

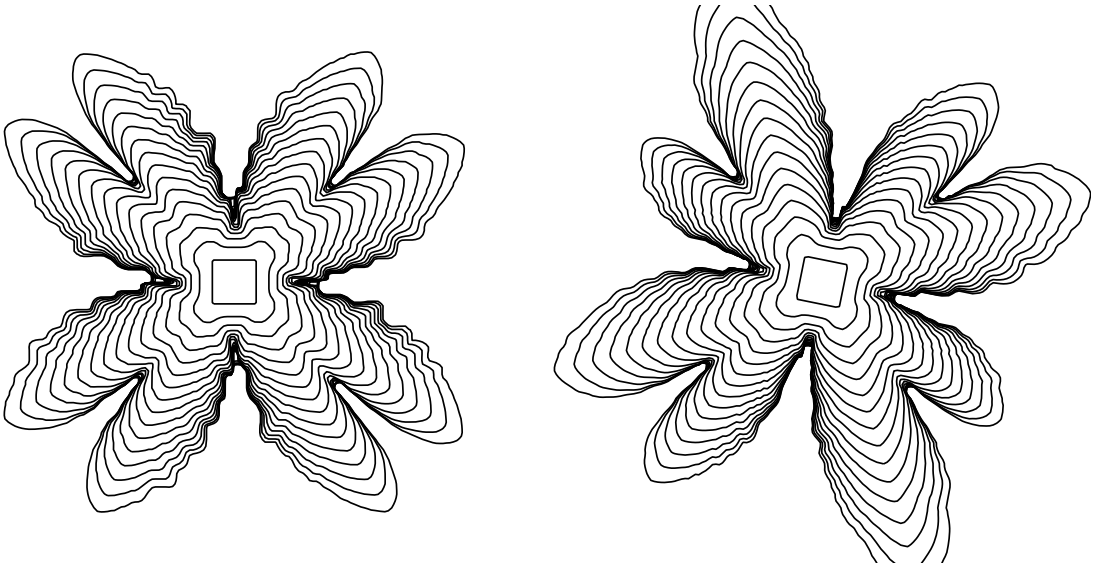

Figure 2: The evolution of a single square crystal of initial side length 0.05 growing with $\alpha = 10^{-8}$, plotted at 2 second intervals aligned with the mesh (left) and rotated by 0.2 radians (right). Since the curvature effect is significantly weaker than in Figure 1, only short facets appear in regions with a relatively weak forcing. The effect of the mesh is more pronounced: the dendrites splitting in half along the diagonal directions are almost certainly mesh artifacts.

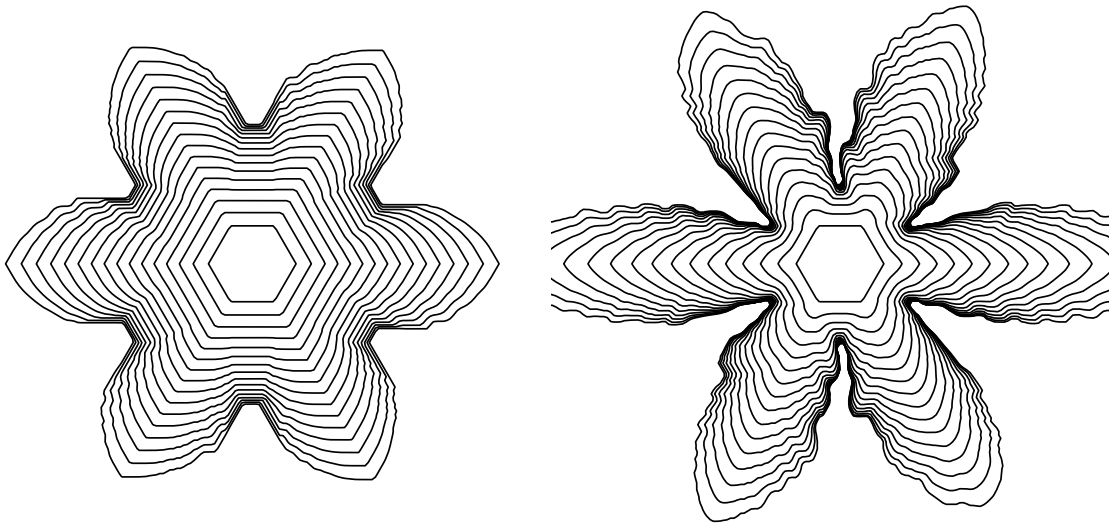

Figure 3: The evolution of a single hexagonal crystal of initial side length 0.05 growing with $\alpha = 2.5 \times 10^{-7}$ (left) and $\alpha = 10^{-8}$ (right), plotted at 2 second intervals. The horizontal dendrites grow faster, indicating an anisotropy caused by the mesh.

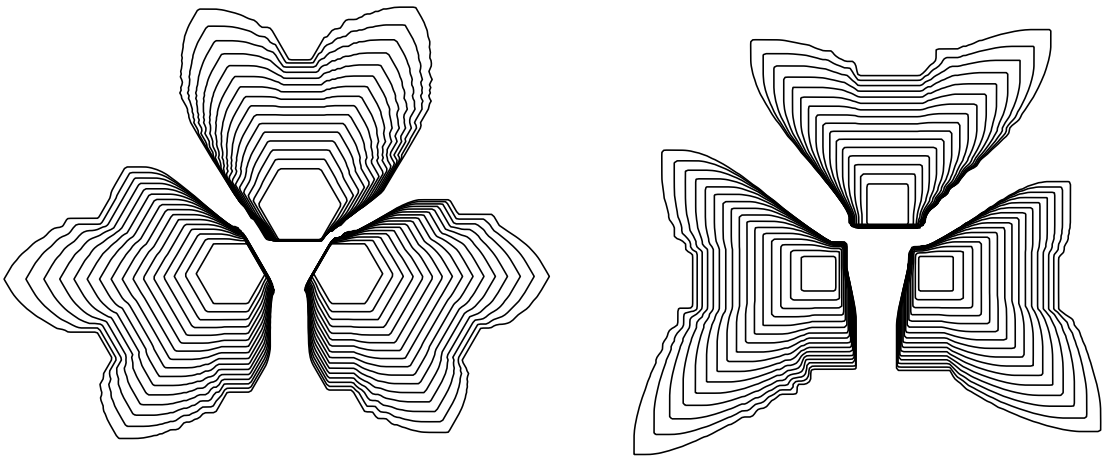

Figure 4: The evolution of three initially hexagonal or square crystals growing with $\alpha = 5 \times 10^{-7}$, plotted at 2 second intervals. Note that the crystals do not merge.

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Faculty of Mathematics and Physics
Institute of Science and Engineering
Kanazawa University
Kakuma town, Kanazawa
Ishikawa 920-1192
JAPAN
E-mail address: `npozar@se.kanazawa-u.ac.jp`