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Facet-breaking for three-dimensional crystals evolving by mean curvature

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We show two examples of facet-breaking for three-dimensional polyhedral surfaces evolving by crystalline mean curvature. The analysis shows that creation of new facets during the evolution is a common phenomenon. The first example is completely rigorous, and the evolution after the subdivision of one facet is explicitly computed for short times. Moreover, the constructed evolution is unique among the crystalline flows with the given initial datum. The second example suggests that curved portions of the boundary may appear even starting from a polyhedral set close to the Wulff shape.

1. Introduction

Motion by crystalline curvature is an anisotropic evolution of a set when the ambient space $\mathbb{R}^N$ is endowed with a convex one-homogeneous function whose unit ball (usually called the Wulff shape) is a polyhedron. It provides a geometric model for physical phenomena in phase transitions and crystal growth where the velocity of the evolving front depends on the orientation of the normal vector and has a finite number of preferred directions, corresponding to the facets of the Wulff shape. We refer for instance to [7] for an overview of this kind of geometric evolutions, and to [3, 16, 24, 25] and references therein for some applications. From the mathematical point of view, the presence of corners and flat regions in the Wulff shape is source of interesting problems, as pointed out in the pioneering papers of Taylor [20, 21, 23] who was also able to compute explicitly the velocity (i.e. the crystalline mean curvature) of the interface (see (4.2)).

The variational nature of this evolution is of basic importance. There is indeed an associated natural free energy, which decreases as fast as possible under crystalline motion by mean curvature, see [1, 2, 23] and Section 3 below. The simplest situation of motion by crystalline curvature in $N = 2$ dimensions has been the object of several recent papers, see for instance [1, 10, 11, 12, 14, 18, 19]. In this case, short-time existence and uniqueness of the evolution has been established, as well as an inclusion principle between the evolving fronts. Moreover, if the initial set E is a polygon compatible with the Wulff shape, its edges translate parallel to themselves during the evolution, so that no edge-breaking occurs. It is interesting to observe that the situation becomes quite different in presence of a space-dependent forcing term [11]. In the present paper we consider motion by crystalline curvature in $N = 3$ dimensions: here the situation is much more complicated, and less is known about the qualitative behaviour of the evolving interfaces. In particular, to the best knowledge of the authors, given an initial set, we can neither definitely predict instantaneous facet-breaking nor understand where subdivisions, if any, take place. In this direction, we refer to the papers [17, 22] for numerical simulations. Furthermore, the issue of short-time existence of a 'smooth' evolution is still open, as well as the construction of a unique weak solution [11] describing the motion after the onset of singularities.

A comparison principle has been established in [13] for some particular evolutions in three dimensions, and generalized in any space dimension and for any convex Wulff shape in [4]. This result implies uniqueness of the evolution. We notice that in [13] the study of the crystalline evolution has been carried out under the assumption that no facet-breaking occurs. Here we compute two examples of facet-breaking for three-dimensional polyhedral surfaces evolving by crystalline mean curvature. Example 1 concerns a cubic Wulff shape $\mathcal{W}_\phi$ and a non convex ϕ-regular initial set E. It turns out that, for proper choices of the lengths of the edges of ∂E, a facet instantly subdivides into two new facets. We explicitly compute the subsequent evolution $t \to E(t)$ for short times: this evolution is unique, i.e. is *the* crystalline evolution of E. Example 2 is more surprising, even if not completely rigorous: here the Wulff shape is a regular orthogonal prism with hexagonal basis, and the initial set E is a convex polyhedron very close to $\mathcal{W}_\phi$. Depending on a certain parameter, there is evidence that a curved portion of the boundary instantly develops. Numerical simulations of all these phenomena will appear in [17]. Such an evolution is expected to be the crystalline evolution of E.

These two examples show several facts. Firstly, subdivision of one facet into new facets seems to be a common phenomenon in three dimensions, as already remarked by Taylor in [22] and by Yunger in [26]. Secondly, since it is natural to look for a short time existence theorem in a suitable class of surfaces, then (if our interpretation of Example 2 is correct) this class must be sufficiently large to include piecewise C^1 surfaces. Notice also that the class of ϕ–regular polyhedra is not stable under crystalline mean curvature flow, even for short times.

We point out that Taylor expects the existence of initial data for which the amount of new subdivisions is not bounded [1, 21]. This could be related to our examples.

The plan of the paper is the following. In Section 2 we define some notation. In Section 3 we recall, following [4], the general definitions of ϕ-regular set and ϕ-regular flow. These definitions concern basically Lipschitz surfaces; we do not restrict ourselves to polyhedral surfaces, in view of Example 2. At the end of Section 3 we partially compute the first variation of the crystalline perimeter. In Section 4 we give some preliminaries on crystalline evolutions of polyhedral sets. In particular, in Definition 4.1 we introduce the class of ϕ-calibrable sets. A ϕ-calibrable set is, roughly speaking, a ϕ-regular polyhedron with each facet of constant ϕ-mean curvature, i.e. which admits a global Cahn–Hoffman vector field having constant divergence on each facet. Theorem 4.3 provides a necessary condition for a set to be ϕ-calibrable, and this will be crucial to construct the examples, which are illustrated in Section 5. We conclude by observing that finding necessary and sufficient conditions on a set E to be ϕ-calibrable would be very useful to understand the class of initial polyhedral surfaces which do not develop new facets for short times.

2. Some notation

In the following we denote by $\cdot$ the standard euclidean scalar product in $\mathbb{R}^3$ and by $|\cdot|$ the euclidean norm of $\mathbb{R}^3$. Given a subset A of $\mathbb{R}$ or $\mathbb{R}^2$, we denote by $|A|$ the Lebesgue measure of A. $\mathcal{H}^k$, for $k = 1, 2, 3$, will denote the k-dimensional Hausdorff measure in $\mathbb{R}^3$. If $E \subset \mathbb{R}^3$, we denote by ∂E the topological boundary of E. By a polyhedral set E we always mean a bounded closed polyhedral set, and by a facet F (resp. an edge l) of ∂E (i.e. of E) we always mean a closed facet (resp. a closed edge); we denote by int(F) (resp. int(l)) the relative interior of F (resp. of l). We assume that all polyhedral sets have a finite number of facets.

Given a polyhedral set E, a facet F of E and an edge l of F, we denote by $\nu_{F,l}$ the euclidean unit normal to int(l) lying in the plane of F and pointing outside F.

We indicate by $\phi : \mathbb{R}^3 \to [0, +\infty[$ a convex function satisfying the properties

$$\phi(\xi) \geqslant \Lambda|\xi|, \qquad \phi(a\xi) = a\phi(\xi), \qquad \xi \in \mathbb{R}^3,\ a \geqslant 0, \tag{2.1}$$

for a suitable constant $\Lambda \in\ ]0, +\infty[$, and by $\phi^o : \mathbb{R}^3 \to [0, +\infty[$, $\phi^o(\xi^*) := \sup\{\xi^* \cdot \xi : \phi(\xi) \leqslant 1\}$ the dual of ϕ. We set

$$\mathcal{F}_\phi := \{\xi^* \in \mathbb{R}^3 : \phi^o(\xi^*) \leqslant 1\}, \qquad \mathcal{W}_\phi := \{\xi \in \mathbb{R}^3 : \phi(\xi) \leqslant 1\}.$$

$\mathcal{F}_\phi$ and $\mathcal{W}_\phi$ are convex sets whose interior parts contain the origin. In this paper we shall assume that ϕ is crystalline, i.e. $\mathcal{W}_\phi$ (and hence $\mathcal{F}_\phi$) is a convex polytope. $\mathcal{F}_\phi$ is usually called the Frank diagram and $\mathcal{W}_\phi$ the Wulff shape.

Let $T^o : \mathbb{R}^3 \to \mathcal{P}(\mathbb{R}^3)$ be the duality mapping defined by

$$T^o(\xi^*) := \tfrac{1}{2}\partial^-(\phi^o(\xi^*))^2, \qquad \xi^* \in \mathbb{R}^3,$$

where $\mathcal{P}(\mathbb{R}^3)$ is the class of all subsets of $\mathbb{R}^3$ and ∂^- denotes the subdifferential in the sense of convex analysis. We observe that T^o is a multivalued maximal monotone operator; moreover

$$T^o(a\xi^*) = aT^o(\xi^*), \qquad a \geqslant 0,$$

and T^o takes $\partial\mathcal{F}_\phi$ onto $\partial\mathcal{W}_\phi$.

One can show that

$$\xi^* \cdot \xi = \phi^o(\xi^*)^2 = \phi(\xi)^2, \qquad \xi^* \in \mathbb{R}^3,\ \xi \in T^o(\xi^*).$$

Given a nonempty set $E \subset \mathbb{R}^3$ and $x \in \mathbb{R}^3$, we set

$$\mathrm{dist}_\phi(x, E) := \inf_{y \in E} \phi(x - y), \qquad \mathrm{dist}_\phi(E, x) := \inf_{y \in E} \phi(y - x),$$

$$d^E_\phi(x) := \mathrm{dist}_\phi(x, E) - \mathrm{dist}_\phi(\mathbb{R}^3 \setminus E, x).$$

At each point x where d^E_ϕ is differentiable, there holds $\nabla d^E_\phi(x) \in \partial\mathcal{F}_\phi$, i.e. the following eikonal equation holds:

$$\phi^o(\nabla d^E_\phi) = 1.$$

Let E be a polyhedral set and F a facet of ∂E. One can check that the function d_ϕ^E is differentiable on int(F) and we set, for $x \in \text{int}(F)$,

$$\widetilde{W}_\phi^F := T^o(\nabla d_\phi^E(x)) \subset \partial \mathcal{W}_\phi.$$

Notice that $\widetilde{W}_\phi^F$ is a convex set independent of $x \in \text{int}(F)$. Moreover $\widetilde{W}_\phi^F$ is a facet of $\partial\mathcal{W}_\phi$ if and only if F is a facet of ∂E parallel to a facet of $\partial\mathcal{W}_\phi$ (i.e. $\widetilde{W}_\phi^F$) and having the same exterior unit normal.

Given a vector field $n : \partial E \to \mathbb{R}^3$, the symbol $\text{div}_\tau\, n$ will denote the tangential divergence of n on ∂E in the sense of distributions. Finally, the crystalline perimeter is the integral functional defined by

$$P_\phi(E) := \int_{\partial E} \phi^o(\nu)\, d\mathcal{H}^2, \tag{2.2}$$

where E is a set of finite perimeter and ν denotes the outward euclidean unit normal to ∂E (both ∂E and ν here must be intended in a geometric measure sense, see [15]). The crystalline perimeter is the natural free energy associated with crystalline motion by mean curvature, see for instance [23], [13] and Section 3 below.

3. General definitions of ϕ-regular set and ϕ-regular flow

The next definition generalizes to the three dimensional crystalline case the notion of smooth compact surface, compare [4].

DEFINITION 3.1 Let $E \subset \mathbb{R}^3$ and $n_\phi : \partial E \to \mathbb{R}^3$ be Borel-measurable. We say that the pair (E, n_ϕ) is *ϕ-regular* if

1. the set ∂E is compact and Lipschitz continuous;
2. $$n_\phi(x) \in T^o\left(\frac{\nu(x)}{\phi^o(\nu(x))}\right) \qquad \mathcal{H}^2\text{-}a.e.\ x \in \partial E;$$
3. there is an open set $A \supseteq \partial E$ such that, for a.e. $y \in A$ there exists a unique $(x, s) \in \partial E \times \mathbb{R}$ so that $y = x + sn_\phi(x)$ and, letting $n_\phi^e(y) := n_\phi(x)$, there holds
$$n_\phi^e \in L^\infty(A; \mathbb{R}^3), \qquad \text{div} n_\phi^e \in L^\infty(A);$$
4. $\text{div}\, n_\phi^e$ admits a trace on ∂E, which we denote by $\text{div}_\tau n_\phi \in L^\infty(\partial E)$. Expressed precisely, for $\mathcal{H}^2$-a.e., $x \in \partial E$, there exists $\lim_{\rho\to 0^+} |B_\rho(x)|^{-1} \int_{B_\rho(x)} \text{div}\, n_\phi^e(y)\, dy = \text{div}_\tau n_\phi(x)$.

As already remarked in the Introduction, such a generality (as in Definition 3.4 below) is needed in view of Example 2 of Section 5, and could be helpful for a short time existence theorem of ϕ-regular flows.

If ∂E is a plane, then div_τ is the usual tangential divergence in the sense of distributions.

The vector field n_ϕ is called the Cahn–Hoffman field [8, 9]; in the case of smooth strictly convex anisotropies ϕ and smooth sets E, n_ϕ is simply given by $T^o(\nabla d_\phi^E)$.

Definition 3.1 slightly differs from Definition 2.1 of [4], where the vector field n_ϕ is directly defined in a tubular neighbourhood of ∂E and satisfies $n_\phi \in T^o(\nabla d_\phi^E)$. We anyway expect that, for a large class of functions ϕ and of ϕ-regular sets, the definitions coincide (see Remark 5.5 below). Notice that in the case of smooth anisotropies ϕ and smooth sets E, n_ϕ is extended in a natural way out of the front, and one can check that $\mathrm{div}_\tau\, n_\phi = \mathrm{div}\, n_\phi$ on ∂E. This essentially follows from the relation $\phi(n_\phi) = 1$.

REMARK 3.2 Let E be a polyhedral set having the following property: given any vertex v of ∂E, the intersection of $\widetilde{W}_\phi^Q$ over all facets Q containing v is non empty. Then it is not difficult to prove that there exists a vector field $n_\phi \in \mathrm{Lip}(\partial E; \mathbb{R}^3)$ such that (E, n_ϕ) becomes ϕ-regular.

Concerning the next definition of intrinsic ϕ-mean curvature we refer to [6, 9, 23].

DEFINITION 3.3 Let (E, n_ϕ) be ϕ-regular. We define the ϕ-mean curvature κ_ϕ of ∂E at $\mathcal{H}^2$-almost every $x \in \partial E$ as

$$\kappa_\phi := \mathrm{div}_\tau\, n_\phi. \tag{3.1}$$

We now introduce the evolution by crystalline mean curvature.

Let $t \in [0, T] \to E(t) \subset \mathbb{R}^3$ be a parametrized family of subsets of $\mathbb{R}^3$. Define

$$d_\phi^{E(t)}(x) := \mathrm{dist}_\phi(x, E(t)) - \mathrm{dist}_\phi(\mathbb{R}^3 \setminus E(t), x).$$

Whenever no confusion is possible, we set $d_\phi(x, t) := d_\phi^{E(t)}(x)$. Let $T > 0$ be given.

DEFINITION 3.4 A *ϕ-regular flow* on the interval $[0, T]$ is a family of pairs $(E(t), n_\phi(\cdot, t))_{t\in[0,T]}$, with $n_\phi(\cdot, t) : \partial E(t) \to \mathbb{R}^3$, which satisfies the following properties:

(1) $(E(t), n_\phi(\cdot, t))$ is ϕ-regular for any $t \in [0, T]$;

(2) the function d_ϕ is Lipschitz continuous on $\mathbb{R}^3 \times [0, T]$, differentiable for a.e. $t \in [0, T]$ and for $\mathcal{H}^2$-a.e. $x \in \partial E(t)$, and such that

$$\frac{\partial d_\phi}{\partial t}(x, t) = \kappa_\phi(x, t), \qquad \text{a.e. } t \in [0, T],\ \mathcal{H}^2\text{-a.e. } x \in \partial E(t). \tag{3.2}$$

In [4] a ϕ-regular flow is defined in a slightly different manner. Essentially (2) is replaced by

(2)′ $d_\phi \in \mathrm{Lip}(\mathbb{R}^3 \times [0, T])$ and

$$\frac{\partial d_\phi}{\partial t}(x, t) = \mathrm{div}\, n_\phi(x, t) + O\big(d_\phi(x, t)\big) \qquad \text{a.e. } (x, t) \in A \times [0, T],$$

where A is a suitable tubular neighbourhood of ∂E.

As a consequence of Corollary 3.4 in [4], it follows that a ϕ-regular flow in the sense of [4] depends only on $E(0)$, i.e. it does not depend on the choice of n_ϕ. We obviously expect that in most cases the two notions coincide. Reasoning as in [4], this would imply that two ϕ-regular flows starting from the same set coincide, and also that a comparison principle holds. In any case the two definitions coincide for the evolution of Example 1 (see Remark 5.5), and this shows that the evolution given in Fig. 4 of the initial set E of Fig. 1 is unique.

Finally, in the polyhedral case and if no new facet creates, the evolution law of Definition 3.4 concides with the one considered in [13, 23].

We conclude this section by sketching the computation of the first variation of the crystalline perimeter (2.2), which motivates, from a variational point of view, the geometric evolution law in Definition 3.4. The computation of the first variation on all ϕ-regular sets and for deformations with a generic initial velocity is of course difficult, because of the nondifferentiability of both the surface and the integrand; see [13, 23] for some discussion in this direction. We will therefore assume further regularity properties on (E, n_ϕ) and on the deformation α.

Let (E, n_ϕ) be ϕ-regular and assume that $n_\phi \in \mathrm{Lip}(A; \mathbb{R}^3)$. Let $\alpha \in \mathrm{Lip}(A \times \mathbb{R}; \mathbb{R}^3)$, with $\alpha(x, s) := x + sg(x)$, for a given $g \in \mathrm{Lip}(A; \mathbb{R}^3)$ which is assumed to be $\mathcal{H}^2$-a.e. differentiable on ∂E. Set $\alpha_s(x) := \alpha(s, x)$ and $\partial E_s := \alpha_s(\partial E)$. Notice that $\alpha_s : A \to \mathbb{R}^3$ is bilipschitz for any $s \in [-s_0, s_0]$, for s_0 sufficiently small. Denote by $\mathcal{P}_\phi$ the measure $\phi^o(\nu)\mathcal{H}^2$ supported on ∂E and set

$$\nu_\phi := \nabla d_\phi^E \quad \text{a.e. in } A,$$
$$X := \{\xi \in \mathrm{Lip}(A; \mathbb{R}^3),\ \xi \in T^o(\nu_\phi) \text{ a.e. in } A\}.$$

Notice that X is non-empty, since $n_\phi \in X$, and every $\xi \in X$ admits divergence on ∂E. Then the following holds:

$$\liminf_{s \to 0} \frac{P_\phi(E_s) - P_\phi(E)}{s} \geqslant \int_{\partial E} g \cdot \nu_\phi \operatorname{div} \xi \, d\mathcal{P}_\phi, \qquad \xi \in X. \tag{3.3}$$

The above inequality can be interpreted as follows: the 'subdifferential' of the functional P_ϕ at E along the field g contains the convex set

$$D(E) := \{\operatorname{div} \xi \ \nu_\phi : \xi \in X\}.$$

Let us prove (3.3). Denote by ν_s the outward euclidean unit normal to ∂E_s. We have

$$P_\phi(E_s) - P_\phi(E) = \int_{\partial E} \phi^o(\nu_s) - \phi^o(\nu) \, \mathrm{d}\mathcal{H}^2 + s \int_{\partial E} \phi^o(\nu) \operatorname{div}_\tau g \, d\mathcal{H}^2 + o(s).$$

Using the regularity assumptions on ∂E and g, and the convexity of ϕ^o, one can check that for $\mathcal{H}^2$-a.e. $x \in \partial E$ and for any $\xi \in X$, there holds

$$\liminf_{s \to 0} \phi^o(\nu_s(x)) - \phi^o(\nu(x)) \geqslant \xi \cdot \frac{\mathrm{d}}{\mathrm{d}s} \nu_{s\,|s=0}.$$

Following [5], Theorem 5.1, we then get

$$\liminf_{s \to 0} \frac{P_\phi(E_s) - P_\phi(E)}{s} \geqslant \int_{\partial E} \xi \cdot (-\nu \nabla g + (\nu \nabla g \cdot \nu)\nu) \, \mathrm{d}\mathcal{H}^2 + \int_{\partial E} \phi^o(\nu) \operatorname{div}_\tau g \, \mathrm{d}\mathcal{H}^2.$$

Observe that $\xi \cdot \nu_\phi = 1$ in A; therefore

$$\liminf_{s\to 0} \frac{P_\phi(E_s) - P_\phi(E)}{s} \geqslant \int_{\partial E} \operatorname{div} g - \nu_\phi \nabla g\, \xi \, \mathrm{d}\mathcal{P}_\phi.$$

Decomposing g as $g = \langle g, \nu_\phi\rangle\xi + (g - \langle g, \nu_\phi\rangle\xi)$, (3.3) follows reasoning as in [5]. Given now $\omega^\xi := \operatorname{div}\xi\ \nu_\phi \in D(E)$, we want to find the field $g^\xi \in X$ which solves

$$\min\left\{\int_{\partial E} g\cdot\omega^\xi\, \mathrm{d}\mathcal{P}_\phi \ :\ g\in X,\ \int_{\partial E}\phi(g)^2\,\mathrm{d}\mathcal{P}_\phi \leqslant 1\right\}.$$

A solution to this problem is given by $g^\xi = -c^\xi \operatorname{div}\xi\ \xi$, where $1/(c^\xi)^2 = \int_{\partial E}\left(\operatorname{div}\xi\right)^2 \mathrm{d}\mathcal{P}_\phi$, and this motivates Definition 3.4.

4. The polyhedral case. ϕ-calibrable sets

Given a ϕ-regular pair (E, n_ϕ), we say that $F \subset \partial E$ is a planar facet of ∂E if, for some $x \in \partial E$, F, if considered as a subset of $T_x\partial E \simeq \mathbb{R}^2$ (where $T_x\partial E$ denotes the tangent plane at x to ∂E defined $\mathcal{H}^2$-a.e. on ∂E), is the closure of a connected component with Lipschitz boundary of $\partial E \cap T_x\partial E$. For $\mathcal{H}^1$-a.e. $s \in \partial F$, let $\nu_F(s)$ be the unit exterior normal to ∂F lying in $T_x\partial E$. By [13], Lemma 9.2, there is a well defined function $c_{\phi,F} \in L^\infty(\partial F)$ which is the trace of $n_\phi \cdot \nu_F$ on ∂F. For any planar facet $F \subset \partial E$, set $\widetilde{W}_\phi^F := T^o(\nabla d_\phi^E)$. We observe that, given a polyhedron E, F a facet of ∂E, l an edge of F and $s \in \operatorname{int}(l)$, if $\nu_F(s)$ points outside E then

$$c_{\phi,F}(s) = \max\{n\cdot\nu_F(s) :\ n \in \widetilde{W}_\phi^F\},$$

and, if $\nu_F(s)$ points inside E, then

$$c_{\phi,F}(s) = \min\{n\cdot\nu_F(s) :\ n \in \widetilde{W}_\phi^F\}.$$

In particular, $c_{\phi,F}(s)$ does not depend on $s \in \operatorname{int}(l)$. So in the following, we will sometimes denote it by $c_{\phi,F,l}$.

Let us define a ϕ-calibrable facet of a ϕ-regular set (E, n_ϕ).

DEFINITION 4.1 Let (E, n_ϕ) be ϕ-regular and let F be a planar facet of ∂E. We say that F is *ϕ-calibrable* if there exists a vector field $n_{\phi,F} \in L^\infty(F;\mathbb{R}^3)$, with $\operatorname{div}_\tau n_{\phi,F} \in L^\infty(F)$, solving the following problem:

$$\begin{cases} n_{\phi,F} \in \widetilde{W}_\phi^F & \mathcal{H}^2\text{-a.e. on } F,\\ \operatorname{div}_\tau n_{\phi,F} = v_F & \mathcal{H}^2\text{-a.e. on } F,\\ n_{\phi,F}\cdot\nu_F = c_{\phi,F} & \mathcal{H}^1\text{-a.e. on } \partial F,\end{cases} \tag{4.1}$$

where the constant v_F is uniquely determined by the Gauss–Green theorem [13, 20] i.e.

$$v_F := |F|^{-1}\int_{\partial F} c_{\phi,F}(s)\,\mathrm{d}\mathcal{H}^1. \tag{4.2}$$

We say that E is *ϕ-calibrable* if there exists a vector field $n_\phi \in L^\infty(\partial E;\mathbb{R}^3)$ with $\operatorname{div}_\tau n_\phi \in L^\infty(\partial E)$, such that the restriction of n_ϕ to each planar facet F of ∂E solves problem (4.1).

The constant v_F defined in (4.2) coincides with the weighted mean curvature introduced by Taylor in the polyhedral case (compare [20, 23]), and $-v_F\ \phi^o(\nu)\nu$ represents the normal velocity of the facet F. One can check that the following property holds.

LEMMA 4.2 Let E be a ϕ-calibrable polyhedral set. Then there exists $n_\phi : \partial E \to \mathbb{R}^3$ such that (E, n_ϕ) is ϕ–regular and each facet of ∂E has constant ϕ-mean curvature.

Proof. See Theorem 9.2 of [13]. □

An interesting problem is to characterize those sets $E \subseteq \mathbb{R}^3$ which admit a vector field $n_\phi : \partial E \to \mathbb{R}^3$ such that (E, n_ϕ) is ϕ-regular, with every facet of constant ϕ-mean curvature. Theorem 4.3 below will provide a necessary condition in order to guarantee the existence of such an n_ϕ, and will be useful to construct the examples of Section 5.

THEOREM 4.3 Let (E, n_ϕ) be ϕ-regular and let F be a ϕ-calibrable planar facet of ∂E. Then the following condition holds:

$$v_P := |P|^{-1} \int_{\partial P} c_{\phi,P}(s)\ \mathrm{d}\mathcal{H}^1 \geqslant v_F, \tag{4.3}$$

for any $P \subseteq F$ with Lipschitz boundary, where

$$c_{\phi,P}(s) := \begin{cases} c_{\phi,F}(s) & \text{if } s \in \partial P \cap \partial F, \\ \sup\ \{n \cdot \nu_P(s) :\ n \in \widetilde{W}_\phi^F\} & \text{otherwise.} \end{cases}$$

Proof. From (4.1) we get $\mathrm{div}_\tau\ n_{\phi,F} = v_F$ on F. If we integrate $\mathrm{div}_\tau\ n_{\phi,F}$ over $P \subseteq F$, using the Gauss–Green theorem, we get

$$|P|\ \mathrm{div}_\tau\ n_{\phi,F} = \int_P \mathrm{div}_\tau\ n_{\phi,F}\ \mathrm{d}x = \int_{\partial P} n_{\phi,F} \cdot \nu_P\ \mathrm{d}\mathcal{H}^1 \leqslant \int_{\partial P} c_{\phi,P}\ \mathrm{d}\mathcal{H}^1,$$

which implies (4.3). □

We expect that condition (4.3) is also sufficient for a facet $F \subset \partial E$ to be ϕ-calibrable, and this is subject of current research. This would suggest that the subdivision condition for a facet F reads as follows: F instantly subdivides if and only if there does not exist a Cahn–Hoffman vector field with constant divergence on F (and with the correct boundary conditions), which becomes equivalent to say that there exists $P \subset F$ with $v_P < v_F$.

REMARK 4.4 The definitions and results of Sections 3 and 4 can be extended without modifications in arbitrary space dimensions and for a generic convex one-homogeneous function ϕ.

5. The examples

Example 1

In this example we fix the Wulff shape to be $\mathcal{W}_\phi := [-1, 1]^3$.

Let E be the set of Fig. 1. Observe that the set E satisfies the assumptions of Remark 3.2. In Proposition 5.2 below we show that, for suitable choices of the lengths of the edges of ∂E, there are

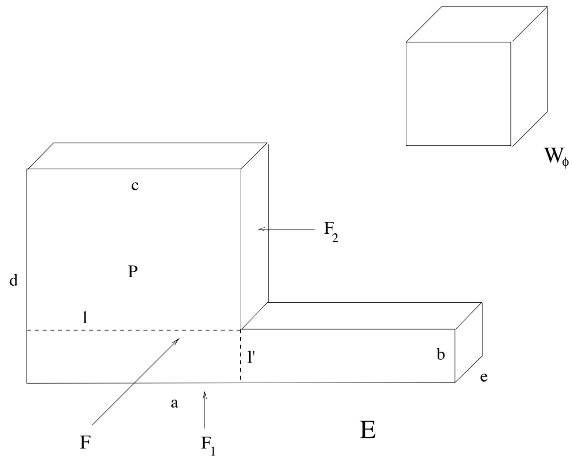

FIG. 1. Example 1: the Wulff shape $\mathcal{W}_\phi$ and the initial set E.

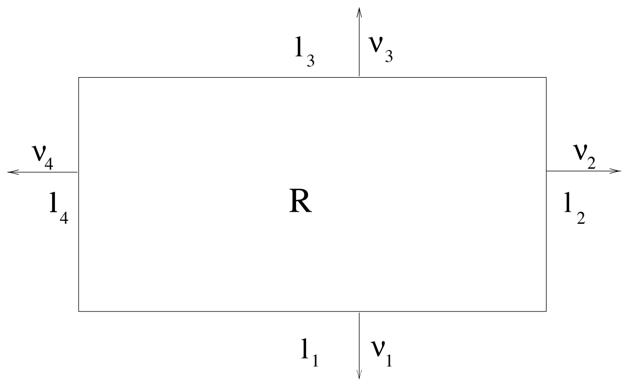

FIG. 2. ϕ-calibrable rectangular facet.

facets of ∂E not satisfying condition (4.3). In addition, using Lemmas 5.3 and 5.4, we prove that in the crystalline evolution starting from E, some facets instantly subdivide. In particular, we observe that the velocity field does not need to be continuous on a facet of the evolving front.

The following lemma shows that a rectangular facet F is always ϕ-calibrable when $\widetilde{W}_\phi^F$ is a rectangle; using this fact, we will show that ϕ-calibrable facets F are not necessarily rectangles.

LEMMA 5.1 Let $R \subset \mathbb{R}^2$ be a closed rectangle with edges $l_1, \dots, l_4$ parallel to the coordinate axes, and let $\nu_i := \nu_{R,l_i}$ be the exterior unit normal to l_i (see Fig. 2). Let $a_i := a_{l_i} \in \mathbb{R}$ $(i = 1, \dots, 4)$ be real numbers with $|a_i| \leqslant 1$. Then there exists a vector field $n = (n_1, n_2) \in$

$C^1(\mathrm{int}(R), \mathbb{R}^2) \cap C(R, \mathbb{R}^2)$ such that

$$\begin{cases} \max\{|n_1|, |n_2|\} \leqslant 1 & \text{in } \mathrm{int}(R), \\ \mathrm{div}\, n = v_R := |R|^{-1} \sum_{i=1}^{4} a_i |l_i| & \text{in } \mathrm{int}(R), \\ n \cdot \nu_i = a_i & \text{in } \mathrm{int}(l_i). \end{cases} \tag{5.1}$$

Proof. For simplicity, fix the origin at the intersection between l_4 and l_1. Given $(x, y) \in R$, we set

$$n_1(x, y) := \frac{a_2 x}{|l_1|} - a_4 \left(1 - \frac{x}{|l_1|}\right), \qquad n_2(x, y) := \frac{a_3 y}{|l_4|} - a_1 \left(1 - \frac{y}{|l_4|}\right).$$

The vector field $n := (n_1, n_2)$ satisfies (5.1). □

In the following we sometimes identify an edge of a polygon with its length.

PROPOSITION 5.2 Let F be the frontal facet of E with edges of length a, b, c, d respectively (see Fig. 1). Then F is ϕ-calibrable if and only if

$$b \geqslant \frac{cd}{c+d}, \qquad c \geqslant \frac{ab}{a+b}. \tag{5.2}$$

Proof. One directly checks that $c_{\phi,F} = 1$ on each edge of ∂F, therefore, by the expression of v_F in (4.2) we get

$$v_F = \frac{2(a+d)}{cd + b(a-c)}.$$

Assume now that F is ϕ-calibrable. Let P be the rectangle in Fig. 1, having edges c and d. Recalling the definition of $c_{\phi,P}$ given in Theorem 4.3, we get $c_{\phi,P} = 1$ on each edge of ∂P. Applying Theorem 4.3 to P and F, we get

$$v_P = \frac{2(c+d)}{cd} \geqslant \frac{2(a+d)}{cd + b(a-c)} = v_F,$$

i.e.

$$\frac{cd}{c+d} \leqslant \frac{cd + b(a-c)}{a+d}.$$

Rearranging terms, we have

$$b \geqslant \left(\frac{cd}{c+d} - \frac{cd}{a+d}\right)\left(\frac{a+d}{a-c}\right) = \frac{cd}{c+d},$$

which is the first inequality of (5.2). The second inequality can be proved in a similar way by applying Theorem 4.3 to F and the rectangle R with edges a and b. Indeed, the inequality

$$v_R = \frac{2(a+b)}{ab} \geqslant \frac{2(a+d)}{cd + b(a-c)} = v_F$$

yields

$$\frac{ab}{a+b} \leqslant \frac{c(d-b)}{a+d} + \frac{ab}{a+d},$$

i.e.

$$\left(\frac{ab}{a+b} - \frac{ab}{a+d}\right)\left(\frac{a+d}{d-b}\right) \leqslant c,$$

which is the second inequality in (5.2).

Assume now that (5.2) holds. We have to prove that F is ϕ-calibrable. Let us consider the rectangle $F \setminus P$. In order to apply Lemma 5.1 to $F \setminus P$, we have to define the constants $a_1, \dots, a_4$. We set these constants equal to 1 on $\partial(F \setminus P) \setminus l'$ and we define $a_{l'}$ in such a way that

$$v_F = v_{F \setminus P},$$

i.e.

$$\frac{1 + a_{l'}}{2} = \frac{(a+d)(a-c)}{cd + b(a-c)} - \left(\frac{a}{b} - \frac{c}{b}\right) = \frac{(a-c)(c+d-cd/b)}{cd + b(a-c)}.$$

We need to check that $|a_{l'}| \leqslant 1$. The condition $a_{l'} \geqslant -1$ is equivalent to $b \geqslant cd/(c+d)$, whereas the condition $a_{l'} \leqslant 1$ is implied by $c \geqslant ab/(a+b)$. Indeed, $(1 + a_{l'})/2 \leqslant 1$ means that

$$(d-b)c^2 - [(d-b)(a+b) + bd]c + ab(d-b) \leqslant 0,$$

and it is easy to check that the above quadratic polynomial is nonpositive when c satisfies the constraints $ab/(a+b) \leqslant c \leqslant a$. We conclude that (5.2) implies $|a_{l'}| \leqslant 1$.

The same argument applies to the edge l. Indeed, for the rectangle $S \subset P$ of edges c and $d - b$, the constant a_l is defined in such a way that $v_F = v_S$, i.e.

$$\frac{1 + a_l}{2} = \frac{(d-b)(a+b-ab/c)}{cd + b(a-c)},$$

and one checks that $(1 + a_l)/2 \in [0, 1]$ when $cd/(c+d) \leqslant b \leqslant d$. Once a_l and $a_{l'}$ have been defined, we can apply Lemma 5.1 three times (separately to the three rectangles partitioning F, reversing the signs of a_l and $a_{l'}$ in the rectangle $P \setminus S$) and get a vector field $F \to \mathbb{R}^2$ satisfying (5.1). By adding a constant third component we get a vector field satisfying (4.1). □

Notice that the vector field $n_{\phi,F}$ constructed in the last part of the proof of Proposition 5.2 is not continuous on F; more precisely the tangential component of $n_{\phi,F}$ along l' jumps across l'.

By choosing for instance $a := 2$, $b := \frac{1}{4}$, $c := 1$, and $d := 1$, it turns out that F is not ϕ-calibrable, since $v_F = \frac{24}{5}$, $v_P = 4$, and inequality (4.3) is violated.

We want now to define a ϕ-regular evolution starting from E, when F is not ϕ-calibrable; notice that, during the evolution, the facet F cannot translate parallel to itself.

We begin with two preliminary lemmas, whose proof is similar to that of Proposition 5.2.

LEMMA 5.3 Let F_2 be the polygon in Fig. 3. The facet F_2 is ϕ-calibrable for any $\epsilon \in\ ]0, e/2[$ if and only if $b \leqslant e \leqslant d$.

Proof. First we compute the constants $c_{\phi,F_2,l}$, where l is an edge of F_2. We have

$$c_{\phi,F_2,\epsilon} = c_{\phi,F_2,d} = c_{\phi,F_2,e} = 1, \qquad c_{\phi,F_2,b} = c_{\phi,F_2,e-2\epsilon} = -1,$$

hence

$$v_{F_2} = \frac{4\epsilon + 2(d-b)}{e(d-b) + 2\epsilon b}.$$

Assume that F_2 is ϕ-calibrable for $\epsilon \in\ ]0, e/2[$. Let Q_1 be the rectangle in Fig. 3, having edges ϵ and b. We have $c_{\phi,Q_1,\epsilon} = c_{\phi,F_2,\epsilon} = 1$, $c_{\phi,Q_1,b} = c_{\phi,F_2,b} = -1$, and $c_{\phi,Q_1,l'} = 1$. Hence applying

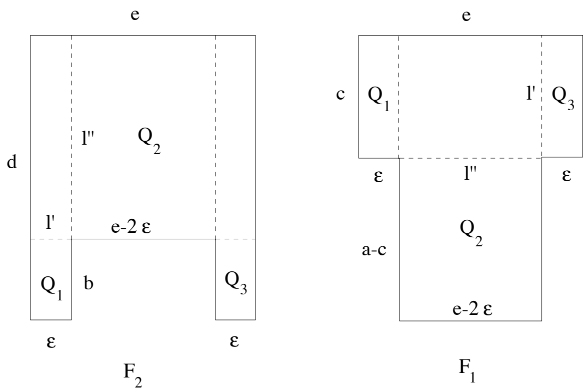

FIG. 3. ϕ-calibrable facets. The side facet F_2 and the lower facet F_1 of $E(t)$.

Theorem 4.3 to Q_1 and F_2, we get $v_{Q_1} = 2/b \geqslant v_{F_2}$, which is equivalent to $b \leqslant e$. The inequality $e \leqslant d$ can be obtained by a similar argument applied to F_2 and the rectangle Q_2 of edges $d - b$ and $e - 2\epsilon$ in Fig. 3. Indeed Theorem 4.3 yields

$$v_{Q_2} = \frac{(e - 2\epsilon) + (2\epsilon - e) + 2(d - b)}{(e - 2\epsilon)(d - b)} \geqslant v_{F_2},$$

which is equivalent to $e - d \leqslant 2\epsilon$. Letting $\epsilon \downarrow 0^+$, we get $e \leqslant d$.

Assume now that $b \leqslant e \leqslant d$. We have to show that F_2 is ϕ-calibrable for $\epsilon \in \,]0, e/2[$. Let us consider the rectangle Q_1. Choose $a_{l'}$ in such a way that $v_{F_2} = v_{Q_1}$. Since

$$v_{Q_1} = \frac{\epsilon - b + b + \epsilon a_{l'}}{\epsilon b} = \frac{1 + a_{l'}}{b},$$

we are imposing

$$\frac{1 + a_{l'}}{2} = \frac{b(2\epsilon + d - b)}{e(d - b) + 2\epsilon b}.$$

Clearly $(1 + a_{l'})/2 \geqslant 0$, and one directly checks that $b \leqslant e$ is equivalent to $(1 + a_{l'})/2 \leqslant 1$.

Similarly, let us consider the rectangle Q_2. We have

$$v_{Q_2} = \frac{2a_{l''}}{e - 2\epsilon}.$$

Imposing $v_{F_2} = v_{Q_2}$ makes the inequality $e - d \leqslant 2\epsilon$ equivalent to $a_{l''} \leqslant 1$, while $a_{l''}$ is always $\geqslant -1$. Applying Lemma 5.1 and reasoning as in Proposition 5.2, we conclude that F_2 is ϕ-calibrable. □

LEMMA 5.4 Let F_1 be the polygon in Fig. 3. The facet F_1 is ϕ–calibrable for any $\epsilon > 0$ sufficiently small if and only if $c \geqslant ae/(a + e)$.

Proof. We have $c_{\phi,F_1} = 1$ on each edge of F_1, hence

$$v_{F_1} = \frac{2(a + e)}{ae - 2\epsilon(a - c)}.$$

Assume that F_1 is ϕ-calibrable and $\epsilon > 0$ is sufficiently small. We have $c_{\phi,Q_3} = 1$ on each edge of Q_3; hence

$$v_{Q_3} = \frac{2(\epsilon + c)}{\epsilon c}.$$

The inequality $v_{Q_3} \geqslant v_{F_1}$ is always satisfied for ϵ sufficiently small. Reasoning in a similar way for the rectangle Q_2, one can check that the inequality

$$v_{Q_2} = \frac{2(a-c) + 2(e-2\epsilon)}{(a-c)(e-2\epsilon)} \geqslant v_{F_1}$$

is always satisfied for ϵ sufficiently small.

Assume now that $c \geqslant ae/(a+e)$. We have to prove that F_1 is ϕ-calibrable for any $\epsilon > 0$ sufficiently small. Choose $a_{l'}$ such that $v_{F_1} = v_{Q_3}$; we have

$$\frac{1 + a_{l'}}{2} = \epsilon \left(\frac{(a+e)}{ae - 2\epsilon(a-c)} - \frac{1}{c} \right).$$

Hence $(1 + a_{l'})/2 \leqslant 1$ for ϵ small enough, and one checks that the inequality $(1 + a_{l'})/2 \geqslant 0$ is equivalent to

$$c \geqslant \frac{ae - 2\epsilon(a-c)}{a+e}.$$

Similarly

$$v_{Q_2} = \frac{2(a-c) + (e-2\epsilon)(1 + a_{l'})}{(a-c)(e-2\epsilon)}.$$

Imposing $v_{F_1} = v_{Q_2}$, we get

$$\frac{1 + a_{l''}}{2} = (a-c) \left(\frac{a+e}{ae - 2\epsilon(a-c)} - \frac{1}{e - 2\epsilon} \right).$$

Then $(1 + a_{l''})/2 \geqslant 0$ whenever $e^2 \geqslant 4\epsilon c$, which is satisfied for ϵ small enough, and one checks that $(1 + a_{l''})/2 \leqslant 1$ is always satisfied for ϵ sufficiently small. □

Now let $a = 2$, $b = \frac{1}{4}$, $c = 1$, and $d = 1$, and choose $e := \frac{1}{2}$. With this choice of the lengths of the edges of ∂E, the facet F is not ϕ-calibrable, whereas the facets F_1 and F_2 are ϕ-calibrable for ϵ sufficiently small.

We are in a position to construct an evolution of the set E of Fig. 1, which actually is *the* evolution of E by crystalline mean curvature; see Remark 5.5. The frontal facet F instantly subdivides into two disjoint facets (the fracture appears along l'), and then each facet translates parallel to itself with velocity given by (4.2). The same applies to the facet opposite to F. In this way we get an evolution $t \to E(t)$ starting from E and defined on a suitable time interval $[0, T]$, with $T > 0$, having shape as in Fig. 4. We need to prove that this evolution corresponds to a ϕ-regular flow starting from E. In order to prove this, we must construct a vector field $n_\phi(\cdot, t) : \partial E(t) \to \mathbb{R}^3$, $t \in [0, T]$, as in Definition 3.4. By Lemma 4.2, it is enough to prove that $E(t)$ is ϕ-calibrable for $t \in [0, T]$, with $T > 0$ sufficiently small. We observe that, for any $t \in [0, T]$, the only facets of $\partial E(t)$ which are not rectangular are F_1 and F_2 of Fig. 3. By applying Proposition 5.2 and Lemmas 5.4 and 5.3, it follows that $E(t)$ is ϕ-calibrable. For $t = 0$, one can construct the field n_ϕ on ∂E, by

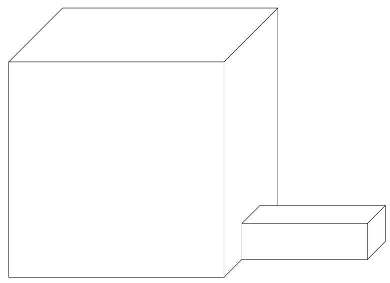

FIG. 4. Example 1: qualitative shape of the evolving set $E(t)$ starting from E for short times.

FIG. 5. Example 1: numerical computation of $E(t)$.

considering the facet F (and similarly the facet opposite to F) as the union of P and $F \setminus P$, and then solve (4.1) independently on the two rectangles, setting $c_{\phi,P,l'} = 1 = -c_{\phi,F\setminus P,l'}$. We observe that, with this definition, the field n_ϕ is not continuous on F: we do not know if there exists a continuous field equivalent to n_ϕ (i.e. with the same divergence and satisfying the same restrictions).

Figure 5 is the result of a numerical computation.

The following remark is crucial and concerns uniqueness of the ϕ-regular flow.

REMARK 5.5 Since the vector field n_ϕ previously defined admits an extension (by lines) in a suitable space–time neighbourhood $A \times [0, T]$ of the evolving front $\partial E(t)$, the map $(E(t), n_\phi(\cdot, t))$ becomes a ϕ-regular evolution in the sense of [4], and is unique in that class.

Example 2.

In this example we fix the Wulff shape to be the regular orthogonal prism with hexagonal basis centred at the origin; the apothem of the hexagonal basis is set equal to 1. Let E be the convex set of Fig. 6. Observe that also in this case E satisfies the assumptions of Remark 3.2. We will prove that, for a proper choice of the parameter $\epsilon > 0$, E is not ϕ-calibrable. Moreover, we expect that its evolution develops curve portions of the boundary, i.e. the set E does not remain a polyhedral set under crystalline mean curvature flow. Assume for simplicity that $r = 1$ in Fig. 6.

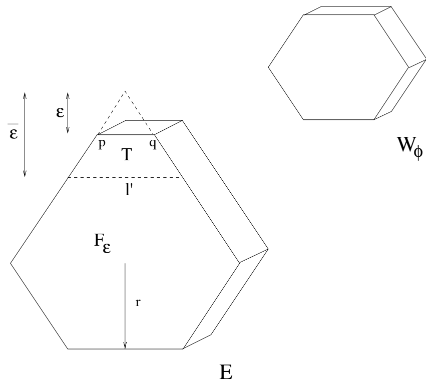

FIG. 6. Example 2: the Wulff shape $\mathcal{W}_\phi$ and the initial set E.

LEMMA 5.6 There exists $\overline{\epsilon} > 0$ such that the frontal facet F_ϵ of ∂E is not ϕ-calibrable for any $\epsilon \in\ ]0, \overline{\epsilon}[$.

Proof. We have $c_{\phi,F_\epsilon} = 1$ on each edge of ∂F_ϵ, and

$$v_{F_\epsilon} = \frac{2(7-\epsilon)}{7-\epsilon^2} \leqslant 2,$$

for any $\epsilon \in [0, 1]$. The function $\epsilon \to v_{F_\epsilon}$ is strictly convex on [0, 1], with $v_{F_0} = v_{F_1} = 2$, and attains its minimum for $\overline{\epsilon} = 7 - \sqrt{42}$, with value $v_{F_{\overline{\epsilon}}} = (7 + \sqrt{42})/7 < 2$. Hence F_ϵ is not ϕ-calibrable for any $\epsilon \in\ ]0, \overline{\epsilon}[$. □

Let us fix $\epsilon \in\ ]0, \overline{\epsilon}[$. An interesting problem is to understand which is the evolution starting from this set. We expect that such an evolution $E(t)$ does not remain a polyhedral set. This is motivated by the following heuristic argument.

One can realize that $F_{\overline{\epsilon}}$ satisfies (4.3) with the choice $c_{\phi,F_{\overline{\epsilon}}} = 1$ on each edge of $\partial F_{\overline{\epsilon}}$. *Assuming* that condition (4.3) is necessary and sufficient for a facet to be ϕ-calibrable, we deduce that $F_{\overline{\epsilon}}$ is ϕ-calibrable. If this is true, there exists a field $n_\phi : F_{\overline{\epsilon}} \to \mathbb{R}^3$ satisfying (4.1). Now let p and q be the points in Fig. 6, and let $n(p)$ (resp. $n(q)$) be the unique vector obtained as the intersection of $\widetilde{W}_\phi^Q$ over all facets Q of ∂E having p (resp. q) as vertex (see Remark 3.2). We define the field n_ϕ on $T := F_\epsilon \setminus F_{\overline{\epsilon}}$ by taking the linear combination of $n(p)$ and $n(q)$ on every section of T parallel to l'. We can perform the same construction for the facet of ∂E opposite to F_ϵ. Since the other facets of ∂E are all ϕ-calibrable by Proposition 5.2, we get a global field $n_\phi : \partial E \to \mathbb{R}^3$ such that the pair (E, n_ϕ) is ϕ-regular.

We observe that, contrary to Example 1, the function $\mathrm{div}_\tau\ n_\phi$ is *not* constant (nor piecewise constant) on F_ϵ, but increases moving away from l' in T. Moreover, as can be shown by a direct computation, $\mathrm{div}_\tau\ n_\phi$ is *continuous* on F_ϵ, i.e. the two definitions of n_ϕ on $F_{\overline{\epsilon}}$ and on T have the same divergence on l'. This suggests that, during an evolution starting from E, the facet F_ϵ does not break into two different facets as in Example 1, but rather bends inside E (with velocity given by $\mathrm{div}_\tau\ n_\phi$). Figure 7 (obtained by a numerical computation) shows the expected shape of

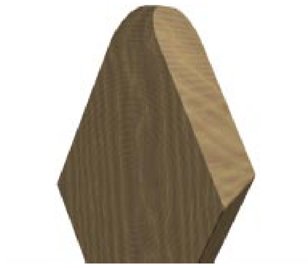

FIG. 7. Example 2: numerical computation of the evolving set $E(t)$ starting from E for short times.

the evolving set $E(t)$ for small positive times. This example suggests that one cannot expect a short-time existence theorem for ϕ-regular flows in the class of polyhedral sets. The problem of predicting where a fracture creates in a planar facet of an evolving set is interesting and deserves further investigation. Numerical computations in this direction will appear in [17].

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