Nucleation and backward motion of discrete interfaces

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Abstract

We use a discrete approximation of the motion by crystalline curvature to define an evolution of sets from a single point (nucleation) following a criterion of "maximization" of the perimeter, formally giving a backward version of the motion by crystalline curvature. This evolution depends on the approximation chosen.

Geometric variational evolutions, in particular curvature-based motions, may be studied using an implicit-time scheme proposed by Almgren, Taylor and Wang. Following the formal consideration that curvature can be seen as the variation of the perimeter, they defined a time-discrete trajectory E^τ_k, where τ is a time step, E^τ_0 is an initial set and E^τ_k is a minimizer of

$$\min\Big\{P(E)+\frac{1}{\tau}D(E,E^\tau_{k-1})\Big\}, \tag{1}$$

where P is the Euclidean perimeter, D is a dissipation term accounting for the L^2-distance of the boundary of E from that of E^τ_{k-1}. We can read (1) as follows: the set E^τ_k "contracts" by minimizing the perimeter subject to a penalization of its "distance" from E^τ_{k-1}. A suitable limit of these time-discrete trajectories gives motion by mean curvature [3]. The same scheme can be repeated taking as P a crystalline perimeter, to obtain motion by crystalline curvature in dimension two [2].

In this paper, we consider the opposite problem of defining a motion when starting from the same discrete schemes for sets which "expand" by *maximizing* the perimeter subject to a penalization of their distance from the previous set. Formally, this involves considering problems of the form

$$\min\Big\{-P(E)+\frac{1}{\tau}D(E,E^\tau_{k-1})\Big\}, \tag{2}$$

which can be seen as a "backward" version of the previous ones if the index k is considered as parameterizing negative time (see [5] Section 10.2). Unfortunately, this problem is ill-posed, giving the trivial infimum $-\infty$ at the first step. Following a suggestion by J.W. Cahn, we consider a discrete approximation of P in the crystalline case, and use it to define a backward crystalline-curvature motion with prescribed extinction point (or, equivalently, nucleation of the motion defined for positive times).

For crystalline curvature flow, the energy to be considered is

$$P(A) = \int_{\partial A} \|\nu\|_1 d\mathcal{H}^{d-1},$$

with domain the family of sets of finite perimeter in $\mathbb{R}^d, d \geq 2$, where ∂A is the reduced boundary of A, ν is the measure-theoretical normal to ∂A, $\|\nu\|_1 = \sum_{i=1}^d |\nu_i|$ and $\mathcal{H}^{d-1}$ is the Hausdorff $(d-1)$-dimensional measure [4]. The approximating energies are

$$P_\varepsilon(A) = \mathcal{H}^{d-1}(\partial A), \qquad A \in \mathcal{A}_\varepsilon$$

with domain all unions of coordinate cubes of centres in $\varepsilon\mathbb{Z}^d$ and side length ε; i.e.,

$$\mathcal{A}_\varepsilon = \Big\{ \bigcup_{i\in I} (\varepsilon i + \varepsilon Q) : I \subset \mathbb{Z}^d \Big\}, \qquad Q = [-1/2, 1/2]^d.$$

The functionals P_ε can be seen as discrete "ferromagnetic" energies (defined directly on subsets I of $\mathbb{Z}^d$) and Γ-converge to P (see [1]). Minimizing movements along P_ε have been studied by Braides, Gelli and Novaga [6] and they give the crystalline curvature flow upon taking $\varepsilon << \tau$.

We consider initial data $E_0^{\tau,\varepsilon,\lambda} = Q_\varepsilon = \varepsilon Q$ (which, in the discrete setting, all correspond to the singleton $\{0\}$), and define iteratively $E_k^{\tau,\varepsilon,\lambda}$ as a minimizer of

$$\min\Big\{ -\frac{1}{\lambda} P_\varepsilon(E) + \frac{1}{\tau} D_\varepsilon(E, E_{k-1}^{\tau,\varepsilon,\lambda}) \Big\}, \tag{3}$$

where

$$D_\varepsilon(E,E') = \sum_{i\in\mathbb{Z}^d\cap\frac{1}{\varepsilon}E} \varepsilon^{d+1} d_\infty\Big(i, \mathbb{Z}^d \cap \frac{1}{\varepsilon}E'\Big) + \sum_{i\in\mathbb{Z}^d\cap\frac{1}{\varepsilon}(E'\setminus E)} \varepsilon^{d+1} d_\infty\Big(i, \mathbb{Z}^d \setminus \frac{1}{\varepsilon}E'\Big), \tag{4}$$

$$d_\infty(i,I) = \min\{\|i-i'\|_\infty : i' \in I\}. \tag{5}$$

Note the new parameter λ, which does not change the nature of the problems and whose introduction can be interpreted as a time-scaling of the trajectories with $\lambda = 1$ (see [5] Chapter 10).

Choice of scalings. We first determine a correct scaling for λ and τ in terms of ε in order to have a non-trivial limit. To this end, we note that the minimal variation of the energy in (3) from the set $E_{k-1}^{\tau,\varepsilon,\lambda}$ corresponds to the addition of an ε-square with no side in common with $E_{k-1}^{\tau,\varepsilon,\lambda}$. The variation is

$$-\frac{2d}{\lambda}\varepsilon^{d-1} + \frac{1}{\tau}K\varepsilon^{d+1} \tag{6}$$

with $0 \neq K \in \mathbb{N}$. This quantity may be negative if and only if

$$1 \leq \frac{2d\tau}{\lambda\varepsilon^2}. \tag{7}$$

The relative scaling of ε, τ and λ must be such that this condition be satisfied.

We treat the case

$$\tau/\varepsilon = \gamma \in (0, +\infty), \qquad \lambda\varepsilon = \alpha \in (0, +\infty), \tag{8}$$

so that (7) corresponds to

$$\frac{1}{2d} \leq \frac{\gamma}{\alpha}. \tag{9}$$

The convergence result. We can now describe the behaviour of the minimizing-movement scheme in (3).

Theorem (nucleation). *Let τ, ε and λ satisfy condition* (8)*; correspondingly, let $E^\tau(t) = E^{\tau,\varepsilon,\lambda}_{\lfloor t/\tau \rfloor}$, with $E^{\tau,\varepsilon,\lambda}_k$ given by* (3) *with initial data $E^{\tau,\varepsilon,\lambda}_0 = \varepsilon Q$, and let*

$$\frac{2d\gamma}{\alpha} \not\in \mathbb{N} \tag{10}$$

be satisfied. Then, for all fixed t, the Kuratowsky limit of the family $E^\tau(t)$ as $\tau \to 0$ is a square of centre 0 *and side length $2\lfloor \frac{2d\gamma}{\alpha} \rfloor t$. In particular:*

(a) (pinning threshold) *if* (9) *is not satisfied, then the motion is trivial: $E(t) = \{0\}$;*

(b) (linear expansion) *if* (9) *and* (10) *are satisfied, then the motion is given by a family of expanding cubes whose sides move with constant velocity $\lfloor \frac{2d\gamma}{\alpha} \rfloor$.*

Remark. (i) if $\frac{2d\gamma}{\alpha} \in \mathbb{N}$, then we obtain that the sets E are contained in the cubes moving with velocity $\frac{2d\gamma}{\alpha}$, and contain the cubes moving with velocity $\frac{2d\gamma}{\alpha} - 1$, but need not be cubes themselves. This is due to the non-uniqueness of the minimal sets in (3);

(ii) contrary to the forward case, in which crystalline motion has been described only in dimension two (see [8]), due to its simpler form the limit can be described in all dimensions d;

(iii) the problem can be set for different distances d_φ (depending on a norm φ) in the place of the ∞-distance in (5). In that case, the sets $E(t)$ are not cubes, but are homothetic to the convex envelope $\mathcal{E}$ of the set of points $i \in \mathbb{Z}^d$ such that

$$d_\varphi(i, 0) \leq 2d\frac{\gamma}{\alpha} \tag{11}$$

(as above, this description does not hold if we have equality in (11) for some i), and expand with constant velocity. Note that, even for the Euclidean distance, such sets are non-trivial polyhedra;

(iv) note that for general distances, the set $\mathcal{E}$ may be of dimension lower than d. For example, in dimension two, and φ a sufficiently asymmetric norm, $E(t)$ may be a linearly growing segment.

We give a brief proof of the theorem as stated in this easier case, and after that comment the more technical points for the changes in the proof in the general case.

Proof. First note that if (9) is not satisfied, then every competing set E in the definition of $E_1^{\tau,\varepsilon,\lambda}$ gives a strictly larger value than the set $E_0^{\tau,\varepsilon,\lambda}$; hence, each discrete trajectory is trivial, and so is their limit.

Suppose now that (9) is satisfied. We then prove that $E_k^{\tau,\varepsilon,\lambda}$ is a (even) checkerboard structure containing εQ; i.e., it is the union of cubes $\varepsilon(i+Q)$ with $i \in \mathbb{Z}^d$ and $\|i\|_1 = |i_1| + \cdots + |i_d|$ even (for short, we say that i is even). Moreover,

$$\{i \in \mathbb{Z}^d : \varepsilon i \in E_k^{\tau,\varepsilon,\lambda}\} = \Big\{i \in \mathbb{Z}^d \text{ even }, \|i\|_\infty \leq \Big\lfloor \frac{2d\gamma}{\alpha} \Big\rfloor k\Big\}. \tag{12}$$

The statement above can be proved inductively by showing that

$$\{i \in \mathbb{Z}^d : \varepsilon i \in E_k^{\tau,\varepsilon,\lambda}\} = \Big\{i \in \mathbb{Z}^d \text{ even }, d_\infty\Big(i, \frac{1}{\varepsilon} E_{k-1}^{\tau,\varepsilon,\lambda}\Big) \leq \Big\lfloor \frac{2d\gamma}{\alpha} \Big\rfloor\Big\}. \tag{13}$$

To this end, it suffices to note that the contribution of the energy of a competitor E corresponding to points i with $d_\infty\big(i, E_{k-1}^{\tau,\varepsilon,\lambda}\big) = j$ for $1 \leq j \leq 2d\gamma/\alpha$ is minimal when no two such points have a nearest-neighbour in E, while if $j > 2d\gamma/\alpha$ it is minimal if E contains no such point. This shows that $E_k^{\tau,\varepsilon,\lambda} \setminus E_{k-1}^{\tau,\varepsilon,\lambda}$ corresponds to a checkerboard structure. Since the contribution of even and odd checkerboard structure outside $E_{k-1}^{\tau,\varepsilon,\lambda}$ is equal, and the even checkerboard structure allows to leave $E_{k-1}^{\tau,\varepsilon,\lambda}$ unchanged, we get the thesis.

Remark. The proof above relies heavily on the structure of the l^∞ distance, for which all sublevel sets in the proof are squares. For a general norm φ this is not true; as a consequence, in particular we might not have that the minimal sets $E_k^{\tau,\varepsilon,\lambda}$ correspond to the same checkerboard structure (even or odd), and they might 'oscillate' between even or odd checkerboards. This may happen only for a finite number of indices k; eventually, they stabilize and after some k_0 theu have the same parity (which may be the odd checkerboard, not containing then the point 0). At this point, we may apply an induction argument as above. Note, however, that in this case the evolving sets are homothetic only in the limit, while the discrete sets are not homothetic at $\varepsilon, \tau, \lambda$ fixed.

The proofs and examples in the general case will appear in [7].

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