Efficient computation of crystal growth using sharp interface models

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(joint work with John W. Barrett, Robert Nürnberg)

In order to compute crystal growth one needs to efficiently track the interface between different phases. In simple situations this results in the problem of computing the solution of a geometric evolution equation involving the curvature of the interface. In this talk, we review a variational formulation for such geometric evolution laws that leads to discretizations with very good mesh properties, and we indicate how these formulations can be extended to situations where the interface evolution is coupled to a bulk equation. For simplicity we state the equations for curves in the plane first and later indicate how the approach can be generalized to higher dimensions.

Given a parameterization $\vec{x}(\rho, t) : I \times [0, T] \to \mathbb{R}^2$, $I := \mathbb{R}/\mathbb{Z}$, of the family of closed curves $\Gamma(t) \subset \mathbb{R}^2$, we note that the L^2- and H^{-1}-gradient flow of length, i.e. the curvature flow and the surface diffusion flow, respectively, can be written as

$$
(1) \qquad \vec{x}_t \,.\, \vec{\nu} = \begin{cases} \varkappa \\ -\varkappa_{ss} \end{cases} , \qquad \varkappa \, \vec{\nu} = \vec{x}_{ss} ,
$$

with $\varkappa$ the curvature of Γ and $\vec{\nu}$ a unit normal. Note that the formulation (1) is independent of the tangential component, $\vec{x}_t \,.\, \vec{x}_s$, of the velocity $\vec{x}_t$. However, when (1) is discretized with the help of piecewise linear finite elements, then the corresponding discrete tangential velocity is no longer arbitrary. In fact, the spatially discrete solutions are such that the polygonal curves $\Gamma^h(t)$, where they are not locally flat, are equidistributed at every time $t > 0$.

On introducing the appropriate spaces $\underline{V}^h$ and V^h of periodic piecewise linear vector- and scalar-valued parametric finite elements, we obtain the following semidiscrete continuous-in-time approximation of (1). Given $\Gamma^h(0)$, for $t \in (0, T]$ find $\Gamma^h(t) = \vec{X}^h(I, t)$, with $\vec{X}^h(t) \in \underline{V}^h$, and $\kappa^h(t) \in V^h$ such that

$$
(2a) \qquad \langle \vec{X}_t^h, \chi \, \vec{\nu}^h \rangle_h^h - \begin{cases} \langle \kappa^h, \chi \rangle_h^h \\ \langle \kappa_s^h, \chi_s \rangle_h \end{cases} = 0 \qquad \forall\, \chi \in V^h,
$$

$$
(2b) \qquad \langle \kappa^h \, \vec{\nu}^h, \vec{\eta} \rangle_h^h + \langle \vec{X}_s^h, \vec{\eta}_s \rangle_m = 0 \qquad \forall\, \vec{\eta} \in \underline{V}^h;
$$

where $\langle f, g \rangle_h := \int_{\Gamma^h(t)} f \,.\, g \, \mathrm{d}s = \int_I f \,.\, g \, |\vec{X}_\rho^h(t)| \, \mathrm{d}\rho$ with $\langle \cdot, \cdot \rangle_m^h$ the mass lumped inner product. It is now straightforward to show that (2b) implies that neighbouring elements of $\Gamma^h(t) = \vec{X}^h(I, t)$ have the same length or are parallel. When introducing fully discrete approximations, it is possible to use semi-implicit time stepping or a fully implicit approach. In the former case, we obtain linear schemes that intrinsically move mesh points tangentially so that e.g. numerical steady states are always equidistributed, while the latter leads to highly nonlinear approximations that truly equistribute at each time level; see [1, 2] and [9], respectively. Both variants are unconditionally stable.

An advantage of our scheme (2a,b), that follows from the formulation (1), is that other geometric evolution laws can be handled easily. For example, nonlinear curvature flow, including the inverse curvature flow, area preserving curvature flow, Willmore flow (or elastic flow) for curves, as well as higher codimension flows of curves in $\mathbb{R}^d$, $d \geq 3$, and geodesic flows of curves flowing on a given manifold, can all be considered; see [1, 2, 10] for details.

The approximation (2a,b) can also be generalized to cover the geometric evolution of curve networks, where different curves move by their given normal velocities and where certain conditions have to hold at triple junctions, where three curves meet at a point. It turns out that the natural generalization of the weak formulation used to derive (2a,b) approximates all the necessary triple junction conditions correctly; see [1, 2].

Replacing the isotropic curve length $|\Gamma| := \int_\Gamma 1 \, ds$ with a weighted length of the form $|\Gamma|_\gamma := \int_\Gamma \gamma(\vec{\nu}) \, ds$, where $\gamma : \mathbb{R}^2 \setminus \{\vec{0}\} \to \mathbb{R}_{>0}$ is a given one-homogeneous anisotropy function, yields the anisotropic analogues of the geometric evolution equations of curvature flow and surface diffusion, i.e.

$$(3) \qquad \vec{x}_t \,.\, \vec{\nu} = \begin{cases} \beta(\vec{\nu}) \,\varkappa_\gamma \\ -(\beta(\vec{\nu}) \, [\varkappa_\gamma]_s)_s \end{cases} , \qquad \varkappa_\gamma \, \vec{\nu} = [\gamma'(\vec{\nu})]_s^\perp \,,$$

where $\vec{\nu} = -\vec{x}_s^\perp$, $\varkappa_\gamma$ is the weighted curvature, and $\beta : S^1 \to \mathbb{R}_{>0}$ is an anisotropic mobility. The finite element approximations based on (2a,b) can now be extended to approximate the flows (3). The fully discrete schemes can be shown to be unconditionally stable for arbitrary smooth convex anisotropies, in the case of a fully implicit time discretization ([9]), and for anisotropies of the form

$$(4) \qquad \gamma(\vec{p}) = \left[\sum_{\ell=1}^{L} [\gamma^{(\ell)}(\vec{p})]^r \right]^{\frac{1}{r}} = \left[\sum_{\ell=1}^{L} [\vec{p} \,.\, G^{(\ell)} \, \vec{p}]^{\frac{r}{2}} \right]^{\frac{1}{r}} ,$$

where $G^{(\ell)} \in \mathbb{R}^{2 \times 2}$, $\ell = 1 \to L$, are symmetric and positive definite, and $r \in [1, \infty)$; see [3, 10].

Moreover, the ideas presented above naturally generalize to the approximation of geometric evolution equations for hypersurfaces in $\mathbb{R}^3$. Examples are the mean curvature flow, nonlinear mean curvature flow and surface diffusion for isotropic (see [4]) and anisotropic surface energies (see [6]), the Willmore flow and Helfrich flow (see [5]), as well as the evolution of surface clusters with triple junction lines and quadruple junction points (see [7]). In all of the isotropic cases, we can show that our semidiscrete continuous-in-time approximations produce triangulations with very good mesh qualities, so called *conformal polyhedral surfaces*; see [4, §4] for details. Such surfaces are characterized by the fact that the two popular notions of discrete vertex normals, given by the directions of steepest descent of area and volume, respectively, coincide; which in turn means that the triangulation cannot be bad. Related properties can be derived for anisotropic surface energies.

Finally, we can also consider situations where the interface evolution is coupled to an equation that needs to hold in a bulk domain. For instance, the evolution of

FIGURE 1. Solid plates and sectored plates.

a solidifying front $\Gamma(t)$ in a Stefan problem with anisotropic Gibbs-Thomson law and kinetic undercooling can be expressed as

$$(5) \qquad \rho\,(\vec{x}_t\,.\,\vec{\nu}) = \beta(\vec{\nu})\,[\alpha\,\varkappa_\gamma - a\,u] \qquad \text{on } \Gamma(t),$$

where u, usually a rescaled temperature, satisfies a heat equation in the bulk domain Ω, with an energy balance at the interface leading to jumps in the gradient of u across $\Gamma(t)$. Coupling our natural parametric finite element approximation of (5) to a finite element approximation of the evolution of u in the bulk, we are able to introduce stable fully discrete schemes which mimic the underlying Lyapunov structure of the continuous problem, see [8]. When u is interpreted as a concentration, then the studied Stefan problem can be used to model the solidification from a supersaturated solution, which is relevant for snowflake growth. An example computation, for a surface energy of the form (4) with a hexagonal prism Wulff shape, can be seen in Figure 1.

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