A minimizing movement approach without using distance function for evolving spirals by crystalline curvature

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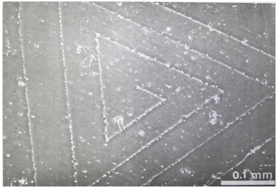
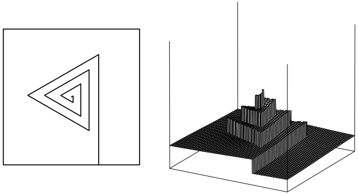
This is a joint work with Y.-H. R. Tsai (Univ. Texas at Austin).

Spirals by crystalline curvature flow

Consider evolution of spiral steps by crystalline curvature flow.
(Physical background: Crystal growth due to screw dislocation (cf. Burton–Cabrera–Frank(1951)))

(a) 



Settings:

- $\Omega \subset \mathbb{R}^2$: bounded domain with smooth boundary
- $a_1, \dots, a_N \in \Omega$: centers of spirals (screw dislocation)
- $W = \Omega \setminus \bigcup_{j=1}^{N} \overline{B_r(a_j)}$: the domain in where spirals are in.
- $m_j \in \mathbb{Z} \setminus \{0\}$: Signed number of steps provided by a_j
  - $|m_j|$: number of steps
  - $m_j > 0$: counter-clockwise rotating when $V_\gamma > 0$
- Evolution equation

$$V_\gamma = -H_\gamma + f$$

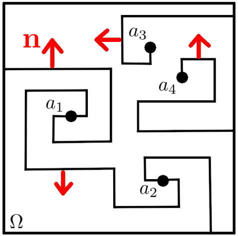
V_γ, H_γ: normal velocity and curvature corresponding to the surface energy density $\gamma \colon \mathbb{R}^2 \to [0, \infty)$.

(Photo(a): I. Sunagawa and P. Bennema, *Morphology of growth spirals: theoretical and experimental*, Preparation and properties of solid state materials **7**, 1982.)

Level set method for spirals

O(2003), O-Tsai-Giga(2015)

To describe the merging of spirals (not interfacial curve), we use the level set method.



$$m_1 = -2, \quad m_2 = 2,$$
$$m_3 = 1, \quad m_4 = 1.$$

Sheet structure function (Kobayashi(2010), Miura–Kobayashi(2015))

$$\theta(x) = \sum_{j=1}^{N} m_j \arg(x - a_j).$$

Level set formulation of spirals: (O(2003), O-Tsai-Giga(2015))

$$\Gamma_t = \{x \in \overline{W};\ u(t,x) - \theta(x) \equiv 0 \mod 2\pi\mathbb{Z}\}, \qquad \mathbf{n} = -\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}$$

Anisotropic curvature and velocity:

$$H_\gamma = -\mathrm{div}\{\xi(\nabla(u-\theta))\} \quad (\xi = \nabla\gamma : \text{Cahn-Hoffman vector}), \qquad V_\gamma = \frac{u_t}{\gamma(\nabla(u-\theta))}$$

(cf. Y. Giga, *Surface Evolution Equations. A Level Set Approach*, Birkhäuser, 2006.)

Crystalline curvature flow for spirals

H_γ is a crystalline curvature $\Leftrightarrow$ Wulff diagram (Equilibrium interface) is a convex polygon

Wulff diagram: $\mathcal{W}_\gamma = \{p \in \mathbb{R}^2;\ \gamma^\circ(p) \le 1\}, \quad \gamma^\circ(p) = \sup\{p \cdot q;\ \gamma(q) \le 1\}$.

$\to$ It is natural to take $\gamma^\circ(p) = \max_{1 \le j \le N_\gamma} \tilde{n}_j \cdot p$, and so is $\gamma (= \gamma^{\circ\circ})$.

Level set equation of crystalline curvature flow for spirals

(E) $$u_t - \gamma(\nabla(u-\theta))\Big(\mathrm{div}\{\xi(\nabla(u-\theta))\} + f\Big) = 0 \quad \text{in } W \times (0,T)$$

with the following assumptions.

- (A1) $\gamma \in C(\mathbb{R}^2)$ is convex,
- (A2) $\gamma > 0$ on S^1,
- (A3) γ is positively homogeneous of degree 1: $\gamma(\lambda p) = \lambda \gamma(p)$ for $\lambda > 0$, $p \in \mathbb{R}^2$
- (A4) γ is piecewise linear: $\gamma(p) = \max_{1 \le j \le N_\gamma} n_j \cdot p$.

Typical example: $\gamma(p) = |p_1| + |p_2| \Rightarrow \mathcal{W}_\gamma = [-1,1]^2$

Aim: propose a numerical method to solve (E).

Pioneering works

- Front-tracking model (ODE system describing to evolution of facets)

  Interface Angenent-Gurtin(1989), Taylor(1991)

  Spiral Imai-Ishimura-Ushijima(1999, $f \equiv 0$), Ishiwata (2014), Ishiwata-O (2019)

- Level set method

  Interface Giga-Giga(2001, 2D), Giga-Požár(2016, 3D) (Crystalline)

  Spiral Smereka(2000), O(2003), O-Tsai-Giga(2015) (isotropic or smooth anisotropic evolution)

- Minimizing movement approach:
  - by Family of interior: Almgren-Taylor-Wang(1993), Luckhaus-Sturzenhecker(1995), Almgren-Taylor(1995), ...
  - with Level set method by signed distance: Chambolle(2004), Chambolle-Morini-Ponsiglione(2017), Oberman-Osher-Takei-Tsai(2011)

Key idea: Apply Chambolle's algorithm with general level set function instead of signed distance.

Chambolle's algorithm(2004)

Let $\Sigma \subset \Omega$ be an interfacial curve. Define the signed distance of Σ by

$$d_\gamma(x,\Sigma) = \begin{cases} -\inf_{y\in\Sigma} \gamma^\circ(y-x) & \text{outside } (\mathbf{n} \text{ direction}) \text{ of } \Sigma, \\ \inf_{y\in\Sigma} \gamma^\circ(x-y) & \text{inside of } \Sigma. \end{cases}$$

Find a minimizer w^* of

$$E(w) = \int_\Omega \gamma(\nabla w)dx + \frac{1}{2h}\|w - d_\gamma(x,\Sigma)\|_{L^2}^2.$$

Then, the first variation of $E(w)$ yields $\frac{\delta E}{\delta w} = -\mathrm{div}(\xi(\nabla w^*)) + \frac{w^* - d_\gamma(x,\Sigma)}{h} = 0$, which implies

$$d_\gamma(x,\Sigma) = -h\mathrm{div}D\gamma(\nabla u^*) = -h(-H_\gamma(\partial\{w^* = 0\})).$$

Then, set $S_h(\Sigma) = \{x;\ w^*(x) = 0\}$ describes the motion of Σ by $V_\gamma = -H_\gamma$ in a short time step $h > 0$.

Difficulty for spirals: Spiral curve is not interfacial curve. $\Rightarrow$ Signed distance cannot be available.

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Proposed algorithm (for spirals)

1. Let Σ_0 be given by $\Sigma_0 = \{x \in \overline{W};\ u_0(x) - \theta(x) \equiv 0 \mod 2\pi\mathbb{Z}\}$ with $u_0 \in C(\overline{W})$.
2. For given u_n $(n \geq 0)$, which possibly is not the distance function), find the minimizer w^* of

$$E_\gamma(w; u_n) = \int_W \gamma(\nabla(w - \theta))dx - \int_W fw dx + \frac{1}{2h}\left\| \frac{w - u_n}{\sqrt{\gamma(\nabla(u_n - \theta))}} \right\|_{L^2}^2 .$$

   Then, w^* formally satisfies

$$-\operatorname{div}\{\xi(\nabla(w^* - \theta))\} - f + \frac{w^* - u_n}{h\gamma(\nabla(u_n - \theta))} = 0$$

$$\Rightarrow\ w^* = u_n + h\gamma(\nabla(u_n - \theta))\Big(\operatorname{div}\{\xi(\nabla(w^* - \theta))\} + f\Big).$$

3. Thus, we set $u_{n+1} = w^*$.

Then, $\Sigma_n = \{x \in \overline{W};\ u_n(x) - \theta(x) \equiv 0 \mod 2\pi\mathbb{Z}\}$ approximates the motion of spirals at $t \approx nh$.

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Existence of minimizer

From analogy of BV semi-norm, define

$$J_\gamma(w) = \sup\left\{-\int_W w\,\mathrm{div}\varphi\,dx - \int_W \nabla\theta\cdot\varphi\,dx;\ \varphi\in C_c^1(W;\mathbb{R}^2),\ \gamma^\circ(\varphi)\le 1\right\}$$

for $w \in L^1(W)$. (cf. Amar, Bellettini, *Ann. Inst. Henri Poincaré sect. C*, 11(1), 91-133 (1994).)

(Claim! $J_\gamma(w) = \int_W \gamma(\nabla(w-\theta))dx$ if $w \in W^{1,1}(W)$.)

Theorem 1 (in preparation)

Assume that (A1)–(A3) hold. Let $h > 0$, $f, g \in L^2(W)$, and $\psi\colon W \to [0,\infty)$ satisfy $a \le \psi \le A$ for constants $A, a > 0$. Then, there exists a unique minimizer $w^* \in L^2(W) \cup BV(W)$ of

$$E_\gamma(w;g) = \begin{cases} J_\gamma(w) - \int_W fw\,dx + \dfrac{1}{2h}\left\|\dfrac{w-g}{\sqrt{\psi}}\right\|_{L^2}^2 & \text{if } w\in L^2(W)\cap BV(W),\\ +\infty & \text{otherwise.}\end{cases}$$

Since $w^* \in BV(W)$ has ∇w in the sense of Radon measure, we set $\psi = \max\{a, \gamma(\nabla(w^*-\theta))\}$ in numerics.

Split Bregman method(1)

- We divide the variables of $E(w;g)$ into "w-part" and "∇w-part" with penalty term: Consider the functional of the form

$$(w,d) \mapsto \underbrace{\int_W \gamma(d-\nabla\theta)dx - \int_W f w dx + \frac{1}{2h}\left\|\frac{w-g}{\sqrt{\psi}}\right\|_{L^2}^2}_{=:F(w,d;g)} + \frac{\mu}{2}\|d-\nabla w\|_{L^2}^2$$

- Consider the Bregman iteration to find $(w^*,d^*) = \arg\min_{(w,d)} F(w,d;g)$ with subject to $d^* = \nabla w^*$. In our case, it is rephrased as the following iteration:

$$(w^{k+1},d^{k+1}) = \arg\min_{(w,d)} \left(\int_W \gamma(d-\nabla\theta)dx - \int_W f w dx + \frac{1}{2h}\left\|\frac{w-g}{\sqrt{\psi}}\right\|_{L^2}^2 + \frac{\mu}{2}\|d-\nabla w - b^k\|_{L^2}^2\right),$$

$$b^{k+1} = b^k + \nabla w^{k+1} - d^{k+1}.$$

Then, $\lim_{k\to\infty}(w^k,d^k) = (w^*,d^*)$ is the desired result.

Split Bregman method(2): alternate iteration

Find the minimizer (w^{k+1}, d^{k+1}) by the following alternate iteration.

1. Initialize $(w_0^k, d_0^k) = (w^k, d^k)$.
2. For given (w_ℓ^k, d_ℓ^k) $(\ell \geq 0)$, find the minimizer

$$w_{\ell+1}^k = \arg\min_w \left\{ -\int_W f w dx + \frac{1}{2h} \left\| \frac{w-g}{\sqrt{\psi}} \right\|_{L^2}^2 + \frac{\mu}{2} \| d_\ell^k - \nabla w - b^k \|_{L^2}^2 \right\}.$$

   It is established by solving the following elliptic PDE:

$$\begin{cases} w - h\mu\psi\Delta w = g + h\psi \left(f - \mu \operatorname{div}(d_\ell^k - b^k) \right) & \text{in } W, \\ \dfrac{\partial w}{\partial \vec{\nu}} = d_\ell^k - b^k & \text{on } \partial W. \end{cases}$$

3. Find the minimizer

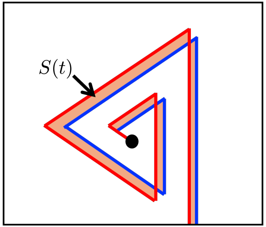
$$d_{\ell+1}^k = \arg\min_d \left\{ \int_w \gamma(d - \nabla\theta) dx + \frac{\mu}{2} \| d - \nabla w_{\ell+1}^k - b^k \|_{L^2}^2 \right\}.$$

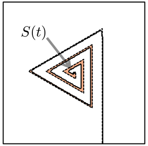
   It is established by calculating the minimizer of integrant directly with (A4).

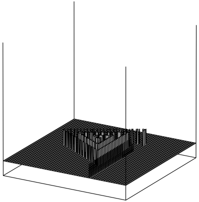
Then, $(w^{k+1}, d^{k+1}) = \lim_{\ell \to \infty} (w_\ell^k, d_\ell^k)$.

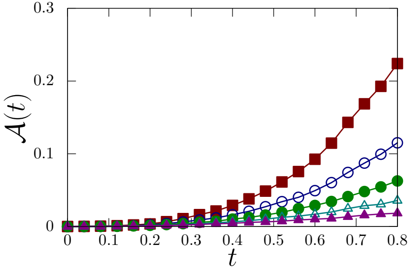
Numerical accuracy

We compute the relative area difference $\mathcal{A}(t) = S(t)/|W|$ between our method and front-tracking model by Ishiwata-O(2019) with several spatial mesh sizes Δx.









Setting: regular triangular spiral

$$\gamma(p) = \max_{0\le j\le 2} n_j \cdot p, \quad n_j = \left(\cos\frac{2j+1}{3}\pi, \sin\frac{2j+1}{3}\pi\right)$$

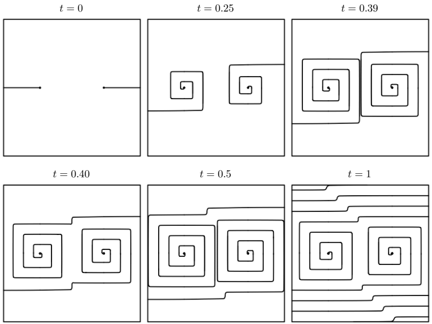
Eq. : $V_\gamma = 1 - 0.01H_\gamma$.

Domain : $[0, 0.8] \times ([-1.5, 1.5]^2 \setminus \overline{B_{2\Delta x}(0)})$

■ : $\Delta x = 0.02$, ○ : $\Delta x = 0.01$,
● : $\Delta x = 0.0067$, △ : $\Delta x = 0.005$,
▲ : $\Delta x = 0.004$.

(Claim: The difference is basically developed from the center.)

Example: merging

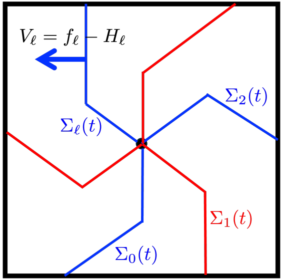


Numerical simulations: co-rotating case.

- Domain: $[0, 1] \times [-1.5, 1.5]^2$.
- Anisotropy: $\gamma(p) = |p_1| + |p_2|$ for $p = (p_1, p_2)$. $\Rightarrow \mathcal{W}_\gamma = [-1, 1]^2$.
- Equation: $V_\gamma = 1 - 0.02 H_\gamma$.
- Centers: $a_1 = (-0.7, 0)$, $a_2 = (0.7, 0)$, $m_1 = m_2 = 1$.

Application: interlace motion

Let $\Sigma(t)$ has m-minor steps denoted by $\Sigma_\ell(t)$ ($\ell = 0, 1, \ldots, m-1$), i.e., $\Sigma(t) = \bigcup_{\ell=0}^{m-1} \Sigma_\ell(t)$, and each $\Sigma_\ell(t)$ evolves by $V_\ell = f_\ell - H_\ell$.



$\Sigma_\ell(t)$ can be described as

$$\Sigma_\ell(t) = \{x \in \overline{W};\ u(t,x) - \theta(x) \equiv 2\pi\ell \mod 2\pi m\mathbb{Z}\}.$$

$$\left(\theta(x) = \sum_{j=1}^{N} m_j \arg(x - a_j), \quad m_j = m \text{ or } -m.\right)$$

Let us denote the level set equation for Σ_ℓ by

$$u_t + F_\ell(\nabla(u-\theta), \nabla^2(u-\theta)) = 0 \quad \text{in } (0,T) \times W.$$

$$(F_\ell(p, X) = -\gamma_\ell(p)\left\{\operatorname{div}(\xi_\ell(p)) + f_\ell\right\}, \quad \text{where } \xi_\ell = \nabla\gamma_\ell.)$$

In other words, u satisfies

$$u_t + F_\ell(\nabla(u-\theta), \nabla^2(u-\theta)) = 0 \quad \text{in a neighborhood of } \Sigma_\ell(t) = \{u - \theta \equiv 2\pi\ell\}.$$

Interlace motion equation

$$u_t + F_\ell(\nabla(u-\theta), \nabla^2(u-\theta)) = 0 \quad \text{in a neighborhood of } \Sigma_\ell(t) = \{u - \theta \equiv 2\pi\ell\}.$$

$$F_\ell(p, X) = -\gamma_\ell(p)\,\{\mathrm{div}(\xi_\ell(p)) + f_\ell\}$$

Now, let $\lambda \in \mathbb{R}/(2\pi m\mathbb{Z}) \to [0,1]$ be a cut-off function such that

$$\lambda(\sigma) = \begin{cases} 1 & \text{if } |\sigma| < \pi - \delta, \\ 0 & \text{if } |\sigma| > \pi + \delta, \end{cases} \qquad \sum_{\ell=0}^{m-1} \lambda(\sigma - 2\pi\ell) = 1.$$

By using λ, we combine all the level set equations as follows:

$$\begin{aligned} u_t &+ \lambda(u-\theta)F_0(\nabla(u-\theta), \nabla^2(u-\theta)) \\ &+ \lambda(u-\theta-2\pi)F_1(\nabla(u-\theta), \nabla^2(u-\theta)) \\ &+ \lambda(u-\theta-4\pi)F_2(\nabla(u-\theta), \nabla^2(u-\theta)) \\ &+ \cdots + \lambda(u-\theta-2(m-1)\pi)F_{m-1}(\nabla(u-\theta), \nabla^2(u-\theta)) = 0 \quad \text{in } (0,T)\times W. \end{aligned}$$

(cf. Y. Giga and Y.-H. R. Tsai, *Hokkaido University Preprint Series in Mathematics* #591, 2003.)

Algorithm for interlace motion

$$u_t + \sum_{\ell=0}^{m-1} \lambda(u-\theta-2\pi\ell) F_\ell(\nabla(u-\theta), \nabla^2(u-\theta)) = 0 \quad \text{in } (0,T)\times W.$$

---

1. Initialize: $u_0 \in C(\overline{W})$ satisfying $\Sigma(0) = \{u_0 - \theta \equiv 0\}$ is given.
2. For given $u_n \in C(\overline{W})$, find minimizers w_ℓ^* of

$$w_\ell^* = \arg\min_{w} \left\{ \int_W \gamma_\ell(\nabla(w-\theta))dx - \int_W f_\ell w dx + \frac{1}{2h} \left\| \frac{w-u_n}{\sqrt{\gamma_\ell(\nabla(u_n-\theta))}} \right\| \right\}$$

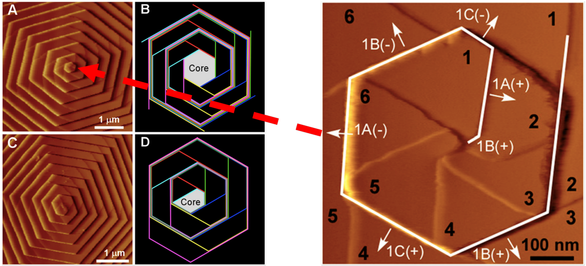
   for $\ell = 0, 1, 2, \ldots, m-1$.
3. Set

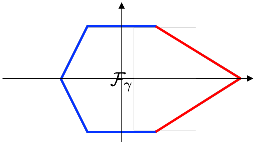
$$u_{n+1} = u_n + \sum_{\ell=0}^{m-1} \lambda(u_n - \theta - 2\pi\ell)(w_\ell^* - u_n).$$

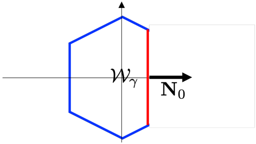
$$\left(\text{Recall:} \quad w_\ell^* - u_n = h\gamma_\ell(\nabla(u_n-\theta)) \{\operatorname{div}(\xi_\ell(\nabla(w_\ell^*-\theta)) + f_\ell\}.\right)$$

The lattice of L-cystine has

- hexagonal anisotropy with 5-usual and 1-low surface energy facets,
- Unit cell of the lattice has 6 layers successively rotated clockwise by $\pi/3$.





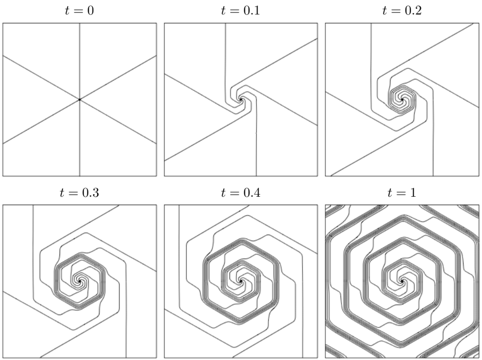


This situation can be expressed by γ whose Frank diagram: $\mathcal{F}_\gamma = \{p;\ \gamma(p) \le 1\}$ is the convex hull of

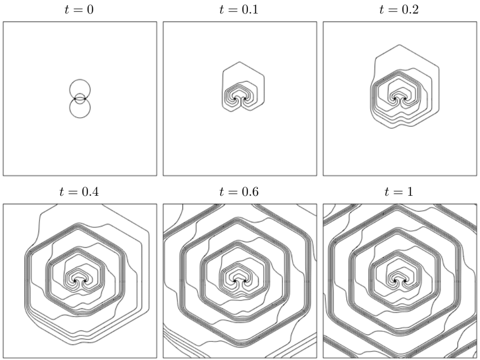
$$\mathbf{N}_0 = (1/a, 0)\ (0 < a < 1), \quad \text{and} \quad \mathbf{N}_j = \left(\cos\frac{\pi j}{3}, \sin\frac{\pi j}{3}\right)\ (j = 1, \dots, 5).$$

(Left Figure: Shtukenberg et al., Illusory loops and spirals, *PNAS* 110, 17195–17198 (2013).)

Numerical simulation of Illusory loops and spirals



Illusory loops (1 center)
Spiral steps form isles.



Illusory spirals (2 centers)
Isle steps form a spiral.

(In above cases we choose $a = 0.5$. Note that $a > 0$ for L-cystine crystal is $a \approx 0.1$.)

Summary

- We proposed an numerical algorithm for evolving spirals by crystalline curvature flow.
- A simple algorithm of minimizing movement approach was established by using general level set function
- Numerical accuracy was obtained by comparing our approach and front-tracking method due to Ishiwata-O(2019).
- As an application of our approach, the case when bunching occurs can be treated (just formal computation).

Remark

- We can choose different anisotropies for eikonal and curvature part.
- The equation with mobility; $\beta V_\gamma = -H_\gamma + f$ can be established by setting

$$u_{n+1} = u_n + \frac{w^* - u_n}{\beta(\nabla(u_n - \theta))} \quad (w^* : \text{ minimizer of } E(w : u_n)).$$

Thank you for your attention.