

ヘレ・ショウ流れ, 結晶成長, 紙の燃焼に対する境界追跡法について¹⁾ On boundary tracking methods for Hele-Shaw flows, crystal growth and combustion of paper

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Abstracts. A simple and fast numerical methods for the classical Hele-Shaw problem, the area-preserving crystalline curvature flow equation, and the closed curve version of Kuramoto-Sivashinsky equation are presented.

1 Introduction

Let $\mathcal{C}(t)$ be a smooth Jordan curve at time t in the plane $\mathbb{R}^2$. In the physical context, $\mathcal{C}(t)$ is a model of interface between a viscous liquid and the air, boundary of crystal, a flame/smoldering front, and so on. The curve $\mathcal{C}(t)$ is parameterized by $\mathbf{x}(u, t)$ for $u \in [0, 1]$ and moves by

$$\dot{\mathbf{x}}(u, t) = V(u, t)\mathbf{N}(u, t) + W(u, t)\mathbf{T}(u, t), \quad (1.1)$$

where $\dot{\mathbf{F}} = \partial \mathbf{F} / \partial t$.

In this paper we follow the so-called direct approach in which the evolution of the position vector $\mathbf{x} = \mathbf{x}(u, t)$ is governed by equation (1.1), especially in the case where the normal $\mathbf{N}$ velocity V is given by the following equations: one phase Hele-Shaw flow equation, crystalline curvature flow equation, and Kuramoto-Sivashinsky equation, while the tangent $\mathbf{T}$ velocity W controls the grid-point spacing to be uniform. Note that the tangential velocity W has no effect on the shape of evolving curve, which is determined by the value of the normal velocity V only. Therefore, one can take $W \equiv 0$ when analyzing analytical properties of the geometric flow driven by (1.1). On the other hand, the impact of a suitable choice of W on the construction of robust and stable numerical schemes has been pointed out by many authors (see e.g., [9, 14] and references therein).

2 Moving Jordan curve and eight examples

Time evolution of a Jordan curve $\mathcal{C}(t)$ is parameterized by $\mathbf{x} : [0, 1] \times [0, T) \rightarrow \mathbb{R}^2$ s.t. $\mathcal{C}(t) = \{\mathbf{x}(u, t); u \in [0, 1]\}$ and $|\mathbf{x}'| > 0$. Here $\mathbf{x}' = \partial \mathbf{x} / \partial u$ and $g(u, t) = |\mathbf{x}'|$ is the local length. We denote $|\mathbf{a}| = \sqrt{\mathbf{a} \cdot \mathbf{a}}$ where $\mathbf{a} \cdot \mathbf{b}$ is the inner product between $\mathbf{a}$ and $\mathbf{b} \in \mathbb{R}^2$. The unit tangent vector is $\mathbf{T} = \mathbf{x}' / g = \mathbf{x}_s$ where s is the arc-length parameter $ds = g du$ and $\mathbf{F}_s = \mathbf{F}' / g$, i.e., $\partial / \partial s = g^{-1} \partial / \partial u$ is the formal definition, since the arc-length s depends on u and t . The unit outward normal vector is $\mathbf{N} = -\mathbf{T}^\perp$ where $(a, b)^\perp = (-b, a)$. The tangential angle θ is defined s.t. $\mathbf{T} = (\cos \theta, \sin \theta)^\top$. The curvature κ is obtained from $\mathbf{T} = \mathbf{x}_s$ and the Frenét formula $\mathbf{T}_s = -\kappa \mathbf{N}$, from which it follows that $\kappa = \theta_s$ or $\kappa = \det(\mathbf{x}_s, \mathbf{x}_{ss})$ where $\mathbf{F}_{ss} = (\mathbf{F}' / g)' / g$ (sign convention is the way that $\kappa = 1$ if $\mathcal{C}$ is a unit circle). See Figure 2.1.

¹⁾Manuscript for 『数値解析学の最前線：理論・方法・応用』, November 8–10, 2017 at RIMS, Kyoto University. This work was partially supported by KAKENHI No.16H03953.

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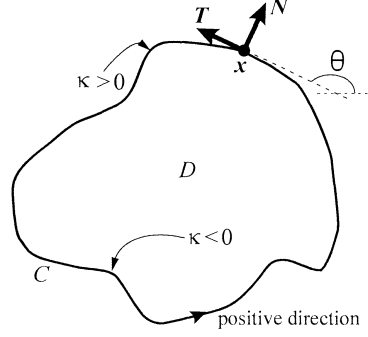


Figure 2.1: Moving Jordan curve

A geometric evolution problem can be formulated as follows: For a given initial Jordan curve $\mathcal{C}^0$, find a family of curves $\{\mathcal{C}(t)\}_{0 \leq t < T}$, starting from $\mathcal{C}(0) = \mathcal{C}^0$ and evolving by the normal velocity V .

In what follows, we show eight examples of various kinds of the normal velocity V .

Example 2.1 A simple example of V is the **Eikonal equation** $V = -1$, which is the L^2 -gradient flow of the enclosed area $\mathcal{A}(t) = \frac{1}{2} \int_{\mathcal{C}(t)} \mathbf{x} \cdot \mathbf{N} ds$, since

$$\dot{\mathcal{A}}(t) = \int_{\mathcal{C}(t)} V ds. \quad (2.1)$$

Example 2.2 Another typical example is the classical **curvature flow equation** $V = -\kappa$, which is the L^2 -gradient flow of the total length $\mathcal{L}(t) = \int_{\mathcal{C}(t)} ds$, since

$$\dot{\mathcal{L}}(t) = \int_{\mathcal{C}(t)} \kappa V ds. \quad (2.2)$$

Then we have the curve-shortening property (**CS-property** in short) $\dot{\mathcal{L}}(t) \leq 0$, and then $V = -\kappa$ is also called the curve-shortening equation.

Example 2.3 The **area-preserving curvature flow equation** $V = \langle \kappa \rangle - \kappa$ is also classical, where $\langle F \rangle = \mathcal{L}(t)^{-1} \int_{\mathcal{C}(t)} F ds$ is the average of F along the curve $\mathcal{C}(t)$. The enclosed area $\mathcal{A}(t)$ is preserved in time (**AP-property** in short), since from (2.1) we have

$$\dot{\mathcal{A}}(t) = \int_{\mathcal{C}(t)} (\langle \kappa \rangle - \kappa) ds = \langle \kappa \rangle \int_{\mathcal{C}(t)} ds - \int_{\mathcal{C}(t)} \kappa ds = 0.$$

By means of CBS inequality, we also have the CS-property $\dot{\mathcal{L}} \leq 0$ which is the same as the classical curvature flow equation $V = -\kappa$ in Example 2.2. Indeed, $V = \langle \kappa \rangle - \kappa$ is the L^2 -gradient flow of $\mathcal{L}$ subject to area-preserving.

Example 2.4 The fourth example is the **Willmore flow equation** $V = \kappa_{ss} + \kappa^3/2$, which is the L^2 -gradient flow of the elastic energy $\mathcal{E}(t) = \int_{\mathcal{C}(t)} \kappa^2 ds/2$, since

$$\dot{\mathcal{E}}(t) = - \int_{\mathcal{C}(t)} \left(\kappa_{ss} + \frac{1}{2} \kappa^3 \right) V ds. \quad (2.3)$$

Example 2.5 The fifth example is the **surface diffusion flow equation** $V = \kappa_{ss}$ which is formally obtained from the Willmore flow equation without the term $\kappa^3/2$. The solution of this equation satisfies the AP-property $\dot{\mathcal{A}}(t) = \int_{\mathcal{C}(t)} \kappa_{ss} ds = 0$. We also have the CS-property $\dot{\mathcal{L}}(t) \leq 0$, and in this sense, the surface diffusion flow and the area-preserving curvature flow are very similar each other.

Example 2.6 As we have seen, the area-preserving curvature flow equation $V = \langle \kappa \rangle - \kappa$ and the surface diffusion flow equation $V = \kappa_{ss}$ have the AP- and the CS-properties. The following **Hele-Shaw flow equation** also has these two properties.

The Hele-Shaw problem is description of a motion of viscous fluid in a quasi two-dimensional space, which was starting from a short paper [5] in 1898 by Henry Selby Hele-Shaw (1854–1941). In his experiment, viscous fluid is sandwiched between two parallel plates with a narrow gap, and the apparatus is called Hele-Shaw cell. He succeeded to visualize stream lines by means of colored water in the cell. In the mathematical context, the Hele-Shaw problem is reduced from Navier-Stokes equations via stationary Stokes approximation, parabolic-shape approximation of the velocity profile, and assumption of the Laplace relation on the boundary, that is, the problem is stated as follows (see [8, 4] in detail):

$$\begin{cases} \Delta p = 0 & \text{in } \mathcal{D}(t), \\ p = \gamma \kappa & \text{on } \mathcal{C}(t), \\ V = -\nabla p \cdot \mathbf{N} & \text{on } \mathcal{C}(t), \end{cases} \quad (2.4)$$

where $\mathcal{D}(t) \subset \mathbb{R}^2$ is region occupied by fluid, $\mathcal{C}(t) = \partial\mathcal{D}(t)$ is the boundary, p is the pressure function, κ is the curvature, $\gamma > 0$ is the surface tension coefficient, $\mathbf{N}$ is the unit outward normal vector, and $V = \dot{\mathbf{x}} \cdot \mathbf{N}$ is the normal velocity. See Figure 2.1.

Thus the Hele-Shaw problem is stated as a kind of moving boundary problems determining unknown function p and unknown fluid region $\mathcal{D}$. It can be described in another way such as follows. Let $\mathbf{u}$ be the velocity vector of two-dimensional fluid. Then the harmonicity of the pressure p is an expression of continuation derived from the Darcy's law $\mathbf{u} = -\nabla p$ and the incompressible condition of fluid $\operatorname{div} \mathbf{u} = 0$, and the normal velocity V is derived from mass conservation law $\dot{\mathbf{x}} = \mathbf{u}$.

When the pressure p and the curve $\mathcal{C}(t)$ are solutions of the Hele-Shaw problem (2.4), then we have the CS-property in the following sense

$$-\dot{\mathcal{L}}(t) = \frac{1}{\gamma} \int_{\mathcal{C}(t)} p \nabla p \cdot \mathbf{N} ds = \frac{1}{\gamma} \iint_{\mathcal{D}(t)} \operatorname{div}(p \nabla p) dxdy = \frac{1}{\gamma} \iint_{\mathcal{D}(t)} |\nabla p|^2 dxdy \geq 0.$$

We also have the AP-property

$$\dot{\mathcal{A}}(t) = - \int_{\mathcal{C}(t)} \nabla p \cdot \mathbf{N} ds = - \iint_{\mathcal{D}(t)} \operatorname{div}(\nabla p) dxdy = - \iint_{\mathcal{D}(t)} \Delta p dxdy = 0.$$

Example 2.7 Let us consider the total interfacial energy $\mathcal{L}_\sigma(t) = \int_{\mathcal{C}(t)} \sigma(\theta) ds$, where $\sigma > 0$ is the interfacial energy density per unit arc-length and θ is the tangential angle as

in Figure 2.1. Then the L^2 -gradient flow of $\mathcal{L}_\sigma$ is $V = -\kappa_\sigma$, where $\kappa_\sigma = (\sigma + \sigma'')\kappa$ is the weighted curvature, since we have

$$\dot{\mathcal{L}}_\sigma(t) = \int_{\mathcal{C}(t)} \kappa_\sigma V \, ds, \quad (2.5)$$

which is regarded as the anisotropic version of (2.2). The equation $V = -\kappa_\sigma$ is called the **weighted curvature flow equation**. The energy density σ is specified by so-called the Wulff shape $\mathcal{W}_\sigma = \bigcap_{\theta \in [0, \pi]} \{\mathbf{x} \in \mathbb{R}^2; \mathbf{x} \cdot \mathbf{N}(\theta) \leq \sigma(\theta)\}$, where $\mathbf{N}(\theta) = (\sin \theta, -\cos \theta)^T$. If σ is a smooth function of θ and $\sigma + \sigma''$ is positive, then $(\sigma + \sigma'')^{-1}$ is the curvature of the boundary of the Wulff shape $\mathcal{W}_\sigma$. When the Wulff shape is a polygon, σ is not smooth and is called crystalline energy density, and the gradient flow of total crystalline energy derive the so-called **crystalline curvature flow equation**, which will be discussed in §5.

Example 2.8 The last example is the case where the normal velocity V is a linear combination of the Eikonal, the classical curvature flow and the surface diffusion flow equations with the coefficients $V^{(0)}$, $\alpha_{\text{eff}} - 1$ and δ such that

$$V = V^{(0)} + (\alpha_{\text{eff}} - 1)\kappa + \delta\kappa_{ss}, \quad (2.6)$$

where $V^{(0)}$ is a constant speed, and α_{eff} and δ are positive parameters. This equation (2.6) is equivalent to, in a certain scale, the so-called **Kuramoto-Sivashinsky equation** for the graph $y = f(x, t)$ of a curved flame front [7, 15] when $V^{(0)} = 1$ and $\delta = 4$:

$$\dot{f} + \frac{1}{2}f'^2 + (\alpha_{\text{eff}} - 1)f'' + 4f'''' = 0, \quad (2.7)$$

where $f' = \partial f / \partial x$, $f'' = \partial^2 f / \partial x^2$ and $f'''' = \partial^4 f / \partial x^4$. One can find the simple scaling argument in [3].

If $\alpha_{\text{eff}} > 1$, then $(\alpha_{\text{eff}} - 1)\kappa$ induces instability, which is similar to the ill-posedness of backward heat equation $\dot{f} = -f''$, and $\delta\kappa_{ss}$ plays a stabilization role of the unstable front. An alternative stabilization method is to use the Willmore flow [10].

3 Numerical scheme for (1.1)

In the direct approach, a moving Jordan curve is approximated by a moving Jordan polygonal curve, say $\Gamma(t)$ at time t , with N vertices labeled $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ in the anti-clockwise order. Let Γ_i be the i -th edge $\Gamma_i = [\mathbf{x}_{i-1}, \mathbf{x}_i]$ ($i = 1, 2, \dots, N$; $\mathbf{x}_0 = \mathbf{x}_N$). Then the moving Jordan polygonal curve at time t is $\Gamma(t) = \bigcup_{i=1}^N \Gamma_i(t)$. Our goal here is to construct a discretization of (1.1) in space, i.e., to derive a system of ordinary differential equations (ODEs in short) for $\Gamma(t)$: for $i = 1, 2, \dots, N$

$$\dot{\mathbf{x}}_i(t) = V_i(t)\mathbf{N}_i(t) + W_i(t)\mathbf{T}_i(t), \quad (3.1)$$

where V_i is the normal $\mathbf{N}_i$ -component of the velocity at $\mathbf{x}_i$, and W_i the tangential $\mathbf{T}_i$ -component of the velocity at $\mathbf{x}_i$.

The right-hand-side of (3.1) consists of several polygonal quantities on Γ at time t , and all of them can be constructed from $\{\mathbf{x}_i\}_{i=1}^N$ through the following steps. In what follows, these are regarded as functions of time t with N -periodic index, i.e., $\mathbf{F}_0 = \mathbf{F}_N$, $\mathbf{F}_{N+1} = \mathbf{F}_1$.

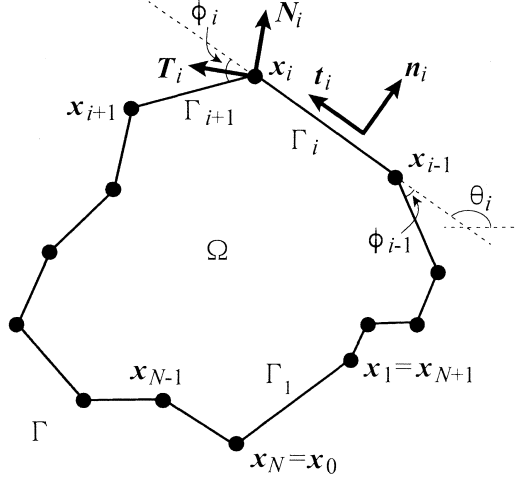


Figure 3.1: Moving Jordan polygonal curve

Step 1 several polygonal quantities (see Figure 3.1)

$r_i = |x_i - x_{i-1}|$: the length of Γ_i ,

$L = \sum_{i=1}^N r_i$: the total length of Γ ,

$t_i = (x_i - x_{i-1})/r_i$: the unit tangent vector on Γ_i ,

$n_i = -t_i^\perp$: the outward unit normal vector on Γ_i ,

$\phi_i = \text{sgn}(\det(t_i, t_{i+1})) \arccos(t_i \cdot t_{i+1})$: the angle between the adjacent edges Γ_i and Γ_{i+1} ,

$T_i = (t_i + t_{i+1})/(2\cos_i)$: the unit tangent vector at x_i , where $\cos_i = \cos(\phi_i/2)$,

$N_i = -T_i^\perp$: the unit outward normal vector at x_i ,

$\kappa_i = (\tan_i + \tan_{i-1})/r_i$: the curvature on Γ_i , where $\sin_i = \sin(\phi_i/2)$, $\tan_i = \sin_i/\cos_i$;

Step 2 the normal velocity $V_i = (v_i + v_{i+1})/(2\cos_i)$ at x_i , where

v_i is a given averaged normal velocity on Γ_i such as $v_i = -\kappa_i$, and so on;

Step 3 the tangential velocity W_i at x_i is defined by one of the followings:

(1) **Uniform Distribution Method**: $W_i = (\Psi_i + c)/\cos_i$ at x_i , where

$$\Psi_i = \sum_{j=1}^i \psi_j, \quad c = - \left(\sum_{j=1}^N \Psi_j / \cos_j \right) / \left(\sum_{j=1}^N \cos_j \right), \quad \psi_1 = 0 \quad \text{and}$$

$$\psi_j = \frac{1}{N} \sum_{l=1}^N \kappa_l v_l r_l - V_j \sin_j - V_{j-1} \sin_{j-1} + \left(\frac{L}{N} - r_j \right) \omega$$

for $j = 2, 3, \dots, N$, and ω will be defined later;

(2) **Crystalline Method:** $W_i = (v_{i+1} - v_i)/(2\sin_i)$ at $\mathbf{x}_i$;

(3) **Curvature Adjusted Method:** an interpolation of (1) and (2);

GOAL (3.1) can be summarized as the following ODEs:

$$\dot{\mathbf{X}} = \mathbf{F}(\mathbf{X}), \quad (3.2)$$

where $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) \in \mathbb{R}^{2 \times N}$, and

$$\begin{cases} \mathbf{F} = (\mathbf{F}_1, \mathbf{F}_2, \dots, \mathbf{F}_N) : \mathbb{R}^{2 \times N} \rightarrow \mathbb{R}^{2 \times N}; \\ \mathbb{R}^{2 \times N} \ni \mathbf{X} \mapsto \mathbf{F}_i(\mathbf{X}) \in \mathbb{R}^2 \ (i = 1, 2, \dots, N). \end{cases}$$

The background of the above steps are the followings.

Step 1 Several polygonal quantities r_i , L , $\mathbf{t}_i$, $\mathbf{n}_i$ and ϕ_i are defined naturally as in Step 1.

- To define the tangent and normal vectors at $\mathbf{x}_i$, we use the angle ϕ_i between the adjacent edges Γ_i and Γ_{i+1} ($\mathbf{t}_i \cdot \mathbf{t}_{i+1} = \cos \phi_i$). As in Figure 3.1, the unit tangent vector $\mathbf{T}_i$ at $\mathbf{x}_i$ are defined by an average of the adjacent corresponding vectors in the sense as in Step 1.
- To define the curvatures on Γ_i and at $\mathbf{x}_i$, we use (2.2) rather than the Frenét formulae, i.e., we recall that the curvature can be defined by the first variation of the total length $\mathcal{L}$ from (2.2). From (3.1), the total length L , and $\dot{r}_i = V_i \sin_i + V_{i-1} \sin_{i-1} + W_i \cos_i - W_{i-1} \cos_{i-1}$, we obtain $\dot{L} = \sum_{i=1}^N \hat{\kappa}_i V_i \hat{r}_i$, where $\hat{r}_i = (r_i + r_{i+1})/2$, and $\hat{\kappa}_i = 2\sin_i/\hat{r}_i$ is the polygonal curvature at $\mathbf{x}_i$. It is a natural definition since the normal velocity V_i at $\mathbf{x}_i$ is the average of the adjacent normal averaged velocities in the sense of Step 2. Then it follows that

$$\dot{L} = \sum_{i=1}^N \kappa_i v_i r_i, \quad (3.3)$$

which is a discretization of (2.2), where κ_i in Step 1 is the polygonal curvature on Γ_i . Note that κ_i is same as the polygonal curvature or the crystalline curvature in a prescribed class of polygonal curves [2] and v_i is not necessarily equivalent to $\dot{\mathbf{x}}_i \cdot \mathbf{n}_i$ (see the next step (2)).

Step 3 Let L_ε be a small perturbation ε of L at $\mathbf{x}_i$ only such as $\mathbf{x}_i + \varepsilon \mathbf{z}$. The $\mathbf{z}$ -directional derivative of L_ε is $dL_\varepsilon/d\varepsilon|_{\varepsilon=0} = \hat{\kappa}_i \mathbf{N}_i \cdot \mathbf{z} \hat{r}_i$. Hence $\mathbf{z} = -\mathbf{N}_i$ is the gradient direction of L at $\mathbf{x}_i$. However, from the enclosed area $A = \sum_{i=1}^N \mathbf{x}_{i-1}^\perp \cdot \mathbf{x}_i / 2$, we have $dA_\varepsilon/d\varepsilon|_{\varepsilon=0} = \tilde{\mathbf{N}}_i \cdot \mathbf{z}$ with $\tilde{\mathbf{N}}_i = r_i \mathbf{n}_i + r_{i+1} \mathbf{n}_{i+1}$, and hence $\tilde{\mathbf{N}}_i$ is not the same direction as $\mathbf{N}_i$ unless $r_i \equiv L/N$. Therefore, $\mathbf{N}_i$ is not the gradient direction of A , and so an error term (comparing with (2.1)) appears as follows:

$$\dot{A} = \sum_{i=1}^N v_i r_i + \text{err}_A, \quad \text{err}_A = \sum_{i=1}^N \left(W_i \sin_i - \frac{v_{i+1} - v_i}{2} \right) \frac{r_{i+1} - r_i}{2}. \quad (3.4)$$

There are two ways to vanish err_A :

- (1) To use W_i satisfying $r_i \equiv L/N$:

This method is called the uniform distribution method (UDM in short). Because of numerical errors, an asymptotic UDM is utilized practically as follows. To obtain the asymptotic UDM, $r_i \rightarrow L/N$ ($t \rightarrow T_{\max} \leq \infty$), we assume that for $i = 1, 2, \dots, N$

$$r_i - \frac{L}{N} = \eta_i e^{-\mu(t)} \quad \left(\sum_{i=1}^N \eta_i = 0, \quad \lim_{t \rightarrow T_{\max}} \mu(t) = \infty \right).$$

Differentiating the both sides and putting $\omega(t) = \dot{\mu}(t)$, we have $\dot{r}_i = U_i$ for $i = 1, 2, \dots, N$, where

$$U_i = \frac{\dot{L}}{N} + \left(\frac{L}{N} - r_i \right) \omega(t), \quad \int_0^{T_{\max}} \omega(t) dt = \infty,$$

and ω is a large value if $T_{\max} = \infty$ as in this paper's case, and we obtain the tangential velocity equation $W_i \cos_i - W_{i-1} \cos_{i-1} = U_i - V_i \sin_i - V_{i-1} \sin_{i-1}$ for $i = 1, 2, \dots, N$. Since these N equations are linearly dependent, imposing the zero-average condition $\sum_{i=1}^N W_i = 0$ yields N linearly independent equations, which can be solved as in Step 3.

- (2) To use $W_i = (v_{i+1} - v_i)/(2\sin_i)$:

This method is called crystalline method which is equivalent to the case $v_i = \dot{\mathbf{x}}_i \cdot \mathbf{n}_i$, and in this case, Γ is restricted in a prescribed class of polygonal curves as mentioned in Step 1.

- (3) This method is an interpolation of (1) and (2) developed by [1, 13].

To solve ODEs (3.2), one can use the following several methods: the Euler method, a semi-implicit method, the classical fourth order Runge-Kutta method, and an iteration method, depending on each problem.

4 The Hele-Shaw flow equation in Example 2.6

The averaged normal velocity v_i in Step 2 will be approximated from the normal velocity of the Hele-Shaw flow equation (2.4) in Example 2.6, by means of the **Method of Fundamental Solutions** (MFS in short) as follows.

For each fixed $t \geq 0$ we solve the following Dirichlet problem:

$$\begin{cases} \Delta p = 0 & \text{in } \Omega(t), \\ p = \gamma \kappa_i & \text{on } \Gamma_i(t) \quad (i = 1, 2, \dots, N). \end{cases}$$

We seek the approximate solution P of the form

$$P(\mathbf{x}) = Q_0 + \sum_{j=1}^N Q_j E_j(\mathbf{x}), \quad E_j(\mathbf{x}) := E(\mathbf{x} - \mathbf{y}_j) - E(\mathbf{x} - \mathbf{z}_j) \quad (\mathbf{x} \in \overline{\Omega}(t)), \quad (4.1)$$

$$P(\mathbf{x}_i^*) = \gamma \kappa_i \quad (i = 1, 2, \dots, N), \quad (4.2)$$

$$v_i = -\nabla P(\mathbf{x}_i^*) \cdot \mathbf{n}_i \quad (i = 1, 2, \dots, N), \quad (4.3)$$

where $E(\mathbf{x}) = \log |\mathbf{x}|/(2\pi)$ is the fundamental solution of the Laplace operator Δ , $\mathbf{x}_i^* = (\mathbf{x}_i + \mathbf{x}_{i-1})/2$ is the mid point on Γ_i , $\{Q_j\}_{j=0}^N$ are unknown coefficients which will be solved below, $\mathbf{y}_j$'s are the singular points defined by

$$\mathbf{y}_j = \mathbf{x}_j^* + d\mathbf{n}_j \quad (j = 1, 2, \dots, N),$$

where $d > 0$ is a parameter controlling accuracy of MFS, and $\mathbf{z}_j$'s are "dummy" points located in $\mathbb{R}^2 \setminus \overline{\Omega}(t)$ which are not equal to the singular points $\{\mathbf{y}_j\}_{j=1}^N$.

Note that P satisfies $\Delta P = 0$ in Ω and is invariant under the trivial affine transformation and the origin shift of the boundary data as well as the original invariant scheme of MFS or so-called the Charge Simulation Method (see [12] and references therein). One can add one more condition which is required for the invariance of the original invariant scheme of MFS. We select the condition such a way that the weighted average of Q_j 's is equal to 0, that is, coefficients $\{Q_j\}_{j=0}^N$ are determined by (4.2) and

$$\sum_{j=1}^N Q_j H_j = 0, \quad H_j = - \sum_{i=1}^N \nabla E_j(\mathbf{x}_i^*) \cdot \mathbf{n}_i r_i, \quad j = 1, 2, \dots, N. \quad (4.4)$$

One can solve this system of $N + 1$ linear equations (4.2) and (4.4) by a standard elimination method.

As mentioned in Example 2.6, AP-property and CS-property hold for Hele-Shaw problem. When the averaged normal velocity v_i on Γ_i is defined by (4.3), if $\text{err}_A = 0$ by UDM, then we have

$$\dot{A} = \sum_{i=1}^N v_i r_i = \sum_{j=1}^N Q_j H_j = 0, \quad (4.5)$$

where H_j 's are in (4.4). Thus AP-property holds in a discrete sense.

We also have the approximated CS-property as follows.

$$\begin{aligned} \dot{L} &= \sum_{i=1}^N \kappa_i v_i r_i = - \sum_{i=1}^N \kappa_i \nabla P(\mathbf{x}_i^*) \cdot \mathbf{n}_i r_i = - \frac{1}{\gamma} \sum_{i=1}^N P(\mathbf{x}_i^*) \nabla P(\mathbf{x}_i^*) \cdot \mathbf{n}_i r_i \\ &= - \frac{1}{\gamma} \sum_{i=1}^N \int_{\Gamma} P(\mathbf{x}_i^*) \nabla P(\mathbf{x}_i^*) \cdot \mathbf{n}_i ds \\ &\approx - \frac{1}{\gamma} \sum_{i=1}^N \int_{\Gamma_i} P(\mathbf{x}) \nabla P(\mathbf{x}) \cdot \mathbf{n}_i ds = - \frac{1}{\gamma} \int_{\Gamma} P(\mathbf{x}) \nabla P(\mathbf{x}) \cdot \mathbf{n} ds \\ &= - \frac{1}{\gamma} \iint_{\Omega} \text{div}(P \nabla P) dx dy = - \frac{1}{\gamma} \iint_{\Omega} |\nabla P|^2 dx dy \leq 0. \end{aligned}$$

Note that, instead of (4.2) and (4.3), if we use

$$[P]_i = \gamma \kappa_i, \quad i = 1, 2, \dots, N, \quad (4.6)$$

$$v_i = -\langle \nabla P \rangle_i \cdot \mathbf{n}_i, \quad i = 1, 2, \dots, N, \quad (4.7)$$

where $\langle F \rangle_i = r_i^{-1} \int_{\Gamma_i} F ds$ is the average of F on Γ_i , and $[F]_i = \langle F \nabla F \rangle_i \cdot \mathbf{n}_i / \langle \nabla F \rangle_i \cdot \mathbf{n}_i$, then we have $\dot{L} \leq 0$ without an approximation. However, in this case we have to solve nonlinear $N + 1$ equations of $\{Q_j\}_{j=0}^N$, and that computational cost is not cheap.

To solve ODEs (3.2), we use the classical fourth order Runge-Kutta method. A precise argument and several numerical experiments can be found in [11].

5 The area-preserving crystalline curvature flow equation in Example 2.7

In the crystalline setting, we use the following additional polygonal quantities (cf. §3):

Step 1 (addition)

$h_i = \mathbf{x}_i \cdot \mathbf{n}_i = \mathbf{x}_{i-1} \cdot \mathbf{n}_i$: the hight function for Γ_i ,

θ_i : the tangent angle satisfying $\mathbf{t}_i = (\cos \theta_i, \sin \theta_i)^T$. See Figure 3.1. All tangent angles $\{\theta_i\}_{i=0}^{N+1}$ can be derived as in the following procedure: Firstly, from $\mathbf{t}_1 = (t_{11}, t_{12})^T$, we have $\theta_1 = -\arccos(t_{11})$ if $t_{12} < 0$; $\theta_1 = \arccos(t_{11})$ if $t_{12} \geq 0$. Secondly, for $i = 1, 2, \dots, N$, we successively compute θ_{i+1} from θ_i as $\theta_{i+1} = \theta_i + \phi_i$. Finally, we obtain $\theta_0 = \theta_1 - (\theta_{N+1} - \theta_N)$, since $\theta_N = \theta_0 + 2\pi$ and $\theta_{N+1} = \theta_1 + 2\pi$ hold.

Note that all the polygonal quantities above and in Step 1 except $\{\theta_i\}_{i=0}^{N+1}$ satisfy the periodic boundary conditions: $F_0 = F_N$, $F_{N+1} = F_1$.

Construction ($h, \nu \Rightarrow \mathbf{x}, \mathbf{t}, \mathbf{n}, r$). The set of vertices $\{\mathbf{x}_i\}_{i=1}^N$ can be constructed from the sets $\{h_i\}_{i=1}^{N+1}$ ($h_{N+1} = h_1$) and $\{\theta_i\}_{i=1}^{N+1}$ ($\theta_{N+1} = \theta_1 + 2\pi$) as follows. Let $\mathbf{t}(\theta) = (\cos \theta, \sin \theta)^T$ and $\mathbf{n}(\theta) = (\sin \theta, -\cos \theta)^T$, and then we have $\mathbf{t}_i = \mathbf{t}(\theta_i)$ and $\mathbf{n}_i = \mathbf{n}(\theta_i)$. Since $h_i = \mathbf{x}_i \cdot \mathbf{n}(\theta_i)$ and $h_{i+1} = \mathbf{x}_i \cdot \mathbf{n}(\theta_{i+1})$, from the sets $\{h_i\}_{i=1}^{N+1}$ and $\{\theta_i\}_{i=1}^{N+1}$ we obtain $\mathbf{x}_i = (h_{i+1}\mathbf{t}_i - h_i\mathbf{t}_{i+1}) / \sin \phi_i$ for $i = 1, 2, \dots, N$. From this the length of the i -th edge can be described as

$$r_i = \frac{h_{i+1}}{\sin \phi_i} - h_i(\cot \phi_i + \cot \phi_{i-1}) + \frac{h_{i-1}}{\sin \phi_{i-1}}.$$

For N -tuples $\mathbf{h} = (h_1, h_2, \dots, h_N)$ and $\phi = (\phi_1, \phi_2, \dots, \phi_N)$ with the periodic boundary conditions $F_0 = F_N$, $F_{N+1} = F_1$, we denote the right hand side of r_i as $D_i(\mathbf{h}, \phi)$, i.e., $r_i = D_i(\mathbf{h}, \phi)$ holds for $i = 1, 2, \dots, N$.

The Wulff polygon and admissibility. Now let us restrict the polygonal curve Γ in an admissible class associated with the N_σ -sided convex polygon, say the Wulff polygon $\mathcal{W}_\sigma$ for an appropriate positive function σ : $\mathcal{W}_\sigma = \bigcap_{i=1}^{N_\sigma} \{\mathbf{x} \in \mathbb{R}^2; \mathbf{x} \cdot \mathbf{n}(\eta_i) \leq \sigma(\eta_i)\}$, where η_i is the tangent angle of the i -th edge of $\mathcal{W}_\sigma$ ($i = 1, 2, \dots, N_\sigma$). Such σ is called crystalline interfacial energy density. The length of the i -th edge is described as $l_\sigma(\eta_i) = D_i(\boldsymbol{\sigma}(\eta), \boldsymbol{\psi})$, where $\boldsymbol{\sigma}(\eta) = (\sigma(\eta_1), \sigma(\eta_2), \dots, \sigma(\eta_{N_\sigma}))$, $\boldsymbol{\psi} = (\psi_1, \psi_2, \dots, \psi_{N_\sigma})$, and $\psi_i = \eta_{i+1} - \eta_i \in (0, \pi)$ for $i = 1, 2, \dots, N_\sigma$ ($\psi_0 = \psi_{N_\sigma}$, $\psi_{N_\sigma+1} = \psi_1$). Note that $\sigma > 0$ should be satisfied $l_\sigma(\eta_i) > 0$ for $i = 1, 2, \dots, N_\sigma$. Let $\mathcal{N} = \{\mathbf{n}_i\}_{i=1}^N$ and $\mathcal{N}_\sigma = \{\mathbf{n}(\eta_j)\}_{j=1}^{N_\sigma}$ be the set of normal vectors on Γ and $\partial\mathcal{W}_\sigma$, respectively. The polygonal curve Γ is called $\mathcal{W}_\sigma$ -admissible if the following two conditions are satisfied.

$$(1) \mathcal{N} \subset \mathcal{N}_\sigma; \quad (2) \frac{(1-\lambda)\mathbf{n}_i + \lambda\mathbf{n}_{i+1}}{|(1-\lambda)\mathbf{n}_i + \lambda\mathbf{n}_{i+1}|} \notin \mathcal{N}_\sigma \quad (i = 1, 2, \dots, N; \mathbf{n}_{N+1} = \mathbf{n}_1; \lambda \in (0, 1)).$$

Let $\Gamma(t)$ be the $\mathcal{W}_\sigma$ -admissible, N -sided and time t -dependent polygonal curve. The curve $\Gamma(t) = \bigcup_{i=1}^N \Gamma_i(t)$, $\Gamma_i(t) = [\mathbf{x}_{i-1}(t), \mathbf{x}_i(t)]$ evolves by prescribed normal velocities:

$$v_i = \dot{\mathbf{x}}_i \cdot \mathbf{n}(\theta_i) = \dot{h}_i \quad (i = 1, 2, \dots, N),$$

which will be defined later. Note that for any ϕ_i there is a $j \in \{1, 2, \dots, N_\sigma\}$ such that $|\phi_i| = \psi_j$ holds.

The energy and the crystalline curvature. The total interfacial crystalline energy is defined by $L_\sigma = \sum_{i=1}^N \sigma(\theta_i) r_i$. Since the time differential of $r_i = D_i(\mathbf{h}, \phi)$ is $\dot{r}_i = D_i(\dot{\mathbf{h}}, \phi) = D_i(\mathbf{v}, \phi)$, where $\mathbf{v} = (v_1, \dots, v_N)$, the time differential of L_σ is

$$\dot{L}_\sigma = \sum_{i=1}^N \sigma(\theta_i) D_i(\mathbf{v}, \phi) = \sum_{i=1}^N v_i D_i(\sigma(\theta), \phi) = \sum_{i=1}^N \kappa_{\sigma i} v_i r_i,$$

where $\kappa_{\sigma i} = D_i(\sigma(\theta), \phi)/r_i$, $D_i(\sigma(\theta), \phi) = \chi_i l_\sigma(\theta_i)$, $\chi_i = (\text{sgn}(\phi_{i-1}) + \text{sgn}(\phi_i))/2$, $\sigma(\theta) = (\sigma(\theta_1), \sigma(\theta_2), \dots, \sigma(\theta_N))$. The $\kappa_{\sigma i}$ is called the i -th crystalline curvature, and the χ_i is called the i -th transition number.

The gradient flow subject to area-preserving. The time differential of enclosed area $A = \sum_{i=1}^N h_i r_i / 2$ is $\dot{A} = \sum_{i=1}^N v_i r_i$ without the error term err_A , since the tangential velocity is given by (2) Crystalline Method in Step 2. As the area-preserving gradient flow of L_σ , we obtain the area-preserving crystalline curvature flow equations

$$v_i = \langle \kappa_\sigma \rangle - \kappa_{\sigma i}, \quad \langle F \rangle = \frac{1}{L} \sum_{i=1}^N F_i r_i \quad (i = 1, 2, \dots, N). \quad (5.1)$$

Now we are ready to set up the problem. Let P_σ^N be a set of all $\mathcal{W}_\sigma$ -admissible, N -sided polygonal Jordan curve in the plane. For a given $\Gamma^0 \in P_\sigma^N$ find a family of curves $\{\Gamma(t) \in P_\sigma^N\}_{0 \leq t < T}$ satisfying $\dot{h}_i = v_i$ ($i = 1, 2, \dots, N$), starting from $\Gamma(0) = \Gamma^0$.

An iteration. Instead of solving ODEs (3.2), we solve the equivalent ODEs $\dot{h}_i = v_i$ by the following discretization

$$\frac{h_i^{m+1/2} - h_i^m}{\tau_m/2} = F_i(\mathbf{h}^{m+1/2}) = \frac{\sum_{j=1}^N k_{\sigma j}^{m+1/2} r_j^{m+1/2}}{\sum_{j=1}^N r_j^{m+1/2}} - k_{\sigma i}^{m+1/2},$$

where $k_{\sigma i}^{m+1/2} = D_i(\sigma(\nu^m), \phi^m)/r_i^{m+1/2}$, $r_i^{m+1/2} = D_i(\mathbf{h}^{m+1/2}, \phi^m)$, and solve this by the iteration as in the following steps.

- (1) $l = 0$; $\mathbf{y}^{(l)} = \mathbf{h}^m$;
- (2) $\mathbf{y}^{(l+1)} = \mathbf{h}^m + \mathbf{F}(\mathbf{y}^{(l)}) \tau_m / 2$;
- (3) If $\|\mathbf{y}^{(l+1)} - \mathbf{y}^{(l)}\| / r_{\max}^m \leq \delta_{\text{tol}}$, then GOTO (5);
- (4) $l := l + 1$; GOTO (2);
- (5) $\mathbf{h}^{m+1} = R^{(l+1)} \tilde{\mathbf{y}}^{(l+1)}$, $\tilde{\mathbf{y}}^{(l+1)} = 2\mathbf{y}^{(l+1)} - \mathbf{h}^m$, $R^{(l+1)} = \sqrt{A^0 / \tilde{A}^{(l+1)}}$.

Here $\delta_{\text{tol}} > 0$ is a tolerance, A^0 is the enclosed area of Γ^0 , $\tilde{A}^{(j)}$ is the enclosed area of a polygon constructed from the heights $\{\tilde{y}_i^{(j)}\}_{i=1}^N$, $\mathbf{y}^{(j)} = (y_1^{(j)}, \dots, y_N^{(j)})$, $\mathbf{F}(\mathbf{y}^{(j)}) = (F_1(\mathbf{y}^{(j)}), \dots, F_N(\mathbf{y}^{(j)}))$, $\tilde{\mathbf{y}}^{(j)} = (\tilde{y}_1^{(j)}, \dots, \tilde{y}_N^{(j)})$, $\|\mathbf{y}^{(l+1)} - \mathbf{y}^{(l)}\| = \max_{1 \leq i \leq N} |y_i^{(l+1)} - y_i^{(l)}|$, and $F_{\max} = \max_{1 \leq i \leq N} F_i$.

The iteration succeeds in showing the convergence $\lim_{l \rightarrow \infty} y_i^{(l)} = h_i^{m+1}$, the AP-property $A^{m+1} = A^m$ and the energy-decaying property $L_\sigma^{m+1} \leq L_\sigma^m$. See [2, 6].

6 The closed curve version of the Kuramoto-Sivashinsky equation in Example 2.8

To approximate (2.6), κ_{ss} is discretized as follows.

Step 1 (addition) $(\kappa_{ss})_i = ((\kappa_{\hat{s}})_{i+1} - (\kappa_{\hat{s}})_{i-1})/(2r_i)$, where

$$(\mathbf{F}_{\hat{s}})_i = \frac{1}{r_i} \left(\frac{\mathbf{F}_{i+1} + \mathbf{F}_i}{2\cos^2_i} - \frac{\mathbf{F}_i + \mathbf{F}_{i-1}}{2\cos^2_{i-1}} \right) \text{ on } \Gamma_i. \quad (6.1)$$

Then the averaged normal velocity on Γ_i can be defined as $v_i = v^{(0)} + (\alpha_{\text{eff}} - 1)\kappa_i + \delta(\kappa_{ss})_i$, $v^{(0)} = V^{(0)}$.

To compute $(\kappa_{ss})_i$, we calculate the gradient flow of $E = \sum_{i=1}^N \kappa_i^2 r_i / 2$, which is a discrete analogue for obtaining the Willmore flow equation from (2.3). Under a direct calculation, we have

$$\dot{E} = - \sum_{i=1}^N \left((\kappa_{ss})_i + \frac{1}{2} \langle \kappa^3 \rangle_i \right) v_i r_i + \text{err}_E, \quad (6.2)$$

where $\langle \kappa^3 \rangle_i = (\kappa_i^+ \kappa_{i+1}^2 + 2\kappa_i^3 + \kappa_i^- \kappa_{i-1}^2)/4$ is an average of κ_i cubed on Γ_i ($\kappa_i^+ = 2\tan_i/r_i$, $\kappa_i^- = 2\tan_{i-1}/r_i$, n.b. $\kappa_i = (\kappa_i^+ + \kappa_i^-)/2$), and err_E is the remaining term.

The term $(\kappa_{ss})_i$ is extracted from (6.2). Note that the difference operator (6.1) is meaningful, since $(\mathbf{t}_{\hat{s}})_i = -\kappa_i \mathbf{n}_i$ holds, which is a discrete version of the Frenét formula $\mathbf{T}_s = -\kappa \mathbf{N}$. Of course, this argument is not the only way to obtain κ_{ss} , for example, $\mathbf{x}_{sss}$ based method is also valid [10].

To solve ODEs (3.2), we use the classical fourth order Runge-Kutta method. A precise argument and several numerical experiments can be found in [3].

7 Conclusion

We showed a simple and fast numerical method for a general moving boundary problems, and especially for the classical Hele-Shaw problem, the area-preserving crystalline curvature flow equation, and the closed curve version of Kuramoto-Sivashinsky equation.

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