#### 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<sup>1)</sup> 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  $\boldsymbol{x}(u,t)$  for  $u \in [0,1]$ and moves by

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

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

In this paper we follow the so-called direct approach in which the evolution of the position vector  $\boldsymbol{x} = \boldsymbol{x}(u,t)$  is governed by equation (1.1), especially in the case where the normal  $\boldsymbol{N}$  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  $\boldsymbol{T}$  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 C(t) is parameterized by  $\boldsymbol{x} : [0,1] \times [0,T) \to \mathbb{R}^2$  s.t.  $C(t) = \{\boldsymbol{x}(u,t); u \in [0,1]\}$  and  $|\boldsymbol{x}'| > 0$ . Here  $\boldsymbol{x}' = \partial \boldsymbol{x}/\partial u$  and  $g(u,t) = |\boldsymbol{x}'|$  is the local length. We denote  $|\boldsymbol{a}| = \sqrt{\boldsymbol{a} \cdot \boldsymbol{a}}$  where  $\boldsymbol{a} \cdot \boldsymbol{b}$  is the inner product between  $\boldsymbol{a}$  and  $\boldsymbol{b} \in \mathbb{R}^2$ . The unit tangent vector is  $\boldsymbol{T} = \boldsymbol{x}'/g = \boldsymbol{x}_s$  where s is the arc-length parameter  $ds = g \, du$  and  $\mathsf{F}_s = \mathsf{F}'/g$ , i.e.,  $\partial/\partial s = g^{-1}\partial/\partial u$  is the formal definition, since the arclength s depends on u and t. The unit outward normal vector is  $\boldsymbol{N} = -\boldsymbol{T}^{\perp}$  where  $(a, b)^{\perp} = (-b, a)$ . The tangential angle  $\theta$  is defined s.t.  $\boldsymbol{T} = (\cos \theta, \sin \theta)^{\mathrm{T}}$ . The curvature  $\kappa$  is obtained from  $\boldsymbol{T} = \boldsymbol{x}_s$  and the Frenét formula  $\boldsymbol{T}_s = -\kappa \boldsymbol{N}$ , from which it follows that  $\kappa = \theta_s$  or  $\kappa = \det(\boldsymbol{x}_s, \boldsymbol{x}_{ss})$  where  $\mathsf{F}_{ss} = (\mathsf{F}'/g)'/g$  (sign convention is the way that  $\kappa = 1$ if C is a unit circle). See Figure 2.1.

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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  $C^0$ , find a family of curves  $\{C(t)\}_{0 \le t < T}$ , starting from  $C(0) = C^0$  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  $\mathcal{A}(t) = \frac{1}{2} \int_{\mathcal{C}(t)} \boldsymbol{x} \cdot \boldsymbol{N} \, ds$ , since

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

**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

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

Then we have the curve-shortening property (**CS-property** in short)  $\hat{\mathcal{L}}(t) \leq 0$ , 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  $\langle \mathsf{F} \rangle = \mathcal{L}(t)^{-1} \int_{\mathcal{C}(t)} \mathsf{F} ds$  is the average of  $\mathsf{F}$  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

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

$$\begin{cases} \Delta p = 0 & \text{in } \mathcal{D}(t), \\ p = \gamma \kappa & \text{on } \mathcal{C}(t), \\ V = -\nabla p \cdot \mathbf{N} & \text{on } \mathcal{C}(t), \end{cases}$$
(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,  $\kappa$  is the curvature,  $\gamma > 0$  is the surface tension coefficient, N is the unit outward normal vector, and  $V = \dot{\boldsymbol{x}} \cdot \boldsymbol{N}$  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 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  $u = -\nabla p$  and the incompressible condition of fluid div u = 0, and the normal velocity V is derived from mass conservation law  $\dot{x} = u$ .

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

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

We also have the AP-property

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

**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  $\theta$  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

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

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  $\sigma$  is specified by so-called the Wulff shape  $\mathcal{W}_{\sigma} = \bigcap_{\theta \in [0,\pi]} \{ \boldsymbol{x} \in \mathbb{R}^2; \ \boldsymbol{x} \cdot \boldsymbol{N}(\theta) \leq \sigma(\theta) \}$ , where  $\boldsymbol{N}(\theta) = (\sin \theta, -\cos \theta)^{\mathrm{T}}$ . If  $\sigma$  is a smooth function of  $\theta$  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,  $\sigma$  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  $\delta$  such that

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

where  $V^{(0)}$  is a constant speed, and  $\alpha_{\text{eff}}$  and  $\delta$  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  $\delta = 4$ :

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

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  $\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N$  in the anticlockwise order. Let  $\Gamma_i$  be the *i*-th edge  $\Gamma_i = [\boldsymbol{x}_{i-1}, \boldsymbol{x}_i]$   $(i = 1, 2, \dots, N; \boldsymbol{x}_0 = \boldsymbol{x}_N)$ . 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  $i = 1, 2, \dots, N$ 

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

where  $V_i$  is the normal  $N_i$ -component of the velocity at  $x_i$ , and  $W_i$  the tangential  $T_i$ component of the velocity at  $x_i$ .

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



Figure 3.1: Moving Jordan polygonal curve

Step 1 several polygonal quantities (see Figure 3.1)

 $r_i = |\boldsymbol{x}_i - \boldsymbol{x}_{i-1}|$ : the length of  $\Gamma_i$ ,

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

 $\boldsymbol{t}_i = (\boldsymbol{x}_i - \boldsymbol{x}_{i-1})/r_i$ : the unit tangent vector on  $\Gamma_i$ ,

 $oldsymbol{n}_i = -oldsymbol{t}_i^{\perp}$ : the outward unit normal vector on  $\Gamma_i$ ,

 $\phi_i = \operatorname{sgn}(\operatorname{det}(\boldsymbol{t}_i, \boldsymbol{t}_{i+1})) \operatorname{arccos}(\boldsymbol{t}_i \cdot \boldsymbol{t}_{i+1})$ : the angle between the adjacent edges  $\Gamma_i$  and  $\Gamma_{i+1}$ ,

 $T_i = (t_i + t_{i+1})/(2\cos_i)$ : 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  $\Gamma_i$ , where  $\sin_i = \sin(\phi_i/2)$ ,  $\tan_i = \sin_i/\cos_i$ ;

<u>Step 2</u> 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  $\Gamma_i$  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  $\boldsymbol{x}_i$ , where  $\Psi_i = \sum_{j=1}^i \psi_j, \ c = -\left(\sum_{j=1}^N \Psi_j/\cos_j\right) / \left(\sum_{j=1}^N \cos_j\right), \ \psi_1 = 0$  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  $\omega$  will be defined later;

- (2) Crystalline Method:  $W_i = (v_{i+1} v_i)/(2\sin_i)$  at  $x_i$ ;
- (3) Curvature Adjusted Method: an interpolation of (1) and (2);

<u>GOAL</u> (3.1) can be summarized as the following ODEs:

$$\dot{\boldsymbol{X}} = \boldsymbol{F}(\boldsymbol{X}), \tag{3.2}$$

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

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

The background of the above steps are the followings.

- **Step 1** Several polygonal quantities  $r_i$ , L,  $t_i$ ,  $n_i$  and  $\phi_i$  are defined naturally as in Step 1.
  - To define the tangent and normal vectors at  $\boldsymbol{x}_i$ , we use the angle  $\phi_i$  between the adjacent edges  $\Gamma_i$  and  $\Gamma_{i+1}$  ( $\boldsymbol{t}_i \cdot \boldsymbol{t}_{i+1} = \cos \phi_i$ ). As in Figure 3.1, the unit tangent vector  $\boldsymbol{T}_i$  at  $\boldsymbol{x}_i$  are defined by an average of the adjacent corresponding vectors in the sense as in Step 1.
  - To define the curvatures on  $\Gamma_i$  and at  $\boldsymbol{x}_i$ , 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  $\boldsymbol{x}_i$ . It is a natural definition since the normal velocity  $V_i$  at  $\boldsymbol{x}_i$  is the average of the adjacent normal averaged velocities in the sense of Step 2. Then it follows that

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

which is a discretization of (2.2), where  $\kappa_i$  in <u>Step 1</u> is the polygonal curvature on  $\Gamma_i$ . Note that  $\kappa_i$  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  $\dot{\boldsymbol{x}}_i \cdot \boldsymbol{n}_i$  (see the next step (2)).

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

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

There are two ways to vanish  $\operatorname{err}_A$ :

(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,  $r_i \to L/N$  ( $t \to T_{\text{max}} \leq \infty$ ), we assume that for  $i = 1, 2, \dots, N$ 

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

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  $\omega$  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  $v_i = \dot{x}_i \cdot n_i$ , and in this case,  $\Gamma$  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  $t \ge 0$  we solve the following Dirichlet problem:

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

We seek the approximate solution P of the form

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

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

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

$$(4.3)$$

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

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

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

Note that P satisfies  $\Delta P = 0$  in  $\Omega$  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

$$\sum_{j=1}^{N} Q_j H_j = 0, \quad H_j = -\sum_{i=1}^{N} \nabla E_j(\boldsymbol{x}_i^*) \cdot \boldsymbol{n}_i r_i, \quad j = 1, 2, \cdots, N.$$
(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  $\Gamma_i$  is defined by (4.3), if  $\operatorname{err}_A = 0$  by UDM, then we have

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

$$\begin{split} \dot{L} &= \sum_{i=1}^{N} \kappa_{i} v_{i} r_{i} = -\sum_{i=1}^{N} \kappa_{i} \nabla P(\boldsymbol{x}_{i}^{*}) \cdot \boldsymbol{n}_{i} r_{i} = -\frac{1}{\gamma} \sum_{i=1}^{N} P(\boldsymbol{x}_{i}^{*}) \nabla P(\boldsymbol{x}_{i}^{*}) \cdot \boldsymbol{n}_{i} r_{i} \\ &= -\frac{1}{\gamma} \sum_{i=1}^{N} \int_{\Gamma} P(\boldsymbol{x}_{i}^{*}) \nabla P(\boldsymbol{x}_{i}^{*}) \cdot \boldsymbol{n}_{i} \, ds \\ &\approx -\frac{1}{\gamma} \sum_{i=1}^{N} \int_{\Gamma_{i}} P(\boldsymbol{x}) \nabla P(\boldsymbol{x}) \cdot \boldsymbol{n}_{i} \, ds = -\frac{1}{\gamma} \int_{\Gamma} P(\boldsymbol{x}) \nabla P(\boldsymbol{x}) \cdot \boldsymbol{n} \, ds \\ &= -\frac{1}{\gamma} \iint_{\Omega} \operatorname{div}(P \nabla P) \, dx dy = -\frac{1}{\gamma} \iint_{\Omega} |\nabla P|^{2} \, dx dy \leq 0. \end{split}$$

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

$$[P]_i = \gamma \kappa_i, \quad i = 1, 2, \cdots, N,$$

$$v_i = -\langle \nabla P \rangle_i \cdot \boldsymbol{n}_i, \quad i = 1, 2, \cdots, N,$$

$$(4.6)$$

$$(4.7)$$

where  $\langle \mathsf{F} \rangle_i = r_i^{-1} \int_{\Gamma_i} \mathsf{F} \, ds$  is the average of  $\mathsf{F}$  on  $\Gamma_i$ , and  $[\mathsf{F}]_i = \langle \mathsf{F} \nabla \mathsf{F} \rangle_i \cdot \boldsymbol{n}_i / \langle \nabla \mathsf{F} \rangle_i \cdot \boldsymbol{n}_i$ , then we have  $\dot{L} \leq 0$  without an approximation. However, in this case we have to solve nonlinear N + 1 equations of  $\{Q_j\}_{i=0}^N$ , 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)

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

 $\theta_i$ : the tangent angle satisfying  $\mathbf{t}_i = (\cos \theta_i, \sin \theta_i)^{\mathrm{T}}$ . See Figure 3.1. All tangent angles  $\{\theta_i\}_{i=0}^{N+1}$  can be derived as in the following procedure: Firstly, from  $\mathbf{t}_1 = (t_{11}, t_{12})^{\mathrm{T}}$ , we have  $\theta_1 = -\arccos(t_{11})$  if  $t_{12} < 0$ ;  $\theta_1 = \arccos(t_{11})$  if  $t_{12} \geq 0$ . Secondly, for  $i = 1, 2, \cdots, N$ , we successively compute  $\theta_{i+1}$  from  $\theta_i$  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 <u>Step 1</u> except  $\{\theta_i\}_{i=0}^{N+1}$  satisfy the periodic boundary conditions:  $\mathsf{F}_0 = \mathsf{F}_N$ ,  $\mathsf{F}_{N+1} = \mathsf{F}_1$ .

**Construction**  $(h, \nu \Rightarrow x, t, n, r)$ . The set of vertices  $\{x_i\}_{i=1}^N$  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  $t(\theta) = (\cos \theta, \sin \theta)^T$  and  $n(\theta) = (\sin \theta, -\cos \theta)^T$ , and then we have  $t_i = t(\theta_i)$  and  $n_i = n(\theta_i)$ . Since  $h_i = x_i \cdot n(\theta_i)$  and  $h_{i+1} = x_i \cdot n(\theta_{i+1})$ , from the sets  $\{h_i\}_{i=1}^{N+1}$  and  $\{\theta_i\}_{i=1}^{N+1}$  we obtain  $x_i = (h_{i+1}t_i - h_it_{i+1}) / \sin \phi_i$  for  $i = 1, 2, \cdots, N$ . 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  $\boldsymbol{\phi} = (\phi_1, \phi_2, \dots, \phi_N)$  with the periodic boundary conditions  $\mathsf{F}_0 = \mathsf{F}_N, \mathsf{F}_{N+1} = \mathsf{F}_1$ , we denote the right hand side of  $r_i$  as  $D_i(\mathbf{h}, \boldsymbol{\phi})$ , i.e.,  $r_i = D_i(\mathbf{h}, \boldsymbol{\phi})$  holds for  $i = 1, 2, \dots, N$ .

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

(1) 
$$\mathcal{N} \subset \mathcal{N}_{\sigma}$$
; (2)  $\frac{(1-\lambda)\boldsymbol{n}_{i}+\lambda\boldsymbol{n}_{i+1}}{|(1-\lambda)\boldsymbol{n}_{i}+\lambda\boldsymbol{n}_{i+1}|} \notin \mathcal{N}_{\sigma}$   $(i=1,2,\cdots,N;\boldsymbol{n}_{N+1}=\boldsymbol{n}_{1};\lambda\in(0,1)).$ 

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

$$v_i = \dot{\boldsymbol{x}}_i \cdot \boldsymbol{n}(\theta_i) = h_i \quad (i = 1, 2, \cdots, N),$$

which will be defined later. Note that for any  $\phi_i$  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  $r_i = D_i(\mathbf{h}, \boldsymbol{\phi})$  is  $\dot{r}_i = D_i(\mathbf{h}, \boldsymbol{\phi}) = D_i(\mathbf{v}, \boldsymbol{\phi})$ , where  $\mathbf{v} = (v_1, \cdots, v_N)$ , the time differential of  $L_{\sigma}$  is

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

where  $\kappa_{\sigma i} = D_i(\boldsymbol{\sigma}(\theta), \boldsymbol{\phi})/r_i$ ,  $D_i(\boldsymbol{\sigma}(\theta), \boldsymbol{\phi}) = \chi_i l_{\sigma}(\theta_i)$ ,  $\chi_i = (\operatorname{sgn}(\phi_{i-1}) + \operatorname{sgn}(\phi_i))/2$ ,  $\boldsymbol{\sigma}(\theta) = (\sigma(\theta_1), \sigma(\theta_2), \cdots, \sigma(\theta_N))$ . The  $\kappa_{\sigma i}$  is called the *i*-th crystalline curvature, and the  $\chi_i$  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  $A = \sum_{i=1}^{N} v_i r_i$  without the error term  $\operatorname{err}_A$ , since the tangential velocity is given by (2) Crystalline Method in Step 2. As the area-preserving gradient flow of  $L_{\sigma}$ , we obtain the area-preserving crystalline curvature flow equations

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

Now we are ready to set up the problem. Let  $P_{\sigma}^{N}$  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

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

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

- (1)  $l = 0; \ y^{(l)} = h^m;$
- (2)  $y^{(l+1)} = h^m + F(y^{(l)})\tau_m/2;$
- (3) If  $||\boldsymbol{y}^{(l+1)} \boldsymbol{y}^{(l)}|| / r_{\max}^m \leq \delta_{\text{tol}}$ , then GOTO (5);

(4) 
$$l := l + 1$$
; GOTO (2);

(5) 
$$\boldsymbol{h}^{m+1} = R^{(l+1)} \widetilde{\boldsymbol{y}}^{(l+1)}, \ \widetilde{\boldsymbol{y}}^{(l+1)} = 2\boldsymbol{y}^{(l+1)} - \boldsymbol{h}^m, \ R^{(l+1)} = \sqrt{A^0 / \widetilde{A}^{(l+1)}}.$$

Here  $\delta_{\text{tol}} > 0$  is a tolerance,  $A^0$  is the enclosed area of  $\Gamma^0$ ,  $\widetilde{A}^{(j)}$  is the enclosed area of a polygon constructed from the heights  $\{\widetilde{y}_i^{(j)}\}_{i=1}^N$ ,  $\boldsymbol{y}^{(j)} = (y_1^{(j)}, \cdots, y_N^{(j)})$ ,  $\boldsymbol{F}(\boldsymbol{y}^{(j)}) = (F_1(\boldsymbol{y}^{(j)}), \cdots, F_N(\boldsymbol{y}^{(j)}))$ ,  $\widetilde{\boldsymbol{y}}^{(j)} = (\widetilde{y}_1^{(j)}, \cdots, \widetilde{y}_N^{(j)})$ ,  $||\boldsymbol{y}^{(l+1)} - \boldsymbol{y}^{(l)}|| = \max_{1 \le i \le N} |y_i^{(l+1)} - y_i^{(l)}|$ , and  $\mathsf{F}_{\max} = \max_{1 \le i \le N} \mathsf{F}_i$ .

The iteration succeeds in showing the convergence  $\lim_{l\to\infty} y_i^{(l)} = h_i^{m+1}$ , the APproperty  $A^{m+1} = A^m$  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),  $\kappa_{ss}$  is discretized as follows.

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

$$(\mathsf{F}_{\hat{s}})_{i} = \frac{1}{r_{i}} \left( \frac{\mathsf{F}_{i+1} + \mathsf{F}_{i}}{2\mathsf{cos}_{i}^{2}} - \frac{\mathsf{F}_{i} + \mathsf{F}_{i-1}}{2\mathsf{cos}_{i-1}^{2}} \right) \text{ on } \Gamma_{i}.$$
(6.1)

Then the averaged normal velocity on  $\Gamma_i$  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

$$\dot{E} = -\sum_{i=1}^{N} \left( (\kappa_{ss})_i + \frac{1}{2} \langle \kappa^3 \rangle_i \right) v_i r_i + \operatorname{err}_E,$$
(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  $\kappa_i$  cubed on  $\Gamma_i$  ( $\kappa_i^+ = 2 \tan_i / r_i$ ,  $\kappa_i^- = 2 \tan_{i-1} / r_i$ , n.b.  $\kappa_i = (\kappa_i^+ + \kappa_i^-)/2$ ), and  $\operatorname{err}_E$  is the remaining term.

The term  $(\kappa_{ss})_i$  is extracted from (6.2). Note that the difference operator (6.1) is meaningful, since  $(\mathbf{t}_s)_i = -\kappa_i \mathbf{n}_i$  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  $\kappa_{ss}$ , for example,  $\mathbf{x}_{ssss}$ 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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