

## **Numerical Methods for Propagating Fronts**

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In many physical problems, a key aspect is the motion of a propagating front separating two components. As fundamental as this may be, the development of a numerical algorithm to accurately track the moving front is difficult. In this report, we describe some previous theoretical and numerical work. We begin with two examples to motivate the problem, followed by some analytical results. These theoretical results are then used as a foundation for two different types of numerical schemes. Finally, we describe the application of one of these schemes to our work in combustion.

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## I. Motivation

### A) Crystal Growth

A relatively straightforward example is the growth of a solid immersed in a supercooled liquid, discussed extensively in Langer [9]. To illustrate, we imagine a solid ice crystal placed in a bath of water that has been supercooled below its freezing point. We limit the discussion to two dimensions and neglect a variety of effects such as convective heat transport, solid impurities and crystalline anisotropy. Let  $\gamma(t)$  be the closed curve representing the boundary between ice and water at time  $t$ , with ice inside the curve. The diffusion equation for the temperature  $T$  holds both inside and outside  $\gamma(t)$ , namely,  $\partial T_{s(l)}/\partial t = c_{s(l)} \nabla^2 T_{s(l)}$ , where  $\nabla^2$  is the two-dimensional Laplacian,  $c_{s(l)}$  is the thermal diffusion coefficient and  $T_{s(l)}$  is the temperature in the solid(s)/liquid(l) region. Conservation of heat flux across the boundary interface must include the heat required to go from solid to liquid, thus  $c_s \partial T_s / \partial n - c_l \partial T_l / \partial n = L V_\gamma$ , where  $\partial / \partial n$  is differentiation in the normal direction,  $L$  is the latent heat of formation and  $V_\gamma$  is the velocity of the boundary  $\gamma(t)$  along its normal vector field. Finally, the thermodynamic boundary condition, which includes the effects of surface tension, is given by the Gibbs-Thomson relation, see Turnbull [23]; at each point  $x^-$  of the boundary  $\gamma(t)$ , we require that

$$T(x^-) = T_M (1 - \epsilon K(x^-))$$

where  $T_M$  is the melting temperature,  $\epsilon$  is a constant and  $K(x^-)$  is the curvature of the boundary  $\gamma(t)$  at  $x^-$ . Thus, if points of negative curvature are concave towards the solid region, they yield a higher temperature than those with positive curvature and this variation in the solidification rate along the boundary as a function of curvature provides intricate growth patterns. For further information, see [9], [10], [13], [14], [16], [20].

## B) Flame Propagation

Much work surrounding the stability/instability of a flame is aimed at understanding the "turbulization" or wrinkling of a flame front and its interaction with the hydrodynamic flow field. The pioneering work in this field is the analysis of a plane flame front by Landau [8]. The flame front is idealized as a surface of discontinuity, i.e., a closed curve  $\gamma(t)$ , separating regions of constant steady-state velocity, density and temperature. In Landau's model, the flame speed  $V_\gamma$  of the curve along its normal vector field is constant. By ignoring all but hydrodynamic effects, flames are shown to be unstable to perturbations in velocity and pressure around a mean state. Since this conclusion is physically unreasonable, Markstein [11] postulated that the flame speed depended on the curvature so that

$$V_\gamma = V^o(1 - \varepsilon K(\gamma))$$

where  $V^o$  is the constant speed of a flat flame,  $\varepsilon$  is a constant and  $K(\gamma)$  is the curvature. The motivation behind such an assumption, loosely speaking, is that parts of the flame front which bend in towards the hot burnt region are subject to greater heat and hence burn faster; slower flame speeds are thus implied for fingers reaching out into cool gas. Using linear stability analysis of this model, Markstein demonstrated the stabilizing effect of curvature. Since then, there have been numerous investigations of flame stability for a variety of combustion models; a comprehensive though now outdated account may be found in Markstein [12], here, we also mention the work of Sivashinsky [22], Frankel and Sivashinsky [4] and Zeldovich [24].

## II. Theoretical Results

Starting with a simple, smooth, closed initial curve  $\gamma(0)$  in  $R^2$ , let  $\gamma(t)$  be the one parameter family of curves, where  $t \in [0, \infty)$  is time, generated by moving the initial curve along its normal vector field with speed  $F$  a given function of the curvature. Let  $\vec{x}(s, t)$  be the position vector which parameterizes  $\gamma(t)$  by  $s$ ,  $0 \leq s \leq S$ ,  $\vec{x}(0, t) = \vec{x}(S, t)$ . The curve is parameterized so that the interior is on the left in the direction of increasing  $s$ . With  $K(s, t)$  as the curvature at  $\vec{x}(s, t)$ , the equations of motion are

$$\vec{n}(s, t) \cdot \frac{\partial \vec{x}(s, t)}{\partial t} = F(K(s, t)) \quad (1)$$

$$\vec{x}(s, 0) = \gamma(0) \quad \text{prescribed}; \quad s \in [0, S] \quad t \in [0, \infty),$$

where  $\vec{n}(s, t)$  is the unit normal vector at  $\vec{x}(s, t)$ . If  $\alpha(s)$  corresponds to arclength, then  $d\alpha = g(s, t)ds$  where  $g(s, t) = (x_s^2 + y_s^2)^{1/2}$ . From the above, one can produce an evolution equation for the metric  $g$ , namely

$$g_t(s, t) = g(s, t) K(s, t) F(K(s, t)), \quad (2)$$

and an evolution equation for the curvature  $K$ , namely

$$K_t(s, t) = - \left[ F_s(K(s, t)) g^{-1}(s, t) \right]_s g^{-1}(s, t) - K^2(s, t) F(K(s, t)). \quad (3)$$

We point out two facts: 1) The case  $F(K)=K$  occurs in the modeling of grain boundaries in metals, and has been studied extensively in Brakke [1] and 2) For  $F(K)=K$ , a recent result by Huisken show that convex surfaces remain smooth as they collapse; the smoothness of non-convex surfaces remains an open question.

Let  $Var(t)$  be the total variation of the front at time  $t$ , defined as

$$Var(t) = \int_0^S |K(s, t)| g(s, t) ds. \quad (4)$$

Then we have the following (see [19]);

**Proposition** Consider a front moving with speed  $F(K)$ , as in Equation (1). Assume that  $\gamma(0)$  is non-convex, so that  $K(s,0)$  changes sign, and assume  $K$  is zero at a finite number of points. Assume that  $F$  is twice differentiable, and that  $K(s,t)$  is twice differentiable for  $0 \leq s \leq S$  and  $0 \leq t \leq T$ . Then

1) if  $F_K(0) \leq 0$  ( $F_K(0) \geq 0$ ), then

$$\frac{dVar(t)}{dt} \leq 0 \quad \left( \frac{dVar(t)}{dt} \geq 0 \right)$$

2) if  $F_K(0) < 0$  ( $F_K(0) > 0$ ) and  $K_s(0) \neq 0$ , then

$$\frac{dVar(t)}{dt} < 0 \quad \left( \frac{dVar(t)}{dt} > 0 \right)$$

for  $0 \leq t \leq T$ .

Remarks: This proposition states that if  $F_K < 0$  wherever  $K=0$ , then the front "flattens out". If  $\gamma(t)$  is convex, the proposition is trivial, since  $Var(t) = \int_0^S K g ds = 2\pi$ . If  $F_K < 0$ , the "energy" of the front dissipates. We also have the following, which applies to a front moving at constant speed:

**Corollary** If  $F_K = 0$ , then the total variation is constant.

We focus on the case  $F(K) = 1 - \varepsilon K$ , where  $\varepsilon$  is a constant. For  $\varepsilon > 0$ ,  $\frac{dVar(t)}{dt} < 0$  and the energy dissipates; for  $\varepsilon = 0$ ,  $\frac{dVar(t)}{dt} = 0$  and the energy is constant. We may rewrite the curvature evolution equation as

$$K_t = \varepsilon K_{\alpha\alpha} + \varepsilon K^3 - K^2 \tag{5}$$

where here we have changed variables and taken the derivative of curvature with respect to

arclength to eliminate the metric  $g$ . This is a reaction-diffusion equation, in which the reaction term ( $\epsilon K^3 - K^2$ ) is mitigated by the diffusion term ( $\epsilon K_{\alpha\alpha}$ ). With  $\epsilon > 0$ , it can be shown that the solution stays smooth for all time. With  $\epsilon = 0$ , we have  $K_t = -K^2$  which is singular at finite  $t$  if the initial curvature is anywhere negative.

This situation is reminiscent of the development of shocks in hyperbolic conservation laws. Consider Burgers equation with viscosity, namely

$$u_t + uu_x = \epsilon u_{xx}. \quad (6)$$

It is well-known, see [5,6], that for  $\epsilon > 0$ , the "viscosity" term produces smooth solution and the energy dissipates smoothly. For  $\epsilon = 0$ , shock discontinuities can develop in the solution, even for smooth initial data, and an "entropy" condition is used to provide a weak solution beyond breakdown. Loosely put, this entropy condition requires that characteristics "enter" shock discontinuities, and the weak solution obtained is the limiting solution of Equation (6) as  $\epsilon \rightarrow 0$ .

In fact, it is easy to see that our equations for a propagating curve can be recast as a single conservation law with viscosity. Suppose we write the propagating curve as a function, that is, let  $y = \phi(x, t)$  be the height  $y$  of the moving curve at a point  $x$  at time  $t$ , drawn in the  $x$ - $y$  plane. Then the equation of motion for a front moving with speed  $F(K) = 1 - \epsilon K$  can be written as

$$\phi_t = (1 + \epsilon \frac{\phi_{xx}}{(1 + \phi_x^2)^{3/2}})(1 + \phi_x^2)^{1/2} \quad (7)$$

Let  $u = \phi_x$ . Then

$$u_t - [G(u)]_x = \epsilon [u_x / ((G(u))^2)]_x \quad (8)$$

where  $G[u] = (1 + u^2)^{1/2}$ . Thus, the equation for the propagating tangent  $\phi_x$  satisfies a Burgers-

type equation with viscosity.

What role does the entropy condition from the shock case play in the propagating curve? Imagine the front as a flame separating a burnt interior from an unburnt exterior; each point is transformed from unburnt to burnt when touched by the propagating front. The entropy condition, loosely speaking, may be stated as follows: Once a particle is burned, it stays burnt. The position of the front at a time  $t$  may be obtained by using Huygens principle: the front is formed by the envelope of all disks of radius  $t$  centered along the initial curve. This solution will be called the "Huygens principle construction".

A different way to look at what is happening is to construct the normals to initial curve, which we shall call ignition curves. Consider the following construction: Starting with the initial curve, allow the front to burn along the ignition curves until there is a collision. Eliminate the curves (characteristics) that collide, and continue moving the front along the remaining curves. As time progresses, the front will consist of a shrinking subset of the original curve, and any point on the solution can be traced back to the initial curve. Conversely, there will be points along the initial curve that do not affect the solution beyond some time, and thus the solution becomes irreversible. Thus, characteristics always trace back to the initial line. Furthermore,  $\frac{dVar}{dt} \leq 0$ , since  $Var(t)$  is the integral of a positive quantity over a set whose length is a non-increasing function of time (here, one evaluates  $Var(t)$  over open intervals where the curvature is defined together with jumps in the tangent at the corners).

These two constructions yield the the same solution. The removal of ignition curves in the propagating flame case corresponds to the elimination of colliding characteristics in the shock case. Furthermore, this weak solution can be shown to be the limiting case of the smooth solution with viscosity as  $\varepsilon \rightarrow 0$ .

The above suggests at least two numerical schemes for following fronts. Most algorithms place marker particles along the front and advance the position of the particles in accordance with a set of finite difference approximations to the equations of motion. Such schemes usually go unstable and blow up as the curvature builds around a cusp, since small errors in the position produce large errors in the determination of the curvature. One alternative is to consider the reformulation equations of motion as a conservation law with viscosity and solve these equations with the techniques developed for gas dynamics. These techniques, based on high-order upwind formulations, are particularly attractive, since they are highly stable, accurate and preserve monotonicity. We have made some preliminary tests of such schemes applied to our problem of propagating fronts in crystals and flames, with extremely encouraging results, and will report on this work elsewhere [17].

Another alternative is to rely on the Huygens principle idea and follow the motion of the *interior* of the "burnt" region, rather than the boundary. These techniques are of the "volume of fluid" type, and it is those we shall discuss and demonstrate below.

### **III. Numerical Methods Based on Volume of Fluid Techniques**

Here, we briefly describe an application of a volume of fluid method (SLIC) for the case  $\varepsilon=0$ . For details, see [3], [15], [17].

We lay down a square grid  $i,j$  of uniform mesh size on the computational domain, and assign a number  $f_{ij}$ ,  $0 \leq f_{ij} \leq 1$  corresponding to the fraction of burnt fluid within cell  $i,j$ . Each cell's material is moved in the direction  $\vec{u}=(u,v)$  by executing a fractional step in each direction. An interface is drawn in the cell representing the boundary of the material, where the orientation of the interface depends on the value of  $f_{ij}$  and the  $f_{ij}$ 's in the cell's neighbors. This interface is then transported in the  $x$  direction a distance  $u \Delta t$  and the

process is then repeated for the sweep in the  $y$  direction, providing new  $f_{ij}$ .

This algorithm can be used to advance a front along its normal vector field using Huygens principle. For the moment, assume that  $F(K)=1$  and consider  $L$  angles,  $\Theta_l=(2\pi(l-1)/L)$ ,  $l=1,\dots,L$ . Given any cell with volume fraction  $f_{ij}^n$ , the material in that cell is moved a distance  $\Delta t$  in each of the  $l$  directions  $(\cos\Theta_l, \sin\Theta_l)$ . As  $L \rightarrow \infty$  and the mesh size goes to zero, this corresponds to drawing a disk of unit radius around the center of the cell. The Huygens principle construction says that the envelope formed by all such disks (that is, for all  $i, j$ ) gives the front advanced a unit distance along its normal field. Thus, let  $f_{ij}^n \Theta_l$  be the array of volume fractions obtained by moving the fractions in the direction  $\Theta_l$  and let  $f_{ij}^n \Theta_0 = f_{ij}^n$ . The new volume fractions approximating the front advanced one time step will be given by

$$f_{ij}^{n+1} = \max_{0 \leq l \leq L} f_{ij}^n \Theta_l.$$

Since  $f_{ij}$  is often either zero or one, careful programming will limit the computing effort to the boundary. The generalization to three dimensions is straightforward.

This numerical method filters out high wavelengths and smooths the solution by limiting the oscillations of the front to the order of one cell width. The method can be extended to a front moving with speed  $F(K)$  by determining the curvature from the volume fractions. A method based on osculating circles has been developed [2]; there, the cell size determines the smallest possible osculating circle and hence bounds the curvature and smooths the solution. In spite of this smoothing, such a curvature algorithm can provide a valuable tool for analyzing a moving front, since the entropy condition naturally generates weak solutions and the mesh size can be systematically refined to allow larger curvatures in a controlled way. Thus, if a mesh size  $h$  is used with maximum allowable curvature  $K_h$ , the algorithm produces a weak solution with this bound; by refining the mesh size, one can

investigate both possible blow up in the curvature and the nature of the solution beyond the singularity.

#### IV. Examples

To begin, we use the above algorithm to follow a kidney bean shape expanding with constant velocity  $F(K)=5$ . In Figure 1A (see [18]), we show the exact solution, found by solving the equations of motion, for a burnt region initially bounded by four joined semi-circles. The position of the front is shown for various values of  $t$ . The concave region sharpens into a corner at  $t=1$ , which then opens up and smooths out. In Figure 1B, we show the results of the application of the Huygens principle algorithm to this problem, with 8 angles and a  $60 \times 60$  mesh of cells. The numerical method follows the development of the corner, and the ensuing weak solution.

Next, we use this algorithm to analyze the competing effects of viscosity and exothermicity on flame propagation (see [20,21]). The setup of the problem is as follows. A fluid swirling in a closed box is ignited halfway up the left wall. The motion of the flame consists of two effects: it burns in a direction normal to itself at a constant speed, and it is advected by the underlying velocity field. Four different experiments were performed. First (A), we study inviscid, constant density flow. In this experiment, the flow is potential (no-slip condition is ignored), and the flame is cold (no expansion upon combustion), thus the flame simply burns and is passively advected by the swirling flow. In the second experiment (B), inviscid flow with exothermicity, the flow is potential but the fluid expands as it burns, thus the pressure in the vessel is increased, changing the hydrodynamic field. In the third experiment (C), we have viscous flow with a cold flame. Here, the no-slip condition on the walls is satisfied, creating counterrotating corner eddies which contort and stretch the flame. Finally, in the last experiment, we have viscous flow with exothermicity.

In the two viscous runs, the flow was started two seconds before ignition so that recirculation zones would have time to develop. The results are shown in Figure 2A-2D. In the inviscid, constant density case, the flame is smoothly advected by the large vortex in the center. In the inviscid, exothermic case, the velocity field produced by volume expansion and the rise in pressure and flame speed cause the flame to spiral in towards the center at a faster rate. In the viscous, constant density case, the flame front is twisted by the eddies that develop in the corners; the flame is carried over the eddies and dragged backwards into the corners. The effect of these eddies is to extend the length of the flame front, bringing it into contact with unburnt fuel and increasing the rate at which the vessel becomes fully burnt. Finally, when both viscous and exothermic effects are combined, the flame is both wrinkled due to the turbulence of the flow (hence increasing the surface area of the flame) and carried by the exothermic field; in addition both the flame speed and pressure increase. The effect of these factors is to greatly decrease the amount of time required for complete conversion of reactants to products.

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