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Level-Set Methods

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A Simple Level-Set Method for Solving Stefan Problem

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1 Abstract

In this report, a simple level-set method for solving Stefan Problems proposed by S. Chen, B. Merriman, S. Osher and P. Smereka will be presented.

2 Introduction

Stefan Problems are problems that involve solving change of phase (gas, liquid and solid) of a pure material. One of the most common examples is melting ice in water. Stefan problem is probably the most simple change of phase model thus far. There are many one-dimension models and one-dimension Stefan Problems are studied in depth. In introduction, classical Stefan Problem formulation will be introduced and talk about a modified that solve change of phase the other way around.

2.1 Physics

Change of phase involves losing and gaining heat/energy in a matter. Therefore temperature plays a big role in classical Stefan Problem formulation. Suppose a simple ice melting in water problem. Knowing that ice starts to melt when it absorbs enough energy and reaches temperature zero degree Celsius; the ice-water interface will remain constant which is zero degree. And since the ice is melting in water, one can imagine that the interface is moving toward the ice with some velocity. In the next subsection, we will formulate the generic (matter of any kind, not just water) classical Stefan Problem.

2.2 Classical Stefan Problem Formulation

Suppose a material has melting temperature T_m, and the material melts gradually creating both its liquid and solid phases with solid-liquid interface Γ. Let $T(t)$ be the temperature function depending on time t and $s(t)$ be the position of interface at time t then we can separate the two phases of the material as:

$$s(t) = \begin{cases} s(t)+, & \text{interface position of solid} \\ s(t)-, & \text{interface position of liquid} \end{cases}$$

Therefore, at the interface, the temperature function can be written as

$$T(s(t)+, t) = T(s(t)-, t) = T_m \tag{1}$$

Next, let $D(t)$ be the finite region that the interface can reach the farthest and let L be the latent heat. Heat must be used as diffusion when it contributes to the change of temperature. Then let k_i be the diffusion coefficient of the material. So the heat flux is

$$Heat\ Flux = -k_i D(t) T(t) \tag{2}$$

To find the total heat flux using equation (2), one needs to take double derivatives for both liquid and solid phases. One can set up equation as below

$$\iint \left[-k_1 D(t) T(s(t)-, t) - k_2 D(t) T(s(t)+, t)\right]\ dx\ dy$$
$$= A(D) \int \left[-k_1 T(t) + k_2 T(t)\right]\ dt$$

Evaluating the integral above, we get our Stefan condition,

$$-k_1 T(s(t)-, t) + k_2 T(s(t)+, t) = LV \tag{3}$$

where k_1 and k_2 are the heat diffusion coefficients for solid and liquid phase and V is the derivative of interface position $s(t)$ which is the velocity of interface evolution. We now have constructed the lower dimension classical Stefan Problem.

2.3 Discussion

While lower dimension Stefan Problem has been studied widely and there are a lot of good models for it, these models are not very accurate when it comes to higher dimension. The model proposed by Chen, Merriman, Osher and Smereka is very effective on higher dimension Stefan Problems. In addition, while classical Stefan Problem usually deals with melting of a material (from solid to liquid), the modified Stefan Problem can work out solidification of a material (from liquid to solid) when a supercooled object is dropped into a liquid. This modified Stefan Problem was successful in modeling many physical features such as dendrite solidification and water-to-ice formation.

3 A Simple Level-Set Method for Solving Stefan Problems

In this section, we will construct a Stefan problem using level-set methods.

3.1 Formulation

Suppose a supercooled object is dropped into a liquid. This time, consider D as a square domain (or box) of a material. Let Ω and Ω^c denote solid and liquid region respectively. Instead of melting, the material undergoes solidification; therefore, the interface evolves outward rather than inward as described in classical Stefan problem formulation. Let

vector $\mathbf{n}$ be the normal vector pointing outward on solid-liquid interface and $\mathbf{x}$ be any point in D. Remember heat contributes to the change of temperature through diffusion form so we can derive temperature equation based on equation (2) in the classical case:

$$\frac{\partial T}{\partial t} = \begin{cases} c_1 \dfrac{\partial T_{solid}}{\partial t} = \nabla \cdot (k_1 \nabla T), & \mathbf{x} \in \Omega \\ \\ c_2 \dfrac{\partial T_{liquid}}{\partial t} = \nabla \cdot (k_2 \nabla T), & \mathbf{x} \in \Omega^c \end{cases} \tag{4}$$

k_1 and k_2 as before are diffusion coefficients and c_1 and c_2 are heat capacities of solid and liquid. By taking divergence of gradient T, we can study temperature rate of change at the interface Γ. Using equation (4) and based on Stefan condition (3), we can write the new Stefan condition as:

$$LV = -\left[k_2 \frac{\partial T_{liq}}{\partial n} - k_1 \frac{\partial T_{sol}}{\partial n}\right] \tag{5}$$

Likewise, L is the latent heat, V is the velocity of the interface and $\frac{\partial T}{\partial n}$ is the normal derivative of T.

In order to accurately model solidification of the material, one has to consider surface tension, anisotropy and molecular kinetic coefficients in temperature equation at the interface. Such relation to temperature is given by classical Gibbs Thomson relation at the interface:

$$T(\mathbf{x}, t) = -\epsilon_c \kappa - \epsilon_v V \tag{6}$$

where ϵ_c is surface tension, ϵ_V is molecular kinetic coefficient and κ is the curvature of the interface. For simplicity, we only consider isotropic case that ϵ_c and ϵ_V equal to 1. Also, without loss of generality, we can set the latent heat to be one. Therefore, at the interface Γ, the

temperature rate of change is divergence of the gradient of T which is the Laplacian of T:

$$\frac{\partial T}{\partial t} = \nabla \cdot \nabla T = \Delta T \tag{7}$$

Therefore, we can update equation (4):

$$\frac{\partial T}{\partial n} = \begin{cases} c_1 \dfrac{\partial T_{solid}}{\partial t} = \nabla \cdot (k_1 \nabla T), & \mathbf{x} \in \Omega \\ \Delta T, & \mathbf{x} \in \Gamma \\ c_2 \dfrac{\partial T_{liquid}}{\partial t} = \nabla \cdot (k_2 \nabla T), & \mathbf{x} \in \Omega^c \end{cases} \tag{8}$$

Modify the Stefan condition (5) we get:

$$V = -\left[\frac{\partial T}{\partial n}\right], \qquad \mathbf{x} \in \Gamma \tag{9}$$

We are done setting up the new Stefan problem. In the next subsection, we will start implementing level-methods onto the new Stefan problem.

3.2 Level-Set Methods Implementation

First we need to construct zero level-set function for this problem. What we want is:

$$\phi(\mathbf{x}, 0) = \begin{cases} +d, & \text{outside the solid} \\ 0, & \text{at the interface} \\ -d, & \text{within the solid} \end{cases} \tag{10}$$

ϕ is signed distance function. Zero level-set function is defined as

$$\Gamma(t) = \{\mathbf{x} \in D : \phi(\mathbf{x}, t) = 0\} \tag{11}$$

The idea of using level-set methods is to move the signed distance function ϕ with updated interface velocity at each grid point and update the temperature at each new position. The best part about using the signed distance function is that we can store all the information in ϕ. Since V is just a normal speed function at the interface and we know that at each grid point the interface evolves differently, we need to determine a vector F that is the extension of normal V. We can write advection equation ϕ_t, normal vector $\mathbf{n}$ and curvature κ in terms of signed distance function ϕ.

$$\phi_t = F|\nabla\phi| \tag{12}$$

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|} \tag{13}$$

$$\kappa = \nabla \cdot \mathbf{n} \tag{14}$$

Using equation (13), we can rewrite equation (9) as

$$V = -[\nabla T] \cdot \mathbf{n} \tag{15}$$

To find velocity extension F, we can also use advection equations formulation using temperature normal derivatives. In Chen, Merriman, Osher and Smereka's paper, extra two coordinates are used to approximate F.

3.3 Reinitialization of Signed Distance Function ϕ

Equations (12), (13) and (14) are dependent of signed distance function ϕ at the interface. Works done by M. Schmidt show that the

advection equation (12) will not be the exact signed distance function after one time step. This will increase the difficulties of computing. The reinitialization of *phi* proposed by M. Schmidt is

$$\phi_t = S(\phi_0)(1 - |\nabla\phi|) \tag{16}$$

where $\phi_0 = \phi(\mathbf{x}, 0)$ is the zero level-set function. We can smooth the sign function S by the equation

$$S_\epsilon(\phi_0) = \frac{\phi_0}{\sqrt{\phi_0^2 + \epsilon^2}} \tag{17}$$

4 Numerical Approaches - Discretization

To solve the partial differential equations and Methods in section three numerically, we need to employee some numerical schemes. For rest of the discretizations we define

$$\begin{aligned}
&\mathbf{x}_{i,j} = ((i-1)h, (j-1)h) \\
&\phi_{i,j} = \phi(\mathbf{x}_{i,j}) \\
&T_{i,j} = T(\mathbf{x}_{i,j}) \\
&i, j = 1, 2, ...
\end{aligned}$$

4.1 Discretization of advection equation (12)

To solve differential equations (12), (13) and (14), for increased accuracy, we use second order ENO method. To avoid the instabilities causing from temporal discretization of these equations, we will use simple TVD-RK type time discretization. To discretize the advection equation (12) we need to compute the extended normal velocity F. F

can be approximated using

$$F_{i,j} = \frac{1}{2}\left[u^1_{i,j}(\frac{\phi_x}{|\nabla\phi|})_{i,j} + u^2_{i,j}(\frac{\phi_y}{|\nabla\phi|})_{i,j} + u^3_{i,j}(\frac{\phi_\eta}{|\nabla\phi|})_{i,j} + u^4_{i,j}(\frac{\phi_z eta}{|\nabla\phi|})_{i,j}\right] \tag{18}$$

The spatial first derivatives of ϕ in the above relation are still approximated by second order ENO. Apply equation (18) we end up solving the right hand side of (18). And *phi* is updaed using RK scheme. The discretization to $|\nabla phi|$ use done by central difference approximation

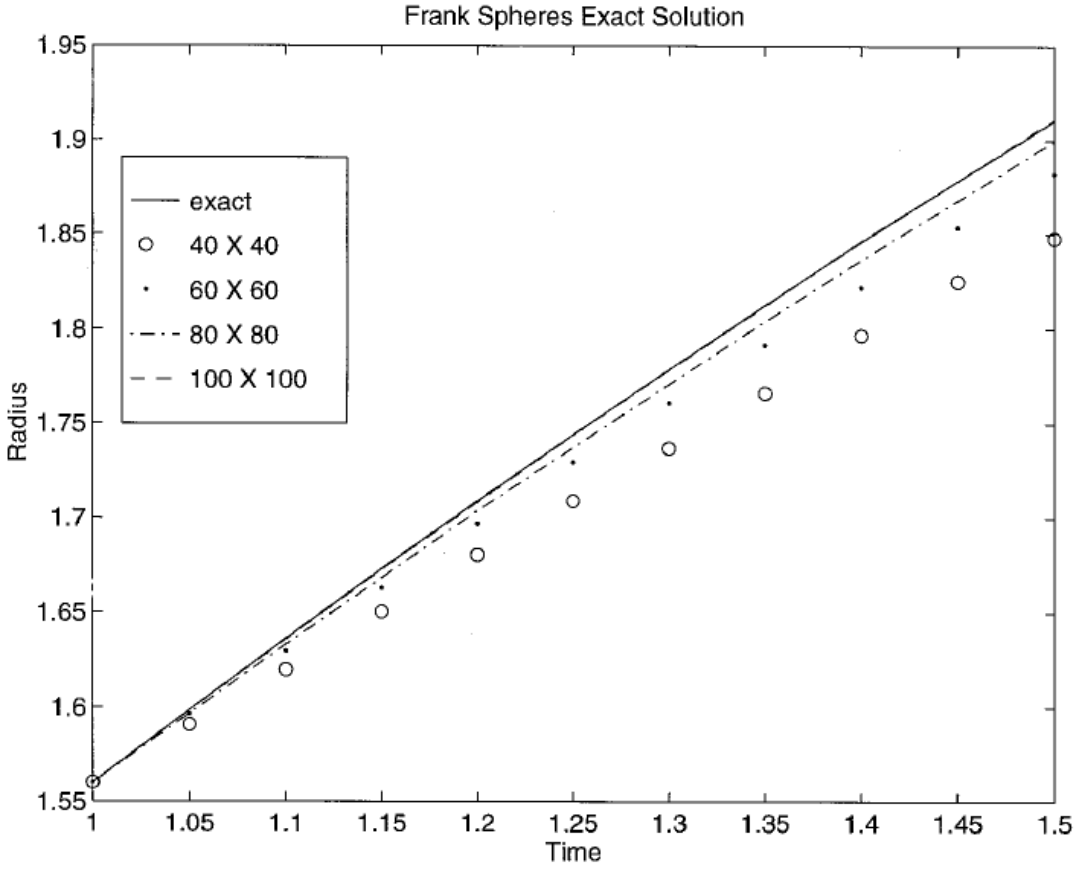
$$|\nabla\phi|_{i,j} = \begin{cases} \sqrt{(\phi_x)^{i.j} + (\phi_y)^2_{i,j}} \\ \sqrt{(\phi_\eta)^{i.j} + (\phi_\zeta)^2_{i,j}} \end{cases} \tag{19}$$

5 Numerical Result

For demonstration we will use a two dimension Stefan problem called *Growing Frank Spheres*. The solid region is a cylinder of radius $R = St^{1/2}$ and the temperature field is $T(r,t)$ is given by

$$T(r,t) = T(s) = \begin{cases} T_\infty\left(1 - \frac{F(s)}{F(S)}\right), & s > S \\ 0, & s < S \end{cases} \tag{20}$$

where $r = \sqrt{x^2 + y^2}$, $s = r/t^{1/2}$ and T_∞ is a constant. The plotted result of exact and approximated solution is shown below. The more grid points we use the more accurate it gets.



6 Conclusion and Future Studies

The process of solving Stefan problems using level-set methods is: 1. construct signed distance function ϕ 2. derive necessary terms for constructing ϕ_t such as curvature (bases on T) 3. update and discretize 4. repeat. This new method of solving Stefan problems can solve more complicated problems that the classical Stefan problem methods cannot such as unstable solid dendrite solidification because level set methods evolve the sharp interface between two phases. In the future, hopefully more real-world applications can be quantified

using this level-set approach.

Bibliography

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Appendex

In all the computations for discretiazation, we take the domain D to be a square box that we set Δx and Δy are uniform mesh grid with side length h. For accuracy, the approximation to $[\Delta t]$ is added with more coordinates as 45 degree rotated x- and y- axis called name η and ζ. Each approximation to the Stefan condition in a derivative of T can be extended away from the front by advection equations:

$$u_i^i + S(\phi\phi_x)u_x^i = 0 \tag{21}$$

where $i = x, y, \eta, \zeta$, $u = \frac{\partial T}{\partial x_i}$ and S is a smooth function. For better accuracy the extra added coordinates look like