

Using level sets to solve the Stefan problem

Nat Wilson

May 11, 2014

1 Introduction

Level set methods provide a means for solving evolving interface problems. They have applications in materials science, fluid dynamics, and computational graphics. The classical Stefan heat flow problem is

$$u = -\lambda_f^{-1} \left(\kappa_1 \frac{\partial T_1}{\partial \mathbf{n}} - \kappa_2 \frac{\partial T_2}{\partial \mathbf{n}} \right) \quad (1)$$

$$\frac{\partial T_i}{\partial t} = \nabla \cdot \left(\frac{\kappa_i}{c_i} \right) \nabla T_i \quad (2)$$

where u is the movement velocity in the normal direction of the interface between two material phases. The temperature gradient governs heat flow, and so the temperature field is solved from (2) given latent heat of fusion λ_f , heat capacity c_i , and thermal diffusivity κ_i (cf. *Chen et al.*, 1997). The problem considered below is the calculation of a solid-liquid phase boundary, such as between ice and water. In such a problem, the interface between the solid and liquid phases is represented by the zero level set of a function $\psi(x_i)$.

Alternative approaches for similar problems include front-tracking, volume of fluid methods, and phase field methods (*Chen et al.*, 1997; *Sethian and Smereka*, 2003). All of these methods have advantages and disadvantages.

Front-tracking These methods explicitly track the coordinates of some set of discrete points on the interface. Because only points on the interface need to be computed, these methods can provide high resolution. Front-tracking is relatively straightforward to do when interface topology is unchanging, but becomes complicated when interfaces may merge or split, or when extended to higher dimensions (*Sethian and Smereka*, 2003).

Volume of fluid By evolving a discrete volume function defined over all grid cells, the volume of fluid method keeps track of the interface location implicitly in terms of fractionally-filled cells. A primary strength of these methods is their conservation of volume over time (*Sethian and Smereka*, 2003). Drawbacks include the requirement of a non-diffusive advection equation to evolve the volume equation, and the added complication of reconstructing an explicit interface location from fractionally-filled cells (*Gerlach et al.*, 2006). Hybrid level-set and volume of fluid schemes exist, e.g. that described by *Sussman and Puckett* (2000).

Phase field Similar to level set methods, phase field methods define a phase function ϕ . This function might be defined to be 1 in one phase, far from the interface, and 0 in a second phase, also far from the interface. Within a distance ϵ of the interface, $0 > \phi > 1$, so that the computational representation of the front isn't sharp. The phase function is evolved in time, and the location of the front is implicitly updated. In order to achieve high accuracy, the space stepping in the vicinity of the front must be much small in the mushy region ($h \ll \epsilon$) (*Sethian and Smereka*, 2003).

Like the volume of fluid and phase field methods, level set approaches automatically and implicitly handle changes in topology. They do not require the high resolution around the front required by phase field methods for accuracy, and there is no need to explicitly compute the interface in order to compute the normal direction or curvature as with volume of fluid methods. They generalize to higher dimensions, however the dimensionality of the level set function ψ is related to the physical dimensionality of the domain as $d_\psi = d_{\text{phys}} + 1$, which translates to greater computational costs associated with evolving the level set function. Approaches to handle this include solving ψ only within a narrow band around the interface and the "Fast Marching Method."

2 Motivation

One field for which the problem of numerically representing the boundary between ice and liquid water is relevant is glaciological and oceanographic study of marine-terminating glaciers and sea ice. Modern glacier dynamics models typically compute stresses within the ice, strain rates, and internal temperatures. It is desirable to couple ice flow models with melt rate parameterizations at the seawater boundary. *O'Leary and Christoffersen* (2013) show that the interaction between melt rates and glacier behaviour is important, however current models do not consider this in an integrated way, and may be limited because their spatial discretization does not admit the inclusion of a moving ice-water interface. The theory behind parameterisations of melt rates at a glacier terminus is beginning to develop to the degree (e.g. *Jenkins*, 2011) that it would be possible to be possible to include them in a model of glacier dynamics.

An important step in approaching this problem is the treatment of the ice-seawater boundary. Particular requirements are that (a) the movement of the front may be in either direction, i.e. both melting and freezing may occur, (b) multipart topologies aren't necessarily likely, but features such as cracks and ridges should be easily represented, and (c) external fields should be used, such as the heat equation or the Navier-Stokes momentum equations. The first requirement discards Fast Marching as an option (cf. *Strang*, 2007).

3 Implementation

The demonstration of the level set method applied to a Stefan problem that is presented here uses the signed-distance function as the level set function

$$\psi = \begin{cases} -d & T < T_{\text{melt}} \\ 0 & T = T_{\text{melt}} \\ d & T > T_{\text{melt}} \end{cases} \quad (3)$$

where d is the distance to the front. The signed distance scheme has been shown to have advantages over other functions such as a squared distance function (*Osher and Fedkiw, 2003*).

The solution consists of the following steps¹:

1. The parabolic heat equation is solved to compute a temperature field according to (2). The coefficient (κ_i/c_i) is computed over each domain, and (2) is solved using finite differences. After experiments with an explicit solver, a Crank-Nicolson implicit scheme was chosen to reduce the number of time steps required for stability:

$$T_j^{n+1} - T_j^n = \frac{\kappa_i}{c_i} \frac{k}{2h^2} (T_{j-1}^{n+1} - 2T_j^{n+1} + T_{j+1}^{n+1} + T_{j-1}^n - 2T_j^n + T_{j+1}^n). \quad (4)$$

The temperature is bounded such that it cannot be above the melting point in the solid domain, defined as where $\psi > 0$, or below the melting point in the liquid domain.

2. The flux function Φ is calculated based on temperature gradients according to (1). This is used to evolve the level set function following the hyperbolic equation

$$\frac{\partial \psi}{\partial t} = \Phi |\nabla \psi|. \quad (5)$$

An explicit Euler scheme is unstable, but periodic reinitialization of the level set function can prevent the solution from running away.

3. To reinitialize the level set function ψ , the elliptic Eikonal equation

$$|\nabla \psi| = 1 \quad (6)$$

is approximately solved. The approximate solver iterates over

$$\frac{\partial \psi}{\partial t} = \text{sgn}(\psi_0) (1 - |\nabla \psi|) + \kappa_n \frac{\partial^2 \psi}{\partial x^2} \quad (7)$$

The first term on the right hand side is the expression suggested by *Sussman et al. (1994)*. Using the sign of the initial level set function ψ_0 has the advantage that the location of the zero level set remains constant over iterations, and doesn't require a buffer in ψ to preserve the zero level set (*Osher and Fedkiw, 2003*). The boundary conditions on the edge of the domain are Neumann boundary conditions.

When iterated forward, (7) may develop numerical asperities that are controlled by a small amount of numerical diffusion in the second term, with diffusivity κ_n . The amount of numerical diffusion required for a bounded solution was greater in the one-dimensional case than in the two-dimensional case.

In the case of the one-dimensional problem, the exact signed-distance function is inexpensive to compute, and can be used to compare with the approximation.

Chen et al. (1997) reinitialize ψ at every time step, however *Sethian and Smereka (2003)* alledge that reinitializing more often than is necessary contributes error to the front position. It would be possible to reinitialize when the residuals in (6) exceed a threshold. Here, reinitialization occurs at a pre-defined interval instead, which is chosen based on the problem.

¹The code implementing these steps is at <https://github.com/njwilson23/Iceberg.jl>.

Grid res.	Residual
25	3.24×10^{-2}
50	1.34×10^{-2}
100	4.51×10^{-3}
200	2.54×10^{-3}

Table 1: Maximum absolute difference between the analytical and numerical result ($L-\infty$ norm) for Experiment 1 with increasing grid resolution. The order of accuracy is ~ 1 .

4. The grid points in the domain are recoloured depending on whether $\psi \leq 0$ or $\psi > 0$, and step (1) repeats, solving the heat equation in each phase domain.

4 Results

4.1 One-phase experiment

The first experiment conducted represents a freezing front progressing through a one-dimensional liquid at the melting temperature. This scenario has a simple exact solution, described by *Hill* (1987). The progression of the freezing front is proportional to the square root of time elapsed

$$X(t) = \sqrt{\frac{2\gamma\kappa_s t}{\rho_s c_s}}, \quad (8)$$

where γ is given by the transcendental equation

$$\alpha e^{\gamma/2} \sqrt{\frac{\pi\gamma}{2}} \operatorname{erf}\left(\sqrt{\frac{\gamma}{2}}\right) = 1 \quad (9)$$

$$\alpha = \frac{L_f}{c_s (T_m - T_s)}$$

(*Hill*, 1987). In the case that latent heat of fusion $L_f = 1$, specific heat of the solid $c_s = 1$, the melting temperature $T_m = 0$ and the temperature is held at $T_s = -1$ at $x = 0$, then $\gamma \approx 0.76896$. I approximate the semi-infinite domain of the analytical problem by a numerical domain over $[0, 1]$, and solve for the freezing front position through $t = 0.5$, at which point the freezing front in the analytical solution nears $x = 1$. A comparison of the analytical and numerical results for increasing grid resolutions is shown in Table 1 and Figure 1. The residuals compared to the analytical solution indicate that the method is approximately first order accurate in space.

4.2 Two-dimensional experiment

A two-dimensional extension of the experiment in 4.1 is performed by extending the functions above to two dimensions. Whereas the front velocity in the one dimensional case was calculated exactly at the interface and linearly interpolated throughout the model domain, in the two dimensional case explicit calculation of the interface is not trivial and defeats the purpose of the level set method. Instead, effective front velocities are

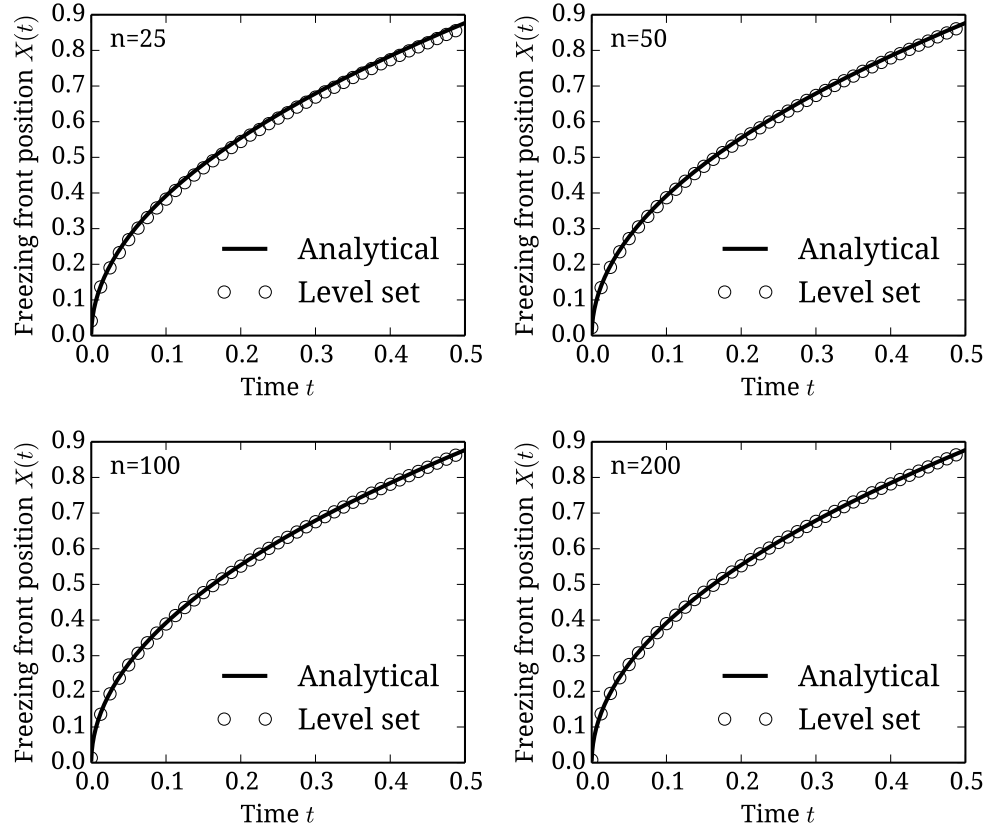


Figure 1: Analytical results compared to the numerical results using the level set method with various numbers of grid points for the one-dimensional one phase scenario on pages 6–14 of *Hill* (1987). An explicit heat equation solver was used and $\Delta t = 5 \times 10^{-5}$ in all runs.

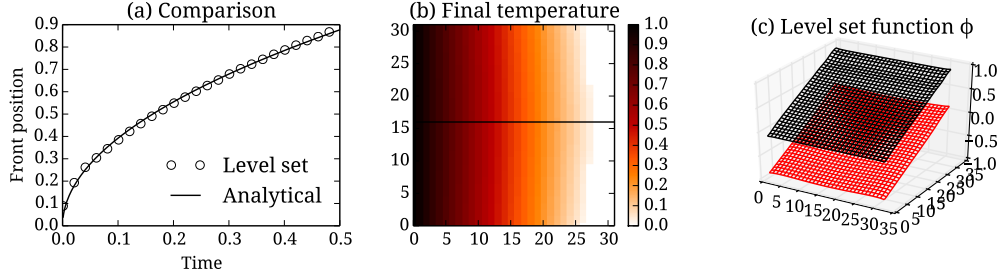


Figure 2: Two-dimensional phase calculation experiment. The problem solved here is identical to the one dimensional problem in 1, but is computed on a 32×32 two-dimensional domain. (a) Comparison of analytical and numerical result. (b) The final temperature field. (c) The initial (black) and final (red) level set functions.

calculated within a narrow band around zero level set, and all other points are set to the average of the front velocities on the band. A better approach would be to interpolate to areas far from the zero level set, or to explore advecting velocities in the direction normal to the interface with an upwinding scheme, as used by *Chen et al.* (1997) and discussed in *Osher and Fedkiw* (2003).

The band for velocity calculation X is determined from the level set function, and chosen to be

$$X_i = \epsilon_\ell < \psi_i < \epsilon_u. \quad (10)$$

By choosing $\epsilon_{\ell,u} = h$, the band calculated for a signed distance function should be 1–2 grid cells wide on either side of the zero level set. To account for small departures from a true signed distance function, $\epsilon_{\ell,u} = 2h$ is used. The solution applies to the problem over the domain $[0, 1]$, $[0, 1]$.

The results for a problem of size 32×32 are shown in Figure 2. Boundary conditions for the heat equation have not been properly coupled along the upper and lower boundaries, and so the phase front propagates more slowly there. Measuring along a line far from the boundaries in the center of the domain, the level set result compares well with the analytical solution (8).

In the current implementation, the reinitialization of the level set function required to satisfy the Eikonal equation (6) consumes nearly half of the time required to compute the solution. This is partly because the method of satisfying the Eikonal equation used here requires the solution of a sparse matrix for every cycle. The method used by *Chen et al.* (1997) does not require this, because they explicitly smooth the level set function rather than computing the implicit heat equation. Also contributing is the simplistic manner in which the velocity function is interpolated which does not yield a smooth result and requires frequent reinitialization.

4.3 Two-dimensional block experiment

As a final experiment that explores the potential for level set methods in higher dimensions by taking full advantage of the two-dimensional model, a pair of overlapping blocks with

Parameter	Experiments 1–2	Experiment 3
L_f	1	4
κ_ℓ	1	1
κ_s	1	1
c_ℓ	1	2
c_s	—	1
ρ_ℓ	1	1
ρ_s	1	1

Table 2: Physical parameters used for Experiments 1–3, described in Sections 4.1–4.3. In Experiments 1–2, the temperature of the solid is the melting temperature, so its heat capacity is irrelevant.

temperature $T = -1$ gradually warm and melt over time in a pool of non-convecting fluid initially with temperature $T = 1$. Parameter details are given in Table 2. The temperature boundaries on the domain are Dirichlet conditions. The level set function is approximately reinitialized at every time step with four cycles of (7) with a pseudo-time step of 0.005.

The temperature gradient at the interface, which starts large, quickly diminishes. Front velocities push the level set function down and gradually round the corners. Some experimentation with the reinitialization routine was required to reduce the effect of numerical diffusion.

No attempt has been made yet to validate this experiment, and an exact analytical solution is expected to be difficult. Solutions for infinite cylinders exist (*Hill*, 1987), and could be used to verify a similar experiment. For now, Experiments 1–2 are a better indicator of accuracy.

5 Conclusions

Level set schemes provide an approach to Stefan problems that benefit from an implicit description of the phase interface. This makes it simple to construct solutions to problems with irregular geometries. For example, holes and intersecting or merging boundaries are included more easily than in a scheme that directly computes the front location. Compared to volume of fluid schemes, the interface geometry is more simply calculated, while compared to phase field schemes, the interface is resolved sharply without requiring high resolution.

Challenges met here in applying the level set scheme largely revolve around accurately and efficiently computing the level set function in time. In the two dimensional models described in Sections 4.2 and 4.3, the global calculation of the level set function to satisfy the Eikonal equation is computationally expensive. Faster schemes for global computation of the level set function exist, and local schemes such as Fast Marching are also possible. Finally, a more careful treatment of the level set time evolution could reduce the need for frequent reinitialization.

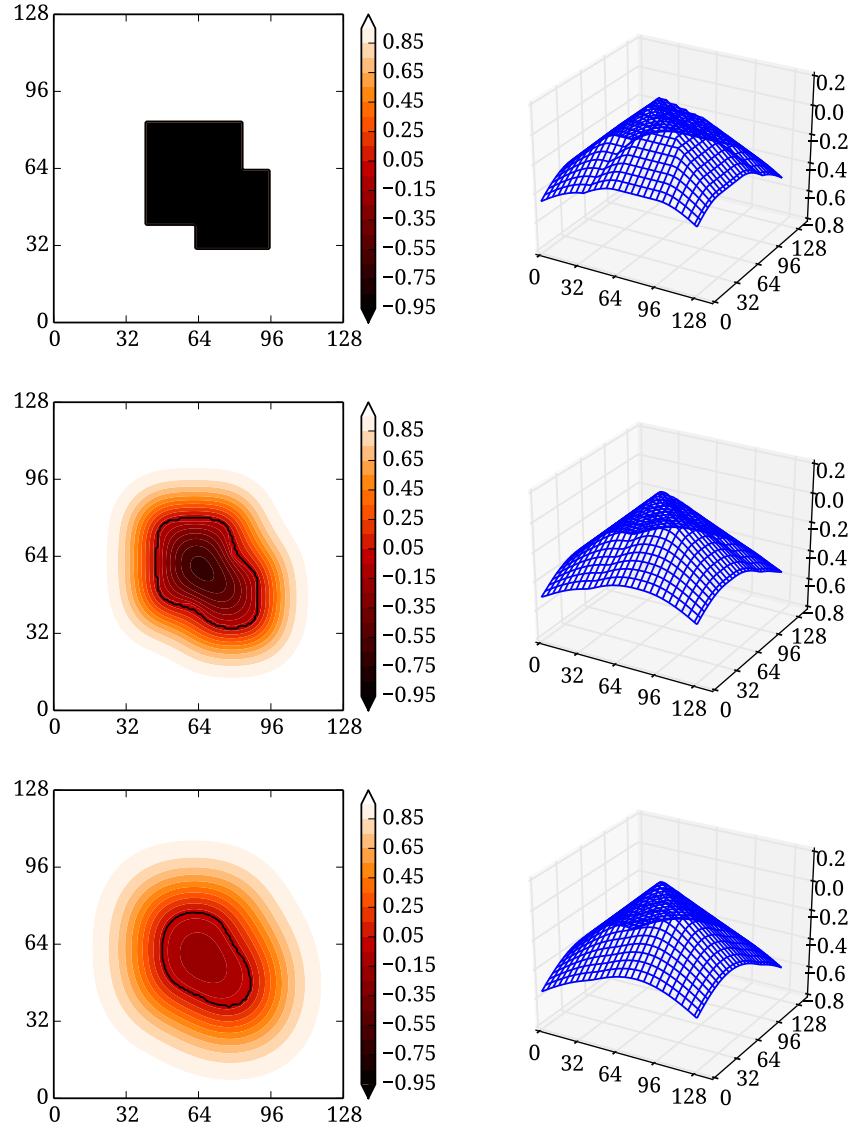


Figure 3: Results of a dimensional block experiment. Snapshots from at $t = 0, 0.005, 0.01$ with the temperature field on the left and wireframes of the level set function on the right.

References

- Chen, S., B. Merriman, S. Osher, and P. Smereka (1997), A simple level set method for solving stefan problems, *Journal of Computational Physics*, 135(1), 8–29.
- Gerlach, D., G. Tomar, G. Biswas, and F. Durst (2006), Comparison of volume-of-fluid methods for surface tension-dominant two-phase flows, *International Journal of Heat and Mass Transfer*, 49(3), 740–754.
- Hill, J. M. (1987), *One-dimensional Stefan problems: an introduction*, Longman Scientific & Technical New York.
- Jenkins, A. (2011), Convection-driven melting near the grounding lines of ice shelves and tidewater glaciers., *Journal of Physical Oceanography*, 41(12).
- O’Leary, M., and P. Christoffersen (2013), Calving on tidewater glaciers amplified by submarine frontal melting., *Cryosphere*, 7(1).
- Osher, S., and R. Fedkiw (2003), *Level set methods and dynamic implicit surfaces*, Springer.
- Sethian, J. A., and P. Smereka (2003), Level set methods for fluid interfaces, *Annual Review of Fluid Mechanics*, 35(1), 341–372.
- Strang, G. (2007), *Computational science and engineering*, Wellesley-Cambridge Press Wellesley.
- Sussman, M., and E. G. Puckett (2000), A coupled level set and volume-of-fluid method for computing 3d and axisymmetric incompressible two-phase flows, *Journal of Computational Physics*, 162(2), 301–337.
- Sussman, M., P. Smereka, and S. Osher (1994), A level set approach for computing solutions to incompressible two-phase flow, *Journal of Computational physics*, 114(1), 146–159.