Efficient Computation of a Sharp Interface
by Spreading via Phase Field Methods

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Abstract. A sharp interface arising from any of the major transition problems (classical or
modified Stefan, etc.) can be smoothed out using the phase field approach as a numerical tool.
The computations in one-dimensional space and n-dimensions with radial symmetry indicate
that this efficient method for dealing with stiff equations results in a very accurate interface
determination without explicit tracking. The methods also provide a numerical verification of
the concept of a critical radius.

I. INTRODUCTION

Numerical computations of moving boundaries have posed important and difficult problems
(see [1] for a survey). For such problems, a variety of methods have been implemented. These
include interface tracking, regularization or "smoothing" of the interface, and numerous
methods designed for special purposes.

In this paper we present a computational technique for a broad class of free boundary
problems based on the ideas of the phase field approach. We apply this technique to a
class of problems which arise from phase transitions and accurately determine the interface
without tracking it separately. In particular, Stefan-type models with or without surface
tension and other effects are approximated very accurately and efficiently with a smooth
system of parabolic equations (see [2] and references in [3]). These ideas are the numerical
counterpart of the theory introduced in Section 4 of [4].

A key feature relevant to efficiency is that the width of the interface (and consequently
the stiffness of the equations) can be changed. This results in execution times which are
reduced by more than one order of magnitude without significant change in the evolution of
the interface. Qualitative details to be described below indicate that this conclusion is not
only self-consistent but is validated when compared with an exact solution. In fact, one can
obtain an accuracy of four digits with an interface diffused to one-fifth of the entire domain.

We have also applied these concepts to study a well-known instability in materials science,
namely the unstable equilibrium at critical undercooling (see section IV). Our results provide
a numerical verification of the onset of this instability and confirm the critical nature of
the magnitude of the surface tension. Most significantly, from our perspective, the results
imply that even in this subtle situation, the interface thickness can be modified without
significantly altering the results. Other aspects of numerics involving the phase field model
have been investigated in [5-7].

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II. THE SHARP INTERFACE MODELS AND THE PHASE FIELD MODEL

In this paper our aim is to compute a solution to a sharp interface problem in a region \( \Omega \subset \mathbb{R}^n \). The problem is to find a function \( u(x,t) \) (i.e. the temperature) and a curve \( \Gamma(t) \subset \Omega \) (i.e. the interface) such that

\[
\begin{align*}
  u_t &= K \Delta u \quad \text{in} \quad \Omega \setminus \Gamma(t) \\
  \nu l &= -K[\nabla u \cdot n]^\pm \quad \text{on} \quad \Gamma(t) \\
  u &= -\sigma \kappa - \alpha \sigma v \quad \text{on} \quad \Gamma(t)
\end{align*}
\]

(2.1) (2.2) (2.3)

where \( l, K, \sigma, \alpha \) are constants (the latent heat, diffusion coefficient, surface tension and relaxation parameter). The variable \( n \) is the normal to the interface (in the direction from \( - \) to \( + \), i.e. solid to liquid) and \( v \) is the (normal) velocity of the interface, \([\nabla u \cdot n]^\pm\) is the jump in the gradient of \( u \).

With \( \sigma \equiv 0 \) in (2.3), this is the classical Stefan model. With finite \( \sigma \) and \( \alpha \), the model is a modification which compensates for surface tension and kinetic undercooling.

The phase field equations may be written as

\[
\begin{align*}
  u_t + \frac{1}{2} \phi_t &= K \Delta u \\
  \alpha \xi^2 \phi_t &= \xi^2 \Delta \phi + \frac{1}{2a}(\phi - \phi^3) + 2u
\end{align*}
\]

(2.4) (2.5)

where \( \xi \) and \( \alpha \) are constant parameters and \( \phi \) is a phase or "order" parameter. The initial and boundary conditions for \( \phi \) must be chosen so that \( \phi = \phi_\pm \) on \( \partial \Omega \) where \( \phi_+, \phi_- \) are the largest and smallest roots of \((2a)^{-1}(\phi - \phi^3) + 2u = 0\), so that \( \phi \approx \pm 1 \).

For the purposes of this paper we assume the philosophical viewpoint that equations [(2.4),(2.5)] are used to approximate [(2.1)-(2.3)], in a scaling limit in which \( \xi, a \) and sometimes \( \alpha \) approach zero. In particular, the scaling relations ([4] p.46) show that the surface tension, \( \sigma \), and the interfacial thickness, \( \xi \), are related by

\[
\sigma = \frac{2}{3} \frac{\epsilon}{\xi a} = \frac{2}{3} \xi a^{-\frac{1}{3}}; \quad \epsilon = \xi a^\frac{1}{3}
\]

(2.6)

For example, in order to approximate the modified Stefan problem [(2.1)-(2.3)] (with nonzero constants \( \sigma \) and \( \alpha \)) one can take \( \xi a^{-\frac{1}{3}} = \frac{2}{3} \sigma = O(1) \) with \( \epsilon \to 0 \).

III. SPREADING THE SHARP INTERFACE

The smoothing of any of the problems of the form [(2.1)-(2.3)] is accomplished by fixing the physical constants \( \sigma \) and \( \alpha \) unless either one is zero, then one adjusts \( \epsilon \), thereby changing the interfacial thickness and the "stiffness" of (2.5), while holding \( \sigma \) fixed in (2.6). One must ensure that the algebraic equation \((2a)^{-1}(\phi - \phi^3) + 2u = 0\) still has three distinct roots. Beyond this constraint, however, one is quite free to choose \( \epsilon \). Of course, the smaller the \( \epsilon \), the closer the approximation to [(2.1)-(2.3)] and also the more points that are needed in order to compensate for the stiffness of the problem.

We consider the spherically symmetric problem in an annular geometry. The boundary conditions \( u_0 \) are set at both parts of the boundary. The initial and boundary conditions on \( \phi \) are then set using the relation \((2a)^{-1}(\phi - \phi^3) + 2u = 0\). E.g. for solidification one has \( \phi_- \approx -1 \) on the inner part and \( \phi_+ \approx +1 \) on the outer.

The results for the modified Stefan problem, with different values for \( \epsilon \), are displayed in Figure 1. With the package used for these computations, an interface which is about 14.7 times wider reduces the computation (C.P.U.) time by a factor of 560. Hence, we observe that the interfacial thickness can be changed considerably without a significant difference in the development of the interface. Other numerical trials show that even a small change in the surface tension effects the motion of the interface.
The self-consistency observed above can be confirmed by comparing our numerical results with an exact calculation. This is possible with the one-dimensional classical Stefan model. In this case the numerical approximation is possible by taking small values for both $\sigma$ and $\epsilon$ in (2.6). For a typical melting or freezing problem (see Figure 2) we find an agreement of three to four digits with an interface which is about one-fifth of the entire domain. For an interface which is about 35% of the entire domain, the agreement is up to two digits. Note that in the one-dimensional problem the curvature is automatically zero by virtue of the geometry. However, the surface tension, $\sigma$, still plays an important role in (2.3) because of the kinetic undercooling term $-\alpha\sigma v$. Thus one expects that the computations should differ significantly as $\sigma$ is changed and $\alpha$ is kept constant.

An essential question with respect to the computations is the number of points which must be placed in the interfacial region. Stated another way, if one has $N$ points in the entire domain, how small may the thickness of the interface, $3\epsilon$, be chosen? We find that 25 points at the interface provide the same or better results than taking several times this number.

IV. THE UNSTABLE EQUILIBRUM AT CRITICAL RADIUS

A good test of the power of these methods can be obtained with an application to the phenomenon of the critical radius. Briefly, if a solid sphere of curvature $\kappa_0$ is surrounded by its melt and the surface tension is $\sigma_0$, then equilibrium will prevail when there is a constant temperature of $\kappa_0 = -\sigma_0 \kappa_0 / \Delta s$. This is an unstable equilibrium configuration which is well known (see [8] p.67) to melt or freeze upon varying any of the parameters. We have obtained numerical confirmation of the onset of this instability and observe it by varying $\sigma_0$ by a few percent. However, a much larger change in the interfacial thickness does not alter the direction or (approximate) magnitude of the interface velocity. Thus, even in this critical physical situation, the interface can be broadened considerably without much change in the evolution of the interface.

![Computed Interfaces of the Modified Stefan Problem](image)

**Figure 1**

*COMPUTED INTERFACES OF THE MODIFIED STEFAN PROBLEM WITH $\sigma = 0.08533$. FROM TOP TO BOTTOM THE CURVES CORRESPOND TO $\epsilon = 0.16628$, $\epsilon = 0.09051$ AND $\epsilon = 0.011313$.***
AN EXACT SOLUTION TO THE CLASSICAL STEFAN PROBLEM AND AN APPROXIMATION USING A PHASE FIELD SYSTEM COMPUTED WITH $\nu = 0.00533$ and $\epsilon = 0.02683$.

FIGURE 2

REFERENCES

7. A. Visintin, Surface tension effects in phase transitions, in [4], 505-538.