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Adaptive method for approximation phase field equation

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Abstract

A moving mesh method is developed for the solution of phase-change problems modelled by the phase-field equation. Numerical result is given for classical Stefan problem and demonstrate the accuracy and effectiveness of the proposed algorithm.

Mathematics Subject Classification: 65M60

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1 Introduction

Numerical study of the free boundaries can be grouped broadly into two categories: one is to solve sharp-interface problems, and the other is phase field equation. Most numerical methods to solve the phase-field equation have used stationary uniform meshes, see, e.g., [1]. However, it is important that the diffused interface is well resolved if the correct dynamics are to be reproduced. As the phase interface moves in time it is clear that an efficient numerical approach must involve some form of mesh adaptivity.

The objective of this work is to develop moving mesh method for solving one dimensional phase-field equation.

2 Modified Stefan Model

The modified Stefan model describes a heat conduction problem and evolution of a sharp interface $\Gamma(t)$ within $\Omega \subset \mathbb{R}^n$. The objective is to find a temperature field u(x, t) and a curve $\Gamma(t) \subset \Omega$ that solve the nondimensional equations

$$\frac{\partial u}{\partial t} = K\Delta u \qquad \qquad x \in \Omega \backslash \Gamma(t), \tag{1}$$

$$Lv = -K \left[\nabla u\right]_{-}^{+} \qquad x \in \Gamma(t), \tag{2}$$

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$$u = -\frac{\sigma}{\Delta s}(\kappa + \alpha \upsilon) \quad x \in \Gamma(t).$$
(3)

Equations (1) and (2) describe the diffusion of heat within the domain and the release of latent heat across the phase-change interface. Here L is the latent heat per unit mass, K is the thermal diffusivity, v is the normal velocity of the interface, and $[\nabla u]^+_-$ is the jump in the normal component of the temperature gradient at the interface. The parameter σ is the surface tension, α denotes a kinetic undercooling coefficient, Δs is the entropy difference between the two phase, and κ is the sum of the principle curvatures at a point of the interface. The classical Stefan model is obtained by setting $\sigma = 0$.

3 Phase-Field(PF) Model

The PF equation are derived using the idea of a phase order parameter p and Landau-Ginzburg theory. A free energy functional F is constructed in terms of the phase order parameter and other thermodynamic variables. For example,

$$F(p,u) = \int_{\Omega} \left[\frac{1}{2} \tau^2 (\nabla p)^2 + f(p,u) \right] dx, \qquad (4)$$

where τ is a length scale and f(p, u) is a free energy density. Various choices of the precise choice of f have been suggested, the most studied of which is the Caginalp potential[1]:

$$f(p,u) = \frac{1}{8a}(p^2 - 1)^2 - 2up.$$
(5)

Both parameters τ ans a are length scales related to the macroscopic physics. In particular, the surface tension σ and the interfacial thickness ϵ are related by

$$\sigma = \frac{2}{3}\varepsilon/a = \frac{2}{3}\tau/\sqrt{a}, \quad \varepsilon = \tau\sqrt{a} \tag{6}$$

A kinetic equation for the phase field is obtained by requiring that F monotonically decreases in time. The simplest choice of this requirement leads to the phase-field equation

$$\alpha \tau^2 \frac{\partial p}{\partial t} = -\frac{\delta F}{\delta p},\tag{7}$$

where $\alpha \tau^2$ is a relaxation time. Direct calculation from the above equation gives

$$\alpha \tau^2 \frac{\partial p}{\partial t} = \tau^2 \Delta p - \frac{1}{2a} (p^3 - 1) - 2u.$$
(8)

The phase equation is conjoined with the heat equation, modified to take into account the liberation of latent heat by the inclusion of an appropriate source term:

$$\frac{\partial u}{\partial t} + \frac{L}{2}\frac{\partial p}{\partial t} = K\Delta u,\tag{9}$$

4 Numerical Results

We now present numerical result in the section. The results are obtained with ODE15S software and adaptive mesh redistribution method which developed in [3]. Consider a classical freezing problem in a semi-infinite plan. We briefly describe the example, the details can be found in [2]. The Neumann solution of the classiccal Stefan problem has the following form

$$u^{(s)}(x,t) = \begin{cases} c_1 \frac{\left[\operatorname{erf}(\beta/2) - \operatorname{erf}(x/(2\sqrt{t+t_0})) \right]}{\operatorname{erf}(\beta/2)} & x \leq s(t) \\ c_2 \frac{\left[\operatorname{erf}(\beta/2) - \operatorname{erf}(x/(2\sqrt{t+t_0})) \right]}{1 - \operatorname{erf}(\beta/2)} & x \geq s(t) \end{cases}$$

where t_0 is a starting time and c_1 and c_2 are constants. The position of the interface is given by

$$s(t) = \beta \sqrt{t + t_0}$$

with $t_0 = 0.15$, $c_1 = -0.085$, $c_2 = -0.015$, L = K = 1, $\beta = 0.396618$. The initial and boundary conditions for the temperature are

$$u(0,t) = c_1, \quad u(1,t) = u^{(s)}(1,t) \text{ and } u(x,0) = u^{(s)}(x,0)$$

Also the initial and boundary conditions for the phase field are

$$p(0,t) = \min_{p} f(p,c_1), \quad \text{closest } to \ -1$$

 $p(1,t) = \min_{p} f(p, u^{(s)}(1,t)), \quad \text{closest to } 1$

and

$$p(x,0) = \begin{cases} p(0,0) \tanh(\frac{s(0)-x}{2\varepsilon}), & x \leq s(0) \\ p(1,0) \tanh(\frac{x-s(0)}{2\varepsilon}), & x \geq s(0) \end{cases}$$

We can see that the mesh points move smoothly and the predict interface position is very accurate. To plotting accuracy the moving grid results are indistinguishable from the Neumann solution. The numerical results are in good agreement with previously published results of Tan et. al. [2]



Figure 1: (1): temperature(left) and phase field (right) at t = 0.2. (2): temperature(left) and phase field (right) at t = 1. (3): mesh trajectories with N = 50(left)and interface position (right).

References

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