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A thermodynamically consistent numerical method for a phase field model of solidification

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ABSTRACT

A discretization is presented for the initial boundary value problem of solidification as described in the phase-field model developed by Penrose and Fife (1990) [1] and Wang et al. (1993) [2]. These are models that are completely derived from the laws of thermodynamics, and the algorithms that we propose are formulated to strictly preserve them. Hence, the discrete solutions obtained can be understood as discrete dynamical systems satisfying discrete versions of the first and second laws of thermodynamics. The proposed methods are based on a finite element discretization in space and a midpoint-type finite-difference discretization in time. By using so-called discrete gradient operators, the conservation/entropic character of the continuum model is inherited in the numerical solution, as well as its Lyapunov stability in pure solid/liquid equilibria.

1. Introduction

The first widely known mathematical theory of solidification is the so-called Stefan model [3]. This theory is a classical example of free-boundary problem, in which a set of Partial Differential Equations (PDE's) need to be solved on a moving domain. These PDE's are coupled through boundary conditions that hold on an unknown solid–liquid interface. Thus, in the Stefan model the fundamental unknowns are the temperature field and the location of the interface. The attractive feature of this theory is that the temperature defines the phases at each point. Wherever the temperature is lower than the solidification temperature we have the solid phase and vice versa. The interface is defined as the lower-dimension geometrical entity in which the temperature equals the equilibrium temperature.

This paradigm broke down when experimental evidence showed that the temperature on the interface does not equal the solidification temperature. Actually, for static interfaces, the difference between those is proportional to the sum of the principal curvatures of the interface at that point [4]. Several decades later, additional experimental evidence showed that for dynamic interfaces, the difference between the equilibrium temperature and the actual temperature on the interface also depends on the interface velocity (this is normally referred to as kinetic undercooling). These facts clearly showed that temperature was not the right quantity to define the phases, and alternative approaches were sought. This lead to the emergence of the phase-field method, in which a new variable called order parameter was introduced to distinguish the phases. The order parameter is defined on the whole domain (both in the liquid and the solid phases) and naturally leads to continuous description of the two-phase system in which diffuse interfaces appear as solutions to the fundamental phase-field

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equations. Therefore, the phase-field method leads not only to a physically sound description of solidification, but also to simpler numerical approximation of the theory, because interface tracking is completely avoided.

There have been several phase-field theories over the years [5–7,2]. We feel that a significant development was the thermodynamic framework for phase-field solidification theories that was developed by Penrose and Fife [1]. In this work, the authors presented a framework to develop phase-field theories that satisfy the fundamental laws of thermodynamics. An example of such a theory was later proposed by Wang et al. [2]. In this paper, we will focus on that theory.

Since modern solidification phase-field theories observe the laws of thermodynamics at the continuous level, it seems desirable to develop numerical algorithms that inherit those properties at the discrete level. This is precisely the objective of this paper. Here we present thermodynamically consistent algorithms that are strictly energy-conserving and entropy-increasing for closed systems. The proposed algorithms are based on our recent work [8–11], which establishes a framework for developing numerical methods that preserve the laws of thermodynamics and symmetries of thermodynamical systems. This idea, which has been previously applied to thermomechanical problems, allows to formulate discrete dynamical systems whose behavior closely resembles that of the corresponding continuum model. Moreover, numerical results indicate that the strict satisfaction of the discrete conservation laws avoids excessive dissipation in the numerical integration which is responsible for the smearing of phase interfaces.

The design of thermodynamically consistent methods ultimately depends on a consistent redefinition of the thermodynamic affinities, in such a way that the correct energy and entropy balance is built, exactly, into the discrete evolution equations. The formulation of such modified derivatives builds upon the so-called discrete gradient operator [12–17], an idea often employed for the design of conserving methods in Hamiltonian mechanics, wee, among many others, [18–23]. In the present work, we start from the thermodynamically based phase field model proposed by Wang et al. [2], and further exploit this idea to construct a discretization which inherits the two laws of thermodynamics.

We note that similar ideas have been previously used to derive unconditionally gradient-stable schemes for isothermal phase-field theories, such as, for example, the Cahn–Hilliard equation which governs the phase separation of immiscible fluids [24–26]. In particular, our algorithms have similarities with those proposed by Du and Nicolaides [27]. Some other recent works in this field include [28–32]. However, the aforementioned works focus on algorithms which inherit the dissipation inequality of an isothermal theory, while this paper proposes algorithms which comply with the two laws of thermodynamics in a non-isothermal fully-coupled thermodynamical system.

We are able to prove that the dynamical system defined by Wang's model is Lyapunov stable close to pure phases. This result further indicates that indeed this theory is sound and suitable for the simulation of solidification problems. Moreover, it will be proved that the newly proposed method inherits this nonlinear stability from the continuum problem. Such feature stems from the thermodynamical consistency of the numerical method, and it is not shared by other discretizations.

An outline of the article is the following. In Section 2 the phase field model for solidification due to Penrose and Fife [1] and Wang et al. [2] is summarized. Its numerical approximation is described in Section 3, where standard methods as well as a new discretization are presented. The strict satisfaction of the laws of thermodynamics by the new method is proved. Section 4 analyzes the Lyapunov stability of the continuum model as well as the discrete model, showing again that the numerical solution inherits this desirable feature. Numerical examples of the performance of the new method are addressed in Section 5. Finally, the article concludes with a summary of results in Section 6.

2. A phase field model for solidification

Phase field models have proven to be a valid approach for the analytical formulation and numerical solution of solidification problems. In this work we propose a discretization of the model described in [2] in which the phase field equations for a solidification model are derived ensuring that all modeling complies with the two laws of thermodynamics. We summarize in this Section Wang's model, and then in Section 3 we will discretize its equations while preserving the conservation laws.

2.1. Balance equations

Consider a solid occupying a volume described by an open set $V \subset \mathbb{R}^d$, with $d = 2$ or 3, and closure $\bar{V}$, which includes a solid and a liquid phase. To describe which parts of the body belong to each of the phases, we introduce an order parameter $\phi : V \to [0,1]$ with value $\phi = 0$ on solid points, $\phi = 1$ on liquid points, and $\phi \in (0,1)$ at the interfaces. In this description, the phase field variable becomes one of the state variables that fully determine the thermodynamic state of every particle of the body.

For every region $\Omega \subseteq V$, let $E(\Omega)$ denote its total energy. Since the energy is an extensive property, it can be expressed as

$$E(\Omega) = \int_\Omega e \, \mathrm{d}v, \tag{1}$$

where e is the energy density.

If no external power is applied on the body, the first law of thermodynamics states that the total change of energy of any subset Ω is due to the thermal power entering through its boundary $\partial\Omega$. If $\boldsymbol{q} : \bar{V} \to \mathbb{R}^d$ is the heat flux and $\boldsymbol{n}$ is the unit outward normal to the boundary $\partial\Omega$, then the first law of thermodynamics reads: