Computational Materials Science 126 (2017) 426–437

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Bracket formalism applied to phase field models of alloy solidification

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ARTICLE INFO

Article history:
Received 23 May 2016
Received in revised form 12 September 2016
Accepted 26 September 2016
Available online 24 October 2016

Keywords:
Phase field
Alloy solidification
Non-equilibrium thermodynamics

ABSTRACT

We present a method for coupling current phase field models of alloy solidification into general continuum modelling. The advantages of this approach are to provide a generic framework for phase field modelling, give a natural and thermodynamically consistent extension to non-isothermal modelling, and to see phase field models in a wider context.

The bracket approach, introduced by Beris and Edwards, is an extension of the Poisson bracket of Hamiltonian mechanics to include dissipative phenomena. This paper demonstrates the working of this formalism for a variety of alloy solidification models including multi phase, multi species with thermal and density dependency.

We present new models by deriving temperature equations for single and more general phase field models, and give a density dependent formulation which couples phase field to flow.

1. Introduction

The phenomena and process of alloy solidification, well described in [1], is now routinely associated with the significant successes of the modelling methods of phase field. Phase field came into being as a computational convenience (if not necessity) to capture the evolution of complex surface structures. More recently it has become possible to compute with physically realistic finite interface regions where the material is neither solid nor liquid, in which case the phase field becomes a physical field in the interface region.

Although it is well known that dissipative phenomena with constant boundary temperature spontaneously change to accommodate a lowering of the Gibbs free energy, the details of such transitions are still obscure for many complex materials. For dynamic modelling, this complexity is reflected in the construction of the Gibb's free energy, which typically includes both physical and non-physical states of matter – an example of the latter being the Gibbs free energy of a solid significantly above its melting temperature. Moreover, current computing resources and methods still struggle to grapple with the highly non-linear partial differential equations that the phase field method produces. Yet, in principle, the modelling of even complex materials using phase field is quite straightforward in outline: specify the global free energy of the physical system and allow the system to evolve spatially and temporally in such a way as to optimally minimise this functional in a thermodynamically consistent way. This manifests itself mathematically by the underlying presence of variational derivatives and diffusion parameters. To illustrate this, given a single phase formulation of the free energy, $F = \int_\Omega f(\phi, \nabla\phi, c, T)\,\mathrm{d}^3x$, in a domain Ω for the thermal-solutal (T, c) solidification of a metal, where $\phi \in [0, 1]$ indicates bulk melt or bulk solid at the extremes, the dynamical equations are typically given as, [2] a variational form for the phase variable

$$\dot{\phi} = -M\frac{\delta F}{\delta \phi}; \tag{1}$$

a conserved variational form for the solute concentration variable, c,

$$\dot{c} = \nabla \cdot D\nabla\frac{\delta F}{\delta c}; \tag{2}$$

and a temperature diffusion equation

$$C\dot{T} = \nabla \cdot \kappa\nabla T + L\dot{\phi}. \tag{3}$$

In the above M is phase mobility, D a solute diffusion parameter, κ thermal conductivity, C, and L are the volumetric heat capacity and volumetric latent heat parameters respectively - all prescribed. Also arising in the right hand side of Eq. (2) can be $\nabla \cdot \mathbf{j}$ where $\mathbf{j}$ is an anti-trapping current that compensates for non-physical effects in isothermal simulations associated with the computationally convenient use of a larger than realistic interface width, [3] – the anti-trapping current is not currently derived from a variational procedure and it is difficult to apply the mathematical analysis to general materials.There is likely to be a problem with a non -variational induced anti-trapping when applied to thermal models if the

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http://dx.doi.org/10.1016/j.commatsci.2016.09.036
0927-0256/

current is not entropically neutral. Thus generation of an anti-trapping current from a variational procedure, if possible, which guarantees zero entropy generation may be advantageous. However, further discussion of this is beyond the scope of this paper.

The presence of $\nabla\phi$ in the free energy indicates a penalty in the free energy, i.e. an increase of free energy if the interface becomes too sharp. It is by no means obvious how three such different looking equations come from a single underlying principle. The form of these equations can be justified either by appeal to a sharp interface model, [4], or by assuming a finite interface and seeking thermodynamic consistency, [5].

This paper is concerned with the application of a generic non-equilibrium thermodynamic method to phase field modelling of alloy solidification. Multiphase models have been described without coupling to a temperature equation, for example by Nestler et al. [6] and, although it might be perfectly feasible to start from this formulation using the methods of, Penrose et al. [5], we are here applying the generic methods of Beris and Edwards [7]. Generic, in the sense that these methods apply to any continuum system with or without dissipative behaviour. Significant non-dissipative examples being: Euler flow and Elasticity; and dissipative examples being: Navier-Stokes, complex fluid modelling and visco-plasticity. This method has more in common with [5] than with [4], keeps the formal structure and the particular physical system concerned quite distinct, and brings to light differences and clarification when compared with other models (including single phase models) in the literature. The most obvious differences in the model are shown here to be in the temperature equation, which may be compared with single phase formulations as described in, [12–15].

The approach detailed here concerns a generalisation of the Poisson bracket for continuous non-dissipative phenomena and will be referred to as the "bracket" formalism. Application of the bracket produces a variational formulation, which in turn produces systems of coupled PDEs. In this sense there is a hierarchy:

Bracket → Variational form → PDEs.

Before embarking on a description of the bracket formalism as applied to phase field dynamics we state some reasons why this method may be preferable to other approaches, the main contender perhaps being the methods of Linear Irreversible Thermodynamics (LIT) [16]. The bracket formalism can be used to derive evolution equations for systems involving any number of coupled phenomena, and to guarantee that the couplings do not violate any principles of mechanics or laws of thermodynamics by construction. In LIT there is no provision for the inclusion of the kinematic of flow (as expressed by the Cauchy momentum equation) and the stress tensor. LIT provides expressions for the viscous or dissipative stresses, but cannot help with the conservative or elastic stresses. The bracket structure dictates the stress that appears in the Cauchy momentum equation, in terms of both conservative and dissipative contributions. Furthermore, these contributions are guaranteed to be mechanically and thermodynamically consistent between all of the coupled evolution equations necessary for the system description. In the bracket approach, the stress tensor field is given via a specification of the free energy functional, which is also something that does not come from LIT. In the phase field application here, we may wish to include flow modelling in a thermodynamically consistent way that will include conservative as well as dissipative phenomena. Indeed, the simple provision for an associated density change with phase already begins this coupling because conservation of mass implies the presence of flow. It is the generality of the bracket that is key here. The bracket formalism encompasses all continuous phenomena and provides a clear distinction between the conservative and dissipative contributions. In Section 7.1 of [7], the authors state their assumption that the Onsager/Casimir reciprocal relations are valid for systems close to equilibrium and that this implies that the lowest order representation of the dissipation bracket, as used here, must be a symmetric bilinear functional. Taking this as our starting point, we show, in agreement with [7], that the bracket formalism appears considerably easier to apply and perhaps less prone to error than other methods. Finally, even in the simplest phase field applications as explored in this paper, by applying the bracket in all generality there appear terms that have previously either been overlooked or neglected. Possibly the most important example of the latter is the correct construction of the temperature field equation.

The structure of the paper is as follows: Section 2 introduces the bracket and illustrates its application to a simple phase field model of solidification and then extends to include a thermal field. The temperature equations differ from the literature and so simulation results are presented which show the effect of the postulated new terms. Section 3 extends the bracket to apply to multi phase and multi species models of alloy solidification. Section 4 discusses previously neglected terms (postulated by a more general dissipative bracket) as providing additional enrichment for alloy modelling. Section 5 extends the single phase and multiphase model to include density. The key feature of this section is the introduction of the Poisson bracket alongside the dissipative bracket. The introduction of density implies a flow field so as to maintain mass conservation, an associated stress tensor, and additional terms to the pressure and temperature field.

The additional terms due to density modelling are easily extended to multiphase field formulations.

2. The bracket and phase field solidification

In this section we review the bracket and illustrate the formalism with single phase solidification modelling.

The bracket formalism is an extension of the Poisson bracket methodology of conservative, discrete particle systems to include dissipative and continuous systems. As is well known for conservative particle systems, dynamical equations are given once the Hamiltonian is prescribed in terms of the position and momentum. For example, for a single particle of mass m in a potential well V the Hamiltonian energy is given in terms of the momentum, $\mathbf{p}$ and position, $\mathbf{x}$ by

$$H(\mathbf{p},\mathbf{x}) = \frac{\mathbf{p}\cdot\mathbf{p}}{2m} + V(\mathbf{x}), \tag{4}$$

and the equations of motion for any variable, Q, by

$$\dot{Q} = \{Q, H\}. \tag{5}$$

In particular when Q represents the position and momentum of the particle:

$$\dot{x}_i = \{x_i, H\},$$

$$\dot{p}_i = \{p_i, H\}. \tag{6}$$

Here the Poisson bracket is specified by the antisymmetric operator (for arbitrary variables A, B)

$$\{A,B\} \equiv \sum_j^3 \left(\frac{\partial A}{\partial x_j}\frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial x_j} \right). \tag{7}$$

This gives as expected

$$\dot{x}_i = \frac{p_i}{m}, \tag{8}$$

$$\dot{p}_i = -\frac{\partial V}{\partial x_i}, \tag{9}$$