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A Newton method with adaptive finite elements for solving phase-change problems with natural convection

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ABSTRACT

We present a new numerical system using finite elements with mesh adaptivity for the simulation of solid–liquid phase change systems. In the liquid phase, the natural convection flow is simulated by solving the incompressible Navier–Stokes equations with Boussinesq approximation. A variable viscosity model allows the velocity to progressively vanish in the solid phase, through an intermediate mushy region. The phase change is modeled by introducing an implicit enthalpy source term in the heat equation. The final system of equations describing the liquid–solid system by a single domain approach is solved using a Newton iterative algorithm. The space discretization is based on a P2–P1 Taylor–Hood finite elements and mesh adaptivity by metric control is used to accurately track the solid–liquid interface or the density inversion interface for water flows.

The numerical method is validated against classical benchmarks that progressively add strong non-linearities in the system of equations: natural convection of air, natural convection of water, melting of a phase-change material and water freezing. Very good agreement with experimental data is obtained for each test case, proving the capability of the method to deal with both melting and solidification problems with convection. The presented numerical method is easy to implement using FreeFem++ software using a syntax close to the mathematical formulation.

1. Introduction

Solid–liquid phase change systems involving melting or freezing processes are encountered in numerous practical applications, ranging from metal casting and thermal energy storage to food freezing. Most of the models consider the conduction as the principal mechanism in describing the heat transfer during melting or solidification (Stefan problem). Recent models include several other important physical phenomena, such as gravity effects, convection in the liquid phase, the presence of a *mushy* region (containing both solid and liquid particles) at the interface between the two phases, etc. For a comprehensive review of such models, see [1].

In particular, it was found that the natural convection in the liquid plays an important role in the heat transfer between phases and the propagation of the melting/solidification front [2–7]. This is specifically the case in recent practical

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applications using phase-change materials (PCM) to store heat energy or to diminish temporary peak temperatures in different technologies (*e.g.* thermal regulation of buildings, passive cooling of electronic devices). Another example of convection dominated phase-change systems is the water freezing, appearing in many environmental applications, such as water transportation, food processing, weather prediction, etc.

In this paper we use a single domain approach to simulate phase-change systems with convection. In the liquid phase, the natural convection flow is simulated by solving the full incompressible Navier–Stokes equations with Boussinesq approximation. The same system of equations is solved in the solid phase by introducing a variable viscosity coefficient taking very large values in the solid (*e.g.* [8]). This model allows the velocity to progressively vanish in the solid through an intermediate *mushy* region, defined accordingly to classical enthalpy methods (*e.g.* [3,9,10]). In enthalpy methods, the phase change is modeled by introducing an enthalpy source term in the heat equation. The phase-change is supposed to occur over a temperature interval setting the width of the mushy region. This temperature interval is also used to regularize discontinuous functions representing the variation of material constants (conductivity, specific heat, latent heat) across the solid–liquid interface.

The main advantage of the single domain approach is that the same system of equations is solved in both liquid and solid phase. In exchange, the numerical method has to tackle two important challenges: properly resolve the convection cells in the fluid region and accurately capture the solid–liquid interface. The former issue is related to the non-linearity in the momentum Navier–Stokes equations, while the latter comes mainly from the very sharp variation of the coefficients of the equations (viscosity, latent heat, etc.) in a small region around the solid–liquid interface. Since most of the numerical methods presented in the numerical heat transfer community use finite difference (FD) or finite volume (FV) methods on a fixed mesh, the general strategy to address these issues is to dramatically increase the mesh resolution in the whole domain. This results is a considerable increase of the computational time, even for two dimensional cases. Finite element (FE) methods offer the possibility to dynamically refine the mesh only in the regions of the domain where sharp phenomena take place (*e.g.* solid–liquid interface, recirculation zones).

FE methods were used in late 1980s to derive mathematically sound numerical algorithms for the Stefan problem (involving Laplace operators). Different modeling approaches were analyzed, from enthalpy-type methods (*e.g.* [11]) to front-tracking methods (*e.g.* [12]). Only recently, adaptive FE methods were proposed for the phase-change problem. A moving mesh technique was developed in [13] and used to simulate melting and solidification problems. The method was based on solving a modified set of equations, including two supplementary partial differential equations modeling the mesh movement between two time steps. An anisotropic mesh adaptation algorithm based on an approximation of a hierarchical error estimator was proposed in [14] for classical two-phase Stefan problem (without convection). A different mesh adaptivity strategy, based on the definition of edge length from a solution dependent metric, was used to deal with the same Stephan problems in three-dimensional simulations. This last adaptivity method, based on solution dependent metrics, was also tested for phase-change systems with convection in [15]. The use of locally adaptive meshes with strong anisotropy proved very effective in reducing the number of computational nodes for phase-change systems.

As a first contribution of the present paper, we introduce an FE method with time-dependent mesh adaptivity by metric control that is effective for a large range of phase-change systems with convection, from melting to solidification. The proposed mesh refinement strategy has the capacity to take into account different metrics and thus the ability to refine the mesh in different regions of interest in the computational domain. In particular, we show that the method is able to simultaneously track several interfaces in the domain, a feature that was not present in previous mesh refinement algorithms. Similar algorithms based on FreeFem++ [16,17] were successfully used for solving different systems of equations with locally sharp variation of the solution, such as Gross–Pitaevskii equation [18,19] or Laplace equations with nonlinear source terms [20].

The second contribution of this paper is the derivation of a Newton algorithm for solving the nonlinear system of equations for the single domain approach of the phase-change system with convection. Newton linearization has been successfully used for fluid dynamics and heat transfer equations (*e.g.* [21]) with the advantage to accelerate computations due to its rapid quadratic convergence. Effective classical or high-order Newton methods for the steady Navier–Stokes equations were proposed in [22,23] using finite-difference methods on non-staggered grids. For the Navier–Stokes–Boussinesq system, a Newton method with explicit treatment of the temperature was briefly introduced in [15]. We derive below a fully-implicit Newton method for the phase-change system based on a finite-element formulation of the Navier–Stokes equations. The advantage of this formulation is to permit a straightforward implementation of different types of non-linearities in the system of equations. For the sake of modularity, we derive and test the Newton algorithm by progressively treating the following non-linearities:

(i) the convective nonlinear term in the Navier–Stokes–Boussinesq equations (test case: natural convection of air in a differentially heated cavity),
(ii) problem *(i)* plus a nonlinear buoyancy term (test case: natural convection of water in a differentially heated cavity),
(iii) problem *(i)* plus the enthalpy nonlinear source term and nonlinear variable viscosity (test case: melting of phase-change material),
(iv) problem *(iii)* plus a nonlinear buoyancy term and nonlinear variation of thermodynamic properties (test case: water freezing).