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A fully coupled finite element formulation for liquid–solid–gas thermo-fluid flow with melting and solidification

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Abstract

Many important industrial processes, such as additive manufacturing, involve rapid mass, flow and heat transport between gas, liquid and solid phases. Various associated challenges, such as the large density ratio between gas and condensed phases, make accurate, robust thermal multi-phase flow simulations of these processes very difficult. In order to address some of the associated challenges, a computational framework for thermal multi-phase flows is developed based on the finite element method (FEM). A unified model for thermal multi-phase flows similar to the models widely used in the manufacturing community is adopted. The combination of the level-set method and residual-based variational multi-scale formulation (RBVMS) is used to solve the governing equations of thermal multi-phase flows. Phase transitions between solid and liquid phases, i.e., melting and solidification, are considered. Interfacial forces, including surface tension and Marangoni stress, are taken into account and handled by a density-scaled continuum surface force model. A robust fully coupled solution strategy is adopted to handle various numerical difficulties associated with thermal multi-phase flow simulations, and implemented by means of a matrix-free technique using Flexible GMRES. The mathematical formulation and its algorithmic implementation are described in detail. Four numerical test cases are presented to demonstrate the capability of the proposed formulation. The first case is a benchmark example of solidification of aluminum in a graphite mold, the second case is a thermo-capillary droplet migration problem, the third case is a spot laser melting problem, and the fourth case is the melting of metal with an interior gas bubble. The computational results are compared with analytical, experimental and simulation data from other researchers, with good agreement in cases where such data is available.

Keywords: Thermal multi-phase flows; Gas–liquid–solid systems; Surface tension; Marangoni stress; Melting; Manufacturing

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1. Introduction

Thermal multi-phase flows occur in many traditional manufacturing processes, such as welding and casting, as well as additive manufacturing processes, such as selective laser melting [1–5]. Although there are several numerical methods available for the simulations of single phase thermal fluid flows in the literature [6–11], accurate simulation

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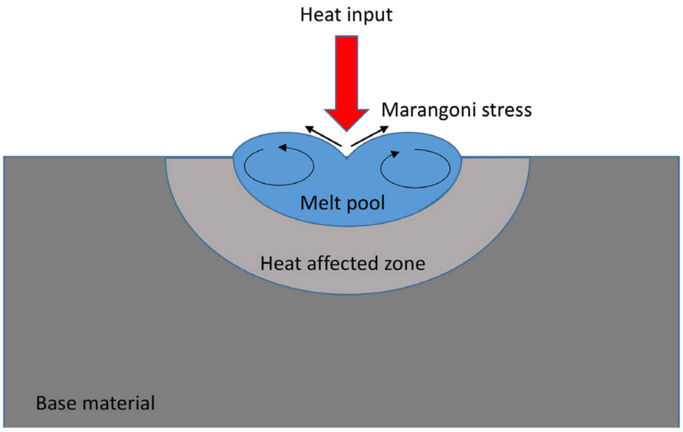

Fig. 1. A 2-D sketch of the melting process, showing the melting pool and the heat affected zone.

and solution strategies of these thermal multi-phase flows that can capture complex multi-physical phenomena in manufacturing processes with large property ratios, still remain a challenging problem.

From the pure fluid mechanics side, the challenges stem from the large density and viscosity ratios between different phases of fluid, pressure discontinuity across the interface, topological interface change, and effects of surface tension and its dependence on temperature. The last of these becomes significantly important for small spatial scales and in the presence of highly curved interfaces and large temperature gradients. In recent decades, a number of techniques have been developed to simulate isothermal multi-phase flow problems. These can be classified into two categories based on how the motion of the interface between different phases is handled: interface-tracking and interface-capturing methods [12,13]. The interface-tracking approaches, including front-tracking methods [14], boundary-integral methods [15], arbitrary Lagrangian–Eulerian (ALE) methods [16], and space–time finite-element methods [17,18], use a deformable mesh that conforms to the moving interface. The main advantage of interface-tracking methods is their ability to achieve high per-degree-of-freedom accuracy near the interfaces. However, when the interfaces form a singularity or change topology, interface-tracking methods become challenging to apply in practice, and require the development of special techniques (see, e.g., [19]). Automatic merging or break-up of interfaces are especially challenging for interface-tracking techniques, which makes 3D multi-phase flow problems notoriously more difficult to solve using this class of methods. On the other hand, interface-capturing methods, such as the volume-of-fluid (VOF) method [20], phase-field methods [21–25], diffuse-interface methods [26,27], front-capturing methods [28], and level set methods [29–33], utilize an auxiliary function defined on the problem domain to describe the interface, and present a practically simpler alternative to the interface-tracking methods. Although interface-capturing methods typically require higher mesh resolution to compensate for lower interface accuracy, these methods are very robust and relatively simple to implement in practice. Because the changes in interface topology do not present a conceptual difficulty for these methods, they have been applied to a broad range of problems including bubble dynamics [34–36], jet atomization [37], and free-surface flows [38–41]. Among these methods, the level set technique is especially popular because of its ability to represent complex interfaces using a smooth implicit function. In principle, this function can be used not only to separate the different fluid phases at their interface, but also to compute the interface normal and curvature that are needed to incorporate the interfacial forces, such as surface tension, in the multi-phase flow model.

As discussed above, great progress has been made in single phase thermal fluid flow and isothermal multi-phase flow simulations in recent years. However thermal multi-phase flows simulations for manufacturing processes are still very difficult. The coupling between thermodynamics and fluid dynamics increases the complexity of thermal multi-phase flow simulations as it involves the interplay of aspects, such as flow, mass, and heat transport, melting, solidification, and interface deformation. These interacting phenomena are illustrated by a typical melting problem shown in Fig. 1. In Fig. 1, a non-uniform heat influx (e.g. from a laser source) melts the solid workpiece into a liquid pool and creates a thermal gradient at the free surface. The dependence of surface tension on temperature gradient thus results in a significant spatial variation of surface tension, manifested in Marangoni stresses at the free surface,