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High-order adaptive arbitrary-Lagrangian–Eulerian (ALE) simulations of solidification

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ABSTRACT

A high-order-accurate method for simulation of solidification is presented. The solidification front is tracked using a triangular, Arbitrary-Lagrangian–Eulerian moving mesh, and a mesh adaption algorithm is used to allow simulations of unsteady problems with large interfacial movement. An improved mesh coarsening algorithm is presented that maintains high quality deforming meshes while reducing the amount of interpolation needed to transfer solutions between meshes. An *hp*-finite element method is used to resolve the thermal and flow fields. This is combined with an A-stable diagonally-implicit Runge–Kutta temporal scheme. The method was demonstrated to give a temporal order of accuracy near 3 by comparing to a 1D analytic solution of melting. The spatial accuracy was calculated to be nearly 5th order for an approximation degree, *p*, equal to 4. Even for this simple case, the mesh adaption algorithm improved the accuracy over a simulation where the mesh only deformed. For a practical demonstration, the algorithm was used to simulate horizontal ribbon growth of single-crystal silicon and was able to resolve solutions where the solid layer thickness decreased by a factor of 20 over the course of the simulation.

1. Introduction

Simulating solidification is important for improving industrial processes such as spin-casting, crystal growth, and mold filling, however it is often difficult because the solid-liquid interface can take on complicated geometries and because the property jumps across the interface make the solution non-smooth. Fixed grid approaches, the most common of which is the phase-field approach (see review [1]), typically allow complicated interfacial geometries to be simulated but with the compromise of reduced accuracy near the interface. Arbitrary-Lagrangian-Eulerian (ALE) moving grid approaches provide greater accuracy near the interface but are less robust for problems with complex interfacial geometries. ALE formulations of solidification were first implemented in the late1970's to early1980's [2–5]. Since that time, many researchers have used this technique [6–13]. An advantage of using an ALE-FEM method is that higher-order spatial accuracy can be obtained by increasing the approximating polynomial degree (*P*). In [6,11] for example, the spectral element method [14,15] was used to obtain exponential convergence for a solidification problem. The drawback to this approach was that it required a quadrilateral or hexahedral mesh. This makes it difficult to use local mesh adaption procedures, thus neither of these works simulated complex interfacial shapes.

The goal of this paper is to develop an adaptive moving grid approach that maintains a high-order of spatial accuracy for solidification problems with complicated interfacial shapes. To allow large interfacial deformations a method for adapting moving meshes [16,17] is used. In [16], it was demonstrated that the adaptive/moving mesh approach could be used for crack propagation problems and for moving body problems with large displacements. However, in [16], it was observed that the mesh coarsening component of the algorithm created an overly coarse mesh and "severely degraded" the quality of the mesh. Other authors [18,19] have obtained good results by "coloring" the vertices before coarsening such that only every other vertex is removed, but this is only applicable to uniform coarsening. Most authors do not discuss whether the coarsening operations are ordered in anyway [20–23]. Another factor is that, while all algorithms collapse an edge to a point, some collapse to a midpoint [16,19,20] while others collapse to an endpoint [18,22,23]. In the following, these various approaches are examined to determine which, if any, can create high-quality coarse meshes.

To enable high-order accuracy, a continuous ALE *hp*-finite element method with triangular elements [24] is used. This method was demonstrated to give high-order accuracy for interfacial flow problems with moderate interfacial deformation. In this work, the approach is extended to solidification and combined with

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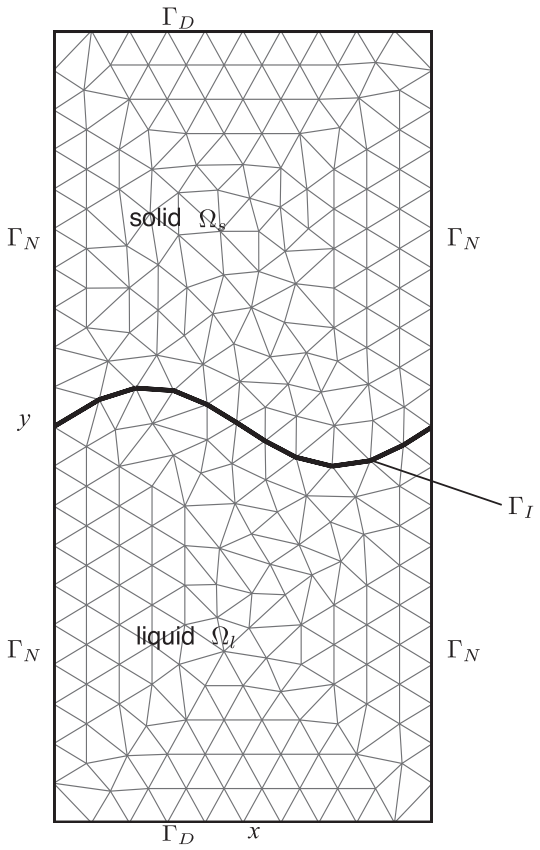

Fig. 1. Schematic showing the physical domain, spatial coordinates, boundary conditions, and typical mesh.

the adaption algorithm so that accurate solidification simulations can be performed with large changes in interfacial shape. An a-posteriori error estimate is used to set the target resolution of the mesh such that both the flow and temperature fields are adequately resolved. Demonstration problems include a solidification problem with an analytic solution where the size of the solid domain changes by a factor of 2 and horizontal ribbon growth where the thickness of the grown solid decreases by a factor of 20.

2. Governing equations

The basic problem is that of a solid and liquid separated by a solidification interface as shown in Fig. 1, which also shows a typical triangular mesh used for the calculations. The domain, Ω, is subdivided into two subdomains, Ω_s and Ω_l, where in all of the following subscripts of s and l denote solid and liquid respectively. The governing equation in the solid is the convection-diffusion equation

$$\frac{\partial \rho_s c_s T}{\partial t} + \frac{\partial \rho_s u_j c_s T}{\partial x_j} + \frac{\partial}{\partial x_j}\left(-k_s \frac{\partial T}{\partial x_j}\right) = 0, \tag{1}$$

where t and x_j are the temporal and spatial coordinates. Indicial notation is used and the problem is 2D so $j \in [1, 2]$. ρ is the density, c is the specific heat, k is the thermal conductivity, u_j is a specified rigid body velocity for the solid, and T is the temperature.

The governing equations in the liquid domain again include the heat equation except u_j is now the liquid velocity which is determined by the Navier-Stokes equations

$$\frac{\partial \rho_l u_i}{\partial t} + \frac{\partial \rho_l u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{i,j}}{\partial x_j} \tag{2}$$

$$\frac{\partial u_j}{\partial x_j} = 0, \tag{3}$$

where p is the fluid pressure and $\tau_{i,j}$ are the viscous stresses. The viscous stresses are given by a Newtonian relationship, $\tau_{i,j} = \mu(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j})$ where μ is the liquid viscosity.

The solid and liquid domains are separated by the solidification interface, Γ_I. Along the interface, the temperature is fixed at the melting temperature, T_m, for both the solid and liquid. This guarantees temperature continuity at the solidification interface. Mass conservation across the interface gives

$$[\![\rho(u_j - x_{j,t})n_{l,j}]\!] = 0, \tag{4}$$

where the double brackets indicate the jump in the quantity across the interface and the subscript with respect to t indicates a time derivative. $x_{j,t}$ is thus the velocity of the points on the interface. n is an outward normal; the change in sign for the jump is included by the opposite directions of the normal as defined from the solid and liquid domains. For this work, it is assumed that the solid and liquid densities are equal so that there is no jump in normal velocity across the interface. As there is also no jump in tangential velocity, the velocity is continuous across the interface. Furthermore, because the solid velocity is specified, the interface is a Dirichlet boundary condition for the flow where the flow velocities are set equal to the solid velocity.

Energy conservation across the interface gives

$$\left[\!\left[\left(\rho c T_m(u_j - x_{j,t}) - k\frac{\partial T}{\partial x_j}\right)n_{l,j}\right]\!\right] = \rho_s(u_j - x_{j,t})n_{l,s,j}L_f, \tag{5}$$

which says that the net energy flux to the interface is responsible for the conversion of solid to liquid with L_f being the latent heat of fusion.

On the boundaries of the domain denoted as Γ_D, Dirichlet boundary conditions are applied for the temperature. On boundaries denoted Γ_N, Neumann boundary conditions are applied. Note that Dirichlet boundary conditions cannot be applied on any boundary that intersects the interface as this would result in incompatible constraints on the temperature ($T = T_m$ or $T = T_{\Gamma_D}$). Boundary conditions must be supplied for the fluid as well and these may be either Dirichlet where both components of the velocity are fixed or Neumann where the stress on the fluid is specified. Initial conditions must be specified for the temperature in both the solid and liquid and for the fluid velocity in the liquid. Specific conditions will be described for each example problem presented.

3. Numerical formulation

To solve the above equations, unstructured triangular grids are generated for Ω_s and Ω_l that share common edges along the interface as shown in Fig. 1. An ALE approach is used where these edges are moved with the interface velocity. To reduce the deformation of the mesh as the interface moves, the remaining vertices in the mesh are also moved. To allow for this motion in the governing equations, the physical coordinates are replaced by unsteady curvilinear coordinates ξ_1, ξ_2, τ as follows

$$x_j = x_j(\xi_1, \xi_2, \tau) \qquad t = \tau. \tag{6}$$

This relation is used to define the mesh metrics, x_{i,ξ_j} as well as the inverse metrics ξ_{i,x_j} and the Jacobian, J, of the transformation, $J = x_{1,\xi_1}x_{2,\xi_2} - x_{2,\xi_1}x_{1,\xi_2}$ where the subscripts of x or ξ denote differentiation.

The field equations are then written in a weak form using the streamwise-upwind-Petrov–Galerkin (SUPG) approach. For the heat