A NUMERICAL FRAMEWORK FOR SOLIDIFICATION AND RESIDUAL STRESS MODELLING IN METALLURGICAL APPLICATIONS

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Quality of foundry products depends on the control of the solidification process; if the phase change is not managed correctly, residual stresses and material shrinkage shall result in loss of product quality. Physical modelling of solidification is particularly challenging: it requires a unified fluid-solid model capable of simulating fluid flow, heat transfer, solidification phase change as well as solid mechanics aspects of the resulting material.
We shall present a physical model capable of following the progress of the melt from injection/pouring of the molten phase into a batch or a continuous casting system and resolving heat transfer, flow of the fluid component, phase change and accumulation of residual stresses in the solid. The model is implemented in OpenFOAM and used to simulate transient 3-D casting process. Such a model is capable of predicting shrinkage and solidification effects and can be used in optimisation of casting systems, mould pressurisation and heat transfer management in foundry applications.
The model is currently validated on fluid and solid mechanics cases and basic fluid-solid interaction with a fixed phase interface.

Introduction

This paper describes a framework for modelling of solidification and residual stress distribution in metallurgical applications. The challenge in the process is in the assembly of a unified model covering both the fluid and solid phase with sufficient fidelity to capture the thermal front and the stress state at the point of solidification, which is the main source of residual stresses, volumetric imperfections and other quality-degrading features of the cast.
The challenge in solidification modelling is its "atypical" model of Fluid-Solid Interaction (FSI), where it is necessary to deploy a single equation set covering the whole process and the complete domain. In essence, this is trivial: conservation laws for mass, momentum and energy readily serve this purpose. However, the problem lies in the chosen constitutive law which needs to cover both the fluid and solid phase. In solids, material accumulates stress with the gradient of displacement, while in fluids the stress is results from the velocity gradient. In consequence, the natural choice of a working variable in solids is displacement or displacement increment and the stress tensor (when accounting for material or geometrical non-linearity), while in fluids the working variable is regularly the velocity $\mathbf{u}$ and pressure p.
The primary objective of this study is the simulation of cast shrinkage and residual stresses. To achieve this, it is necessary to follow the development of stress history from the point of solidification to final state, accounting for thermal stresses in the solid and temperature-dependent material properties. In solidification, a *mushy region* is assumed, with material properties of the solid shell and liquid melt dependent on temperature, and the progress of solidification is followed by a liquid fraction variable.
In what follows, we shall present the choice of appropriate working variable, conservation laws and constitutive relations covering the full range of solidification physics. The new model is validated on canonical cases of solid mechanics, fluid flow and conventional fixed interface fluid-solid interaction, in preparation for solidification studies.

Model Formulation: Solid Phase

A trivial solid mechanics model is a linear elastic model with constant material properties and displacement $\mathbf{d}$ as the working variable [1]. This, however, is not applicable to solidification, due to the presence of material non-linearity (temperature and solidification-dependent material properties) and geometric non-linearity (large deformations and rotations). Thus, the stress model formulation used in this study is the Large Deformation Stress Model in the incremental form, with the displacement increment $\delta\mathbf{d}$ chosen as a working variable [2]. The model is formulated as follows.

Non-Linear Stress Model

The choice of the solid phase model is driven by the need to account for all non-linearities in the system and at the same time align the formulation with the fluid flow model. In fluids, the choice of working variables is naturally the $(p, \mathbf{u})$ pair and we shall aim to achieve the same.
Second Piola-Kirchoff stress tensor increment $\delta\mathbf{\Sigma}$ is defined as:

$$\delta\mathbf{\Sigma} = 2\mu_s \delta\mathbf{E} + \lambda\, tr(\delta\mathbf{E})\mathbf{I}, \tag{1}$$

where μ_s and λ are the Lamé's coefficients, defined in terms of the material modulus of elasticity E and is the Poisson's ratio ν.
Green-Lagrangian strain tensor increment $\delta\mathbf{E}$ is defined as:

$$\delta\mathbf{E} = \frac{1}{2}\left[\nabla\delta\mathbf{d} + (\nabla\delta\mathbf{d})^T + \nabla\delta\mathbf{d}\bullet(\nabla\mathbf{d})^T + \nabla\mathbf{d}\bullet(\nabla\delta\mathbf{d})^T + \nabla\delta\mathbf{d}\bullet(\nabla\delta\mathbf{d})^T\right]. \tag{2}$$

In preparation to the model combination, introducing $\delta\mathbf{d} = \mathbf{u}\,\Delta t$ and writing $\delta\mathbf{\Sigma}$ the stress model can be rewritten in terms of $\mathbf{u}$, yielding the final form of the Green-Lagrangian strain tensor increment:

$$\begin{aligned}\delta\mathbf{\Sigma} = {} & \mu_s\,\Delta t\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^T + \nabla\mathbf{u}\bullet(\nabla\mathbf{d})^T + \nabla\mathbf{d}\bullet(\nabla\mathbf{u})^T + \Delta t\left(\nabla\mathbf{u}\bullet(\nabla\mathbf{u})^T\right)\right] \\ & + \lambda\,\Delta t\, tr\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^T + \nabla\mathbf{u}\bullet(\nabla\mathbf{d})^T + \nabla\mathbf{d}\bullet(\nabla\mathbf{u})^T + \Delta t\left(\nabla\mathbf{u}\bullet(\nabla\mathbf{u})^T\right)\right]\mathbf{I}.\end{aligned} \tag{3}$$

Integration formulas for displacement, strain and stress are used to accumulate the solid stress as a function of displacement (increment) and read:

$$\mathbf{d} = \mathbf{d}_0 + \int_0^t \mathbf{u}\, dt \approx \mathbf{d}_{old} + \mathbf{u}\Delta t \approx \mathbf{d}_{old} + \frac{1}{2}(\mathbf{u}_{old} + \mathbf{u})\Delta t, \tag{4}$$

$$\mathbf{E} = \mathbf{E}_0 + \int_0^t \delta\mathbf{E}, \tag{5}$$

$$\mathbf{\Sigma} = \mathbf{\Sigma}_0 + \int_0^t \delta\mathbf{\Sigma}, \tag{6}$$

where $\mathbf{d}_0$, $\mathbf{E}_0$ and $\mathbf{\Sigma}_0$ represent the initial displacement, strain and stress. At each time instance, the Cauchy stress $\boldsymbol{\sigma}$ can be recovered as:

$$\boldsymbol{\sigma} = \frac{1}{det(\mathbf{F})}\,\mathbf{F}\bullet\mathbf{\Sigma}\bullet\mathbf{F}^T, \tag{7}$$

where $\mathbf{F}$ is the deformation gradient tensor

$$\mathbf{F} = \mathbf{I} + (\nabla\mathbf{d})^T. \tag{8}$$

Linear momentum conservation law in the total Lagrangian formulation reads:

$$\int_{V_0} \rho_0 \frac{\partial\mathbf{u}}{\partial t}\, dV_0 = \oint_{S_0} \mathbf{n}_0\bullet(\mathbf{\Sigma}\bullet\mathbf{F}^T)\, dS_0 + \int_{V_0} \rho_0 \mathbf{f}_b\, dV_0, \tag{9}$$

where V_0, S_0, $\mathbf{n}_0$ represent the initial configuration of the system. This is remarkably similar to the fluid formulation of the momentum equation, barring the absence of the pressure gradient term.
The standard stress formulation of the above equation uses the $\mathbf{I}$ part of the $\mathbf{F}$ tensor to create the implicit terms and treats the rest as an explicit correction, accounting for model non-linearities.

Papadakis Solid Pressure Term Formulation

The non-linear solid stress model suffers from a particular failure mode, where the Poisson's ratio ν reaches the value of 0.5: the second Lamé coefficient λ tends to infinity.

$$\lambda = \frac{E}{3(1-2\nu)}; \;\; \nu = 0.5 \rightarrow \lambda \rightarrow \infty, \tag{10}$$

While $\nu = 0.5$ may be unrealistic for solids, in fluids it describes the state of incompressibility and the model failure for $\nu = 0.5$ must be circumvented. Note that realistic solids are never considered incompressible, meaning that λ remains bounded.
The following pressure manipulation is introduced by Papadakis into the $\nabla\bullet[\Delta t\,\lambda tr(\nabla\mathbf{u})]$ term in Equation 3, recognising that the pressure p is related to the trace of the stress tensor and divergence of the velocity field $\nabla\bullet\mathbf{u}$.
Introduction of the solid pressure term in the non-linear model yields a solid continuity equation, with the bulk modulus K:

$$K = \rho\frac{\partial p}{\partial \rho} = \frac{2}{3}\mu_s + \lambda = \frac{E}{3(1-2\nu)}, \tag{11}$$

defining the pressure (in the solid region!) as:

$$p = -\frac{1}{3} tr(\sigma) = -K \nabla \cdot \mathbf{d} \tag{12}$$

and yielding the final form of the linear stress equation

$$\sigma = -\left(p + \frac{2}{3}\mu_s \nabla \cdot \mathbf{d}\right) \mathbf{I} + \mu_s \left[\nabla \mathbf{d} + (\nabla \mathbf{d})^T\right] \tag{13}$$

The continuity equation is manipulated in terms of velocity $\mathbf{u}$. For a linear elastic material, the equation set reads:

$$\mathbf{u} = \frac{\partial \mathbf{d}}{\partial t}, \tag{14}$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) - \nabla \cdot \mu_s \left[\nabla \mathbf{d} + (\nabla \mathbf{d})^T\right] = -\left(1 + \frac{\mu_s}{3K}\right) \nabla p, \tag{15}$$

$$\nabla \cdot (\rho \mathbf{u}) = -\frac{\rho}{K} \frac{\partial p}{\partial t}. \tag{16}$$

For the non-linear material, the starting form is somewhat more complex (Equation 9); manipulation of the divergence term reads:

$$\Delta t\, \lambda tr(\nabla \mathbf{u}) = -\Delta t \left(p + \frac{2}{3}\mu_s \nabla \cdot \mathbf{u}\right), \tag{17}$$

whereas the solid continuity equation preserves the same form as in the linear case. With the above modification, the system is ready for the use in a blended solid-fluid model, using the $(p, \mathbf{u})$ as the primitive variables.

Thermal Stress Model

Curiously, within the same framework, thermal stresses can be handled in a straightforward manner. In linear elasticity, thermally induced stress is:

$$\sigma_T = 3\, K \alpha_E (T - T_0) \mathbf{I}, \tag{18}$$

where α_E is the thermal expansion coefficient and T_0 the reference temperature. This is clearly inconvenient for the formulation of displacement increment. As the spherical stress is extracted into the solid pressure, thermal stress can be accounted for as a change-of-volume term:

$$\frac{\rho}{K} \frac{\partial p}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 3\alpha_E \frac{\partial T}{\partial t}. \tag{19}$$

This is physically consistent and numerically convenient: any alternative formulation does not satisfy the integral volume increase in the solid. Physically, the *r.h.s.* of Equation 19 accounts for the volumetric expansion of a heated solid, as a part of the solid continuity equation.

Model Formulation: Fluid Phase

Fluid equations can assume the easiest form of the incompressible laminar flow with buoyancy effects, using the decomposition of the pressure into the dynamic and quasi-hydrostatic component [3]:

$$p_d = p - \rho\, \mathbf{g} \cdot \mathbf{x}, \tag{20}$$

where ρ is the density, $\mathbf{g}$ is the gravitational acceleration and $\mathbf{x}$ is the position vector, yielding a reformulated balanced momentum source term:

$$-\nabla p + \rho \mathbf{g} = -\nabla p_d - (\mathbf{g} \cdot \mathbf{x}) \nabla \rho, \tag{21}$$

The final form of the fluid phase equation set reads:

$$\nabla \cdot (\rho \mathbf{u}) = 0 \tag{22}$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) - \nabla \cdot (\mu \nabla \mathbf{u}) = -\nabla p_d + \mathbf{g} \cdot \mathbf{x} \nabla \rho \tag{23}$$

Model Formulation: Unified Non-Linear FSI Model

Formulation of the solid and fluid models are now well aligned. The total Lagrangian formulation in the incremental approach used the pressure p and velocity $\mathbf{u}$ as the base variable and match perfectly with the fluid model both in working variables and model layout. Therefore, conventional "fluids solution techniques" should be applicable to both.

As the working variables match perfectly between the solid model (Equation 16, Equation 9) and the fluid model (Equation 22, Equation 23), it remains to derive the combined model. Blending is performed using the liquid fraction variable α, combining governing equations for the fluid and the solid phase. The fluid model is recovered for $\alpha = 1$, while the other extreme of $\alpha = 0$ indicates solid behaviour. Presence of a mushy region is indicated by $0 \le \alpha \le 1$, assuming a linear combination of the two.

Some Validation Cases

In the first instance, the combined model shall be tested for "pure" fluid flow and solid mechanics. As the formulation and solution algorithm originates from the fluids, the flow validation cases are omitted. For solid mechanics, basic tests have been performed for: linear and non-linear elasticity and linear thermo-elasticity for cases with analytical solutions. In parametric studies of mesh refinement, time-step size and discretisation settings, the model performs perfectly across all cases, with examples of thermal expansion of a heated solid shown in Figure 1.
Conventional fluid-solid interaction cases can also be modelled without difficulty. In such cases, there exists a step change in the fluid fraction indicator α, delimiting the boundary between the fluid and solid. Examples of a travelling pressure wave in an elastic pipe and a fluid jet hitting an elastic membrane are shown in Figure 2.

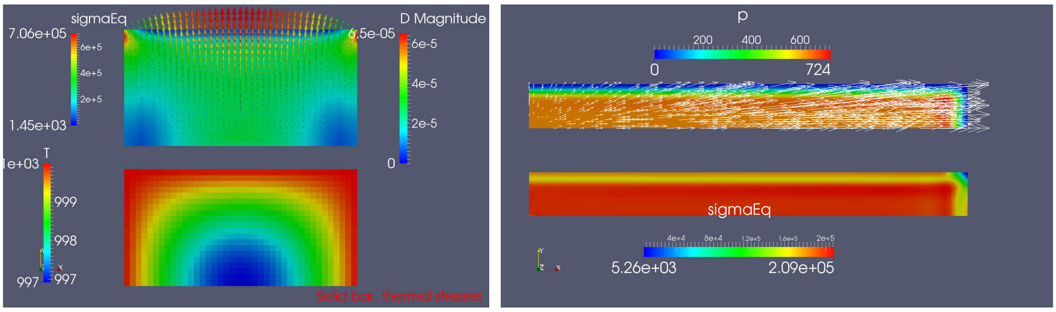

Figure 1: Combined FSI model for cases of thermal expansion of a solid brick and bar.

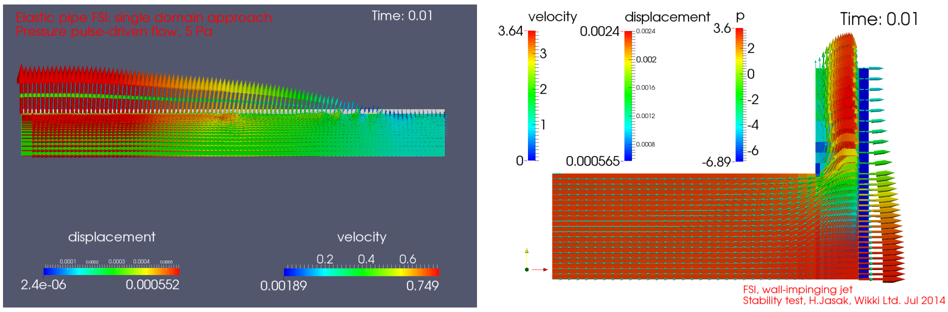

Figure 2: Conventional FSI cases: wave propagation in an elastic pipe and a jet impacting an elastic membrane.

The model can now be considered ready for solidification applications, with extensive validation and verification still in progress.

Conclusion and Future Work

This paper describes a combined model for fluid-solid interaction cases in the unified modelling approach, with the pressure p and velocity $\mathbf{u}$ chosen as the working set of variables. The solid model accounts for material and geometric non-linearities, include the novel handling of thermal stresses and is formulated in terms of the momentum and continuity equation to avoid the Lamé coefficient singularity at Poisson's ratio of $\nu = 0.5$. The fluid model is a conventional single-phase transient laminar non-Newtonian flow model.
The blended fluid-solid model uses a fluid fraction variable α to indicate the phase state and is capable of modelling the mushy zone solidification. At this stage the combined model is validated in the cases of pure fluid flow, various cases of linear and non-linear thermo-elasticity and simple fluid-solid interaction. The work towards a validated and verified solidification model continues and will be reported in further publications.

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