Finite element methods for problems with solid-liquid-solid phase transitions and free melt surface

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Modeling and computation of a process with solid-liquid-solid phase transitions and a free capillary surface is discussed. The main components of the model are heat conduction, a free melt surface, a moving phase boundary, and its coupling with the Navier-Stokes equations. We present two different approaches for handling the phase transitions by applying in a FE method, namely an energy conservation based approach, and a sharp interface approach with moving mesh. By combining both methods, we benefit from the advantages of the respective approach. The methods are applied to a problem where material is accumulated by melting the tip of thin steel wires using laser heating.

1 Introduction

In production of micro-components made of metallic wires, an accumulation process is often included. Conventionally, a multilevel cold-forming process is used. Unfortunately, the upset ratio defined by the quotient of upsetting length and wire diameter is strictly limited even in macro scale, and decreases a lot if the multilevel process is transferred to micro-components. Therefore, a two-level process based on laser melting is used. The top of a thin steel wire is molten by laser heating forming a material accumulation that solidifies again after the laser is switched off. The process benefits from size effects, namely the ratio of surface to volume causing surface tension become dominant compared to gravity [5].

This process can be modeled by coupling Navier-Stokes equations with a free surface and a Stefan problem. We present two methods for handling the phase transitions. The first one is based on energy conservation with mushy-region elements (enthalpy method) [3], and the second one applies a moving mesh method with a sharp interface [2]. Both approaches show advantages in different aspects, and are integrated in a FEM software. For problems including only on the Navier-Stokes equations with free capillary surface, research has already been done [1].

2 Mathematical model

The time dependent domain $\Omega(t) = \Omega_s(t) \cup \Omega_l(t) \cup \Gamma_S(t) \subset \mathbb{R}^3$ consists of a solid subdomain $\Omega_s(t)$, a liquid subdomain $\Omega_l(t)$ and a solid-liquid interface $\Gamma_S(t)$, as shown in Figure **1**, where initially $\Omega_l(0) = \emptyset$ and $\Gamma_S(0) = \emptyset$. In non-dimensional units, the scaled PDE-system is given by

$$\partial_t u + u \cdot \nabla u - \nabla \cdot \left(\frac{1}{\mathrm{Re}} \mathrm{D}(u) - p \mathrm{I_d} \right) = f_u(T) \qquad \text{in } \Omega_l(t), \quad (1)$$

$$\nabla \cdot u = 0 \qquad \text{in } \Omega_l(t), \quad (2)$$

$$\partial_t T + u \cdot \nabla T - \frac{1}{\mathrm{RePr}} \Delta T = f_{T,l} \qquad \text{in } \Omega_l(t), \quad (3)$$

$$\partial_t T - \frac{1}{\mathrm{RePr}} \frac{\kappa_s \rho_l c_{p,l}}{\kappa_l \rho_s c_{p,s}} \Delta T = f_{T,s} \qquad \text{in } \Omega_s(t), \quad (4)$$

with the boundary and initial conditions

$$u \cdot \nu = V_{\Gamma_C} \cdot \nu \quad \text{on } \Gamma_C(t), \qquad \frac{1}{\mathrm{RePr}} \partial_\nu T = g_R(T) \quad \text{on } \Gamma_C(t),$$

$$\sigma \nu = \frac{1}{\mathrm{We}} K \nu \quad \text{on } \Gamma_C(t), \qquad \frac{1}{\mathrm{RePr}} \frac{\kappa_s}{\kappa_l} \partial_\nu T = g_R(T) \quad \text{on } \Gamma_R(t),$$

$$u(\cdot, 0) = 0 \quad \text{in } \Omega_l(0),$$

$$T(\cdot, 0) = T_0(\cdot) \quad \text{in } \Omega(0), \qquad \frac{1}{\mathrm{RePr}} \partial_\nu T = 0 \quad \text{on } \Gamma_N(t).$$

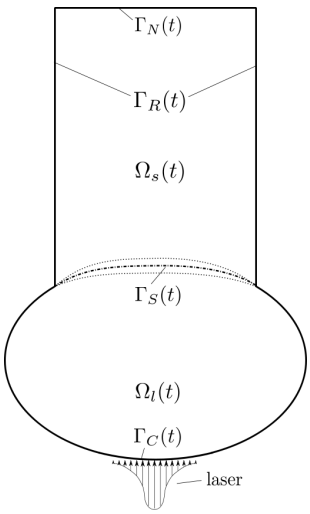

Fig. 1: Domain geometries

V_{Γ_C} denotes the velocity of the free boundary, Re the Reynolds number, Pr the Prandtl number, We the Weber number, K the sum of the principle curvatures and $\sigma := \frac{1}{\mathrm{Re}} D(u) - p\mathrm{I_d}$ is the stress tensor. The temperature is scaled so that $T_{\mathrm{melt}} = 0$.

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2.1 Phase transition approach I: Energy conservation

The first approach bases on the Stefan problem that formulates the energy balance in the whole domain and is given by

$$\partial_t H + u\nabla H - \frac{1}{\mathrm{RePr}}\Delta T = 0 \qquad \text{in } \Omega_{l,s}, \qquad \text{where} \quad T = \alpha(H) := \begin{cases} \frac{1}{c_s}H, & H < 0 \\ 0, & H \in \left[0, \frac{1}{\mathrm{Ste}}\right] \\ H - \frac{1}{\mathrm{Ste}}, & H \geq \frac{1}{\mathrm{Ste}} \end{cases}$$

describes the temperature-enthalpy relation. Ste denotes the Stefan number and $u \equiv 0$ in Ω_s. In general, this approach leads to a mushy-region describing the interface $\Gamma_S(t)$. For the calculation of the fluid flow by FEM, it is a-priori not clear how to treat the mushy-region elements numerically. For simplification, we therefore assume these elements to be solid as long as the temperature at one of its nodes is less than the melting temperature.

2.2 Phase transition approach II: Moving mesh with a sharp interface

The second method is a moving mesh approach with a sharp interface. For this approach, conditions for u, T and for the normal velocity of the interface V_{Γ_S} are prescribed on $\Gamma_S(t)$

$$\begin{aligned} u \cdot \nu &= \left(1 - \frac{\rho_s}{\rho_l}\right) V_{\Gamma_S} \cdot \nu, \\ u - u \cdot \nu\, \nu &= 0, \\ T &= 0, \\ \frac{1}{\mathrm{RePr}}\left[(\nabla T)_l - \frac{\kappa_s \rho_l c_{p,l}}{\kappa_l \rho_s c_{p,s}}(\nabla T)_s\right] &= \frac{1}{\mathrm{Ste}} V_{\Gamma_S}. \end{aligned}$$

The Stefan condition in the last equation reflects thermal energy balance which is used to obtain the movement of the interface $\Gamma_S(t)$. In a corresponding FE method, the mesh is now moved accordingly to the movements of $\Gamma_S(t)$ and the capillary surface $\Gamma_C(t)$. A detailed description of the method is given in [2].

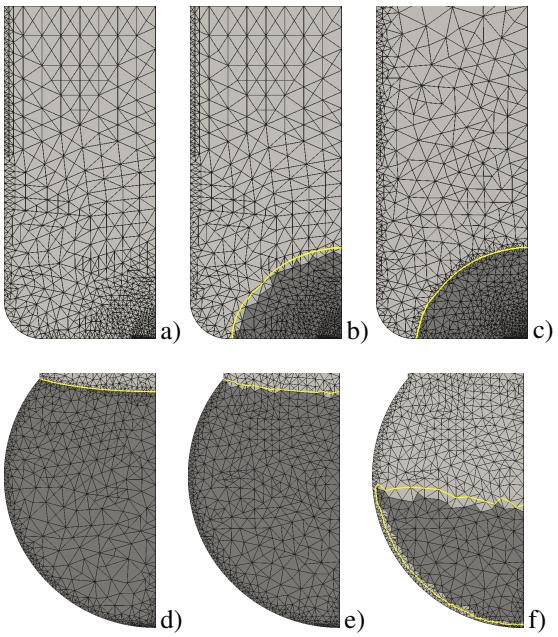

Fig. 2: Visualization of simulation results: The dark gray indicates the molten and the light gray indicates the solid material. Both domains are separated by $\Gamma_S(t)$. In **a** the initial state of the solid component is given, **b** and **c** visualize the first change of method, and **d** and **e** the second change after the laser is switched off. **f** shows the typical characteristics of temperature-isolines during the solidification process.

3 Finite Element Simulations

Both methods for treating the phase transitions during the process are combined and included in the FE-software `NAVIER` [1]. During nucleation of the liquid phase, the approach based on energy conservation is applied to the problem. Due to our simplification of the mushy region, sudden phase changes of elements at the free capillary surface can result in oscillations and non-physical behavior.

To avoid these problems, we switch to the moving mesh method after a sufficient subdomain of the component has been molten. Therefore, a sharp solid-liquid interface $\Gamma_S(t)$ is obtained by interpolation and a new mesh containing this interface is generated by `TRIANGLE` [4]. Due to its movement, the mesh quality can decrease, so including a remeshing procedure is mandatory.

Unfortunately, the moving mesh approach cannot handle the solidification process because of the different relation between triple point and mesh movement in contrast to the relation during the melting process. Hence, after the laser is switched off and the direction of the movement of the interface changes, the method is switched to the first method again to simulate the solidification process. In contrast to the melting process, the change of the geometry during solidification is very small and no oscillation arise due to phase changes of whole elements. The important steps and simulation results are shown in Fig. **2**.

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