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Non-residual-based stabilization formulation for liquid-solid phase-change flows including macrosegregation scenarios

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We present a variational multiescale (VMS) finite element method algorithm to solve liquid-to-solid phase-change problems, including macrosegregation. If $\nabla^s \boldsymbol{u} = \frac{1}{2}(\nabla \boldsymbol{u} + [\nabla \boldsymbol{u}]^T)$ is the symmetrized velocity gradient, the conservation governing equations solved in $Q = \Omega \times \Upsilon$ are the linear momentum, the continuity, the energy equation and the concentration of species given by:

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} - \nabla \cdot (2\mu \nabla^s \boldsymbol{u}) + \nabla p + \boldsymbol{\mathcal{K}}_\varepsilon(f_s, \boldsymbol{u}) = \boldsymbol{f},$$
$$\nabla \cdot \boldsymbol{u} = 0,$$
$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \boldsymbol{u} \cdot \nabla T - \kappa \Delta T = \rho L \frac{\partial f_s}{\partial t}$$
$$\frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \nabla c_l = 0,$$

with $\boldsymbol{f} = \rho \boldsymbol{g}\left(1 - \beta_T(T - T_r) - \beta_c(c_l - c_r)\right)$ the volumetric force term modeling the coupling between the linear momentum equation and the temperature and concentration fields through a double diffusion mechanism, including natural heat and mass convection. The liquid-solid phase change phenomena is described with a modified Carman-Kozeny model:

$$\boldsymbol{\mathcal{K}}_\varepsilon(f_s, \boldsymbol{u}) = \frac{C_0 \mu f_s^2}{\lambda^2[(1 - f_s)^3 + \varepsilon]}\boldsymbol{u},$$

with $C_0 > 0$, λ the interdendritic space, and the numerical parameter $\varepsilon > 0$ used to avoid numerical singularity when $f_s = 1$. The liquid concentration c_l is calculated by the equation

$$c_l = \frac{c}{1 - (1 - r)f_s},$$

and the solid fraction f_s by using the phase diagram and the level rule.

The VMS framework allows equal-order interpolation for all variables and convective dominant scenarios. The formulation has a dynamic term-by-term structure, which reduces the number of stabilization terms to the minimum, ensuring optimal order of convergence of the solved fields [1]. Since the problem involves coupling of the velocity, pressure, temperature and species concentration fields, the resolution algorithm of the equations is important. This work proposes an orthogonal and dynamic term-by-term stabilization to approximate numerically liquid-solid phase change flows, including macrosegregation scenarios [4]. We present convergence test to highlight the optimal convergence order of the stabilized formulation used, the validation of the method with classical numerical and experimental benchmarks, and the approximation of a Pb-Sn binary alloy problem that generates convection plumes.

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