

3D adaptive finite elements with high aspect ratio for the computation of dendritic growth with convection

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In phase field models of solidification, the location of the solid and liquid phases in the computational domain is described by introducing an order parameter, the phase field, which varies smoothly from one in the solid to zero in the liquid through a slightly diffused interface. The solidification process of binary alloys is controlled by the local concentration of the alloy and the temperature. The concentration is altered by the existing flows in the melt. With temperature being a given constant, the model corresponds to coupling the phase-field equation, the concentration equation and the compressible Navier-Stokes equations.

The main difficulty when solving numerically phase field models is due to the very rapid change of the phase field and the concentration field across the diffuse interface, whose thickness has to be taken very small (between 1 and 10 nm) in comparison to the dimension of the computational domain (approximately 1mm) in order to correctly capture the physics of the phase transformation. A high spatial resolution is therefore needed to describe the smooth transition.

The computational time and the number of grid points can be drastically reduced using adaptive finite elements with high aspect ratio. Adaptive algorithm aims to build successive tetrahedral meshes with large aspect ratio such that the relative estimated error of the concentration c in the $L^2(0, T; H^1(\Omega))$ norm is close to a preset tolerance TOL , Ω being the computational domain and T the final time of the simulation. For this purpose, we introduce an error indicator which measures the error of the concentration c in the directions of maximum and minimum stretching of the tetrahedron. The goal of the adaptive algorithm is then to equidistribute the error indicator in the directions of maximum and minimum stretching, and to align the directions of maximum and minimum stretching with the directions of maximum and minimum error. The applied technique allows to perform the simulations of dendritic growth of several dendrites with interface thickness being of the order of 10^{-3} of the domain size with less than 200.000 mesh points, thus making the simulations possible on the standard workstations.

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