3D direct simulation of growth and development during phase change using high performance computing

Luisa Silva**,** Hugues Digonnet [ς]

* Institut de Calcul Intensif, Ecole Centrale de Nantes, Nantes, 44321, Nantes.
Email: luisa.rocha-da-silva@ec-nantes.fr

* Institut de Calcul Intensif, Ecole Centrale de Nantes, Nantes, 44321, Nantes.
Email: hugues.digonnet@ec-nantes.fr

This work aims to better understand and predict structure development during phase change in material science, by building a specific numerical application. Simulation capabilities developed are based on a multiphase formulation, which includes temperature and eventually non-crystallographic branching computations, at the scale of the microstructure.
An implicit boundary method, of the phase-field type, provides the solid/liquid interface displacement by solving an hyperbolic convective-redistancing problem. Energy and orientation/misorientation solvers provide the local value of the interface growth velocity. All are based on linear discretizations and stabilized finite element methods. Such a complex physics is solved in a reasonable time using adaptive anisotropic meshing and parallel computing. Algorithms implemented and results obtained in 2D and 3D structure development illustrate the methodology, the latter being compared to experimental and other numerical cases issued from the literature.

Keywords: Solidification, growth kinetics, adaptive level-set methods, high performance computing