Phase-field modeling of solute precipitation / dissolution using MOOSE: A finite element method

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Phase field model is believed as a successful method to compute interfacial problems without explicit computing of the moving interface instead of level set method. The dynamic of solid-liquid interface controlled by solute precipitation and/or dissolution due to chemical reaction at the interface were simulated in this study. The simulation was solved by finite element method and implemented using MOOSE, a framework developed by Idaho National Laboratory to solve partial differential equation by preconditioned Jacobian-Free Newton-Krylov (PJFNK) solution approach. MOOSE is able to help domain scientists to easily implement the equations and solve the solution by finite element methods instead of writing very complicated codes.

Two-dimensional reaction-limited and diffused-limited dendrite growth cases were setup to demonstrate the relationship between reaction and diffusion. Random noise was introduced in order to generate sidebranch of dendrite under an anisotropic precipitation environment. Some dissolution cases are also created with convection term added. There are still some difficulties to simulate the solid finger effect under diffusion-limited precipitation case, and the relationship of different results from the finite element and finite difference method are not quite clear. However, the phase field model results in this study were still reasonable agreement with the results from other methods.