UNIVERSITY of HOUSTON

Department of Mathematics

Scientific Computing Seminar

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Numerical Simulation of the Formation of Spherulites in Polycrystalline Binary Mixtures

Monday, April 25, 2022
3 PM- 3:50 PM
Room 646 PGH

Abstract: We consider a space-time adaptive splitting scheme for the numerical simulation of the formation of spherulites in polycrystallization processes described by a two-field phase field model. The phase field model consists of a coupled system of evolutionary processes for the local degree of crystallinity ϕ and the orientation angle Θ one of them being of first order total variation flow type. The splitting scheme is based on an implicit discretization in time which allows a decoupling of the system in the sense that at each time step minimization problems in ϕ and Θ have to be solved successively. The discretization in space is taken care of by a standard finite element approximation for the problem in ϕ and Θ an Interior Penalty Discontinuous Galerkin (IPDG) approximation for the one in Θ. The adaptivity in space relies on equilibrated a posteriori error estimator for the discretization errors in ϕ and Θ in terms of primal and dual energy functionals associated with the respective minimization problems. The adaptive time stepping is dictated by the convergence of a semismooth Newton method for the numerical solution of the nonlinear problem in Θ. Numerical results illustrate the performance of the adaptive space-time splitting scheme for two representative polycrystallization processes.

* The results are based on joint work with Basanta Pahari and James Winkle.

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This seminar is easily accessible to persons with disabilities. For more information or for assistance, please contact the Mathematics Department at 743-3500.