11c Developing Quantitative, Multi-Scale Models for Melt Crystal Growth

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The quantitative prediction of incompressible flows, heat transfer, and solute segregation would be of great utility for understanding and developing microgravity crystal growth experiments. In fact, the successful development of such models will enable two modes of use --- as diagnostic aids to explain experimental observations in Earth-bound and microgravity environments and as predictive tools to assess processing operations in these differing environments.

For such models, methods are needed to provide quantitatively realistic boundary conditions depicting furnace-level heat transfer to codes developed to solve for incompressible flow of the melt, heat transfer, and solidification. This presentation focuses on the development of a multi-scale, multi-physics model for melt crystal growth. A global model, CrsyVUn, that computes high-temperature, furnace heat transfer, is coupled with a local model, Cats, that solves for heat transfer, incompressible melt flow, and melt-crystal interface shape. These models are solved using an iterative scheme to compute a self-consistent solution. Sample results demonstrate the need for such an approach vis-a-vis simpler solution strategies that employ one-way coupling of the models.

We discuss several mathematical and computational issues arising from the coupling of these nonlinear models. The framework of fixed-point iterations is employed to assess the convergence behavior of a modular, block Gauss-Seidel iteration of the independent models. Certain choices of coupling the models that are physically reasonable are shown to result in algorithms that will never converge, demonstrating that notions based on physical intuition may not be useful for predicting algorithm performance. Finally, we present recent work implementing approximate-Newton algorithms using strongly coupled iterations. These methods promise convergence rates approaching quadratic and far greater robustness compared to the loosely coupled, block Gauss-Seidel approach.