Control problems in crystal growth processes

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Crystal growth processes involve many different related physical mechanisms, which interact on very different spatial and temporal scales. Mathematically, this is expressed by a hierarchy of weakly coupled models of pdes. In model-based simulation this weak coupling of the different components in the models can be used to derive algorithms which relate microscopic crystal properties to macroscopic growth parameters. Model-based optimization is 'dual' to the model-based simulation in the sense that its hierachy is directed from specific microscopic to more general macroscopic pde models. Output variables of the different models in the simulation loop take now the role of gains, and input variables those of control parameters. In this spirit model-based optimization and design of crystal growth processes are formidable tasks whose solution not only neccesitates interdisciplinary efforts of applied mathematicians and process engineers. It moreover also serves as prototyping test application for the development and specification of new mathematical and numerical approaches in the emerging field of optimization problems with systems of coupled nonlinear pdes.

As model design applications we discuss control of the crystal melt considering as mathematical model the Boussinesq approximation, and control of solidification for a sharp interface model. In addition to numerical examples we also present the first steps towards a rigorous analysis of the underlying optimization problems.