Zusammenfassung des Projektes:

"Optimization problems governed by Cahn-Hilliard variational inequalities"

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Optimierung mit partiellen Differenzialgleichungen

Summary:

The aim of this project is to develop efficient numerical methods to *control interface evolution* governed by Cahn-Hilliard variational inequalities. The applications range from quantum dot formation in *crystal growth* of heteroepitaxial *thin films* and *grain growth* to void evolution in microelectronic devices. In all these applications a certain location of phases or special properties of the interface distribution are of importance.

The Cahn-Hilliard model is a conserved phase field model based on a diffuse (not sharp) interface. The underlying free energy is related to the interfacial thickness and includes an obstacle potential. The model is usually formulated as a non-standard *variational inequality of fourth order*. The current state of the art provides numerical simulation mainly to study the evolution and various appearing phenomena. They are not fast enough to be used as a simulation solver for control purposes. Hence an efficient method has to be developed for the Cahn-Hilliard model. The semi-implicit time discretization of this Cahn-Hilliard model can be viewed itself as a control problem with possibly *nonlinear constraints, control box constraints* and a highly *complex cost function*, which includes semi-norms and non local behaviour of the control function. Hence the evolution of interfaces can be simulated by a sequence of optimization problems, where the inputs change with time. The control of interface evolution can be seen as a process of *nested optimization*. This will be the starting point for our numerical approach. In order to solve the control problem corresponding to the Cahn-Hilliard model we wish to study the application of the *primal-dual active set strategy* and/or a *semi-smooth Newton method*. While on the first glance the optimization formulation falls into the class, where convergence is guaranteed, it is not obvious whether all convergence conditions are fulfilled. This is one of the first issues which has to be clarified. Here, due to the time stepping local convergence is sufficient. The next question to clarify is how to apply the primal-active set strategy efficiently due to the semi-norms in the cost function. Issues as *preconditioning, adaptivity and efficient time stepping* must be approached. The goal is to derive a mesh independent, *superlinear convergent* method where the dependence on the interfacial thickness is moderate. In practical applications the Cahn-Hilliard variational inequality has to be coupled either to an elliptic system or to a nonlinear heat equation. Hence, when efficient methods are developed for Cahn-Hilliard variational inequalities, these have to be generalised to the extended versions.

The final goal is to solve *optimal control problems* in which the extended versions of the Cahn-Hilliard variational inequality act as constraints. In addition to the *highly nonlinear constraints* the cost functional is often *non-convex* and gradient based. First we

plan to study this optimal control problem, which falls into the class of MPEC's, analytically. We wish to derive first and second order optimality conditions as well as the *existence of Lagrange multipliers*. In a second step it is planned to design and implement a fast solver for the optimal control problem with superlinear convergence. Since it does not seem promising to obtain smoothness of the solution operator concerning the variational inequality and of the remaining constraints, we target the application of a semi-smooth Newton-type method also for this overall control problem. *Optimal design problems* involving Cahn-Hilliard variational inequalities shall also be an issue.