Model Validation and Optimum Experimental Design of Partial Differential Equations

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Mathematical models are of great importance for manufacturing and engineering. Besides providing a scientific insight into processes, the mathematical models are used in process optimization and control. However, the results from simulation and optimization will only be reliable if an underlying model precisely describes a given process. This implies a model validated by experimental data with sufficiently good estimates for model parameters. Often many expensive experiments have to be performed to obtain sufficiently good estimates of the parameters. The number of experiments can be drastically reduced by computing optimal experiments.

In recent decades, powerful and efficient methods for model calibration and design of optimal experiments for ordinary differential equation (ODE) models have been developed. First steps towards model validation of partial differential equations (PDE) have been made by semi discretization in space, which transforms the PDE into a huge system of ODEs. In this case, it is not possible to use modern methods for PDE constrained optimization. Consequently, it is hardly possible to solve the problem on standard computers.

To cope with this problem, we combine modern methods for PDE constrained optimization with established approaches for model validation. The optimum experimental design problem is not of standard type. In order to consider the finite measurement time points, the problem is formulated as a multistage optimization problem. Furthermore, the evaluation of the objective function requires the computation of derivatives. Despite these problems, this dissertation successfully adapts the adjoint approach for the computation of the reduced gradient. Furthermore, the thesis presents a positive definite approximation of the second order derivatives, which can be computed very efficiently by adjoint PDEs.