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Numerical Methods for Nonlinear Parameter Estimation and Optimum Experimental Design in Differential Equation Systems

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Abstract

We consider process models given by nonlinear ordinary differential equations, differential algebraic equations or partial differential equations with initial and boundary conditions. Developing quantitatively correct models is typically a difficult and time consuming procedure that requires the solution of challenging optimization problems at several stages. In particular nonlinear parameter estimation and nonlinear optimum experiment problems have to be solved.

The talk reviews the well proved so-called Boundary Value Problem Methods for parameter estimation in large-scale differential algebraic equation systems and reports on recent developments. As versatile realization a direct multiple shooting method is described. The properties and performance of a class of Generalized Gauss Newton methods for the resulting structured constrained regression problems is discussed.

Direct approaches for the solution of state constrained optimal control problems arising in nonlinear optimum experimental design for parameter estimation and model discrimination are presented. For the treatment of uncertainty sequential procedures combined with robust optimization methods are suggested.

Benchmark problems as well as industrial applications including chemical reaction kinetics and transport and degradation processes for xenobiotics in soil are discussed in order to demonstrate the features and the scope of applicability of the methods.