Optimization-Based Model Validation – a Mathematical Technology of High Economic Impact

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Abstract: Validated dependable mathematical models are of ever growing importance in science and engineering, and today also driven by a serious demand of the industry. Apart from providing scientific insight into complex nonlinear processes, mathematical models are fundamental for process simulation, optimization and control. In this context the new paradigmatic concept of "digital twins" may be worth mentioning, which is becoming more and more attractive among researchers from different industrial companies, and is advocated by NASA, GE, Siemens and others. Its idea is that every new system, product or a physical or economical process should be accompanied by a "digital twin", which comprises an ensemble of mathematical models and algorithms. This collection of models, analysis and solution algorithms a virtual avatar or virtual double would ideally accompany the process from the "origin" through its life time, "grow" together with this process, and be used among others to analyze data, predict malfunctioning and perform optimal operation. However, the application of mathematical models for the simulation, and even more for the optimization and control of complex engineering processes requires their thorough validation and calibration by parameter and state estimation based on process data, which should preferably be obtained by optimized experiments, and optimized measurement designs. For the latter, very efficient numerical methods for the complex non-standard optimal control problem of optimal experimental design for dynamic processes were developed, which have proven to be a powerful mathematical technology of high economic impact in industrial practice – often cutting experimental costs by a factor of 5 to 10!

The talk will address new developments in optimization methods for validation and calibration of models, in particular the design of robust optimal experiments based on a second order sensitivity analysis of parameter estimates and design of optimal experiments for PDE models.

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