

## VPLAN - A Tool for Optimization Based Modeling

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In this talk we present our approach of optimization based modeling, discuss our mathematical and numerical methods, show our implementation in the software package VPLAN and present its application to examples from industry. We consider industrial processes, e.g. from chemical industry, which are modeled by nonlinear systems of differential equations. To calibrate the models against experimental data, we use tailored methods for parameter estimation based on the boundary value problem optimization approach with multiple shooting and generalized Gauß-Newton methods. A sensitivity analysis yields the statistical uncertainty of the estimate, described by the variance-covariance matrix which depends on the experimental settings. The task of minimizing the uncertainty leads to optimum experimental design problems. These are non-standard constrained optimal control problems. We discuss our numerical approaches for the solution based on the direct approach of optimal control, Quasi-Newton-type optimization methods and a tailored derivative evaluation. We have implemented our methods for model validation in the software package VPLAN using PARFIT and DAESOL and providing a virtual laboratory for simulation, parameter estimation and optimum experimental design. We give an introduction to the structure and the features of this software and discuss application strategies and results for practical problems from our industrial and academic partners.