Model-based Optimizing Control-
from a vision to industrial reality

mobocon

Lehrstuhl für Systemdynamik
und Prozessführung

UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386

IWR
Interdisciplinary Center
for Scientific Computing

Workshop on Model-based Optimizing Contol

From a vision to industrial reality

June 9-10, 2016, Heidelberg

SEVENTH FRAMEWORK
PROGRAMME

erc
European Research Council
Established by
the European Commission

Venue

Address

Mathematikon
Room 5.104
Im Neuenheimer Feld 205
69120 Heidelberg

How to get here

Take the train to Heidelberg main station. Exit the station to the north and continue with lines 21 or 24 towards Handschuhsheim. Exit at stop Bunsengymnasium and cross the road to the main entrance of the Mathematikon.

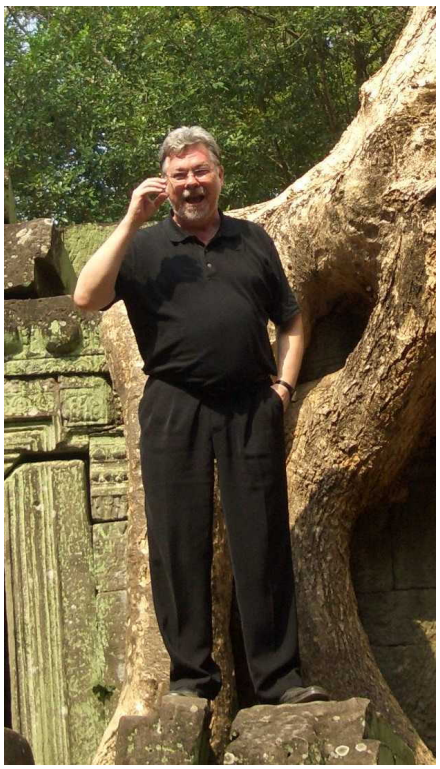
Organization

"Model-based Optimizing Control - from a vision to industrial reality" (MOBOCON) is a European research project co-financed by the European Commission in the 7th Framework Programme (ERC Advanced Grant).

The goal of this project is to overcome obstacles for the industrial application of optimization-based control by developing methods for the enhanced robustness and failure tolerance and for the reduction of the modeling effort as well as by developing new concepts for the interaction with the plant operators.

For more information, visit
http://www.mobocon.eu/CMS/index.php/project.html.

Prof. Dr. Sebastian Engell, Process Dynamics and Operations Group of the Department of Biochemical and Chemical Engineering of TU Dortmund, (Principal Investigator) and Prof. Dr. Hans Georg Bock, Interdisciplinary Center for Scientific Computing of Universität Heidelberg, (Co-Investigator) have been selected for this ERC Advanced Investigator Grant by the expert panel of the European Research Council.

The two researchers have already been closely cooperating in the field of optimization-based control for years. The goal of this project is to overcome obstacles for the industrial application of optimization-based control by developing methods for the enhanced robustness and failure tolerance and for the reduction of the modeling effort as well as by developing new concepts for the interaction with the plant operators. In addition, the idea of optimizing control will be extended to the start-up and shut-down of plants where discrete switches take place.

The project includes experimental validation and demonstration, in particular for a reactive distillation column in pilot plant scale in cooperation with the Fluid Separations Group at TU Dortmund headed by Prof. Andrzej Gorak.

Workshop Program

Thursday, June 9

08:30	Registration
09:00	H. G. Bock: Welcome
09:15	S. Engell: mobocon - an overview
09:35	W. Gao: Fusion of data and models to enable a reliable real-time optimization
10:10	D. Hasskerl: Multi-rate state estimation applied to a model of a reactive distillation process
10:45	Coffee break
11:15	A. Potschka: Backward step control
11:50	R. Paulen: Guaranteed parameter estimation for nonlinear dynamic systems
12:25	L. Wirsching: Fast NMPC with Multi-Level Iterations
13:00	Lunch break
14:00	Modeling day on Optimization http://www.modellierungstag.de
18:00	Dinner

Friday, June 10

09:00 S. Subramanian: Robust and optimal operation of an industrial polymerization reactor under model uncertainties and measurement errors

09:35 C. Leidereiter: Efficient numerics for robust Multi-Stage NMPC with application to a biochemical benchmark problem

10:10 A. Tatulea-Codrean, C. Lindscheid: do-mpc - A platform for the development and implementation of robust NMPC solutions in industry

10:45 Coffee break

11:15 H. C. La: The theory and numerics of dual control with application to a biochemical benchmark problem

11:55 A. Meyer: A Multi-Level Iteration mode based on the trapezoidal rule with application to a biochemical benchmark problem

12:25 J. Gutekunst: NMPC for models with periodic stages

13:00 Lunch break

14:00 R. Lemoine: An approach for speeding up the online Design of Optimal Experiments and its application to the Simulated Moving Bed process

14:35 R. Hashemi: Optimizing control and state estimation of a continuous polymerization process

15:10 Coffee break

15:40 S. Thangavel: Improving performance of robust economic NMPC using dual control: Application to chemical reaction systems

16:15 Closing remarks

16:30 End of the workshop

Talk abstracts

Thursday, June 9, 2016

Fusion of data and models to enable a reliable real-time optimization

Weihua Gao, weihua.gao@bci.tu-dortmund.de

The presentation deals with real-time optimization, i.e. the optimization of stationary operating points of complex systems, in particular chemical plants. In real-time optimization, and in model-based optimization in general, the mismatch between the model that is used in the optimization and the true behaviour of the system of which the performance is optimized is a fundamental issue.

In model-based real-time optimization, plant-model mismatch can be handled by applying corrections to the cost functions and to the constraint functions in an iterative optimization procedure. The corrections modify the gradients of the cost function and of the constraints as well as the values of the constrained functions based upon measurements at past operating points. This procedure leads to iterative convergence to the true optimum of the plant in the presence of plant-model mismatch. One of the major challenges in the application of this approach is the estimation of the plant gradients from noisy measurement data, in particular if

several optimization variables have to be considered. We propose a new real-time optimization scheme that explores the inherent smoothness of the plant mapping to obtain a reliable optimization scheme. The basic idea is to combine the quadratic approximation approach used in derivative-free optimization techniques with the iterative gradient-modification optimization scheme. The gradients can then be computed from the quadratic approximation instead of finite differences between observations. The convergence of the scheme is analyzed and simulation studies for the optimization of a ten-variable synthetic example and a reactor benchmark problem with considerable plant-model mismatch are shown. It is demonstrated that the scheme in much less vulnerable to measurement noise and converges faster than finite-difference based approaches.

Multi-rate state estimation applied to a reactive distillation process

Daniel Haßkerl, daniel.hasskerl@bci.tu-dortmund.de

In chemical plants one key factor for the reliable functioning of model based optimizing control is to have complete information on the current state of the underlying process. If the system is observable, an estimation of the full state of the process can be performed by state estimation methods. In order to make the best possible use of all available measurements, recent formulations of state estimators include measurement information at different sampling intervals – called multi-rate sampling. In the example process, a pilot-scale reactive distillation (RD) column, different sampling instances have to be considered as fast temperature measurements and slower product concentration measurements from near-infrared spectroscopy (NIR) are available. We have investigated two different multi-rate state estimation techniques for DAE-systems, the Extended Kalman Filter (EKF) and the Particle Filter (PF) and have applied these techniques to the large-scale process model of the reactive distillation pilot plant. The performance of the two state estimation techniques was investigated in simulation studies. The EKF and PF show a similar performance. Because the EKF can be implemented in real-time and achieves the required accuracy of the estimation, the EKF is considered for the future work.

Backward step control

Andreas Potschka, potschka@iwr.uni-heidelberg.de

This talk focuses on progress for the fundamental and widely used numerical methods of Newton-type: Backward step control is a novel step size selection method for the globalization of convergence of Newton-type methods for nonlinear root finding problems.

The advantages of the globalization strategy comprise a simple yet efficient implementation and a rigorous convergence analysis based on generalized Newton paths. Under reasonable assumptions, the results of the convergence analysis include full steps in the vicinity of a solution, a lower step size bound, a priori guarantees for the nonlinear decrease of the residual norm, and convergence to a distinguished root, namely the end point of the generalized Newton path emanating from the initial guess. The last property is a tremendous advantage for practitioners also in optimization, because it reduces the sensitivity of the result of the computation with respect to initial guesses. Moreover, because the algorithm and its theory can be stated in a Hilbert space setting, the method is especially appealing for large-scale problems that originate from discretizations of infinite dimensional problems, e.g., in optimal control.

In addition, the framework delivers suitable relative termination tolerances for inexact residual minimizing Krylov-Newton methods. We conclude the talk with numerical results for a boundary value problem resulting from optimal control and the minimal surface partial differential equation.

Guaranteed parameter estimation for nonlinear dynamic systems

Radoslav Paulen, radoslav.paulen@bci.tu-dortmund.de

This talk is concerned with guaranteed parameter estimation of nonlinear dynamic systems in a context of bounded measurement error. The problem consists of finding, or approximating as closely as possible, the set of all possible parameter values such that the predicted values of certain outputs match their corresponding measurements within prescribed error bounds. A set-inversion algorithm is applied, whereby the parameter set is successively partitioned into smaller boxes and exclusion tests are performed to eliminate some of these boxes, until a given threshold on the approximation level is met. Such exclusion tests rely on the ability to bound the solution set of the dynamic system for a finite parameter subset, and the tightness of these bounds is therefore paramount. Equally important in practice is the time required to compute the bounds, thereby defining a trade-off. In this talk, we discuss such a tradeoff by comparing various bounding techniques based on Taylor models with either interval or ellipsoidal bounds as their remainder terms. We also investigate the use of optimization-based domain reduction techniques in order to enhance the convergence speed of the set-inversion algorithm, and we implement simple strategies that avoid recomputing Taylor models or reduce their expansion orders wherever possible. We additionally discuss the problem of optimal experiment design in the context of guaranteed parameter estimation. Finally several case

studies are presented, which show the applicability and benefits of the presented methodologies.

Fast NMPC with Multi--Level Iterations

Leonard Wirsching, leonard.wirsching@iwr.uni-heidelberg.de

Model Predictive Control has matured as an advanced feedback control approach, and attracts more and more interest for application in both industry and academia. A crucial issue for this purpose, in particular for the control of nonlinear processes, is the availability of algorithms that provide feedback quickly and allow fast sampling rates.

The algorithmic framework of Multi-Level Iterations (MLI) has been developed with exactly these aspects in mind and allows both fast sampling rates and quick feedback as soon as current state information is available. The main idea is to efficiently construct and evaluate approximate tangential predictors for feedback control generation while avoiding as much as possible expensive function and derivative evaluations.

In this talk, we present in detail the framework of MLI, give different advantageous aspects of fast feedback, briefly contrast MLI with similar approaches, report numerical experiences and give ideas on the adaptive choice of levels.

Robust and optimal operation of an industrial polymerization reactor under model uncertainties by multi-stage output feedback NMPC

Sankaranarayanan Subramanian,
sankaranarayanan.subramanian@bci.tu-dortmund.de

Nonlinear Model Predictive Control (NMPC) is highly appealing to the industries because it can be applied to nonlinear systems, has the ability to address economic objectives and achieves satisfaction of safety and environmental constraints. NMPC uses the nonlinear model of the system to forecast its future behavior and finds a sequence of control inputs by solving an optimization problem. The first input element in the control sequence is applied to the plant and the optimization problem is solved online again at the next sampling interval in a receding horizon fashion. Since the scheme is model-based, its performance depends on the accuracy of the model. Robust NMPC scheme that can achieve constraint satisfaction under uncertainty is a practical necessity and the robust scheme must be non-conservative so that there is no compromise on the performance. Multi-stage NMPC is a non-conservative robust scheme which predicts different evolutions of the plant for different realizations of the uncertainties in the form of a scenario-tree. The important aspect of the approach is that the feedback information is explicitly considered in the problem formulation by adapting the control inputs to the different evolution of the system resulting from different realizations of the uncertainty. Hence the decisions taken at every time step acts as recourse to counteract the effects of uncertainties and makes the approach non-conservative.

Another practical problem is the unavailability of full state information at every time step. Using the available measurements and the model, state estimates can be obtained using estimation schemes such as Extended Kalman Filter. The error in the current and the future estimates are then taken into account in the output feedback multi-stage NMPC algorithm. In this talk, the standard multi-stage NMPC scheme and the robust output feedback scheme based upon multistage optimization will be discussed. Simulation results of the proposed schemes for an industrial polymerization reactor will be presented to demonstrate the efficiency of the approach.

Efficient numerics for robust Multi-Stage NMPC with application to a biochemical benchmark problem

Conrad Leidereiter, conrad.leidereiter@iwr.uni-heidelberg.de

In the field of nonlinear model predictive control under uncertainty we use a robustification approach based on a multi-stage formulation. More precisely, we describe the evolution of the uncertainty as a scenario tree.

A main challenge of the scenario tree formulation is the exponential growth of the number of scenarios for possible parameter realizations. Hence, the solution of the resulting optimization problem in every nonlinear model predictive control iteration becomes a bottleneck for the computation.

As the optimization problem exhibits a particular structure originating from the scenario tree, we exploit the structure in our numerical method. A dual decomposition approach on the constraints that couple the scenarios can be used to solve the decomposed problem in a massively parallel fashion.

Embedded in a multi-level iteration scheme we take advantage of sequentially solving or approximating the solution of similar problems.

Applying the robustification approach using multi-level iteration schemes and efficient structure-exploiting numerics makes it possible to give fast feedback which is required for the control of complex systems.

In this talk we showcase our approach as efficient numerical method for the control of a biochemical reactor.

do-mpc - A platform for the development and implementation of robust NMPC solutions in industry

Alexandru Tatulea-Codrean, alexandru.tatulea-codrean@bci.tu-dortmund.de,
Clemens Lindscheid, clemens.lindscheidt@bci.tu-dortmund.de

Linear model predictive control has found widespread application in industry, especially in the process industry but increasingly there is interest also in other domains. Its nonlinear counterpart NMPC has been discussed intensely in the research community and there are also prototypical real applications. However it remains true that NMPC has not yet widely spread in industry, thus the potential of better handling nonlinearities and better prediction accuracy that come with the use of nonlinear models is not tapped.

What are the main reasons that prevent NMPC from making an industrial breakthrough and becoming the new predictive control standard? In this talk we will present our point of view on this matter. Additionally we will introduce a software platform that aims at bridging the gap between academia and industry by facilitating the rapid and efficient development and deployment of robust NMPC strategies for complex biochemical and chemical processes: The *do-mpc* platform.

do-mpc is a software tool that builds upon state-of-the-art algorithms for optimization and simulation that are integrated via an interfaces to software packages for automatic differentiation and optimal control. Due to the modular structure of *do-mpc*, the development and testing of NMPC solutions is facilitated because different components of the overall solution – plant models, optimization models, optimization algorithms, state estimators can be combined freely and easily and partial

solutions can be reused.
In order to support the transition from testing to real world applications, *do-mpc* can be used in a development chain that starts with the integration of nonlinear models and ends with a data visualization feature which can be used at the real plant. Different kinds of models such as ODE and DAE systems and different modelling tools such as JModelica and Python/CasADi can be integrated. A library of reliable NMPC and state estimation algorithms is offered to the users. With the modular design of do-mpc the transition from a simulation study to a deployed and tested application can be facilitated and development time can be reduced. Standard communication interfaces can be easily integrated to connect the NMPC solution to the plant infrastructure. A novel concept for data visualization facilitates the monitoring, diagnosis and improvements of the NMPC algorithms, both in development and during operation. We illustrate all parts of the *do-mpc* development chain using the example of a multistage NMPC solution for a CSTR.

The theory and numerics of dual control with application to a biochemical benchmark problem

Huu Chuong La, huu.chuong.la@iwr.uni-heidelberg.de

Dual control refers to strategies that strike a balance between control and estimation. Combined with nonlinear model predictive control, dual control offers advanced feedback methods for optimal control problems under uncertainties. We present dual control from a new perspective, namely, the interplay between the performance control task and the information gain task in connection with optimal experimental design. A new approach to dual control is proposed in which the covariance matrix of the estimates is weighted by the derivatives of the optimal nominal objective value with respect to unknown parameters and initial states. Most notably, we discuss the theoretical background of this approach and provide probabilistic bounds for the controller performance with respect to the original objective function. As applications, we investigate a moon lander problem and a batch bioreactor problem. Numerical results demonstrate the superiority of dual control over nominal control for ensuring feasibility, optimizing economic objectives and enhancing robustness. We also carry out an analysis of the relationship between the performance control task and the information gain task in order to assess when the extra effort for dual control is justified.

A Multi-Level Iteration mode based on the trapezoidal rule with application to a biochemical benchmark problem

Andreas Meyer, andreas.meyer@iwr.uni-heidelberg.de

Nonlinear model predictive control (NMPC) has become an increasingly popular control approach. However, its application to time-critical systems requiring fast feedback still presents a major computational challenge. The multi-level iteration (MLI) approach has been successfully applied for real-time capable NMPC of dynamic processes described by ordinary differential equations (ODEs) or differential-algebraic equations (DAEs). The common realization of MLI is based on the direct multiple shooting method to discretize the ODE/DAE constrained optimal control problems (OCPs). In every NMPC iteration the arising nonlinear program is approximated by a local quadratic subproblem (QP). To provide feedback very fast, the QP data is updated only partially depending on the computational costs and the approximation quality of the existing data. One distinguishes between four modes in which different components are recalculated. In this contribution we motivate a novel mode mainly applicable for OCPs with process dynamics which yield a sparse Jacobian for the right hand side. In this mode we use a trapeziodal rule to obtain a sparse QP, which can be solved efficiently by an appropriate QP solver. We apply our algorithm to a biochemical benchmark problem and present numerical results.

NMPC for models with periodic stages

Jürgen Gutekunst, juergen.gutekunst@iwr.uni-heidelberg.de

Applying Nonlinear Model Predictive Control (NMPC) for online feedback generation of dynamic models with periodic stages poses additional difficulties compared to NMPC for systems with only one stage and steady state behavior. The systems we are characterized by periodically occurring operating stages, each of them usually described by an Ordinary Differential Equation (ODE).

Examples for models with periodic stages can be found in chemical engineering with the Simulated Moving Bed process or in the energy sector with a power producing flying kite.

Optimal Control for such systems leads to periodic steady state solutions. Standard tracking approaches can fail for such periodic steady state solutions.

We will present a purely economic NMPC approach for such models, which adds a periodicity constraint to the optimal control problem that is solved at each sampling time. This periodicity constraint approach gives rise to desirable properties of the resulting NMPC feedback method.

First, it ensures recursive feasibility of subsequent occurring optimal control problems. Second, there is the possibility to add a weighting factor to the part of the objective that corresponds to the contribution of the periodic part of the predicted trajectory, which can be used to prevent greedy behavior.

The resulting method is applied in combination with the multi-level iteration scheme to numerical case studies.

An approach for speeding up the online Design of Optimal Experiments and its application to the Simulated Moving Bed process

Roberto Lemoine, roberto.lemoine@bci.tu-dortmund.de

Accurate predictive models are the basis of optimization and model-based control of chemical engineering processes. Typically, the model equations are formulated by process experts and the model parameters are determined by means of experiments in the laboratory or in small scale plants. To obtain accurate parameters may require a considerable amount of experimental work but nonetheless the parameters of the real plant may deviate from the values that were determined from small-scale experiments due to nonidealities of the equipment, the influence of the geometry and time-varying influences such as fouling and material aging Therefore it is important to detect changes in parameters which are critical for predicting the performance of the process and to correct their values. This requires that the measurements that are obtained from the process during its operation contain enough information to estimate the parameters with an acceptable accuracy. This can be achieved by means of online dynamic Optimal Experiment Design (OED). The objective of online OED usually is to minimize some measure of the error covariance matrix of the parameters. However, the optimization of the objective function of dynamic OED can be very time consuming for large-scale systems with several control inputs and several measurements, making it unrealistic to apply the OED online. We here propose an approach for reducing the numbers of the degrees of freedom and of the measurements that are involved in the OED optimization problem in order to improve the numerical efficiency.. The performance of the method is demonstrated for the

estimation of the adsorption parameters of the individual columns in a Simulated Moving Bed plant.

Optimizing control and state estimation of a continuous polymerization process

Reza Hashemi, reza.hashemi@bci.tu-dortmund.de

While traditionally following some predefined set points or trajectories is the main goal in the control of chemical processes, from the management point of view, other criteria such as minimizing the production costs or maximizing the product output are more important. The concept of optimizing control consists of formulating the control problem as an optimization of economically relevant criteria under constraints on the operation conditions or product quality parameters, rather than tracking set-points of process variables.

In this talk, we show simulation results of implementing an optimizing controller for a modular tubular reactor which has been designed for the production of water soluble acrylic acid-based polymers. The polymerization process is described by a set of pde and exhibits steep fronts of the state variables along the reactor so that advanced discretization methods must be used to simulate and optimize the process. The resulting ode model has 1600 states. The goal of our controller is to maximize the product output while the product quality, which is defined by the weight average molecular weight and the residual monomer concentration of the produced polymer, is kept within the given bounds. The simulation results show that the controller increases the throughput and can keep the quality constraints within the desired bounds. In a changeover scenario the controller aims at minimizing the amount of off-spec products in the transition phase and then maximizing the throughput of the new product after this phase. The process model is an explicit part of the optimizing controller and therefore the states are needed to initialize the model and hence the state estimation is an

important part of the optimizing controller. In this work, we show that the Particle Filtering is a better choice for this purpose compared to the Extended Kalman Filter.

Improving the performance of robust economic NMPC by dual control: Application to chemical reaction systems

Sakthi Thangavel, sakthi.thangavel@bci.tu-dortmund.de

In this talk we explain the concept of dual control and how it can be used in economic robust nonlinear model predictive in order to improve its performance. Nonlinear model predictive control (NMPC) is one of the most promising advanced control approaches for processes with multiple inputs, outputs and constraints. Besides the efficacy of modern optimization solvers that provide fast and reliable solutions to the constrained optimization problems, the handling of uncertainties present in the model parameters remains the most challenging problem in the real time application of NMPC. Several robust NMPC schemes with different level of conservatism have been developed in order to deal with uncertain model parameters that are present in the model equations. The multi stage approach developed in our group achieves a low degree of conservatism compared to other robust approaches as it incorporates the presence of recourse and therefore models the presence of feedback in the future. A scenario tree of possible realization of the uncertain parameters is used to represent the possible evolutions of the process and a multi-stage decision problem is formulated.

An intrinsic disadvantage of any robust MPC scheme is that the constraints must always be met for the most critical model in the set. Hence lack of knowledge on model parameters directly reduces the performance. By reducing the range of the uncertainty of the parameters a drastic improvement in the economic performance can be achieved. Minimization of the uncertainty range can in principle be achieved by online parameter estimation.

The resulting range of uncertainty depends on the inputs to the plant and it can be minimized by using tools for optimal design of dynamic experiments. On the other hand, the optimal inputs from the point of view of parameter estimation usually are not the economically best inputs. The dual control problem aims at a balance between finding the optimizing inputs for the economical criterion and inputs that excite the process enough to obtain tighter bounds on the uncertain parameters. The dual control formulation in multi-stage robust NMPC framework takes into account the future reduction of the range of the uncertainties of the uncertain parameters that the probing control actions will provide over the prediction horizon. The formulation of the optimization problem and results obtained by applying dual robust multi-stage NMPC in comparison to robust multi-stage NMPC without parameter estimation and dual control to a chemical reaction system will be presented in this talk.