23rd IFIP Conference on Modelling and Optimization

Invited Session

Optimization of Dynamic Systems in Chemical Engineering I

Organizer: L. T. Biegler, Carnegie Mellon University (USA), lb01@andrew.cmu.edu

1. *Adaptive Shooting Methods for Dynamic Optimization – Concepts, Algorithms and Applications* - R. Hannemann, A. Hartwich, Wolfgang Marquardt, and Lynn Würth, RWTH Aachen (D), marquardt@lpt.rwth-aachen.de

2. *The Lifted Newton Method and its Use for Large Scale Dynamic Optimization and NMPC in Chemical Engineering* - Jan Albersmeyer and Moritz Diehl, University of Heidelberg (D) and KU Leuven (B), jan.albersmeyer@iwr.uni-heidelberg.de

3. *Optimization Problems in Advanced Operating Modes of Continuous Chromatography*, Malte Kaspereit – MPI Magdeburg (D), kaspereit@mpi-magdeburg.mpg.de

4. *On the Optimality of Superstructures for Simulated Moving Bed Processes* - Sebastian Sager, Yoshiaki Kawajiri, L. T. Biegler, University of Heidelberg (D) and Carnegie Mellon University (USA), lb01@andrew.cmu.edu

Abstracts of all of these talks are given below.

Adaptive Shooting Methods for Dynamic Optimization – Concepts, Algorithms and Applications

R. Hannemann, A. Hartwich, Wolfgang Marquardt, and Lynn Würth
Process Systems Engineering
Center for Computational Engineering Science
RTWH Aachen University, D-52074 Aachen, Germany

This talk will review some of the work on the development of adaptive shooting methods for the solution of optimal control problems carried out in our research group in recent years. The basic feature of the shooting method is an adaptive choice of the control vector parameterization in a shooting type of solution strategy. The control variables are adaptively discretized by multi-scale basis functions to resolve local detail with an appropriate number of parameters. Furthermore, the control switching structure of the solution is automatically detected during the refinement process of the adaptation of the control vector parameterization which gives insight into the solution features facilitating the interpretation of the result. The such detected structure is exploited to reprarameterize the single-stage into a multi-stage problem with a close to minimal number of control vector parameters. First and second order derivatives are computed by novel and highly efficient numerical algorithms exploiting forward as well as backward mode differentiation. Our numerical method conceptually links single-shooting and multiple type shooting on the one hand as well as direct and indirect methods on the other. The robustness and performance of the algorithms will be illustrated by different kinds of examples from chemical engineering of different complexity. The implementation has been proven to be very robust and highly efficient for large-scale optimal control problems with up to 15000 differential-algebraic equations with a number of control variables and many inequality path and endpoint constraints. Some extensions of the algorithm to cover real-time applications in nonlinear model-predictive and neighboring extremal control will be briefly discussed together with illustrating examples.

The Lifted Newton Method and its Use for Large Scale Dynamic Optimization and NMPC in Chemical Engineering

Jan Albersmeyer and Moritz Diehl

We present a new full space exact Hessian SQP algorithm for large scale dynamic optimization that makes heavily use of two ingredients. We start by a process simulator (the DAE solver DAESOL-II (1)) that is able to generate adjoint sensitivites by the principle of internal numerical differentiation. Thus, a gradient computation is available at the cost of about five process simulations. Second, we work in the framework of Bock and Plitt's direct multiple shooting method (2) by introducing intermediate but constrained "node" variables into the optimization problem. It is a well known technique for reducing nonlinearity and increasing robustness of the optimization procedure, in particular for boundary value problems e.g. with end point quality constraints.

By a combination of both ingredients, we are able to derive a full space exact hessian SQP method that iterates in the very large space of all node variables, yet needs to evaluate only the same amount of derivatives as would be needed in a single shooting approach. This is similar to Schlöder's Trick (3) which was however only applicable to least squares objective functions and not yet combined with adjoint techniques for derivative generation. By a smart programming trick, the algorithm can easily be derived by "lifting" a standard single shooting SQP method, thus avoiding the tedious programming work usually avoided with new variants of direct multiple shooting. The algorithm is advantageous in case of large process models with few degrees of freedom. We present also an extension to online optimization in nonlinear model predictive control, and demonstrate its performance at examples from chemical engineering.

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Optimisation Problems in Advanced Operating Modes of Continuous Chromatography

Malte Kaspereit
Max Planck Institute for Dynamics of Complex Technical Systems,
Sandtorstr. 1, D-39106 Magdeburg, Germany

Chemical processes most generally consist of a reaction step (synthesis) and a subsequent resolution of reactants and products (separation). The separation step can be very difficult (and expensive), in particular in the production of valuable pharmaceuticals and fine chemicals. In this context, chromatographic processes are an important option. Chromatography is performed using columns containing a stationary phase. The figure below shows two general process options – discontinuous batch chromatography (single column, periodic injection of small feed amounts; left), and Simulated Moving Bed (SMB) chromatography (periodic switching of multiple columns, continuous feed; right). Due to its superior economic performance, the SMB process is receiving more and more attention.

However, the design of chromatographic processes cannot be performed on the basis of intuition, but requires optimisation schemes to determine suitable parameters. Mathematical process models are computationally expensive, since they typically involve a set of non-linear PDEs coupled by the involved thermodynamic equilibria. Occuring phenomena like shock fronts often necessitate a fine spatial discretisation (up to several thousand grid points per column). Furthermore, the process includes discrete events.

Due to the computational efforts related this, optimisations of SMB processes could be performed only recently. Different strategies have been proposed; for example, genetic algorithms [1], sequential quadratic programming (SQP) [2], a two-level approach [3], and the use of feedback control [4]. Besides standard SMB configurations, currently different advanced operating modes are subject to investigations. These allow to further increase the economic performance of SMB processes and to broaden the range of applications. Examples for advanced operating concepts include:

- combinations of SMB and complementary separation processes,
- additional periodic variation of parameters (e.g., column configuration, flow rates, feed concentration),
- introduction of gradients with respect to solvent strength or temperature,
- implementation of chemical reactions within SMB processes.

However, optimisation of such processes remains a challenge; only few results have been published. Mainly, processes with periodic variations (see above) have been considered using genetic algorithms [5]. More recently, non-linear optimization with full discretisation [6] was applied successfully to several of the above process options. In the presentation, an overview will be given on optimisation problems related to (continuous) chromatographic processes. After an introductory review of fundamental principles and modelling approaches, recent developments with respect to advanced operating modes for SMB processes and optimisation problems will be explained using concrete examples.

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On the Optimality of Superstructures for Simulated Moving Beds

Sebastian Sager, Yoshiaki Kawajiri and Lorenz T. Biegler

The past decade has seen a variety of operating modifications for Simulated Moving Bed (SMB) processes, including Three-Zone, VARICOL, and PowerFeed. In recent studies, we have shown that these can all be embedded within a superstructure optimization problem with time-variant flow rates. Moreover, the resulting dynamic optimization problem has yielded a number of interesting and useful insights on novel SMB operations. In many cases these solutions have a 'bang-bang' character, i.e., the feed, desorbent, extract and raffinate streams appear in only one location. Remarkably, this occurs even though the optimization is performed without an introduction of binary decision variables. In this study we analyze and present conditions where 'bang-bang' solutions are optimal. We also demonstrate cases where these conditions do not hold and where 'bang-bang' solutions are suboptimal. To show that these properties are independent of the column model and solution strategy, we demonstrate both 'bang-bang' and 'non-bang-bang' cases for two different column models and two optimization environments.