4th KoMSO Challenge Workshop
"Online & Offline Optimal Control of Chemical and Biotechnological Processes"

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Authors:
A. Badinski (BASF SE, Scientific Computing)
S. Sauer (University of Heidelberg, IWR)

List of Invited Speakers

Hans Georg Bock, *IWR Heidelberg, Germany*
Sebastian Engell, *TU Dortmund, Germany*
Rudibert King, *TU Berlin, Germany*
Alexander Mitsos, *RWTH Aachen, Germany*
Costas Pantelides, *Process Systems Enterprise Limited London, UK*
Per Rutquist, *Tomlab Optimization AB, Sweden*
Tor Steinar Schei, *Cybernetica AS, Norway*
Kai Sundmacher, *Otto-von-Guericke-University Magdeburg, Germany*

Executive Summary

Model-based optimization (i.e. online & offline optimal control) is defined here as a technology using mathematical models to improve dynamical processes with numerical algorithms. This technology has already been successfully applied for chemical and biotechnological processes. However, during the workshop it was generally agreed that much more can be done. Several strategies for how to successfully apply this methodology more widely were presented and discussed. These strategies address both technical and non-technical challenges. The most important technical challenges when applying modeling solutions to practice are (i) to increase the efficiency of the model building process, (ii) to accomplish the transferability and reusability of models, and (iii) to consider uncertainties of various kinds in modeling and optimization. The most important non-technical challenge is to increase the awareness for modeling and optimization as a central asset for the company's success. The experience of companies like Procter & Gamble shows that when adopting a coherent modeling strategy company-wide, these challenges can successfully be addressed.

1. Overview of KoMSO

The Committee for Mathematical Modeling, Simulation and Optimization (KoMSO) is a strategic alliance founded after the *Strategietag Mathematik 2020*, a component of the Strategy Dialogue for Mathematics established by the German Federal Ministry of Education and Research during the Year of Mathematics 2008. KoMSO organizes challenge workshops on a regular basis; see also www.komso.org.

2. Objectives of workshop

The 4th KoMSO workshop was co-organized by BASF and took place at the Feierabendhaus at BASF on the 23rd of January 2014. Eight invited experts from academia and industry from Germany, Great Britain, Norway and Sweden came together with additional 70 participants from BASF, other industries and academic institutions.[1]

The workshop had three objectives:

- Discuss challenges and share experiences of applying online / offline optimal control to real world dynamic processes in chemistry and biotechnology,
- identify roadmaps for better algorithms, software and modeling workflows (e.g. model building -> offline optimal control -> model reduction -> online optimal control), and
- plan future activities towards exploiting the potential of this technology.

3. Identified Challenges and Solution Approaches

Four categories of technical challenges were identified: *applications*, *numerics*, *software & workflow*, and *methodology*. The main conclusions are stated in the following.

3.1 Applications

Model building is often very time-consuming and the limiting step in applying model-based optimization to practical applications. The decision for the appropriate model complexity is often difficult, e.g. deciding when to neglect reactions in complex networks or when to include non-log normal weight distributions in polymerization reactions. Different model assumptions can lead to a large number of model candidates that have to be tested systematically. To address this point for process models in biotechnology, Prof. King presented and discussed a methodology that allows an automatic generation of physically

[1] http://www.komso.org/fileadmin/Redakteure/Startseite/Downloads/Booklet_KoMSO_CW.pdf

reasonable model candidates from experimental data. Prof. Pantelides suggested starting from a sophisticated first principles “master model”, which is often too complicated to be optimized, and to use such a model to automatically derive less complex sub-models tractable for particular optimization tasks; he illustrated this idea with a pipeline network. Focusing on large micro-kinetic models, Prof. Sundmacher showed and discussed a general scheme for model reduction that can be integrated in standard modeling workflows.

In applying modeling solutions to practical problems, the discrepancy between model and reality often changes over time due to fouling, equipment degradation and failure or other uncertainties in the process. This underlines the importance of online methodologies (i.e. online parameter estimation, online design-of-experiment, online optimization and online adaptation of controller model).

Optimization problems are often embedded in a complex environment, e.g. a single batch reactor is integrated into a reactor network with a common heat system and down-stream process. The potential benefits rely on the degree to which the environment is considered. However, the model complexity increases drastically so that advanced modeling tools become indispensable. Strategies here are to use standard model libraries as pointed out by Dr. Schei and automatically derived models as developed and used by Prof. Pantelides. A method using hierarchical models was presented by Prof. Sundmacher and can be applied to similar questions.

3.2 Numerics

Models used for optimization have to satisfy more conditions than models used for simulations. Models with (implicit) switches and delays are frequently used for simulations but cannot straightforwardly be used with derivative-based optimization methods. Dr. Potschka and Prof. Bischof suggested a modeling tool that provides feedback about the differentiability of the model and gives solution strategies to the modeler. Dr. Rutquist suggested a hybrid approach that may choose between exact derivatives and finite differences. However, when exact derivatives are available, no technical reasons were found to prefer this hybrid approach.

For nonlinear model predictive control (NMPC), models have to be solved in a very short time. This is particularly challenging for models with strong coupling, with many degrees of freedom and with switched dynamics and constraints. Prof. Bock gave examples from different industries that show the capability of state-of-the-art algorithms from academia, e.g. multiple-shooting methods developed at the IWR, Heidelberg. Collocation methods were mentioned as an alternative for specific problems but were considered less suited for rapidly changing processes.

Numerical robustness of various kinds is seen as critical for the successful application of optimization methods. For example, for the modeling and optimization of large distillation columns, substantial modeling effort goes into the initialization of flow sheets to satisfy the respective algebraic equations. A robust and automated method for such problems was presented and discussed by Prof. Pantelides.

3.3 Software and Workflow

The efficiency of the modeling workflow is highly important for model-based solutions in a rapidly changing environment. Different measures are proposed. First, an intuitive and universal model building tool (see 2.1) speeds up the process of model building. Second, a unified language is demanded to facilitate the transfer of models across units and to guarantee the (re-)usability of models by people with different backgrounds. A unified language also allows the use of different simulation and optimization algorithms. Thirdly, a model database is seen as an asset to preserve the knowledge associated with previously developed models. To address these points, Prof. Pantelides advocated the strategy of a general purpose modeling software platform that is used company-wide. Interfaces between the most common modeling and optimization software packages are proposed as an alternative. However, due to the complexity of this issue no agreement was reached about a common modeling language or interface (see Sec. 5). MOSAIC[2] is an attempt in this direction.

3.4 Methodology

The challenge of dealing with model uncertainties is one of the most urgent concerns. If uncertainties are structural ("What mechanism underlies the observed data?"), validating and discriminating numerous model candidates is important (Sec. 2.1). When the model structure is determined, parameter uncertainties often remain. To account for the parameter uncertainty in the context of NMPC, Prof. Engell suggested the use of scenario trees in combination with multi-stage optimizing control. Prof. Mitsos outlined and discussed how to address the uncertainty issue in offline optimization with global and robust optimization algorithms.

[2] http://www.mosaic-modeling.de/

4. Conclusions and Recommendations

The most important challenges when applying modeling solutions to practice are (i) to increase the efficiency of the model building process, (ii) to accomplish the transferability and reusability of models, (iii) to consider uncertainties of various kinds in modeling and optimization, and (iv) to increase the awareness for modeling and optimization as a central asset for the company's success. To address these challenges, the following recommendations were made:

- Establish a professional modeling, simulation and optimization platform with full access to the numerical algorithms that is open to industry and academic partners,
- publish and disseminate success stories illustrating the benefits of model-based optimization,
- define a unified modeling language was not seen to be practicable in the past; therefore define a unified interface standard between the most common modeling and optimization software packages taking into account requirements specific to optimization, and
- Strengthen the collaboration between industries, commercial modeling companies and academia to use synergies in method and software development.

Contact

Dr. Alexander Badinski
BASF SE Ludwigshafen

T: +49 (0)621 – 60-94746
F: +49 (0)621 – 3480690
alexander.badinski@basf.com

Dr. Anja Milde
KoMSO Coordination Office
IWR – Interdisciplinary Center for Scientific Computing
Im Neuenheimer Feld 368
69120 Heidelberg
Germany

T: +49 (0)6221 – 54-8886
F: +49 (0)6221 – 54-8810
komso@iwr.uni-heidelberg.de