ANNUAL SEMINAR IN OPTIMIZATION AND SYSTEMS ENGINEERING 2012

The Center of Excellence in Optimization and Systems Engineering at Åbo Akademi University organizes a one-day seminar on Thursday November 29th in Auditorium Ringbom, Axelia II, Biskopsgatan 8, Åbo, Finland.

Invited speaker
Professor Stratos Pistikopoulos
Imperial College London, UK

Professor Stratos Pistikopoulos from the Centre for Process Systems Engineering at Imperial College London is giving two invited lectures with topics in modeling, optimization and control.

Prof. Pistikopoulos is a Professor and Director of Research in the Department of Chemical Engineering at Imperial College London. During the years 2001-2009, he was also the Director of the Centre for Process Systems Engineering (CPSE). He holds a PhD from Carnegie Mellon University (USA) and was with Shell Chemicals (Amsterdam, the Netherlands) before joining Imperial in 1991. He has authored/co-authored over 250 major research journal publications in the areas of modeling, control and optimization of process and systems engineering applications, 8 books and two patents. A Fellow of the Institution of Chemical Engineers, Co-Editor of the Book Series in Process Systems Engineering (Wiley-VCH), Co-Editor of the Book Series on Computer Aided Chemical Engineering (Elsevier) and Computers & Chemical Engineering (CACE) Journal, on the Editorial Board of the Journal of Global Optimization (JOGO), Industrial and Engineering Chemistry Research (I&ECR), Energy Systems and the Journal of Computational Management Science (CMS). Professor Pistikopoulos has been a Founder/Co-Founder of two spin-off companies from Imperial, Process Systems Enterprise (PSE) Ltd. and Parametric Optimization Solutions (ParOS) Ltd. In 2007, Prof. Pistikopoulos was a co-recipient of the prestigious Mac Robert Award and Gold Medal from the Royal Academy of Engineering; in 2008 he received an Advanced Investigator Award from the European Research Council, and in 2009 he delivered the Bayer Lecture in Process Systems Engineering at Carnegie Mellon University, USA. He is the recipient of the 2012 Computing in Chemical Engineering Award of the Computing and Systems Technology (CAST) Division of the American Institute of Chemical Engineers (AIChE).

The seminar continues in the afternoon with presentations by some of PhD students active within the Center of Excellence in Optimization and Systems Engineering.

The seminar is open to anyone interested. **For registration and more information visit the OSE group's website at www.abo.fi/ose.**

OSE OPTIMIZATION AND SYSTEMS ENGINEERING

Åbo Akademi University

TIME SCHEDULE

10.00 **Professor Tapio Westerlund**
Chairman of the OSE group
Opening statement

10.05 **Professor Stratos Pistikopoulos**
Multi-parametric programming and explicit model predictive control – a progress report

10.50 **COFFEE BREAK**

11.10 **Professor Stratos Pistikopoulos**
Modeling, optimization and advanced control of biomedical systems

12.00 **LUNCH BREAK**

13.30 **Axel Nyberg, PhD student**
The quadratic assignment problem

13.50 **Otto Nissfolk, PhD student**
A metaheuristic optimization algorithm for binary quadratic problems

14.10 **Anders Skjäl, PhD student**
Two approaches to underestimating quadratic functions

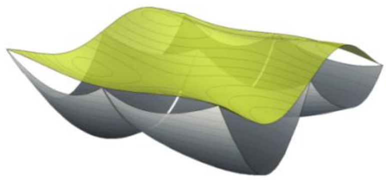
14.30 **COFFEE BREAK**

15.00 **Johan Pensar, PhD student**
A Bayesian score for LDAGs

15.20 **Amir Shirdel, PhD student**
System identification in the presence of trends and outliers

15.40 **Mikael Nyberg, PhD student**
State splitting in continuous time STN-models

KEYNOTE LECTURES IN MODELING, OPTIMIZATION AND CONTROL



At this year's seminar in Optimization and Systems Engineering, the invited speaker Professor Stratos Pistikopoulos from Imperial College London will hold two lectures connected to OSE research.

Multi-parametric programming and explicit model predictive control – a progress report

Multi-parametric programming provides a complete map of solutions of an optimization problem as a function of, unknown but bounded, parameters in the model, in a computationally efficient manner, without exhaustively enumerating the entire parameter space. In a Model-based Predictive Control (MPC) framework, multi-parametric programming can be used to obtain the governing control laws – the optimal control variables as an explicit function of the state variables. The main advantage of this approach is that it reduces repetitive on-line control and optimization to simple function evaluations, which can be implemented on simple computational hardware, such as a microchip, thereby opening avenues for many applications in chemical, energy, automotive, and biomedical equipment, devices and systems.

In this presentation, we will first provide a historical overview of the key developments in multi-parametric programming and control. We will then describe a number of key application areas, where this technology shows a lot of potential and discuss key challenges and directions for future research. We will critically address the question of the suitability of explicit/multi-parametric control as part of the advanced model-based control technology portfolio of the future.

Modeling, optimization and advanced control of biomedical systems

The MOBILE 'Modeling, Control and Optimization of Biomedical Systems' Project is an Advanced Grant awarded by the European Research Council (ERC) carried out at the Centre for Process Systems Engineering (CPSE) at Imperial College London. The objective of MOBILE is to derive novel intelligent computer model-based systems for the automation of drug delivery, which ensure personalized health care, flexibility to adapt to changing patient characteristics, incorporation of the physicians performance criteria, safety of the patient and reduced side-effects by optimizing the drug infusion rates.

In this presentation, we will present an overview of MOBILE. In particular, its overall modeling, optimization and advanced control approach will be described, which relies on novel multi-parametric/explicit model predictive control technology and implemented in the context of three biomedical systems

a) anesthesia and hemodynamic variables,
b) insulin delivery and
c) chemotherapy for leukemia.

More information about the Centre for Process Systems Engineering at Imperial College London can be found on the website ***imperial.ac.uk/centreforprocesssystemsengineering***

ABSTRACTS FOR THE PRESENTATIONS

Axel Nyberg, PhD student

THE QUADRATIC ASSIGNMENT PROBLEM

The quadratic assignment problem, QAP, is a notoriously challenging combinatorial problem originally presented by Koopmans and Beckmann in 1957. The QAP has gained a lot of attention from researchers around the globe. These problems arise in numerous research fields, *e.g.* economics, scheduling, engineering, archeology, biotechnology and design to name a few. Even though the QAP is well-studied it is still one of the most difficult combinatorial optimization problems to solve to optimality. Instances with only a few locations (*i.e.* n=30) are still considered extremely difficult. My talk will be a short overview of some recent methods used to solve larger instances as well as a presentation of a few QAPs from different fields.

Otto Nissfolk, PhD student

A METAHEURISTIC OPTIMIZATION ALGORITHM FOR BINARY QUADRATIC PROBLEMS

A new metaheuristic approach is presented in order to acquire good solutions to binary quadratic problems. The algorithm is based on an iterative two-stage selection of variables to optimize. First the algorithm goes through the vector of binary variables of length n and chooses the m first variables ($m<n$) with a value of one and optimizes over them, then proceeds to the m next variables with values of one and selects them for optimization. In these optimization steps the solution can either improve or stay the same. Once the algorithm has passed through the whole vector without improvement it randomly chooses m variables with values of one to optimize and does this for a specified number of iterations.

Anders Skjäl, PhD student

TWO APPROACHES TO UNDERESTIMATING QUADRATIC FUNCTIONS

I will present two recently described methods for convex underestimation. The first method is a variant of the nondiagonal αBB methods I have been studying. The second method traces back to questions in algebra about characterizing positive polynomials. Positive polynomials on a compact semialgebraic set can be decomposed as polynomial terms containing squares and the defining polynomials of the set. This characterization can be used for describing both the underestimation and the convexity property as semidefinite constraints and minimizing the L^1 distance between function and underestimator. The domains of the methods are C^2 functions and polynomials, respectively. I compare differences and similarities between the methods when applied to the important case of quadratic functions.

Johan Pensar, PhD student

A BAYESIAN SCORE FOR LDAGS

An LDAG is a directed acyclic graph for which labels have been added to the edges. A probabilistic graphical model based on an LDAG has a more refined dependence structure than a traditional Bayesian network as the labels are interpreted to reflect statements of context-specific independence. Efficient Bayesian learning of LDAGs is enabled by introducing an LDAG-based factorization of the Dirichlet prior for the model parameters such that the marginal likelihood can be calculated analytically. In addition to the marginal likelihood, a novel prior distribution for the models is introduced in order to handle the added flexibility. The adjustable nature of the prior allows us to balance the complexity of the graph towards its ability to follow the data.

Amir Shirdel, PhD student

SYSTEM IDENTIFICATION IN THE PRESENCE OF TRENDS AND OUTLIERS

In experimental system identification, it is important to eliminate outliers and trends in the data, as these might otherwise deteriorate the identification accuracy. Normally, the process measurements are first preprocessed to remove outliers and trends, and a model is then identified using the processed data. This approach is, however, not optimal, because before a system model has been identified it may be hard to separate the effects of outliers and trends from the effects due to excitations by the known inputs. In this work we study a procedure for simultaneous identification of a system model and unknown outliers and piecewise changing offsets and trends. This is achieved by modeling the outliers and trends as signals whose second differences are sparse, *i.e.*, have only few nonzero values. The system identification problem can therefore be formulated as a least-squares problem with a sparsity constraint. The problem is solved using L^1-regularization with iterative reweighting, which can be solved efficiently as a sequence of convex optimization problems. Simulated examples demonstrate that by the proposed method accurate system models can be identified using experimental data containing unknown trends and outliers.

Mikael Nyberg, PhD student

STATE SPLITTING IN CONTINUOUS TIME STN-MODELS

Generalized frameworks for modeling batch processes have been developed for several decades. One widely used framework is the State-Task Network (STN) formulation. The standard STN formulations assume complete equipment connectivity between stages in a multi-stage model. In reality it is not uncommon to have limited equipment connectivity. Even though there are approaches dealing with limited connectivity they share two drawbacks: the suggested formulations i) increase the number of binary variables and ii) prohibit splitting and merging of batches. State Splitting is a novel formulation that addresses both problems found in earlier formulations. This approach can be used in both continuous and discrete time and the proposed formulation uses linear constraints without introducing new binary variables. In this presentation the State Splitting approach will be described shortly. Thereafter, a State Splitting formulation for a continuous time STN formulation, using common time points, is presented. Finally some computational results, comparing State Splitting with an earlier method for limited equipment connectivity, will be shown and discussed.

The Optimization and Systems Engineering group at Åbo Akademi University is an interdisciplinary research group within the Division of Natural Sciences and Technology. Appointed a Center of Excellence within research at the university for the period 2010-2014, the group focuses on theory, methods and algorithms in systems engineering, optimization and statistics, as well as their applications in science and engineering.

For more information please contact Professor Tapio Westerlund (Process Design and Systems Engineering), Professor Göran Högnäs (Mathematics), Professor Jukka Corander (Statistics) or Professor Hannu Toivonen (Industrial Systems Engineering), or visit www.abo.fi/ose.