NEWSLETTER JANUARY 2012

#1

CENTER OF EXCELLENCE IN

OPTIMIZATION AND SYSTEMS ENGINEERING

Professor Ignacio Grossman from Carnegie Mellon University, USA, was the plenary speaker of the annual seminar in Optimization and Systems Engineering arranged at Åbo Akademi University in December 2011.

Read more about the seminar on page 2.

INSIDE THE NEWSLETTER

Åbo Akademi University

OSE
OPTIMIZATION AND SYSTEMS ENGINEERING

ANNUAL OSE SEMINAR 2011

Above: Professor Ignacio Grossmann and Professor Tapio Westerlund, chairman of the OSE group, discussing at the seminar (left). A focused audience during professor Grossmann's presentation (right). Below: OSE group members giving presentations. From the left, Mikael Nyberg, Otto Nissfolk, Henrik Nyman, Ray Pörn, Axel Nyberg and Andreas Lundell.

The annual seminar in Optimization and Systems Engineering at Åbo Akademi University, hosted by the OSE group, took place on December 8th 2011 in Axelia II, Turku. At the seminar 2010, professor Christodoulos Floudas from Princeton University, USA, was the plenary speaker. This year, the OSE group was fortunate to be able to welcome professor Ignacio Grossmann from Carnegie Mellon University, USA, as the main speaker.

Professor Grossmann has received a great number of awards and honors and is one of the most cited authors in computer science and chemical engineering. He was included in the distinguished group "One hundred engineers of the modern era" selected by the American Institute of Chemical Engineers (AIChE) in 2008. The persons in this group were chosen based on their technical achievements, leadership of the profession, or pioneering work at the frontiers of technology. Professor Grossmann has also received an honorary doctorate from Åbo Akademi University in 2002.

At the seminar, professor Grossmann held two lectures regarding the use of optimization models for design and operation of process systems, as well as disjunctive problems in nonconvex optimization.

After the plenary talks, the seminar continued with presentations of current research performed in the OSE group.

All presentations given at the seminar are available for download on the OSE group's website **www.abo.fi/ose**.

LECTURES AT THE SEMINAR

Prof. Ignacio Grossmann, Carnegie Mellon University, USA
- Discrete and continuous optimization models for the design and operation of sustainable and robust process systems
- Relaxations for convex nonlinear generalized disjunctive programs and their application to nonconvex problems

Andreas Lundell, PhD
- A reformulation framework for global optimization

Ray Pörn, PhD
- On the construction of finite Blaschke products with prescribed critical points

Henrik Nyman, PhD student
- Labeled graphical models

Mikael Nyberg, PhD student
- A novel approach to include limited equipment connectivity in state-task network models

Anders Skjäl, PhD student
- A generalization of classical αBB underestimation to include bilinear terms

Otto Nissfolk, PhD student
- Solving rank-1 quadratic assignment problems

Axel Nyberg, PhD student
- MILP formulations for the quadratic assignment problem

Amir Shirdel, PhD student
- Identification of switching systems by support vector regression

2011
THE YEAR IN REVIEW

HIGHLIGHTS

Jan 12th Docent Iiro Harjunkoski, is co-author of the article "State-of-the-art review of optimization methods for short-term scheduling of batch processes" listed as the most cited article published in the journal Computers and Chemical Engineering in the last five years.

June 6–9th The 3rd Nordic-Baltic Biometric Conference, NBBC11, was held in Turku. The conference was hosted by the Statistics Unit, University of Turku and Department of Mathematics, Åbo Akademi University.

June 7th The OSE-article: "Global Solution of Optimization Problems with Signomial Parts, Discrete Optimization, 5, Issue 1, February 2008, pp. 108-120" reached fifth place of the list "Top 25 Hottest Articles" in Discrete Optimization during the period January to March 2011.

Oct 10th The article "Detection of recombination events in bacterial genomes from large population samples" was accepted for publication in the Nucleics Acids Research (NAR) which is one of the leading journals in the area of computational molecular biology.

Dec 8th The annual seminar in Optimization and Systems Engineering took place in Turku.

VISIT TO PRINCETON UNIVERSITY

PhD student Anders Skjäl was invited to visit Professor Christodoulos Floudas' research group in Princeton University, USA, for the period 28.3–8.4 2011. Professor Floudas is a member of the International Scientific Panel of the OSE group and was the plenary speaker at the annual OSE seminar in 2010. As a result of the research visit, progress has been made on a nondiagonal version of the αBB underestimator for nonconvex optimization.

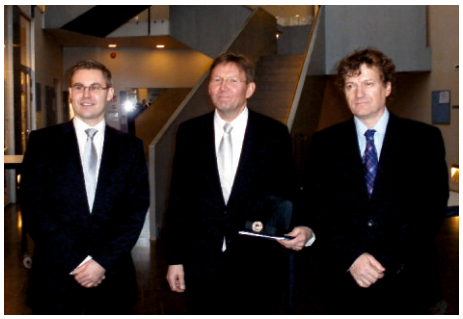
RESEARCH STAY AT UNI. OF TWENTE

Post doc researcher Mikael Kurula is since February 2011 active at the Department of Applied Mathematics at the University of Twente in the Netherlands. There he is mainly working together with professor Hans Zwart on existence proofs for solutions of partial differential equations. The University of Twente was founded in 1961 and it is situated in the city of Enschede by the German border. The university has about 9 000 students and 3 300 scientific staff, and it is the only Dutch university with a campus.

GAMS SEMINAR

Dr Michael Bussieck from GAMS Development Corporation talked about new developments in the GAMS modeling framework on a seminar arranged by the OSE group on December 1st 2011. The research collaboration with Dr Bussieck has among other things led to the AlphaECP solver implementation in GAMS.

PUBLIC THESIS DEFENSE



Toni Lastusilta defended his thesis with the title "GAMS MINLP Solver Comparisons and Some Improvements to the AlphaECP Algorithm" on December 2nd 2011. Professor Zdravko Kravanja, University of Maribor, Slovenia, acted as opponent and professor Tapio Westerlund as custos.

2011 ACHIEVEMENTS

ADVANCES IN SOLVING QAPS

PHOTO: NIKLAS HÄGEN, MFAA

Using novel reformulation techniques developed within the OSE group, PhD student Axel Nyberg and professor Tapio Westerlund managed to solve four previously unsolved quadratic assignment problems in the problem library QAPLIB.

More information about the QAPLIB can be found from www.seas.upenn.edu/qaplib.

STATISTICAL METHODS FOR STUDYING MENINGOCOCCUS

The bacterium meningococcus is a major cause of death among children in industrialized countries and it has caused meningitis epidemics in Africa and Asia. Professor Jukka Corander's research group has developed sophisticated stochastic algorithms that can be used for modeling large sets of genome data.

The mathematical models show that in the meningococcal populations there are subgroups no longer causing meningitis or other diseases. These results are of significance for vaccine research and may provide for a greater understanding of the complex evolution of meningococcus.

The result was published in the Journal of the Royal Society Interface and is a continuation of the project whose results were previously published in Science in 2009 regarding the antibiotic resistance development in the pneumococcus.

SELECTED PUBLICATIONS 2011

MONOGRAPHY

Högnäs, G. and A. Mukherjea. Probability Measures on Semigroups. Convolution Products, Random Walks and Random Matrices. 2nd ed. Springer Science+Business Media, New York, 2011, p. 430.

PEER-REVIEWED PAPERS

Arov, D., M. Kurula, and O. Staffans. "Canonical state/signal shift realizations of passive continuous time behaviors". In: Complex Analysis and Operator Theory 5 (2 2011), pp. 331–402. issn: 1661-8254. doi: 0.1007/s11785-010-0128-8.

Cheng, L.,T. Connor, D. Aanensen, B. Spratt, and J. Corander."Bayesian semi-supervised classification of bacterial samples using MLST databases". In: BMC Bioinformatics 12.1 (2011). issn: 1471-2105. doi: 10.1186/1471-2105-12-302.

Corander, J., T. R. Connor, C. A. O'Dwyer, J. S. Kroll, and W. P. Hanage. "Population structure in the Neisseria, and the biological significance of fuzzy species". In: Journal of The Royal Society Interface (2011). doi: 10.1098/rsif.2011.0601.

Johansson, A., P. Santtila, J. Corander, P. Jern, B. von der Pahlen, M. Varjonen, and K. Sandnabba. "Controlling anger in self-reported sober and alcohol intoxicated states: Moderating effects of trait anger and alcohol consumption". In: Scandinavian Journal of Psychology 52.4 (2011), pp. 382–388. issn: 1467-9450. doi: 10.1111/j.1467-9450.2011.00880.x.

Karelahti, J., P. Vainiomäki, and T. Westerlund. "Large scale production planning in the stainless steel industry". In: Industrial and Engineering Chemistry Research 50.9 (2011), pp. 4893–4906. doi: 10.1021/ie101376b.

Kurula, M. and O. Staffans. "Connections between classical and generalised trajectories of a state/signal system". In: Complex Analysis and Operator Theory 5 (2 2011), pp. 403–422. issn: 1661-8254. doi: 10.1007/s11785-010-0129-7.

Lastusilta, T., L. G. Papageorgiou, and T. Westerlund. "A comparative study of solving the problem of module identification in a complex network". In: Chemical Engineering Transactions 24 (2011), pp. 319–324. doi: 10.3303/CET1124054.

Marttinen, P., W. P. Hanage, N. J. Croucher, T. R. Connor, S. R. Harris, S. D. Bentley, and J. Corander. "Detection of recombination events in bacterial genomes from large population samples". In: Nucleic Acids Research 40.1 (2012), e6. doi: 10.1093/nar/gkr928.

Opmeer, M. R. and O. J. Staffans. "Coprime factorization and optimal control on the doubly infinite discrete time axis". In: SIAM Journal of Control Optimization 50 (2011), pp. 266–285. doi: 10.1137/110823742.

Orozco-terWengel, P., J. Corander, and C. Schlötterer. "Genealogical lineage sorting leads to significant, but incorrect Bayesian multilocus inference of population structure". In: Molecular Ecology (2011). issn: 1365-294X. doi: 10.1111/j.1365-294X.2010.04990.x.

Östman, F. and H. T. Toivonen. "Torsional system parameter identification of internal combustion engines under normal operation". In: Mechanical Systems and Signal Processing 25.4 (2011), pp. 1146–1158. issn: 0888-3270. doi: 10.1016/j.ymssp.2010.11.001.

Östman, F. and H.T. Toivonen. "Adaptive cylinder balancing of internal combustion engines". In: Control Systems Technology, IEEE Transactions on 19.4 (2011), pp. 782–791. issn: 1063-6536. doi: 10.1109/TCST.2010.2052925.

Pitkänen, L.K., M. Tamminen, A. Hynninen, A. Karkman, J. Corander, A. Kotilainen, and M. Virta. "Fish farming affects the abundance and diversity of the mercury resistance gene mera in marine sediments". In: Microbes and Environments 26.3 (2011), pp. 205–211. doi: 10.1264/jsme2.ME11119.

Pörn, R., O. Nissfolk, F. Jansson, and T. Westerlund. "The Coulomb glass – modeling and computational experience with a large scale 0-1 QP problem". In: 21st European Symposium on Computer Aided Process Engineering. Ed. by E.N. Pistikopoulos, M.C. Georgiadis, and A.C. Kokossis. Vol. 29. Computer Aided Chemical Engineering. Elsevier, 2011, pp. 658–662. doi: 10.1016/B978-0-444-53711-9.50132-2.

Sirén, J., P. Marttinen, and J. Corander. "Reconstructing population histories from single nucleotide polymorphism data". In: Molecular Biology and Evolution 28.1 (2011), pp. 673–683. doi: 10.1093/molbev/msq236.

Skjäl, A., A. Lundell, and T. Westerlund. "Global optimization of C^2 constraints by convex reformulations". In: Chemical Engineering Transactions 24 (2011), pp. 373–378. doi: 10.3303/CET1124063.

Smýkal, P., N. Bacová-Kerteszová, R. Kalendar, J. Corander, A. Schulman, and M. Pavelek. "Genetic diversity of cultivated flax (Linum usitatissimum L.) germplasm assessed by retrotransposon-based markers". In: TAG Theoretical and Applied Genetics (2011), pp. 1–13. issn: 0040-5752. doi: 10.1007/s00122-011-1539-2.

Tamminen, M., A. Karkman, J. Corander, L. Paulin, and M. Virta. "Differences in bacterial community composition in Baltic Sea sediment in response to fish farming". In: Aquaculture 313.1–4 (2011), pp. 15–23. issn: 0044-8486. doi: 10.1016/j.aquaculture.2011.01.020.

Toivonen, H. T., A. Meinander, T. Asaoka, M. Westerlund, F. Pettersson, A. Mikhailov, J. E. Eriksson, and H. Saxén. "Modeling reveals that dynamic regulation of c-FLIP levels determines cell-to-cell distribution of CDd95-mediated apoptosis". In: Journal of Biological Chemistry 286.21 (2011), pp. 18375–18382. doi: 10.1074/jbc.M110.177097.

Westerlund, T., A. Lundell, and J. Westerlund. "On convex relaxations in nonconvex optimization". In: Chemical Engineering Transactions 24 (2011), pp. 331–336. doi: 10.3303/CET1124056.

Westerlund, T., A. Lundell, and J. Westerlund. "Some notes on convex relaxations". In: AIDIC Conference Series. Ed. by S. Pierucci. Vol. 10. Aidic Servizi Srl, 2011, pp. 383–392. doi: 10.3303/ACOS1110042.

ABOUT THE OSE RESEARCH GROUP

GROUP LEADERS

Optimization
Professor Tapio Westerlund
Chairman of the OSE group
Process Design and Systems Engineering
Department of Chemical Engineering

Systems engineering
Professor Hannu Toivonen
Industrial Systems Engineering
Department of Information Technologies

Systems theory
Professor Göran Högnäs
Mathematics and Statistics
Department of Natural Sciences

Mathematical statistics
Professor Jukka Corander
Mathematics and Statistics
Department of Natural Sciences

INTERNATIONAL SCIENTIFIC PANEL

Forming a basis for the international collaboration, the OSE group has an international scientific panel consisting of top researchers in the field. The members are:

Professor Ignacio Grossmann
Carnegie Mellon University, Pittsburgh, USA

Professor Christodoulos Floudas
Princeton University, Princeton, USA

Professor Efstratios Pistikopoulos
Imperial College of Science, Engineering and Medicine, London, UK

Professor Leo Liberti
École Polytechnique, Computer Science Department, Paris, France.

Professor Montaz Ali
School of Computational and Applied Mathematics, University of Witwatersrand, Johannesburg, South-Africa.

FOR MORE INFORMATION, VISIT THE OSE GROUP'S WEB SITE AT **WWW.ABO.FI/OSE**

NEW PHD STUDENTS

Amir Shirdel (left) joined the OSE group in April 2011 as a PhD student in Systems Engineering. The topic of his research is "Robust system identification" and it is performed under the supervision of professor Hannu Toivonen.

Andreas Anckar (right) became the newest member of the OSE group when he was accepted as a PhD student starting from January 2012. His thesis is done at the Department of Mathematics under the supervision of professor Göran Högnäs. The title of the research is "The Hausdorff Dimension of Invariant Measures for Iterated Function Systems".

IN THE MEDIA

Jan 21st Advances in solving Quadratic Assignment Problems within OSE is presented in Meddelanden från Åbo Akademi 1/2011.

Feb 2nd OSE Research presented in Åbo Akademi University News Bulletin 1/2011.

March 4th The Finnish national public-service broadcasting company YLE reported about the research in the spreading of polio published in The New England Journal of Medicine by professor Corander's research group.

Nov 25th Professor Ralf Östermark and post doc researcher Andreas Lundell were interviewed about their respective research in Meddelanden från Åbo Akademi 17/2011.

ABOUT THIS ISSUE

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Text: Andreas Lundell and Tapio Westerlund

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