

CENTER OF EXCELLENCE IN OPTIMIZATION AND SYSTEMS ENGINEERING



PHOTO: MIKAEL NYBERG

Invited plenary speaker at the annual seminar in Optimization and Systems Engineering 2013 was professor Leo Liberti from École Polytechnique Paris. The seminar was held at Forum Marinum on November 15th.

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HIGHLIGHTS FROM THE OSE GROUP

CONFERENCES

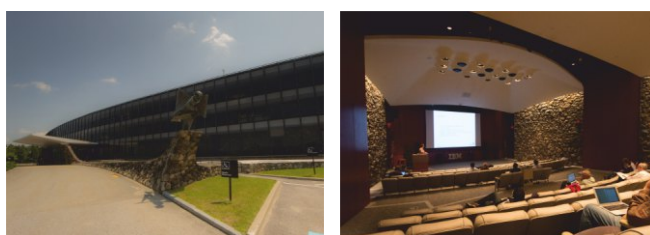
ESCAPE 23 HELD IN FINLAND

The 23rd European Symposium on Computer Aided Process Engineering was held at Lappeenranta University of Technology June 9-12 2013. The OSE group was represented in the national organizing committee by professor Tapio Westerlund. Several post doctoral researchers and PhD students from the OSE group were also present during the conference.

The ESCAPE conference series aims to bring together researchers and practitioners of computer-aided process engineering. Prof. Christodoulos Floudas (Princeton University, USA), a member of the International scientific panel of the OSE group, was a plenary speakers at the conference. Other plenary speakers included professor G.V. Rex Reklaitis (Purdue University, USA) and professor Constantinos Pantelides (Imperial College London, UK).

CPAIOR 2013

Post doctoral researcher Andreas Lundell and PhD student Axel Nyberg participated in the 10th International Conference on Integration of Artificial Intelligence and Operations Research Techniques in Constraint Programming (CPAIOR) organized at IBM Research in Yorktown Heights, New York, USA, 18-22 May 2013. Plenary speakers included Ralph Gomory, one of the most known researchers in integer programming.



IBM T. J. Watson Research Center, Yorktown Heights, NY, USA

INFORMS 2013

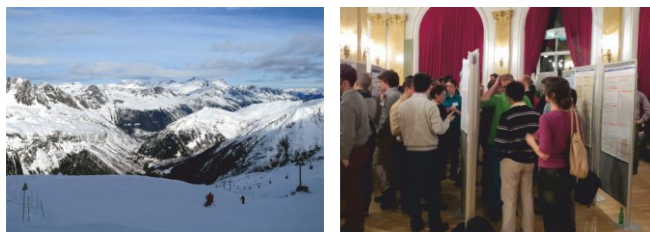
Post doctoral researcher Andreas Lundell participated in INFORMS Annual Meeting 2013 in Minneapolis, USA on October 6-9, with the talk *Reformulation-based global optimization of nonconvex MINLP problems*. The conference is one of the largest in the OR community with about 4 000 participants and a total of 72 sessions.



The Mississippi river runs through the centre of Minneapolis

MCMSki IV

PhD students Johan Pensar and Henrik Nyman participated in the four-day conference MCMSki IV in Chamonix, France, in the beginning of January 2014. As revealed by the name, the focus of the conference is on MCMC and skiing. The days were mainly filled with talks, however, the schedule also allowed for some skiing in the French Alps. In the evenings, well-attended poster sessions were held.



The poster session during the conference

SOME SELECTED OSE NEWS ITEMS

- JAN 16 2013** Professor Jukka Corander informed about breakthroughs in the analysis of resistant bacteria through the means of statistical data analysis at an Academy of Finland breakfast meeting. The results were published in a paper in the journal *Genome Biology*
- APRIL 29 2013** Post doctoral researcher Andreas Lundell was awarded a research prize from the Ruth and Nils-Erik Stenbäck foundation at the Finnish Society of Science and Letters annual ceremony in Helsinki.
- NOV 15 2013** The annual seminar in Optimization and Systems Engineering took place at Forum Marinum in Turku.
- JAN 22 2014** Åbo Akademi University announced that professor Christodoulos Floudas from Princeton University, USA, a member of the OSE group's International Scientific Panel, is to be conferred as Doctor honoris causa at the conferral ceremony on May 23rd, 2014.

NEW RESEARCH PROJECT IN HIGH PERFORMANCE COMPUTING

Professor Ralf Östermark's research group has initiated a multi-disciplinary research project. The research is conducted as a doctoral program in financial accounting and optimization systems in accounting together with doctor of technology Eero Immonen. The Finnish network also consists of researchers from VTT Technical Research Centre of Finland, Thermal and Flow Engineering laboratory at ÅAU and Process Flow Ltd - one of the leading Finnish engineering firms specialized in process dynamics. The research idea is to integrate the financial and technological dimensions of the firm using high performance computing (HPC) methodology. In particular, the technology - for example ship building, blast furnaces - is connected to the financial dimension in a multi-period setting using HPC. This integration allows quantification of the risk surface applying stochastic methodology (e.g. Monte Carlo Analysis, Value at Risk and Real Option theory). The multi-disciplinary research plan has been strongly recommended by leading Finnish and Swedish experts in accounting/finance, economics and engineering.

The computational HPC platform developed by prof. Östermark since 1999 is one of the corner stones of the research project. A number of cutting edge nonlinear programming algorithms, delivered by the leading research groups in USA and Germany and from IBM, have been connected as support libraries to the HPC platform. The system has been extensively tested in difficult NLP, MINLP and GDP problems on single and parallel processors. The platform and its support libraries operate on the new massively parallel supercomputer Cray XC30 at CSC/Helsinki and in single processor mode at the Linux mainframe computer at ÅAU. Scalability has been demonstrated with all available processors on the Cray XC30.

More information can be found at www.abo.fi/ose/ralfostermark.html

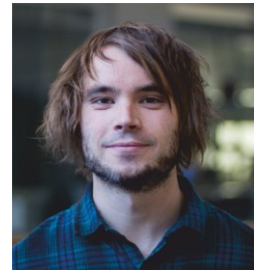
UPCOMING THESIS DEFENSES

Some Reformulations for the Quadratic Assignment Problem

MSc. Axel Nyberg will defend his PhD thesis in process design and systems engineering on March 28th at 12 PM in Auditorium Salin, Axelia II. Opponent is professor Hans Mittelmann from Arizona State University, USA and professor Tapio Westerlund acts as custos.

"The QAP is often referred to as a facility location problem where the goal is to determine the best placing of facilities on a predefined set of locations. As with many other combinatorial optimization problems, QAPs arise in a number of different fields. A few real world examples include: hospital layout planning, airport gate assignment, keyboard configurations and turbine balancing in power plants. The versatility of the fields of application where QAPs are found is one of the reasons why they are important to study. Despite its relatively old age, the QAP is a notoriously difficult problem and instances with only 30 locations are still unsolved using all the methods presented in the literature. In its normal form, the QAP is highly nonlinear with nothing but bilinear terms in the objective function.

My thesis is a summary of four papers. In the first three papers, reformulations for the QAP and a few techniques to improve them are presented. The objective function of the QAP is reformulated to a new form which then is discretized to a mixed integer linear programming formulation. In this way, some instances were solved to proven optimality for the first time ever. The fourth paper shows how the same reformulations can be applied to a multiechelon supply chain problem, in order to improve the model considerably."

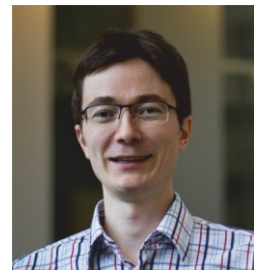


On the Use of Convex Underestimators in Global Optimization

MSc. Anders Skjäl will defend his PhD thesis in applied mathematics on April 10th at 12 PM in Auditorium Salin, Axelia II. Opponent is professor David Bogle from University College London, UK, and professor Tapio Westerlund acts as custos.

"My thesis gives a broad introduction to nonconvex mathematical programming and the use of convex underestimators. Complexity theory provides valuable perspectives on the hardness of optimization. I review basic concepts from complexity theory in one chapter, especially ideas pertaining to optimization and approximation. Many problem formulations appearing in application fields are partly nonconvex or unstructured and accordingly hard to optimize. If a global optimum or verified bounds on the optimum are desirable, one may opt for the *global optimization* approach; to strive for the best solution although success cannot be guaranteed beforehand.

To solve unstructured problems one will normally utilize branch-and-bound methods. I outline the steps of a generic branch-and-bound algorithm in nonlinear programming. The lower bounding step, where a problem is approximated with a more tractable problem, is currently the most prominent application for convex underestimators. My own contributions to the field are included in the form of five peer-reviewed articles. My research has focused on extending α BB convexification methods to include nondiagonal perturbations. The term *nondiagonal* comes from the inclusion of nondiagonal elements in the Hessian matrix of the perturbation. These constant elements β_{ij} correspond to bilinear terms $\beta_{ij}x_i x_j$. A piecewise linear term is added to improve the tightness of the underestimation, it does not affect the convexity."



ANNUAL OSE SEMINAR 2013



Techniques based on graph theory was the central topic of the plenary lectures given at the annual seminar in Optimization and Systems Engineering 2013 by professor Leo Liberti from École polytechnique in Paris, France, currently active at IBM Thomas J. Watson Research Center in New York, USA. Professor Liberti is also a member of the OSE group's International Scientific Panel. The 2013 seminar took place at Forum Marinum, Turku on November 15th.

Prof. Liberti held the following two keynote presentations:

- Symmetry in mathematical programming
- Distance constraints in Euclidean geometry

In the first presentation, a class of symmetry breaking methods based on reformulation techniques were illustrated. These may be used as an efficient presolving step of branch-and-bound based methods. In the second presentation, the topic was a significant problem in distance geometry connected to graph theory, with applications in protein conformation, wireless sensor network design and robotic control.

Professor Liberti has published more than 150 papers on mathematical programming, global and combinatorial optimization, distance geometry, bioinformatics, and industrial systems applications. He is also the author and editor of several books in optimization including "Distance Geometry: Theory, Methods and Applications" coedited with A. Mucherino, C. Lavor and N. Maculan, Springer New York, 2013, and "Global Optimization: from Theory to Implementation" coedited with N. Maculan, Springer Berlin, 2006.

At the seminar presentations of current research performed in the OSE group were also given by PhD students active in the group. All presentations are available on the OSE group's website www.abo.fi/ose.

PREVIOUS SEMINARS



PRESENTATIONS AT THE SEMINAR

MORNING SESSION

CHAIRMAN: PROFESSOR TAPIO WESTERLUND

PROFESSOR LEO LIBERTI

- Symmetry in mathematical programming
- Distance constraints in Euclidean geometry

AFTERNOON SESSION

CHAIRMAN: DR ANDREAS LUNDELL

MIKAEL NYBERG, PHD STUDENT

- Weather routing – using dynamic programming to win sailing races

JOHAN PENSAR, PHD STUDENT

- Marginal pseudo-likelihood: a Bayesian approach for learning the graph structure of a Markov network

ANDERS SKJÄL, PHD STUDENT

- Complexity theory for the global optimizer

AMIR SHIRDEL, PHD STUDENT

- Trend and system identification with orthogonal basis function

AXEL NYBERG PHD STUDENT

- Applications of the quadratic assignment problem

OTTO NISSFOLK, PHD STUDENT

- Reformulation of 0-1 quadratic programs

HENRIK NYMAN, PHD STUDENT

- Stratified Gaussian graphical models

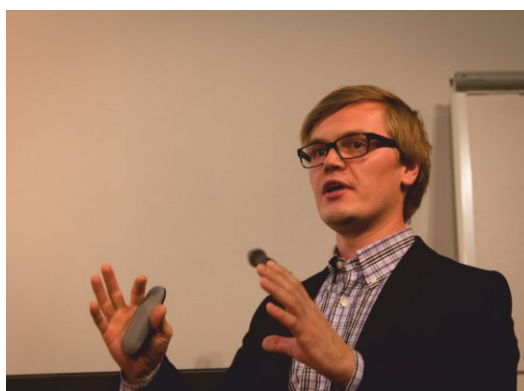
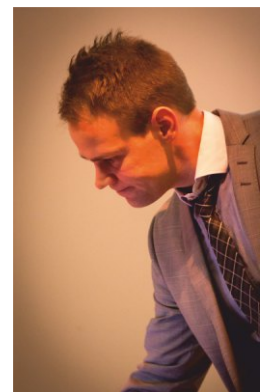


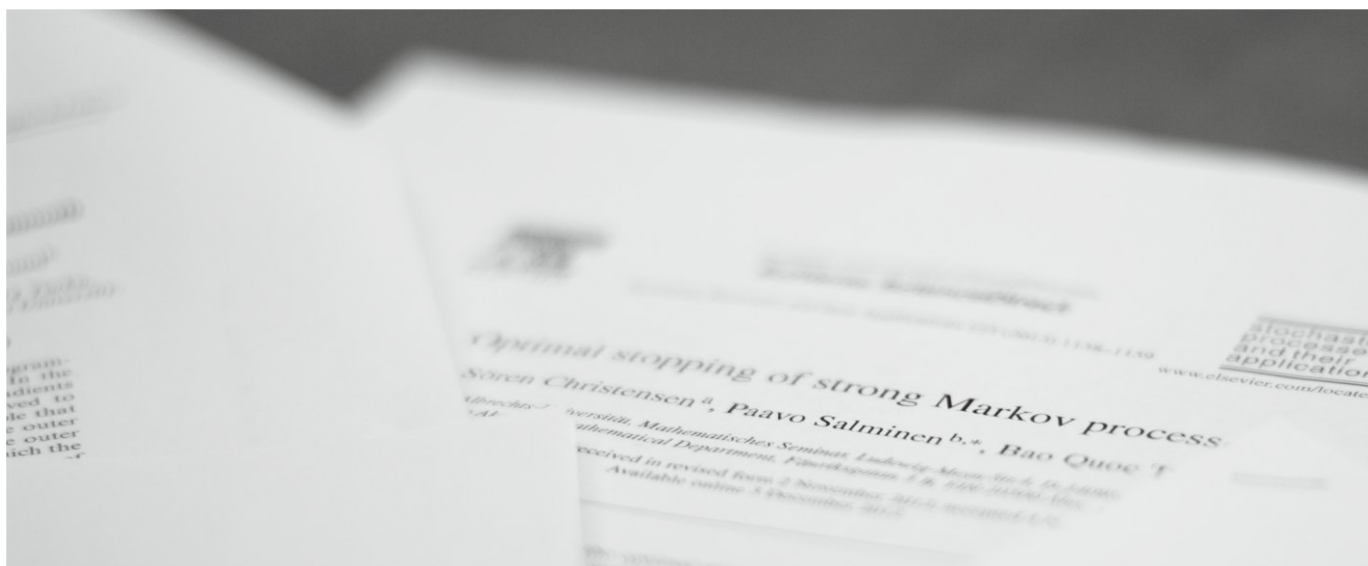
Professor Högnäs asks a question during the plenary



Dr Karmitsa and professors Liberti and Westerlund

Pictures from the seminar. From the upper left: Johan Pensar, Anders Skjäl, Mikael Nyberg, Andreas Lundell, Axel Nyberg, Amir Shirdel, Otto Nissfolk, Henrik Nyman





PEER-REVIEWED PAPERS

Been, M. de, W. van Schaik, L. Cheng, J. Corander, and R. J. Willems. "Draft genome sequence of *Enterococcus faecium* PC4.1, a Clade B strain isolated from human feces". In: *Genome Biology and Evolution*. Available online (2013). doi: 10.1093/gbe/evt111.

Blomstedt, P., R. Gauriot, N. Viitala, T. Reinikainen, and J. Corander. "Bayesian predictive modeling and comparison of oil samples". In: *Journal of Chemometrics* 28.1 (2014), pp. 52–59. issn: 1099-128X. doi: 10.1002/cem.2566.

Cheng, L., T. R. Connor, J. Sirén, D. M. Aanensen, and J. Corander. "Hierarchical and spatially explicit clustering of DNA sequences with BAPS software". In: *Molecular Biology and Evolution*. Available online (2013). doi: 10.1093/molbev/mst028.

Christensen, S., P. Salminen, and B. Q. Ta. "Optimal stopping of strong Markov processes". In: *Stochastic Processes and their Applications* 123 (2013), pp. 1136–1159.

Eronen, V.-P., M. M. Mäkelä, and T. Westerlund. "On the generalization of ECP and OA methods to nonsmooth convex MINLP problems". In: *Optimization* (2013). Available online iFirst June 6th 2013. doi: 10.1080/02331934.2012.712118.

Jääskinen, V., V. Parkkinen, L. Cheng, and J. Corander. "Bayesian clustering of DNA sequences using Markov chains". In: *Statistical Applications in Genetics and Molecular Biology*. Available online (2013). doi: 10.1515/sagmb-2013-0031.

Jääskinen, V., J. Xiong, J. Corander, and T. Koski. "Sparse Markov chains for sequence data". In: *Scandinavian Journal of Statistics*. Available online (2013). issn: 1467-9469. doi: 10.1111/sjos.12053.

Kuikka, S., J. Vanhatalo, H. Pulkkinen, S. Mäntyniemi, and J. Corander. "Experiences in Bayesian inference in Baltic Sea management". In: *Statistical Science*. In press (2013).

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Willems, A. M. Earl, and M. S. Gilmore. "Emergence of epidemic multi-drug resistant *Enterococcus faecium* from animal and commensal strains". In: *mBio* 4 (2013). doi: 10.1128/mBio.00534-13.

Lundell, A., A. Skjäl, and T. Westerlund. "A reformulation framework for global optimization". In: *Journal of Global Optimization* 57.1 (2013), pp. 115–141. issn: 0925-5001. doi: 10.1007/s10898-012-9877-4.

Lundell, A. and T. Westerlund. "The reformulation-based GO algorithm for solving nonconvex MINLP problems – some improvements". In: *Chemical Engineering Transactions* 32 (2013), pp. 1321–1326. doi: 13.3303/CET1332221.

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Marttinen, P., J. Gillberg, A. Havulinna, J. Corander, and S. Kaski. "Genome-wide association studies with high-dimensional phenotypes". In: *Statistical Applications in Genetics and Molecular Biology*. In press (2013).

McNally, A., L. Cheng, S. R. Harris, and J. Corander. "The evolutionary path to extra intestinal pathogenic, drug resistant *Escherichia coli* is marked by drastic reduction in detectable recombination within the core genome". In: *Genome Biology and Evolution* (2013). doi: 10.1093/gbe/evt038.

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Nyberg, A. and T. Westerlund. "Tightening a discrete formulation of the quadratic assignment problem". In: *Chemical Engineering Transactions* 32 (2013), pp. 1309–1314.

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Shepherd, M. A., V. M. Fleming, T. R. Connor, J. Corander, E. J. Feil, C. Fraser, and W. P. Hanage. "Historical zoonoses and other changes in host tropism of *Staphylococcus aureus*, identified by phylogenetic analysis of a population dataset". In: *PLoS ONE* 8.5 (2013). doi: 10.1371/journal.pone.0062369.

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Weiss, G. and O. Staffans. "Maxwell's equations as a scattering passive linear system". In: *SIAM Journal on Control and Optimization* 51.5 (2013), pp. 3722–3756. doi: 10.1137/120869444.

CONFERENCE PROCEEDINGS

Corander, J., T. Janhunen, J. Rintanen, H. Nyman, and J. Pensar. "Learning chordal Markov networks by constraint satisfaction". In: *Advances in Neural Information Processing Systems*. Ed. by C. J. C. Burges, L. Bottou, M. Welling, Z. Ghahramani, and K. Q. Weinberger. Vol. 26. 2013, pp. 1349–1357.

Lundell, A. and T. Westerlund. "Refinement strategies for piecewise linear functions utilized by reformulation-based techniques for global optimization". In: *23rd European Symposium on Computer Aided Process Engineering*. Ed. by A. Kraslawski and I. Turunen. Vol. 32. *Computer Aided Chemical Engineering*. Elsevier, 2013, pp. 529–534. doi: 10.1016/B978-0-444-63234-0.50089-0.

Nissfolk, O. and T. Westerlund. "A metaheuristic optimization algorithm for binary quadratic problems". In: *23rd European Symposium on Computer Aided Process Engineering*. Ed. by A. Kraslawski and I. Turunen. Vol. 32. *Computer Aided Chemical Engineering*. Elsevier, 2013, pp. 469–474. doi: 10.1016/B978-0-444-63234-0.50079-8.

Skjäl, A. and T. Westerlund. "Comparison of two convex underestimation methods for quadratic functions". In: *23rd European Symposium on Computer Aided Process Engineering*. Ed. by A. Kraslawski and I. Turunen. Vol. 32. *Computer Aided Chemical Engineering*. Elsevier, 2013, pp. 535–540. doi: 10.1016/B978-0-444-63234-0.50090-7.

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Christensen, S. and P. Salminen. "Riesz representation and optimal stopping with two case studies". In: arXiv 1309.2469 (2013), pp. 1–24. url: <http://arxiv.org/pdf/1309.2469.pdf>.

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Salminen, P. and B. Q. Ta. "Differentiability of excessive functions of one-dimensional diffusions and the principle of smooth fit". In: arXiv 1310.1901 (2013), pp. 1–22. url: <http://arxiv.org/pdf/1310.1901.pdf>.

PHD AND MASTER'S THESES

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Eklund, T. "Ett stokastiskt dynamiskt system med tillämpning på datorgrafik". MSc.thesis. Åbo Akademi University, 2013.

Kronqvist, J. "Development of measurements and control algorithms with industrial applications". MSc. thesis. Åbo Akademi University, 2013.

Nyberg, A. "Some reformulations for the quadratic assignment problem". PhD thesis. Åbo Akademi University, 2014. isbn: 978-952-12-3019-6.

Skjäl, A. "On the Use of Convex Underestimators in Global Optimization". PhD thesis. Åbo Akademi University, 2014. isbn: 978-952-12-3018-9.

KEY FIGURES 2010-2014

PERSONNEL

- 7 professors
- 6 post doc researchers
- 20 PhD students (8 directly funded)

PUBLICATIONS

- 1 monograph
- 6 PhD theses and 12 master's theses
- 4 book chapters
- 96 peer-reviewed journal articles
- 20 articles in conference proceedings
- 4 reports

ABOUT THE OSE RESEARCH GROUP

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

The Optimization and Systems Engineering (OSE) group at Åbo Akademi University is an interdisciplinary research group focusing on theory, methods and algorithms in systems engineering, optimization and statistics, and their applications in science and engineering.

OSE bridges the systems engineering, systems theory and mathematical disciplines at Åbo Akademi University and the OSE group represents the kernel of expertise in this field at the University. The group was appointed a Center of Excellence within research at the university for the time-period 2010–14.

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
Department of Chemical Engineering,
Carnegie Mellon University, Pittsburgh, USA

PROFESSOR CHRISTODOULOS FLOUDAS
Department of Chemical and Biological Engineering,
Princeton University, USA

PROFESSOR STRATOS PISTIKOPOULOS
Department of Chemical Engineering,
Imperial College London, UK

PROFESSOR LEO LIBERTI
Laboratoire d'informatique,
École Polytechnique, Paris, France

PROFESSOR MONTAZ ALI
School of Computational and Applied Mathematics,
University of the Witwatersrand,
Johannesburg, South-Africa

NEW PHD STUDENT



MSc. Jan Kronqvist has been accepted as a PhD student in the OSE group as of January 2014. His thesis is connected to extensions of the Extended cutting plane method for solving convex MINLP problems and is supervised by professor Tapio Westerlund.

GROUP LEADERS

The steering group of the research group was in 2013 extended to include also professor Paavo Salminen. Professor Göran Högnäs retired from his position at ÅAU during 2013, but continues to be an active researcher within the group as well as a member of the steering group.



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 EMERITUS GÖRAN HÖGNÄS
Mathematics and Statistics
Department of Natural Sciences



MATHEMATICAL STATISTICS
PROFESSOR JUKKA CORANDER
Mathematics and Statistics
Department of Natural Sciences



PROBABILITY THEORY
PROFESSOR PAAVO SALMINEN
Mathematics and Statistics
Department of Natural Sciences

ABOUT THIS ISSUE

LAYOUT: Andreas Lundell
TEXT: Andreas Lundell and Tapio Westerlund

OPTIMIZATION AND SYSTEMS ENGINEERING

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