

CAPD e-Newsletter, October 2009

<http://capd.cheme.cmu.edu>

Dear CAPD member,

We hope this newsletter will have information that is of interest to you.

Best regards, Ignacio Grossmann

- The CAPD Newsletters can now be accessed thorough the webpage <http://capd.cheme.cmu.edu/newsletters.html>. All registered users of CAPD can access these by using their email addresses as userid and password. If you do not have that information, please contact Laura Shaheen at lr23@andrew.cmu.edu . We also welcome any suggestions you may have for our webpage <http://capd.cheme.cmu.edu> .

- Please take note that the next Annual Review Meeting will take place on March 8-9, 2010. This will be followed by the meeting of the special group on Enterprise-wide Optimization on March 10.

- Prior to the CAPD Meeting, we will have the first meeting of the Energy Systems Initiative on Sunday March 7. This initiative will be led by Larry Biegler, who will contact you in January about this meeting.

- New MINLP Cybersite.

We want to let you know that we just launched the CMU-IBM Cyberinfrastructure Collaborative site for MINLP: <http://www.minlp.org>

We hope you will be able to contribute MINLP problems to this new cybersite. The major goal of this site is to create a library of optimization problems in different application areas in which one or several alternative models are presented with their derivation. In addition, each model has one or several instances that can serve to test various algorithms. While we are emphasizing MINLP models, you may also wish to submit MILP and NLP models that are relevant to problems that can be formulated as MINLP problems. The site is intended to provide a mechanism for researchers and users to contribute towards the creation of this library of optimization problems, and to provide a forum of discussion for algorithm developers and application users where alternative formulations can be discussed as well as performance and comparison of algorithms. The site also provides extensive information on various resources, meetings and bibliography.

If you have any comments or suggestions, please send them to:

minlp@andrew.cmu.edu

- The short-course Optimization Modeling and Integrated Process Operations is scheduled for May 20-26, 2010: <http://capd.cheme.cmu.edu/shortcourse/index.html>. The short course is organized in two parts consisting of 6 modules which can be taken in any combination (e.g. 1, 2 3 or all 6):

I. Optimization Modeling to be taught from Thursday through Saturday (May 20-22) will focus on modeling and algorithms with applications to process optimization, process synthesis and molecular design:

- a) Nonlinear programming (Biegler, Thursday, May 20)
- b) Mixed integer and disjunctive programming (Grossmann, Friday, May 21)
- c) Global optimization and optimization under uncertainty (Sahinidis, Saturday, May 22)

II. Integrated Process Operations to be taught from Monday through Wednesday (May 24-26), will focus on three major decision levels in plant and enterprise-wide optimization:

- d) Mixed-integer models for planning and scheduling (Grossmann, Monday, May 24)
- e) Process dynamics and control (Ydstie, May 25)
- f) Differential/algebraic models for real time optimization (Biegler, Wednesday, May 26)

The material in each module is independent and self-contained and can be taken in any combination. A detailed description of the topics covered in the course is given in: http://capd.cheme.cmu.edu/shortcourse/shortcourse_details.htm. Recall that CAPD members receive a 25% discount.

- Enterprise-wide Optimization <http://egon.cheme.cmu.edu/ewocp/>

The meeting of the EWO group took place on September 29. The group is currently composed of the following companies: ABB, Air Products, BP, Dow Chemical, ExxonMobil, NOVA Chemicals, PPG, Praxair and Total. The next meeting of the EWO will take place on Wednesday, March 10. Slides on presentations of these meetings can be found in: http://egon.cheme.cmu.edu/ewocp/slides_meetings.html; slides on seminars on EWO can be found in: http://egon.cheme.cmu.edu/ewocp/slides_seminars.html

- Congratulations to Jeff Sirola who has been named recipient of the 2009 Lawrence B. Evans Award in Chemical Engineering Practice, which will be presented to him at the AIChE Meeting in Nashville. The award is to recognize his outstanding technical and engineering contributions to process synthesis, and for his exceptional service and dedication to the profession.

<http://www.aiche.org/uploadedFiles/CEP/Issues/2009-10/100944.pdf>

- Faculty News

- Larry Biegler, Ignacio Grossmann and Art Westerberg were selected recipients of the 2009 Warren Lewis Award for Excellence in Education by AIChE.

- Andreas Waechter and Larry Biegler were awarded the INFORMS Computing Prize for the Mathematical Programming (2006) paper that describes the IPOPT algorithm. At the recent INFORMS meeting, Andreas and Larry gave a joint presentation at the awards session and described recent advances related to this algorithm and code.

- Larry Biegler is spending part of the fall semester at the University of Wisconsin, Madison as the Hougen Visiting Professor. In addition to a named seminar, Larry is giving a short course on Nonlinear Programming and Dynamic Optimization and

interacting with colleagues in Chemical Engineering, Industrial Engineering and Computer Science at Wisconsin. Over the past month, Larry presented seminars at the Technical University of Berlin and Computing Research Institute, Purdue University. He also taught a short course at the Max Planck Institute on Dynamic Process Systems in Magdeburg, Germany.

- Ignacio Grossmann gave the plenary lectures “Scope for the Application of Mathematical Programming Techniques in the Synthesis and Design of Sustainable Processes” at the FOCAPD Meeting in Breckenridge, and “Research Challenges in Planning and Scheduling for Enterprise-wide Optimization of Process Industries,” at the PSE-2009 meeting in Salvador, Brazil. He also gave the seminars “Optimal Synthesis and Planning of Sustainable Processes,” at INTEC, Santa Fe, Argentina, PLAPIQUI, Bahia Blanca, and Department of Chemical Engineering, National University of Singapore. He taught a short course on enterprise-wide optimization at PLAPIQUI, in Bahia Blanca, Argentina. He also gave the seminar “Mathematical Programming Approaches to Enterprise-wide Optimization of Process Industries,” at the Fields Institute, University of Toronto. Ignacio was appointed for a three year term as Section 3 Search Executive of the National Academy of Engineering.

- Nick Sahinidis chaired the committee that awarded the Beale-Orchard-Hays Prize for the Mathematical Programming Society during the International Symposium on Mathematical Programming in Chicago, August 2009. He also edited a volume for *Optimization Methods and Software* with 19 papers devoted to global optimization vol. 24, issues 4-5, 2009.

- Erik Ydstie visited NTNU in Trondheim to be at the Annual Integrated Operations Workshop to discuss how to integrate PSE tools in the operation of the oil and gas fields in the North Sea. He also gave a three day short course on Adaptive Control Systems to final year students in the Cybernetics Department. Michael Wartmann is spending the semester at the Technical University in Delft with Prof. Dirk van Jansen to work on modeling and enhanced oil recovery with the Shell Research group. Erik Ydstie’s research in the area of solar cells was bolstered by the award of an NSF grant to develop a new high speed process to produce Silicon wafers for solar cells. The research is mostly experimental and includes support to develop a laboratory test system to validate the concept.

- Student and Visitor News

- Congratulations to Fengqi You who has passed his Ph.D. examination on October 22. He will be joining Northwestern University as an Assistant Professor in 2011 after he completes a postdoctoral fellowship at Argonne National Lab.

- Congratulations to Mohit Aggarwal who joined Air Products in Allentown.

- Congratulations to Sebastian Terrazas-Moreno and Rodrigo Lopez Negrete for having passed their Ph.D. proposals.

- The following PSE students successfully passed their Ph.D. qualifying exam: Robert Smith, working for Larry Biegler and Myung Jhon, Vijay Gupta, working for Ignacio Grossmann, Yan Zhang working for Nick Sahinidis, Juan Du and Rocco Panella working for Erik Ydstie.

- Elvis Ahmetovic, who spent one year in Ignacio's group as a Fulbright Scholar working in the area of process water networks, returned to the University of Tuzla, Bosnia, in mid-September.

- Welcome to Professor Zhen Gao from Northeastern University of China, who will be visiting Nick Sahinidis' group for a year.

-Webpages. The following sites might be of interest to you:

Virtual library on Process Systems Engineering:

<http://cepac.cheme.cmu.edu/pasilectures.htm>

You can access webpages of all PSE faculty in the Americas in:

<http://cepac.cheme.cmu.edu/country.htm>

Papers to be presented by CAPD faculty at AIChE Meeting, Nashville:

Larry Biegler's group:

Anshul Agarwal, Lorenz T. Biegler and Stephen Zitney , "A Trust-Region Algorithm for the Optimization of PSA Processes using Reduced Order Modeling"

Sesha H. Vemuri, Parag Jain, Dehee Kim, Lorenz T. Biegler and Myung S. Jhon, "Transport and Reaction Processes in Non-Homogeneous Porous Media for Fuel Cell Applications"

Ravindra S. Kamath, Ignacio E. Grossmann and Lorenz T. Biegler, "Optimal Integrated Design of Air Separation Unit and Gas Turbine Block for IGCC Systems"

Parag Jain, Lorenz T. Biegler and Myung S. Jhon, "Fuel Cell System Integration via Reduced Order Methods"

Sree Rama Raju Vetukuri, Lorenz T. Biegler and Andrea Walther, "A General Nonlinear Programming Algorithm for the Optimization of Problems with Dense Constraint Jacobians"

Rui Huang, Sachin C. Patwardhan and Lorenz T. Biegler, “Nonlinear Observer Based Robust and Offset Free Nonlinear Predictive Control of Air Separation Units in Power Plants”

Weijie Lin, Lorenz T. Biegler and Annette Jacobson, “Parameter Identification and Dynamic Optimization of Seeded Suspension Polymerization Process”

Shivakumar Kameswaran and Lorenz T. Biegler, “Numerical Regularization for Singular Optimal Control Problems”

Estimation of the Arrival Cost in MHE Using Particle Filters, Rodrigo Lopez-Negrete de la Fuente, Sachin C. Patwardhan and Lorenz T. Biegler

Rui Huang, Sachin C. Patwardhan and Lorenz T. Biegler, “Online Model Maintenance and Robust Adaptive Nonlinear Model Predictive Control”

Soo Kim, Parag Jain, Lorenz T. Biegler and Myung S. Jhon, “Inverse Modeling of Solid Oxide Fuel Cells”

Peter Heidebrecht, Kai Sundmacher and Lorenz T. Biegler, “Experimental Design of Dynamic Temperature-Programmed Reduction (TPR) Experiments”

Rodrigo Lopez-Negrete de la Fuente, Salvador Garcia-Munoz and Lorenz T. Biegler, “Nonlinear Programming Based Methods for PCA Parameter Estimation using Data with Missing Elements”

Robert L. Smith, Pil Seung Chung, Parag Jain, Lorenz T. Biegler and Myung S. Jhon, “Molecular Modeling of Proton Transport in Polymer Electrolyte Membrane”

Ignacio Grossmann’s group:

Grossmann, I.E. and G. Guillén-Gosálbez, “Optimal Synthesis and Planning of Sustainable Processes”

You, F., E. Capon, I.E. Grossmann and J.M. Pinto, “Fast Computational Strategies for Large Scale Distribution-Inventory Planning of Industrial Gases under Demand Uncertainty”

Kamath, R.S., I.E. Grossmann and L.T. Biegler, “Optimal Integrated Design of Air Separation Unit and Gas Turbine Block for IGCC Systems”

Terrazas-Moreno, S., I.E. Grossmann and J. Wassick, “Optimal Design of Reliable Integrated Chemical Production Sites”

Alattas, A., I.E. Grossmann and I. Palou-Rivera, “Optimal Model-Based Production Planning for Refinery Operations,”

Lima, R.M., I.E. Grossmann and Y. Jiao, “Planning and Long-Term Scheduling of a Single-Stage Multi-Product Continuous Process with Complex Recycling Structure”

Karuppiah, R., M. Martin and I.E. Grossmann, “A Simple Heuristic for Reducing the Number of Scenarios in Two-Stage Stochastic Programs”

Rocha, R., I.E. Grossmann and M.V.S. Poggi de Areagao, “Cascading Knapsack Inequalities: Hidden Structure in Some Inventory-Production-Distribution Problems”

Ruiz, J.P. and I.E. Grossmann, “Strengthening Lower Bounds in the Global Optimization of Bilinear and Concave Generalized Disjunctive Programs”

Tarhan, B. and I.E. Grossmann, “Improving Dual Bound for Stochastic MILP Models Using Sensitivity Analysis”

Ahmetovic, E. and I.E. Grossmann, “General Superstructure and Global Optimization Model for the Design of Integrated Process Water Networks”

Castro, P., I. Harjunoski and I.E. Grossmann, “Optimal Scheduling Under Variable Electricity Cost and Power Availability”

Castro, P., I. Harjunoski and I.E. Grossmann, “Scheduling Algorithm for Large Scale Multiproduct Plants”

Nick Sahinidis’ group:

Yan Zhang, Panagiotis Vouzis and Nick Sahinidis,
[\(496a\) Risk Assessment for CO2 Geologic Sequestration](#)

Apurva Samudra and Nick Sahinidis,
[\(463b\) Framework for Computer-Aided Molecular Design](#)

Luis Miguel Rios and Nick Sahinidis,
[\(183e\) Derivative-Free Optimization: A Review of Algorithms and Comparison of Software Implementations](#)

Panagiotis Vouzis, Joe Elble and Nick Sahinidis,
[\(437c\) Iterative Methods for Solving PDEs On a Graphics Processing Unit](#)

YoungJung Chang and Nikolaos V. Sahinidis,
[\(380c\) Process Design with Robust Stability Under Parametric Uncertainty](#)

Shweta B. Shah and Nick Sahinidis,
[\(485ah\) Secondary Structure Aided Protein Structure Alignment](#)

Keith Zorn Jr. and Nikolaos Sahinidis,
[\(422i\) Reformulation Linearization Techniques: An Application to Hartree-Fock Calculations](#)

YoungJung Chang and Nikolaos V. Sahinidis,
[\(380c\) Process Design with Robust Stability Under Parametric Uncertainty](#)

Erik Ydstie's group:

Erik Ydstie, "Two Port Representation of Process Systems"

Michael Wartmann and Erik Ydstie, "Optimality of Process Networks"

Juan Du and Erik Ydstie, "The Impact of Zero Dynamics on the Stability of Inventory Control Systems"

Balaji Sukumar, Jovan Illic, Bruce Krogh and Erik Ydstie, "Modeling and Control of Chemical Looping Combustion"

- Upcoming meetings

INFORMS Annual Meeting 2009, October 11-14, 2009
San Diego Convention Center and Hilton San Diego, San Diego, California
<http://meetings.informs.org/sandiego09/>

AIChE 2009 Annual Meeting, November 8-13, 2009
Gaylord Opryland Hotel, Nashville, TN
<http://www.aiche.org/Conferences/AnnualMeeting/index.aspx>

European Workshop on MINLP
April 12 - 16, 2010
Marseille, France
<http://www.roadef.org/forums/index.php?action=vthread&forum=1&topic=746>

ESCAPE-20
June 6-9, 2010
<http://www.aidic.it/escape20/>

Nonlinear Optimization, Variational Inequalities and Equilibrium Problems
July 2 - 10, 2010
<http://www.dis.uniroma1.it/~erice2010/>

9th IFAC Symposium on Dynamics and Control of Process Systems (DYCOPS-9) July 5-7, 2010, Leuven, Belgium <http://www.dycops2010.org>

Computational Management Science

July 28-30, 2010

<http://www.univie.ac.at/cms2010/>

CHISA 2010: 19th International Congress of Chemical and Process Engineering

ECCE-7: 7th European Congress of Chemical Engineering

August 29 to September 2, 2010

Prague, Czech Republic

<http://www.chisa.cz/2010/>

Distillation & Absorption 2010, Sep 12-15, 2010

Eindhoven University of Technology

The Netherlands

<http://www.da2010.nl/>

Complex Systems Design & Management 2010

October 27 - 29, 2010

Paris, France

<http://www.csdm2010.csdm.fr/>