CENTER FOR ADVANCED PROCESS DECISION-MAKING

New Directions for Process Systems Engineering

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Erik Ydstie's Group

GENERAL NEWS

Gary Powers. We deeply regret to inform our CAPD members that Professor Gary Powers died on July 23, 2007. Gary was a leading researcher in process systems engineering and a major force in the CAPD. He did pioneering research in process risk assessment and in process synthesis. He was also an outstanding educator and was one of the most popular and well-liked professors in the department. He was always the smiling face in any group and was supportive of all those around him. Gary will be sorely missed. He is survived by his wife Susan and their six children. Gary received degrees from the University of Michigan (BS ChE, 1967) and from the University of Wisconsin (PhD ChE, 1971). He served on the faculty of MIT before joining Carnegie Mellon in 1974.

In his memory an undergraduate scholarship will be established. Donations may be sent for the Gary J. Powers Scholarship Fund, c/o Toni Mciltrot, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15222-5488.

Pfizer: new member of CAPD. We would like to welcome our newest member of the CAPD, Pfizer, Inc of Groton, Connecticut. The contact will be Dr. Salvador Garcia, Senior Scientist, Data Analysis and Applied Chemometrics in Pfizer Global Research and Development.

Nikolaos Sahinidis. We are very pleased to welcome Nick Sahinidis to the CAPD, whose addition strengthens our optimization efforts and expands them to molecular design problems. His work at the molecular level (X-ray imaging, bioinformatics and molecular design) complements ongoing CAPD activities at the process level. He has recently joined the Department of Chemical Engineering on August 1, 2007. Nick was a Professor of Chemical and Biomolecular Engineering at the University of Illinois at Urbana for 16 years. He obtained his Ph.D. from Carnegie Mellon University in 1990 under the direction of Ignacio. Nick's current research interests are at the interface between computer science and operations research, with applications in chemical, biological, and engineering systems. His research has focused heavily on the development of theory, algorithms, and software for global optimization of mixed-integer nonlinear programs. His BARON global optimization software has found applications in fields ranging from computational chemistry to energy modeling. Nick has served on eight editorial boards, including the Journal of Global Optimization, Optimization and Engineering, and Industrial & Engineering Chemistry Research. He is active in several professional societies, including AIChE, INFORMS, and the Mathematical Programming Society. His research activities have been recognized by several awards, including the 2004 INFORMS Computing Society Prize, and the Beale-Orchard-Hays Prize from the Mathematical Programming Society in 2006. Since returning to CMU, Nick gave a semi-plenary talk on "Optimization in the New Biology" at the 2nd International Conference on Continuous Optimization that took place August 12-16, 2007 at McMaster University in Hamilton, Ontario.

Ignacio Grossmann received the Kun Li Award for Excellence in Education, at graduation. This award is selected by the seniors for the faculty member who, in their view, had the greatest impact. We should note that Gary Powers was a frequent recipient of this award. Ignacio was inspired by Gary's style of teaching and interacting with students.

Ignacio gave a keynote lecture on Enterprise-wide Optimization at the 2nd International Conference on Modeling, Simulation and Applied Optimization, Petroleum Institute, Abu Dhabi, in March, 2007. He participated in the Workshop on Global Optimization, at the Fields Institute, University of Toronto, May, 2007. He also gave a joint plenary lecture with Rafiqui Gani, "Process Systems Engineering and CAPE–What Next?" at the ESCAPE-17 meeting in Bucharest, Romania.

Larry Biegler has been selected recipient of the 2007 CACHE Award for Excellence in Computing in Chemical Engineering Education. This award, sponsored by the CACHE Corporation, is presented for significant contributions in the development of computer aids for chemical engineering education. Larry was recognized for leadership in the development of strategies and methods for process optimization, particularly for the pioneering implementation of the successive quadratic programming (SQP) method in the process simulator FLOWTRAN that has allowed many students to optimize process flowsheets.

Larry was invited to give a number of keynote and plenary talks at conferences this spring and summer. These included:

- "Sensitivity-based NMPC with delayed optimization," (with V. Zavala), invited speaker at Workshop on Nonlinear Model Based Control - Software and Applications (NMPC-SOFAP, 2007), Loughborough, England, April, 2007
- "Large-scale Nonlinear Programming: An Integrating Framework for Enterprise-Wide Dynamic Optimization," invited keynote speaker at ESCAPE-17, Bucharest, May, 2007
- "Parameter Estimation of Dynamic Systems: Simultaneous Collocation and Large-scale Nonlinear Programming," invited speaker at Statistics for Dynamical SystemsWorkshop, Centre de Recherche Mathematiques, Montreal, Canada, July, 2007
- "Efficient Nonlinear Programming Algorithms for Chemical Process Control and Operations," invited plenary speaker, International Foundation on Information Processing (IFIP) Conference on Systems Modeling and Optimization, Cracow, Poland, July, 2007
- "Optimization Methods for Chemical Process Engineering," invited plenary speaker, International Conference on Continuous Optimization (ICCOPT), Hamilton, Ontario, August, 2007

Erik Ydstie has been selected recipient of the 2007 AIChE Computing in Chemical Engineering CAST Award which recognizes outstanding contributions in the application of computing and systems technology to chemical engineering.

Erik presented a lecture on process networks at the University of Rhode Island in May. He presented papers at the DYCOPS conference in Cancun Mexico and at the MOPTA conference on optimization at McMaster University in Hamilton, Canada. He will also present papers at the Reduced Order Modeling Workshop in Leicester, England at the end of August. Erik is now on sabbatical leave. He is spending the leave as CEO of Industrial Learning Systems. ILS currently has five employees working with Emerson on developing passivity based and adaptive control systems for power plants. During his sabbatical Erik will finish writing a new undergraduate textbook on process control. The book will contain no mention of Laplace transforms. Erik continues his work on scale-up and design with Alcoa on the carbothermic aluminum project. Erik is in the process of developing a program aimed towards the manufacture and application of solar cells. A new process for continuous casting of wafers is under development, and he is also developing new approaches for making dye-sensitized solar cells with polymer backing. The later work is carried out in cooperation with Sudhir Narajan, a new Post Doc who joined the research group in March 2007.

Steinar Hauan has declined his participation in activities of the CAPD, effective May 1, 2007.

This year the Chemical Engineering Department recruited a class of 30 graduate students, which has produced the addition of a large number of students in the PSE area. It is a pleasure to welcome the following new Ph.D. students to the PSE group: **Rui Huang** from Zhejiang University, **Lin Weijie** from Tsinghua University, and **Sree Rama Raju Vetujori** from Jawaharlal Nehru Tech. University will be working with Larry Biegler; **Ravi Kamath**, from IIT-Bombay, and **Adam Malacina** from IIT-Chicago, will be working under the joint supervision of Larry and Ignacio; **Abdulamrahman Alattas** from the Petroleum Institute in Abu Dhabi and Colorado School of Mines, **Sylvain Mouret** from Ecole Polytechnique in Paris and **Juan Ruiz** from Instituto Regional in Rosario Argentina, will be working with Ignacio Grossmann; **Michael Wartmann** from University of Stuttgart will be working for Erik Ydstie on optimal control of networked systems. The M.S. students are **Gaurav Bansal** from Coimbarore Inst. of Tech., Anna University will be working with Larry and **Vishnu Chapalamadugu** from Dr. B.V. Raju Institute of Technology will be working with Erik.

Congratulations to **Yoshiaki Kawajiri,** student of Larry Biegler, who defended his Ph.D. thesis in June.

Congratulations to **Christy White** and **Kendell Jillson**, who graduated with PhD's in April and **Vishnu Chapamaladugu** who graduated with an MS. Christy was employed by HTR, Kendell continues as a PostDoc at CMU to complete some modeling and control work on IGCC processes. Vishnu has taken a position at NOVA Chemicals.

Victor Zavala and **Brian Baumrucker** spent the summer at ExxonMobil Chemicals at Baytown, TX and Air Products, Allentown, PA, respectively. Victor was working on NMPC applications with detailed process models while Brian was exploring and extending complementarity models for gas pipeline optimization.

Bora Tarhan spent the summer at ExxonMobil upstream in Houston. He worked with Vikas Goel and Amr El-Bakry on a stochastic optimization model for off-shore oilfields. **Fengqi You** spent the summer at Dow Chemical in Midland. He worked with John Wassick on stochastic optimization models for supply chain. **Eduardo Dozal** spent three months at Bayer working on supply chain problems..

Professors Arturo Jimenez and his student **Jose Maria Ortega Ponce** from Instituto de Celaya in Mexico, who collaborated with Ignacio Grossmann in the area of heat exchanger network synthesis, completed their visit in June. **Daniela Drummond** from University of Campinas in Brazil has joined Ignacio's group as a visitor. She will be working in scheduling of paper machines. **Roger Rocha** from PETROBRAS has joined Ignacio's group as a visitor. He will be working in the area of planning and scheduling in collaboration with Professor John Hooker.

Sudhir Ranjan, Sukumar Balaji, Chengtao Wen, Richard Chan and **Keyu Li** have joined the Ydstie research group as PostDocs. Sudhir os working on solar cells, Bala is working on the Alcoa project and Chengtao, Richard and Keyu are working on power plant control through ILS. **Juan Du** is working on computational fluid mechanics, modeling and control of particulate and fluid bed processes.

The Ydstie group webpage is being renovated and will be back on-line in September. The Industrial Learning Systems can be found at: http://www.ilsystems.net

CAPD e-News. We sent on April 26 our e-newsletter. As we indicated previously, we now issue on a yearly basis two extensive newsletters with detailed descriptions of the projects in August and January, while the two others are brief e-Newsletters in April and October that contain short announcements as well as information that we think will be useful to the CAPD members. We would appreciate receiving feedback or suggestions for improving the e-Newsletter.

2007 ANNUAL REVIEW MEETING

On the first day we had research overviews of the faculty, six excellent industrial presentations and a poster session. The dinner this year took place at Monterey Bay Fish Grotto Restaurant. On the second day, we had the presentations by last year students as well a special session on Modeling Systems (see below).You can access an electronic version of the agenda, list participants and slides presented at the 2007 CAPD Annual Review Meeting in: `http://www.cheme.cmu.edu/internal/capd2007.zip`
Please take note that the next Annual Review Meeting will take place on **March 10-11, 2008.**

ENTERPRISE-WIDE OPTIMIZATION INTEREST GROUP

The special interest group on Enterprise-wide Optimization is part of the project **"Computational Models and Algorithms for Enterprise-wide Optimization (EWO) of Process Industries"** that has been funded by the Pennsylvania Infrastructure Technology Alliance. The current participating companies are ABB, Air Products, BP America, Dow Chemical, ExxonMobil, and NOVA Chemicals. These companies have supplied case studies that are being undertaken by the EWO faculty and students. The project involves a total of 7 Ph.D. students, and 5 faculty (CMU: **Larry Biegler**, **Ignacio Grossmann**, **John Hooker**; Lehigh: **Jeff Linderoth, Larry Snyder**; UPitt: **Andrew Schaeffer**). The next meeting of this group will take place on **November 13, 2007**. The EWO meeting will start on November 12 with breakout groups, and on November 13 there will be academic and industrial presentations. The membership fee to this group is $12,500 for members of the CAPD. A description of the EWO project can be found in http://egon.cheme.cmu.edu/ewocp/

2007 CAPD SHORT COURSE http://capd.cheme.cmu.edu/shortcourse.html

The course this year was scheduled this year on June 6-12, 2007, and there were a dozen participants. For next year we will offer a new modified short course with the participation of Nick Sahinidis. The dates will be **June 12-18, 2008**. The specific format of that course will be published in the next e-Newsletter.

Recall that CAPD members receive a 25% discount. The course includes workshops where participants obtain hands-on experience formulating problems and using various software packages. Course materials include extensive notes, the GAMS software, and our textbook "Systematic Methods of Chemical Process Design." If you are interested in attending this course next summer, please contact Toni McIltrot at 412-268-3573, or e-mail: tm2l@andrew.cmu.edu.

PAN AMERICAN ADVANCED STUDY INSTITUTE ON EMERGING TRENDS IN PSE

Ignacio Grossmann will be organizing with Frank Doyle, Jaime Cerda and Argimiro Secchi the Pan American Advanced Studies Institute (PASI) on emerging trends in Process Systems Engineering on August 12-21, 2008, in Hotel Costa Galana, Mar del Plata, Argentina. The proposed workshop is aimed at advanced graduate and post-doctoral students, and will emphasize the latest developments and research challenges in the emerging areas of *sustainability, energy, biological systems, multiscale systems, and enterprise-wide optimization*. The PASI workshop will be a follow-up to the successful PASI on Process Systems Engineering that took place on in Iguazú, Argentina, in 2005. A website will soon be created to display information about this meeting.

VIRTUAL LIBRARY ON PROCESS SYSTEMS ENGINEERING

The Pan American Study Institute on Process Systems Engineering that was organized by **Ignacio Grossmann** took place in Iguazu, Argentina on August 16-25, 2005. The workshop addressed four major areas: Optimization, Process and Product Design, Process and Supply Chain Operations, and Process Dynamics and Control. A major outcome of the PASI conference was the development of virtual library on Process Systems Engineering covering the four areas. The library consists of the Powerpoint slides of the presentations, background articles, as well as exercises and MATLAB and GAMS computer files for various applications, and a practice exam with solutions. The virtual library can be found in, http://cepac.cheme.cmu.edu/pasilectures.htm

WEBSITES/PROCESS SYSTEMS DIRECTORY

We are happy to report that the CAPD newsletter is distributed in electronic form. We would appreciate receiving feedback from our member companies of our CAPD website, **http://capd.cheme.cmu.edu.** This website provides a number of interesting items including information about individual groups, industrial success stories, software available from the group, etc. Work is under way to update and modify our website. Other websites of interest are Erik's http://mongol.cheme.cmu.edu/, Ignacio's http://egon.cheme.cmu.edu, Larry's http://dynopt.cheme.cmu.edu, and Nick's http://www.andrew.cmu.edu/user/ns1b/ Also, the department maintains the website of CEPAC (Chemical Engineering Pan American Collaboration), the organization that has been formed to promote collaboration between the US and Argentina, Brazil and Chile. You can find in http://cepac.cheme.cmu.edu/country.htm a listing of all universities and researchers with links in the process systems area in the US, Argentina, Brazil, Canada, Mexico and Chile.

EXECUTIVE SUMMARY

Larry Biegler's Group

Since the last newsletter, a number of advances have been made in application of large-scale optimization, particularly for dynamic systems. The past few months have seen the following applications.

Dynamic optimization tools, ultimately for on-line use, have been applied that are centered on IPOPT, which continues to be developed at IBM. These have seen a number of applications ranging from detailed fuel cell models, advanced chromatographic separation, polymer reactors and processes, gas pipeline networks and nonlinear model predictive control. **Victor Zavala** has made strong advances in parameter and system identification for large-scale polymerization processes, and has developed a very efficient parallel computation approach. This is described in a preprint below. In addition, Victor has developed optimization formulations for Nonlinear Model Predictive Control (NMPC) and Moving Horizon Estimation (MHE) that exploit the simultaneous approach as well as recent NLP features in IPOPT. As a result, large dynamic optimization problems used for NMPC and moving horizon estimation (MHE) have *on-line computation costs reduced by two orders of magnitude!* A paper that describes the theoretical properties of this work is listed below. Related to this work is the development of specialized decomposition strategies within the IPOPT framework**. Brian Baumrucker** has developed interesting optimization formulations that incorporate complementarity constraints and allow a class of discrete decisions to be modeled within NLP problems. This approach is not restricted to particular NLP solvers and has been demonstrated on a variety of process applications. A preprint that describes this approach is listed below. Finally, for periodic adsorption applications**, Yoshi Kawajiri** is currently exploring optimization strategies for Simulated Moving Bed applications, the liquid-solid analog of PSA. In previous work, he has shown substantial improvements in productivity for these systems through an efficient dynamic optimization formulation. As a follow-on to this work, a preprint is listed that describes extended optimization formulations for this challenging problem.

Enabling Software From Larry Biegler's Group

Highlights of **Larry Biegler's group** include further development of the interior point nonlinear programming algorithm, IPOPT, in a number of directions. **Andreas Wächter**, now at IBM, developed a novel and very efficient barrier (interior point) NLP method, based on many of our earlier SQP concepts. In the general purpose framework, it adopts a sparse decomposition of the KKT matrix, and has been tested on thousands of applications with up to a quarter of a million variables. It has also been used to solve problems that incorporate a number of specialized decomposition strategies and for a wide variety of applications with several million variables. IPOPT is available under an Open Source software license and the source code can be downloaded from http://www.coin-or.org/Ipopt/index.

Carl Laird, now at Texas A&M, and **Andreas Wächter** have rewritten IPOPT as an object-oriented code written in C++. The resulting C++ package was released for public distribution last August and is seeing regular updates by Andreas. The code contains a much simpler interface to modeling environments as well as a more efficient implementation of the algorithm. Finally, the object-oriented code allows for greater flexibility, especially in adopting additional linear solvers and advanced decomposition strategies.

The IPOPT code has already been interfaced to a number of modeling systems including:

- **GAMS** –This system has been a standard optimization platform at CMU and is widely used in industry. IPOPT has been linked to GAMS by colleagues at GAMS development using the COIN-OR interfaces. The MUMPS sparse linear solver was used in the standard release, although versions are available that allow any sparse matrix solvers to be applied (subject to 3rd party licenses). Moreover, GAMS provides exact first and second derivatives and exploits the full capabilities of IPOPT.
- **AIMMS** –This GAMS-like system has a number of extended features including a full graphical user interface for the development of specific user applications. Moreover, it provides exact first and second derivatives and exploits the full capabilities of IPOPT. **Yi-dong Lang** has nearly completed the interface to this system and is currently testing the interface. A similar interface to GAMS is also planned for January.
- **AMPL** – This GAMS-like system is the standard development platform in the Biegler group, has been available for the past two years and can be downloaded from the COIN-OR webpage. It has extensive features for linking to MATLAB and other environments in Unix and Windows. It also provides exact first and second derivatives and exploits the full capabilities of IPOPT.
- **CAPE-OPEN** – IPOPT has been developed under the MINLP object class and has been demonstrated with the CO-Tester. A paper that describes this interface along with a reprint is listed below.
- **Bonmin** – As described below, joint work with researchers at IBM, Tepper as well as Ignacio's and Larry's groups have integrated IPOPT and CBC to develop a public domain MINLP code. Developed principally

by Dr. Pierre Bonami, the code has been tested on a suite of convex and nonconvex MINLP problems and is being public released.

In addition, Carl has extended this approach to apply internal decompositions that take advantage of linear decomposition schemes of the KKT matrix in IPOPT. This allows a seamless interface to different sparse linear solvers as well as advanced decomposition schemes. This has been prototyped on Schur complement decompositions of the KKT matrix for block bordered diagonal structures. This strategy has been demonstrated on a large-scale Errors-in-Variables-Measured (EVM) parameter estimation problem, which is described in a preprint below.

Yi-dong Lang has developed a user-friendly version of dynamic optimization methods. In particular, they have extended these codes to exploit sparsity and are using them to tackle dynamic optimization problems including batch polymerization, crystallization and parameter estimation. This software, called *DynoPC,* runs under Windows with a GUI interface. It has been distributed to several CAPD members and parts of it can now be downloaded on the same website as IPOPT. Currently, this approach is being extended to include updated versions of IPOPT and will be enhanced further by the development of a number of interfaces to optimization modeling platforms including CAPE-OPEN.

Ignacio Grossmann's Group has been involved in the following developments:

In the area of optimization **Juan Pablo Ruiz**, in a new project, has been developing preliminary work on the global optimization of Bilinear Generalized Disjunctive Programming. The main idea has been to strengthen the estimation of the lower bound by applying ideas of the recent PhD thesis of Nick Sawaya. In collaboration with **Francois Margot, Pietro Belotti and Larry Biegler,** the open source code *couenne* for the global optimization of MINLP problems. Current work has been concentrating on nonconvex NLP problems. **Aldo Vecchietti**, work on LOGMIP for disjunctive programming is being incorporated as a commercial option in GAMS (http://www.ceride.gov.ar/logmip/).

In the area of process synthesis **Ramkumar Karuppiah** has completed the paper on bioethanol in collaboration with **Cargill** and **Mariano Martin**, as well as the calculations for the multieffect columns which combined with heat integration reduced the steam consumption by more than 50%. Ram is also completing his Ph.D. thesis. **Ravi Kamath**, in a new project, has developed a comprehensive superstructure for the optimization of IGCC plants, and developed models for the gasifier and utility plant. **Jose Maria Ponce Ortega** and **Arturo Jimenez** have extended the MINLP synthesis model for heat exchanger networks so as to handle isothermal streams as well as streams with change of phase. They have also extended Yee's retrofit model for simultaneous process optimization. **Jose Caballero** gave a presentation at ESCAPE on flowsheet optimization with implicit models and complex cost and size functions using process simulators. **Ricardo Lima** has been applying a computational strategy based on aggregated models for optimizing superstructure for separation processes based on crystallization. **Gonzalo Guillen** has developed a bicriterion optimization of process flowsheets and process networks in which the two criteria being optimized are economics and the Eco-indicator 99 as a measure of sustainability.

Muge Erdirik has completed a scheduling model of parallel reactors connected with finishing lines, and where the reactors work simultaneously as groups. Muge is also completing her Ph.D. **Bora Tarhan**, has completed the development of a Lagrangean branch and bound method for solving a multistage stochastic programming model for the design and planning of oil infrastructure planning under uncertainties in the sand quality, size of the reservoir and breakthrough time. **Fengqi You** has incorporated a probabilistic inventory models with safety stocks for optimizing the economics and responsiveness of process supply chains, and developed a solution strategy for solving the corresponding bi-criterion optimization problem. **Sylvain Mouret,** in a new project, has developed a novel continuous time model for crude oil scheduling that relies on time slots, and obtains very quickly good solutions for the original MINLP model. **Abdul Attalas,** in a new project, has been testing refinery planning models with fixed yields and swing cuts, as a first towards the incorporation of aggregated nonlinear models for the CDU. **Pedro Castro** has completed a manuscript for the simultaneous batching and scheduling of batch processes with sequence dependent changeovers. In a collaboration with **Antonio Flores-Tlacuahuac** from Mexico, he has developed a Lagrangean decomposition scheme for solving problems related to simultaneous scheduling and control. Finally, **Rosanna Franco** has been developing interfaces for the new MINLP model for heat excnager

networks for isothermal streams and tfor the global optimization of integrated water systems by Ramkumar Karuppiah.

Nick Sahinidis' Group

Nick's work falls into two main thrusts: (1) optimization theory, algorithms, and software and (2) applications of optimization to problems in biology, chemistry, engineering, and medicine. Research in optimization addresses the development of algorithms and software for: (a) global optimization of NLPs and MINLPs, (b) optimization of black-box models, and (c) linear programming. On the applications side, current activities address: (a) crystallographic computing, (b) protein structural alignment, (c) metabolic network modeling and design, and (d) design of compounds with desired properties.

Enabling Software From Nick Sahinidis' Group

Nick continues the development of BARON, primarily in collaboration with his former student **Mohit Tawarmalani**, who is currently an Associate Professor at Purdue's Krannert School of Management. In addition, students in Nick's group address theoretical and computational issues in global/local optimization. Their results are, from time to time, incorporated into BARON. The BARON software is currently available commercially under GAMS and AIMMS. In addition, a full blown version of the GAMS/BARON system is available entirely for free under the NEOS server for optimization. More information about BARON can be found at http://www.andrew.cmu.edu/user/ns1b/baron/baron.html.

Software for bioinformatics is also developed and maintained by Nick's group:

- CMOS: software implementing the Xie and Sahinidis algorithm for solving the contact map overlap problem for aligning the 3D structures of proteins
- R3: software implementing the Xie and Sahinidis residue-rotamer reduction for predicting the structure of protein side chains
- SBH: software implanting the Chang and Sahinidis algorithm for finding all near-optimal solutions of the combinatorial problem in DNA sequencing by hybridization

Nick's web site at http://www.andrew.cmu.edu/user/ns1b/group/biosoftware.html provides these codes as on-line solvers.

STATUS OF RESEARCH PROJECTS

Larry Biegler's Group

General Frameworks for Large Scale Optimization Strategies and Applications

Researcher: Victor M. Zavala (Ph.D. started Fall, 2004)

As a result of several generations of Ph.D. students, we now have a number of very efficient NLP algorithms including rSQP, full-space SQP, parameter estimation, data reconciliation and multiperiod optimization. As described above, the most recent incarnation is IPOPT, with continuing development by Andreas Wächter. This code has become a core algorithm for many of the research projects described below. In his PhD thesis, Carl Laird has applied IPOPT and the AMPL interface to develop a novel source detection strategy for municipal water networks as an important application for barrier methods. This optimization problem is developed to detect attacks on networks and to determine optimal control and remediation strategies. By exploiting the structure of these networks, discretized problems that represent actual municipal networks with up to 300,000 variables could be solved in only a few CPU seconds. More recently, this approach has been extended, by using an MIQP strategy, to a more robust one that promotes unique solutions. Using an efficient pre-processing step, small subproblems can be derived and attack scenarios can be identified more precisely and efficiently. This approach is described in the preprint below.

Finally, the new version of IPOPT continues to updated and maintained. Designed in C++, this code is object oriented and flexible to deal with a wide variety of linear solvers, new barrier algorithms, and a variety of globalization strategies and decomposition approaches. Moreover, as noted above, the new code provides a much easier interface to modeling environments. Carl has expanded the IPOPT code to accommodate in the following ways:

- Multi-scenario problems are essential to deal with process optimization under uncertainty and have a structure that can be decomposed through Schur complements and can be completely parallelized on distributed memory machines. Carl has obtained some excellent results with this decomposition that validate these properties.
- More recently, Victor has demonstrated this approach on a large-scale parameter estimation problem, executed on parallel processors and show essentially perfect speedups with this approach. A preprint that describes this approach is listed below.
- The structure of IPOPT has been expanded to deal with NLP sensitivity. This approach very quickly provides an estimate of the solution of a perturbed NLP problem. As a result, it is very useful for quickly solving a sequence of problems that change only slightly from the previous one. This is applied below to develop a very fast strategy for Nonlinear Model Predictive Control (NMPC).

Mathematical Programs with Equilibrium Constraints (MPECS)

Researchers: **Juan Arrieta (Ph.D. completed April, 2007)**
Brian Baumrucker (Ph.D. started Fall, 2004)
Gaurav Bansal (MS started Fall, 2006)

MPECs represent an exciting new field in mathematical programming. While applications of MPECs have long been recognized in game theory, transportation planning, economics and engineering design, little work has been done in developing efficient algorithms for their solution In process engineering, these problems stem from bilevel and multilevel optimization problems as well as optimization of hybrid (discrete and continuous) systems. Included in this class are optimization problems with phase equilibrium constraints, as in equilibrium stage processes.

The MPEC problem is essentially a nonlinear programming problem augmented by complementarity conditions. The addition of these conditions leads to a violation of convergence assumptions for most nonlinear programming algorithms (e.g., linear independence of the constraint gradients) and can cause these algorithms to fail. On the other hand, the barrier method described above has a straightforward extension to these problems. As a result, complementarity constraints can be incorporated with little additional cost in the algorithm. In fact, all of the features that contribute to the efficient performance of IPOPT can be invoked directly for the solution of the MPEC problems. The resulting algorithm based on IPOPT has been developed further and refined for a number of challenging dynamic optimization applications in process engineering. Our work in this area includes the following:

This project builds on the Ph.D. work of Arvind Raghunathan. In his research, he has incorporated the MPEC formulation into the IPOPT code, now called IPOPT-C, along with algorithmic modifications to treat the complementarity constraints more efficiently. This code has been interfaced to the AMPL modeling system and has been tested on a set of library MPEC problems. Our results show that this implementation compares well against competing barrier algorithms such as LOQO. Arvind tested this approach on a number of process optimization problems with phase equilibrium constraints. These include distillation optimization problems with disappearing vapor and liquid phases on equilibrium stages, dynamic systems with switching conditions, such as overflows and phase disappearance in distillation columns and metabolic network systems.

For the latter, we have considered parameter estimation problems for dynamic fermentation systems for wine production. These results show that this approach leads to better and more uniform performance than the smoothing approach used in our previous studies. Related work initiated by **Juan Arrieta** deals with modeling and optimization of dynamic biological systems that are based on cellular models. Such systems are large-scale extensions of MPECs. Moreover, they have interesting modeling features since state dependent constraint functions with discontinuities also need to be treated through MPEC formulations. **Gaurav Bansal** has recently taken over

this project and is expanding the capabilities of these formulations along with the consideration of larger, extended models for yeast fermentation.

In extending MPEC optimization formulations, **Brian Baumrucker** is currently considering the development of good MPEC formulations that model discrete decisions. He has explored these with the ROMeo real-time optimization package along with formulations for complementarity conditions within real-time optimization models. In particular, he has shown that penalty-based NLP formulations have worked very well on these models. Moreover, with these formulations, one is able to decouple problem-specific optimization algorithms from the optimization model and rely on general purpose optimization solvers. In addition to the ROMeo comparison described above, he has investigated complementarity formulations in distillation columns with mass transfer limitations. This extended MPEC work is described in a preprint listed below.

Simultaneous Optimization of Differential-Algebraic (DAE) Systems

Researchers: **Juan Arrieta Camacho (Ph.D. completed April, 2007)**
Victor Zavala (Ph.D. started Fall, 2004)
Rui Huang (Ph.D. started Fall, 2006)
Weijie Lin (Ph.D. started Fall, 2006)
Yi-dong Lang (Jiansu Research Institute, Nanjing, China)
Euclides Almeida Neto (Petrobrás, Rio de Janeiro, Brazil)

The topic on simultaneous solution and optimization strategies for large-scale, dynamic optimization problems incorporates a number of projects. In the past, we have applied this approach to optimization problems for batch reactors, process dynamics and tray-by-tray batch distillation and large-scale dynamic flowsheeting models. Moreover, we have tackled dynamic examples successfully with this approach that cause any sequential dynamic optimization method to fail. It can occur in open-loop unstable systems that arise in optimal control and nonlinear MPC, dynamic parameter estimation and the optimization of runaway reactors. Prof. Antonio Flores, a research colleague from the University of Iberoamericana, has demonstrated the advantages of this approach on a number of challenging polymerization processes. Moreover, the following research projects are currently being addressed in our group.

Dynamic Optimization Platforms

We have developed two complementary modeling frameworks for dynamic optimization, one based on reduced space and one on full space. First, over the past four years Yi-dong Lang has developed a stand-alone Windows modeling system for dynamic optimization called ***DynoPC***. Written for Windows with a Visual Basic user interface and with heavy integration of graphical, simulation and automatic differentiation tools, this software package incorporates our advances in dynamic optimization, particularly IPOPT and the elemental decomposition. This program continues to be distributed to interested research groups both in academia and industry and can be downloaded from http://coin-or.org Current developments with *DynoPC* include ESO interfaces that are compliant with recently developed CAPE-Open protocols. This leads to an interface compatible with a number of existing process models and modeling environments. In the last year, **Euclides Almeida** has joined our group as a visiting researcher from Petrobras. He is currently working on combining the EMSO interface, a modeling interface similar to gPROMS, with DynoPC. The resulting package will be used to solve challenging industrial problems in dynamic real-time optimization (DRTO). A key feature of this approach is the diagnosis of dynamic optimization solutions, along detailed explanation of algorithmic performance, probing and exploration of solutions and an extensive examination facility to deal with elucidation and correction of possible failures of DRTO problems.

Second, we have been using IPOPT in a full space framework linked to the AMPL modeling environment. As detailed in many of the studies listed below, this framework has been extremely powerful and flexible in solving a wide variety of problems. A MATLAB framework has been coupled to the AMPL modeling language and domain specific prototypes have already been developed and work very well. In addition, Johan Akesson from Lund University has developed a Modellica framework that works with IPOPT and AMPL. In a recent study, he was able to optimize an open-plate reactor with over 100,000 variables in about an hour of CPU time.

Large-scale Parameter Estimation for Polymerization Processes

In a project funded by ExxonMobil Chemicals, **Victor Zavala** has begun to develop multi-stage dynamic optimization problems for grade transition and nonstandard operations. For this, he has developed a detailed reactor model of a polyolefin reactor, which includes a complete kinetic description that is used for parameter estimation using actual process data. Using AMPL and IPOPT, Victor has extended this model to multiple data sets as well as EVM problems (where errors in both inputs and outputs are considered). Applying this approach to a large number of data sets, Victor was able to estimate kinetic parameters quite well; the scatter of the data was reduced by an order of magnitude, compared to previously fitted models. This approach is described in a reprint listed below. Moreover, using the NLP sensitivity approach described above, Victor has recently shown that the covariance matrix from a maximum likelihood formulation can be extracted easily from IPOPT using a few additional back-solves of the KKT matrix. This allows statistical inference to be added efficiently to parameter estimation studies.

Weijie Lin has recently joined the group and is working on process model development for an advanced polymer product. The approach is similar to the moment models developed by Victor, but with more complex features dealing with the polymer structure. Weijie's preliminary work has shown the importance of parameter estimation for this large-scale model in order to demonstrate structurally dependent features (e.g., gel effect, cage effect, glass effect) on the polymer reactions. This also allows her to develop MW distributions of the complex polymer network.

Nonlinear Model Predictive Control Strategies

In less than two decades, Nonlinear Model Predictive Control (NMPC) has evolved from a conceptual framework to an attractive, general approach for the control of constrained nonlinear processes. These advances were realized both through better understanding of stability and robustness properties as well as improved algorithms for dynamic optimization. The above dynamic optimization algorithms have been applied extensively in Nonlinear Model Predictive Control (NMPC). This strategy is also being extended to large-scale models for polymerization processes. In addition, we recently adapted the *real-time iteration* approach developed in the context of multiple shooting (Diehl et al. (2006); Bock et al. (2006)) to a collocation-based approach with a full space nonlinear programming solver. Over the past year, we show that straightforward sensitivity calculations from the KKT system also lead to a real-time iteration strategy, with both shifted and non-shifted variants. This leads to an NMPC strategy called the Advanced Step NMPC Controller. Demonstrated on a large-scale polymer process, the Advanced Step Controller leads to on-line calculation effort that is reduced by over two orders of magnitude. As described in a preprint below, we have been developed a general Lyapunov-type stability analysis for this approach that demonstrates nominal stability, input to state stability and robustness margins to noise and model mismatch. This recent development has been extended to moving horizon estimation (MHE) for parameter and state identification and yields the same dramatic improvements in performance. This result was recently presented in a keynote paper at the DyCOPS meeting and will be included in the next newsletter. Finally, **Rui Huang** has recently joined the group and is extending this approach to distillation control and advanced power plant systems. His preliminary work has demonstrated that the Advanced Step NMPC also reduces on-line calculation time by about two orders of magnitude.

Large-Scale Optimization for Fuel Cell Models

Researchers: Parag Jain (Ph.D. started Fall, 2005, joint with Prof. M. S. Jhon)

In his thesis project, Cong Xu initiated the investigation of optimization problems arising in fuel cell applications, including Direct Methanol Fuel Cells (DMFCs) and Hydrogen PEM fuel cells. In particular, he has extended simple DAE models for fuel cells to consider optimal flow patterns and minimization of contamination effects due to membrane crossover, and he has extended these models to consider sensitivity and optimization calculations. In particular for DMFCs, we have compared and critically assessed several literature models and have explored the crossover phenomenon. By applying our dynamic simulation and optimization tools, they were able to develop dynamic feeding strategies for these systems that greatly reduce contamination due to methanol crossover. The results show that the optimal design of DMFCs can be achieved without pulsed operation. Here crossover is significantly reduced and the power density is correspondingly increased. The efficiency of these processes can also be improved through flowsheet optimization strategies as well as heat integration of the process units. This approach is based on conventional flowsheet optimization schemes within Aspen/Plus along with simultaneous optimization

and heat integration strategies. The application to fuel cell based processes leads to interesting trade-offs between the fuel cell, the rest of the flowsheet and the heat recovery system.

Dynamic optimization has also been applied by Shiva Kameswaran to develop ramping strategies for fuel cell power plants. In a project funded by Fuel Cell Energy, Inc. and DOE, Shiva has demonstrated significant improvements in maintaining power levels with more energy efficient operation. Using AMPL and IPOPT, he has incorporated detailed models of the entire power plant and has demonstrated this approach both for parameter estimation and optimal control. A reprint that describes this approach is listed below. Finally, **Parag Jain** has extended previous modeling and optimization work for Hydrogen PEM Fuel Cells. He has applied a comprehensive two-dimensional computational model of a PEM fuel cell that accounts for major transport processes including membrane electrode assembly (MEA) and gas distribution channels. Additionally a water transport model in the membrane has been developed and incorporated into the full PEM fuel cell model. Using AMPL and IPOPT, Parag is using this model to develop a detailed optimization case study. The results of this work will be presented at the AIChE meeting this November; a preprint of this work will be included in the next newsletter.

Dynamic Optimization for Semi-Closed Process Models
Student: **Sree Ram Raju Vetukuri (PhD started Fall, 2006)**
Collaborator: **Prof. Andrea Walther (Technical University of Dresden)**

This project explores the application of recent developments in automatic differentiation and nonlinear programming to semi-closed process models, including systems solved with DAE integrators. This sequential optimization approach for dynamic systems has been the competing strategy to the simultaneous optimization approach adopted in our group. It has advantages for problems where error control is especially important, where many time steps are needed and where these need to be adjusted frequently during the integration. Recent years have seen the development of efficient sensitivity strategies to obtain accurate first and even second derivatives for use in dynamic optimization algorithms. However, this approach becomes inefficient when there are many degrees of freedom. For instance, in the optimization of Pressure Swing Adsorption units, Ling Jiang developed an efficient sequential dynamic optimization approach. However, when several hundred inputs were considered in the model, the optimization required hundreds of CPU hours.

This bottleneck has recently been addressed by a recent SQP-type algorithm that uses exact right hand sides of the KKT equations, along with Jacobian-vector and Hessian-vector products, but computes only inexact Jacobians. Using leading edge technology in automatic differentiation, these quantities can be computed orders of magnitude faster than with the standard sequential approach. Profs. Andreas Griewank and Andrea Walther have recently developed a globally convergent SQP that uses inexact Jacobians, called TR1. Based on a composite trust region strategy, this approach has recently been applied to periodic adsorption processes as well. A preprint that describes this approach is listed below. Sreeram Vetukuri has recently joined the group and has extended this approach using ADOL-C for automatic differentiation and CVODES for sensitivity calculations of first and second derivatives, and interfacing to TR1. Preliminary results on a small SMB system show the potential of this algorithm for reducing CPU time.

Reduced Order Models for PDE-based Units in Power Plant Flowsheets
Researcher: **Yi-dong Lang (Jiansu Research Institute, Nanjing, China)**
Students: **Anshul Agarwal (Ph.D. started Fall, 2005)**
Adam Malacina (Ph.D. started Fall, 2006)

Process simulation has become an essential capability that spans most tasks in process engineering, design and analysis. Simulation programs such as Aspen Plus, Pro/II and HYSYS are integrated into core engineering design activities. However, due to computational limitations, current process simulators usually deal with lumped parameter models that often do not capture detailed spatial characteristics of process units, including fluid flow and transport processes. As a result, they can suffer accuracy limitations and the loss of predictive capability. To overcome this difficulty, we are working with NETL on the Advanced Process Engineering Co-Simulation (APECS) project. Within this framework, process flowsheeting models (in Aspen Plus) have been successfully combined with computational fluid dynamics (CFD) models (using Fluent) to model multiphase systems, such as gasifiers and turbines within power plants. Current efforts are also focused on the inclusion of other distributed parameter custom models. In particular, an important, and challenging, application for this activity is the FutureGen Cycle, a 275 MW

coal-fired power plant that includes hydrogen generation and CO2 recovery, and requires multi-phase, spatially distributed models within its simulation environment.

To extend these NETL activities, we are developing and applying integrated optimization strategies that provide powerful tools for model development and process improvement. So far, these optimization problems are small-scale and efficient, and robust optimization algorithms are available that can be implemented easily. These features have led to the relatively easy and widespread adoption of optimization strategies. On the other hand, optimization strategies for CFD and distributed parameter models have seen far less development and this currently represents an important and challenging research activity. For APECS, which incorporates these models, we believe that optimization strategies will perform a key role in the development of advanced energy processes, such as the FutureGen Cycle. To provide a vehicle for the research tasks in this project, we consider the model components of the FutureGen Cycle flowsheet. This process includes a number of unit operations for coal gasification and byproduct (e.g., ash/slag and sulfur) separation; multiphase CFD models are needed for this purpose. Yi-dong Lang has been working with colleagues at Fluent Corp. to develop reduced order CFD models based on Proper Orthogonal Decomposition (POD) and Principal Components Analysis (PCA). This approach allows for a tremendous reduction in computing effort for the process flowsheet. Yi-dong has considered a PCA based approach coupled with an efficient experimental design approach along with a neural network solver to determine an input output model. Using an NETL-based Fluent combustor model, he has developed accurate reduced order models (ROMs) that capture the behavior of the Fluent model over a wide input range, but with require about two orders of magnitude less execution time. As a result, these models are quite suitable to incorporate within FutureGen process flowsheet. **Adam Malacina** has recently joined the group and is currently extending Yi-dong's approach to a FutureGen gasifier model, also developed in Fluent.

Further downstream of the gasifier in the FutureGen process, the byproduct gases CO2 and hydrogen are separated and CO2 is sequestered. These separations can be performed effectively by pressure swing adsorption (PSA) units, which operate dynamically and require the calculation (and subsequent optimization) of cyclic steady state behavior. Such models were considered in the PhD thesis of Ling Jiang. While her optimization approach was very successful for large-scale PSA units, it still required many hours of CPU time, and therefore requires custom reduced order models (ROMs). Over the past year, **Anshul Agarwal** has been developing reduced order models for these units as well using a novel space-time discretization to develop the ROM using a POD-based approach. A key advantage of this approach is that very small models are developed that can be discretized in time (using collocation on finite elements) and solved with AMPL and IPOPT. Preliminary results by Anshul show that this strategy can lead to very efficient optimization strategies. This approach will be presented at the AIChE meeting in November and a preprint will be included in the next newsletter.

Optimization and Control of Periodic Adsorption Processes
Student: Yoshi Kawajiri (Ph.D. completed July, 2007)

Simulated Moving Bed (SMB) chromatography was developed in the 1960s as a realization of continuous chromatographic separation. Since then, SMB has been gaining attention in food, sugar, and petrochemical applications. In more recent years, SMB has been recognized as an attractive technology for enantiomeric separations in the pharmaceutical industry. An SMB system is realized by connecting multiple columns in a cycle. The feed and desorbent are supplied continuously between columns, and at the same time extract and raffinate products are withdrawn. Counter-current operation is "simulated" by switching these inlet and outlet streams intermittently in the direction of the liquid flow. As with PSA this system is characterized by a Cyclic Steady State (CSS), where the concentration profiles in the columns change dynamically but repeat the same pattern in every cycle.

Yoshi Kawajiri recently completed his PhD. In his research, he has been investigating efficient optimization strategies for SMB systems. Here optimization methods can be based on the single-discretization approach to discretize the Partial Differential Equations (PDEs) only in the spatial domain and then integrate the resulting Differential Algebraic Equations (DAEs) in time. On the other hand, the full-discretization approach discretizes the PDE both in time and spatial domain, leading to a large-scale Nonlinear Programming (NLP) problem. Yoshi has compared both approaches and found that the latter approach has shown tremendous improvements in the productivity of SMB systems. Moreover, these were obtained almost two orders of magnitude faster than with the single discretization (sequential) method used in gProms. The approach was applied to optimization of SMB

systems with steady and time-varying feeds (i.e., PowerFeed), both for linear and nonlinear isotherms. This efficient approach also allows us to consider the design and control much more complex SMB systems. The results of Yoshi's approach have been detailed in a number of papers included with previous newsletters. In particular, Yoshi has developed two superstructure SMB systems, one for a single step and the second over a full cycle, that allow for the optimization of a number of novel, recently reported designs, as well as some new ones. These superstructures lead to well-defined and easily solved problem formulations and lead to innovative designs with improvements in productivity. Moreover, through the formulation and solution of multi-objective optimization problems, we confirm that our approach has the potential to find more advantageous operating schemes than the standard SMB, PowerFeed, or other advanced, but fixed, operating schemes. These results are described in the preprints listed below.

Ignacio Grossmann's Group

Open-Source Code for MINLP Optimization

New developments: **Open source code *couenne***

Post-doctoral fellow: **Pietro Belotti (Tepper)**
Collaborators: **Larry Biegler, Francois Margot (Tepper)**

This project has been a collaboration with researchers at IBM (Andreas Wächter, Joantahn Lee, Pierre Bonami). The main objective has been to take the next step beyond the open source code *bonmin* for MINLP problems (see http://egon.cheme.cmu.edu/ibm/page.htm). In particular the goal has been to develop a global optimization code for solving MINLP problems.

In this project Pietro Belotti is extending the Bonmin code for handling nonconvex problems. The goal is to develop both approximate as well as rigorous methods that rely on the use of convex envelopes. The rigorous method relies on a spatial branch-and-bound method for bilinear, linear fractional and concave separable functions. Efforts for developing code generating parametric linear upper and lower convex envelopes are under way. Parametric linear convex envelopes are obtained by breaking a nonlinear expression into compositions of simple operators for which convex linearizations are known. By introducing additional variables, a linear convex envelope of the original expression can be obtained. This polyhedral envelope is a function of the upper and lower bounds on the variables and it becomes a tighter approximation when upper and lower bounds on the variables are moved closer. This can be exploited in a branch-and-cut algorithm by branching on continuous variables, i.e. splitting the domain of its possible values. These parametric convex envelopes can also be used to generate an infinite number of valid linear cuts, raising interesting questions regarding cut selection and cut strategy when integrated in a branch-and-cut framework. These ideas are being implemented in the software package *Couenne* with input from Leo Liberti at the Ecole Polytechnique in Paris. Pietro has been able to test his code with about 50 test nonconvex NLP problems, most with dozen variables and few with hundreds and thousands. In most of the cases he was able to obtain the global optimum in reasonable time

Algorithms for Nonlinear Disjunctive Programming

New Developments: **Preliminary work for bilinear GDP problems**

Student: **Juan Pablo Ruiz [started Jan 2007]**
Research collaborator: **Aldo Vecchietti [Researcher at INGAR]**

Nicolas Sawaya

Nick defended his Ph.D. thesis in November 2006 and joined ExxonMobil, Corporate Research. WE summarize here the last part of his work as it has served as a basis for the work of Juan Pablo Ruiz.

In the last part of his Ph.D. thesis Nick was able to establish a nice theoretical connection between the generalized disjunctive programming (GDP) model that we have been considering and the disjunctive model by Balas. This is non-trivial because the major difference is that the GDP model includes Boolean variables for establishing the truth of the disjunctions and logic relations between the discrete decisions. The major point that emerged from Nick's analysis is that if we formulate the linear GDP problem by explicitly adding the OR constraint on the Boolean variables,

$$
\begin{aligned}
&Min\ Z = \sum_{k \in K} c_k + d^T x \\
&s.t. \qquad Bx \geq b \\
&\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ A^{jk} x \geq a^{jk} \\ c_k = \gamma_{jk} \end{bmatrix} \qquad k \in K \\
&\underline{\vee}_{j \in J_k}\, Y_{jk} \qquad k \in K \\
&\Omega(Y) = True \\
&x^L \leq x \leq x^U \\
&Y_{jk} \in \{True, False\} \qquad j \in J_k, k \in K \\
&c_k \in \mathbf{R}^1 \qquad k \in K
\end{aligned}
$$

then if we define the continuous variable λ_{jk}, to represent the Boolean variable Y_{jk}, and convert the logic constraints into inequalities, the following formulation can be obtained:

$$
\begin{aligned}
&Min\ Z = \sum_{k \in K} c_k + d^T x \\
&s.t. \qquad Bx \geq b \\
&\bigvee_{j \in J_k} \begin{bmatrix} \lambda_{jk} = 1 \\ A^{jk} x \geq a^{jk} \\ c_k = \gamma_{jk} \end{bmatrix} \qquad k \in K \\
&\sum_{j \in J_k} \lambda_{jk} = 1 \qquad k \in K \\
&H\lambda \geq h \\
&x^L \leq x \leq x^U \\
&0 \leq \lambda_{jk} \leq 1 \qquad j \in J_k, k \in K \\
&c_k \in \mathbf{R}^1 \qquad k \in K
\end{aligned}
$$

The above model corresponds to a continuous disjunctive program in an intermediary form between its disjunctive and conjunctive normal forms in which the integrality of the variables λ_{jk}, is guaranteed. Having this formulation establishes a direct link with Balas' work where one can then apply the wealth of theoretical results that he has developed. Among these, a major result is to realize that the convex-hull model by Lee and Grossmann is part of a larger family of MIP reformulations. These depend ultimately on the number of basic steps that are applied from conjunctive to disjunctive normal form. To use simple words, what is means is that by intersecting constraints within the disjunctions, one can obtain stronger relaxations. Nick illustrated this first with a small network problem, in which the recursive intersection of disjunctions yields a single disjunction where each term corresponds to one structural alternative in the topology. He has also illustrated this with strip packing problems involving 4, 25 and 31 rectangles. By intersecting disjunctions corresponding to the largest "bottleneck rectangles" he could solve the 4 rectangle problem as an LP! In the 25 rectangle problem the lower bound was increased from 9 (convex hull) up to

27, with 31 being the optimal solution. In the 31crecatangle problem the lower bound was increased from 10.64 up to 33, with 33 being the optimal solution. Needless to say, these results are truly exciting.

Juan Ruiz

The project of Juan is concerned with the global optimization of Generalized Disjunctive Programs that involve bilinearites in the constraints. These problems arise for instance in the design of pooling problems, in the synthesis of integrated water treatment networks, or generally, in the synthesis of process networks with multicomponent flows. Juan's work has as a major objective to improve the computational efficiency of disjunctive spatial branch and bound methods by making use of the recent theoretical developments of Nick Sawaya to obtain tighter relaxations. The basic approach consists of first relaxing the bilinear terms in the GDP using convex envelopes by McCormick, and introducing them as part as the disjunctive set. Since the corresponding relaxation leads to a linear GDP problem, the next step then consists in performing basic steps which involve intersecting disjunctions in order to obtain tighter relaxations as outlined in Balas' theory. Of course there are many options that are possible on how to perform the intersections. To address this issue Juan has developed several rules that for instance eliminate intersections when one can prove a priori that they will not lead to tighter relaxations. Nevertheless, this is still a major research question that he is examining.

Juan has applied his reformulation procedure to two examples., In the case of a water treatment network the bilinearities arise in equations outside the disjunctions, so that the intersection of disjunctions with the convex envelopes leads to potentially stronger relaxations. This was confirmed in an instance where Juan managed to improve the lower bound by 25% which in turn translated in a 50% reduction in the spatial branch and bound search (399 nodes to 204 nodes). In the case of a pooling network, where the bilinearities arise within the disjunctions the strength of relaxations is expected to be lower. This was again confirmed with an instance in which the lower bound was improved by only 1% and the number of nodes was reduced from 746 down to 683. Juan will be presenting this work for his Ph.D. qualifying exam. After Juan completes his qualifier he will study in greater depth the impact of various types of intersections in order to understand in what cases the relaxations can be expected to improve.

Aldo Vecchietti: LOGMIP and DICOPT

Aldo and his students at INGAR in Argentina have been developing the LogMIP code, which is as an extension of the GAMS modeling language for posing logic/disjunctive problems. The syntax developed involves the use of IF THEN ELSE statements to represent the disjunctions, including embedded ones. The definition of disjunctions over sets and subsets can also be specified. As for the propositional logic, the special constructs ATLEAST, ATMOST, EXACTLY are defined to specify that the sum over a subset of variables with a given cardinality is at least, at most or equal to one. Also, LogMIP can now accept logic propositions in symbolic form without the need of translating them into linear inequalities.

For solving linear disjunctive/hybrid problems LOGMIP can automatically generate the convex hull relaxation and big-M transformation for linear problems. Aldo has also automated the logic-based OA algorithm by Metin Turkay, which is suitable for nonlinear GDP process network problems. In collaboration with GAMS, Aldo has been developing a version that will be commercialized later in the fall. In the meantime LogMIP Website provides the possibility of downloadingb the code: http://www.ceride.gov.ar/logmip/.

Aldo has added a capability in DICOPT for handling more effectively infeasible NLP subproblems. What Aldo has done is to allow the addition of linearizations of the infeasible NLP subproblems. This option is rigorous for the case of convex MINLP problems. For nonconvex problems there is the risk of cutting off optimal solutions. To solve problems in GAMS with linearization in infeasible NLPs the following option must be defined: infeasder 1. By default infeasder is 0. In this case DICOPT runs like the previous version (just with the integer cut with NO linearization on the infeasible points). This new option has shown to significantly improve the performance of DICOPT in several problems, which often did not converge with the old version..

Global Optimization of Integrated Process Water Systems

New developments: **Completed manuscript for generic multiscenario problems**

Students: **Ramkumar Karuppiah [Ph.D. started Jan 04]**

Ram's project has dealt with the global optimization for the synthesis of process water systems that integrate the water reuse section for processes with the distributed water treatment section for a given number of pollutants. The initial objective has been to find for given sets of processes and given treatment units the optimal configuration of the system that minimizes the use of freshwater, or more generally that minimizes the total cost. Ram has assumed for the processes units that they are either characterized by fixed contaminant loads, or by variable loads that obey mass exchange constraints in terms of concentrations. For the treatment units fixed recoveries are specified. Ram has considered the extension to synthesis for multiple scenarios in order to handle uncertainties in the contaminant loads and recoveries in the treatment units. This work he has generalized to generic multiscenario problems.

For the synthesis of the integrated water system, Ram developed a superstructure that involves for a given number of process units and treatment units all possible alternatives for interconnection of process and treatment units, and mixing and splitting of streams. The model corresponds to an NLP model with bilinearities in the mixers given by the product of flows times concentrations in ppm of the contaminants. Ram developed a global optimization algorithm that relies on combining spatial branch and bound search, with piecewise linear approximations. The motivation is that piecewise linearizations improve the quality of the lower bound, but they do it at the expense of introducing additional 0-1 variables. For this reason it is sensible to still use a spatial branch and bound search, but strengthened by piecewise linearizations for a fixed (modest) number of intervals. To strengthen the quality of the lower bound, Ram derived a valid cut that represents overall mass balances for each of the contaminants. This cut has proved to be extremely effective to a point where adding it to the original formulation and using BARON requires similar times as the special purpose spatial branch and bound algorithm.

As a next step in his research, Ram considered the extension of the above problem to the case when the water system must operate under multiple scenarios in which the loads in the units as well as the recoveries in the treatment units are uncertain, and therefore change in each scenario. This problem gives rise to a two-stage stochastic programming problem. The first stage costs include the investment cost for piping which depends on the maximum flowrate allowable in a pipe, and the design cost of each treatment unit, which is dependent on the maximum flow of wastewater handled by that treatment unit. The operating costs of the network appear in the second stage, which include the cost of obtaining freshwater for use in the process units, the cost of pumping a certain flow of water through the pipes and the operating costs in the treatment units. The difficulty of the global optimization for the nonconvex multiscenario problem is that the MINLP becomes much larger. Furthermore, 0-1 variables must be introduced for the piping in order to control the potential complexity in the configurations for each period. Ram developed a solution method that is based on a branch and cut algorithm. The basic idea consists in performing a spatial branch and bound where cuts are generated at each node using a Lagreangean decomposition scheme. These cuts are obtained by globally optimizing each scenario independently. These cuts are then added to the original problem that is convexified by constructing convex envelopes for the non-convex nonlinear terms leading to an MILP that is solved to predict a rigorous lower bound to the global optimum. A heuristic is used for the generation of good upper bounds. These lower and upper bounds are converged within a specified tolerance in a spatial branch and bound algorithm. Ram considered a problem with 2 process units and 2 treatment units and 10 scenarios. The MINLP model involved 28 binary variables, 868 continuous variables, 1044 constraints and 490 non-convex terms. The application of the proposed algorithm yields an expected cost of $651,653.06, which is the global solution to the problem. The lower and upper bounds converge within 1% tolerance at the root node of the branch and bound tree. The proposed algorithm takes a total of 62.8 CPU secs to solve.

Ram was able to generalize the above cited branch and cut algorithm for generic multiscenario problems, which was submitted for publication and recently accepted in JOGO. The paper contains rigorous proofs on the validity and strength of the lower bounds generated by the proposed method.

Optimal Design of Corn-based Ethanol Plants

New developments: **Manuscript completed on 65% reduction in steam consumption**

Students: **Ramkumar Karuppiah [Ph.D. started Jan 04]**
Visitor: **Mariano Martin (Salamanca), Andreas Peschel (RWTH Aachen)**

This project was initiated with the exchange student Andreas Peschel and Ramkumar Karuppiah in collaboration with Cargill. Mariano Martin has continued recent work with the help of Ramkumar. The objective has been two-fold: a) Develop short-cut models for corn-based ethanol plants; (b) Develop a superstructure optimization model to determine the extent to which the design of these plants can be improved.

In the first phase of this work, a simplified model was developed for the "dry-grind" process for the corn-based bio-ethanol plant. In such plants, fuel ethanol is produced using corn-kernels as the feedstock. Fuel grade ethanol has to be 100 % pure before it can be blended with gasoline to be used in automobiles. However, conventional distillation columns produce an azeotropic mixture of ethanol and water (95 % ethanol – 5 % water), which has to be purified further for making fuel ethanol. The main challenge in the way of producing fuel ethanol commercially is that the process is very energy intensive and requires large amounts of steam and electricity for use in the rectifiers to get an azeotropic mixture of ethanol and water and requires the use of expensive molecular sieves to get 100 % pure ethanol. Furthermore, the waste spillage from the fermentation units, which is rich in volatile organic compounds, and the other wastewater streams in the plant have to be treated before disposal, which, in turn requires energy intensive units like centrifuges and dryers.

In order to optimize the design of a bio-ethanol plant, Andreas, and Ram developed a model to predict the performance of the flowsheet that includes grinding, scarification, fermentation, centrifugation and drying operations. A superstructure was also postulated in which some of the major alternatives include separation by molecular sieves and or corn grits, and different ways to accomplish the drying for the dried grains solids, the cattle feed by-product. The process units are interconnected to each other through network feed flows and other utility streams. The objective is to optimize the structure, determining the connections in the network and the flow in each stream in the network, such that we minimize the energy requirement of the overall plant while trying to maximize the yields. The optimization produced a 65% reduction in steam consumption, which lead to a decrease of manufacturing cost from $1.50/gal to $1.28/gal. This was largely achieved by using multi-effect distillation in the "beer" column and in the azeotropic column, as well as heat integration. In this way, the production of "bio-ethanol" as a sustainable source of fuels is significantly improved in terms of the economics and energy efficiency. The manuscript describing this work has been completed and is listed in the references.

Optimal Synthesis of Integrated Gasification Combined Cycle (IGCC) Systems

New developments: **Superstructure and models for agsification and utility plant**

Student: **Ravi Kamath [Ph.D. started Jan 2007]**

This is a new project within the newly established Institute of Energy System that is being funded through NETL. The objective is develop a comprehensive synthesis model for IGCC plants, with the possibility of polygeneration and CO_2 sequestration.

Integrated Gasification Combined Cycle (IGCC) technology for future power plants has attracted great interest because of its capacity to not only achieve a higher thermal efficiency but also capture CO_2 more economically than a conventional coal-fired plant. However, IGCC technology has higher capital costs than coal-fired plants and is economically viable only if operated with CO_2 capture. Ravi's project will aims at evaluating the techno-economic performance of an IGCC plant. The problem assumes that we aregiven a type (rank, quality, composition, physical state) of coal, net output power, location of site, ambient conditions for utilities like air and water and other requirements like co-production of hydrogen or chemicals and extent of carbon capture. The objective is to determine the optimal structural configuration and operating parameters of the IGCC plant that minimize the

investment and operating cost, while meeting the constraints for environmental emissions. An important related decision will be the minimum amount of CO_2 to be captured.

Ravi has developed a comprehensive superstructure that includes potential alternative technologies. The goal is to determine the optimal configuration and operating parameters for the IGCC flowsheet by formulating a mixed-integer nonlinear programming (MINLP) problem. Because of the large number of alternatives, MINLP model leads to a large-scale combinatorial problem. We intend to apply the methodology developed by Mark Daichendt that involves optimizing the entire flowsheet at different levels of complexity using a combination of simple and detailed models. As a first step, Ravi has developed simplified models for the two most important sections of the IGCC plants which are coal gasification and utility section. For coal gasification he has developed a model based on Gibbs energy minimization that can be modified to match the performance of real gasifiers. He has obtained very good results for the Shell entrined gasifier in which the prediction of the main eight speciaes is in close agreement with a published mode. Ravi has also developed an MINLP model for combined cycles that extends the work by Bruno. Here again Ravi has obtained good results in terms of predicting optimal topologies for combined cycles. The next major step in Ravi's project will be to integrate these models with new models for acid gas cleaning and air separation unit to eventully tackle the optimization of the entire superstructure. Ravi will present his qualifying exam based on this work.

MINLP Flowsheet Optimization with Process Simulators

New developments: Submission of paper decribing use of simulators in MINLP flowsheet optimization

Collaborators: Jose Caballero [Associate Prof., Univ. Alicante]

While most of the work with Jose Caballero has concentrated on thermally integrated separation sequences, one additional piece of work has been the incorporation of process simulators for MINLP optimization in process flowsheets.

A major motivation for the work has been that in Process Synthesis, GDP and MINLP models are limited to moderated size problems. The reasons are that the number of equations implied in chemical process models can be very large with hundreds or even thousands of integer (binary, Boolean) variables and with a large number of nonlinear and nonconvex equations that can prevent not only to finding the optimal solution but even finding a feasible point. Also, a rigorous modeling approach requires the use of process simulators that include state of the art models. Although most process simulators have optimization capabilities, they are able to deal only with problems involving continuous variables and smooth constraints with continuous domains. Therefore, complex cost models or detailed sizing models included in some simulators cannot be used. For this reason Jose has investigated different algorithms to integrate GDP and MINLP algorithms with existing process simulators in order to include complex cost and/or size functions, or in general complex equations defined over discontinuous domains. These functions can be in the form of explicit equations or implicit blocks (input-output black box relations). The structural optimization of process flowsheets (topology optimization) will be addressed at a later stage.

Jose has investigated three different algorithms using an MINLP reformulation of the original disjunctive problem: BB, OA and LP/NLP-BB. The basic idea relies on working in the reduced space of the decision and convergence variables in order to define the linearization in the MILP master problem. The bottleneck of all the procedure is in the time spent by the NLP that is related mainly to the time used in estimating accurate derivatives. The public version of HYSYS.Plant was used and the NLP subproblems were solved using CONOPT and SNOPT (external to HYSYS) through an activeX client-server application. All the process is controlled by MATLAB . Cost and size models were also developed in MATLAB as third party implicit models or through explicit equations. Jose was able to solve several problems including discontinuous costs in heat exchanger networks and natural gas plant, equipment choices in di-methyl ether plant. The problems were all solved with reasonable computational times (about 2,000 CPU sec largest problem). Jose found that the size of the master problem using implicit equations is greatly reduced in comparison with an equation oriented approach. Also, relaxing blocks of equations, instead of each equation individually, (i.e. by a big M reformulation) seemed to produce better relaxation gaps. The paper describing this work is listed in the section on references.

Synthesis of Crystallization Processes

New developments: **New methodology for initialization and superstructure optimization**

Post-doctoral fellow: **Ricardo Lima (started July 2006)**

Ricardo has been studying the development of superstructures for the optimization of the separation of p-xylene from a mixture of mixed xylenes using crystallization. On previous work, Ricardo has proposed a MINLP model and a two-level decomposition. The MINLP model describes a superstructure for the global crystallization process, involving a sub-superstructure for the crystallization stage and several additional separation stages. In the MINLP model the integer variables are associated with equipment and with disjunctions related with solubility predictions. The two-level decomposition consists on the solution of an aggregated and a detailed model, to overcome the convergence difficulties associated with the optimization of global MINLP model. Recent work has established the two-level decomposition as an initialization and approximation methodology, with a stop criterion based on the intersection of the upper bound defined by the aggregated model and the lower bound defined by the detailed model. The proposed methodology does not guarantee global optimality. Nevertheless, the addition, on each iteration, of integer cuts applied only on the integer variables associated with the equipment imposes the exploration of different combination of units. The results have shown that the aggregated model provides good starting points for the detailed model, and that generally the best solution is obtained before the stop criterion. Lately, the study of feeds containing different p-xylene compositions suggested the development of an improved superstructure and MINPL model. The new superstructure includes alternatives to deal with feed compositions of p-xylene ranging from 21% to 98%. Preliminary results, in terms of process flowsheet and product recovery, are in agreement with descriptions in the literature. The flowsheets obtained show that the sub-superstructure for the crystallization is able to cope with the existence of two crystallization stages at different temperature levels.

Design for Sustainability

New development: **Bi-criterion formulation for maximizing NPV and minimizing Eco-indicator 99**

Post-doctoral fellow: **Gonzalo Guillen**

This is a new project in which Gonzalo, a postdoc with a Fulbright fellowship, is trying to incorporate sustainability considerations in the synthesis and design of chemical processes. The aim of this project is to develop a set of quantitative tools based on mixed-integer modeling techniques that will facilitate the adoption of more sustainable alternatives for a wide range of problems arising in PSE. As a first step, Gonzalo studied the way to incorporate environmental concerns in the synthesis of chemical processes. During these last months, he has focused on extending this preliminary methodology to embrace the entire chemical supply chain (SC). Furthermore, he has also been working on incorporating the main sources of uncertainty that affect the assessment of the environmental performance of the network into the problem formulation.

Specifically, Gonzalo has formulated the design and planning of sustainable chemical SCs as a stochastic multi-objective mixed integer linear problem that aims to maximize the NPV and minimize the probability of exceeding a specific Eco-indicator 99 level. The stochastic model has been converted into its deterministic equivalent by applying concepts from chance-constrained programming. The calculation of the Pareto set of the resulting deterministic bi-criterion MILP has been further reformulated as a parametric MILP. This problem has been solved by a new decomposition technique based on parametric programming theory, which decomposes it into two levels and iterates between them. This method provides the entire Pareto set of the problem in a fraction of the CPU time required by standard methods for multi-objective optimization. Gonzalo has illustrated the capabilities of the proposed modeling framework and solution technique through a case study of a petrochemical SC operating in Europe. The Pareto set for this problem includes a set of SC configurations and planning decisions that represent the optimal compromise between benefit and environmental impact. These robust solutions provide valuable insights into the design problem and allow controlling the variability of the environmental performance in the space of uncertain parameters. Gonzalo is currently working on extending this technique to allow the control of the individual impact measures included in the Eco-indicator 99.

Design and Planning of Deep-Water Oilfield Development under Uncertainty

New Developments: **Implementation of Lagrangean branch and bound method**

Students: **Bora Tarhan (Ph.D. started January 2005)**

The project of Bora Tarhanfollows the line of work of Vikas Goel for the design and planning of gas and oil fields under uncertainty.

As a first step Bora has addressed a different stochastic optimization problem that in principle is simpler to model in order to prepare the ground for the complex gas and oil field problem. The problem is as follows. A network of candidate processes is given over a specified time horizon that is described by multiple time periods in which product demands are specified. It is assumed that major uncertainties are involved in the yields of each process, which are described by probability distribution functions. We consider that the uncertainty can be reduced with the potential investment in pilot plants, which delays the introduction of a process but provides more accurate process information on the yields. In addition, it is assumed that once a process is installed, the uncertainties in the yields decrease with time to reflect the experience and improved understanding in the operation of the process. The problem then consists in making planning decisions for process selection, capacity expansions, and possible investment in pilot plants in order to maximize the expected net present value over the specified time horizon. In order to capture all the complex trade-offs, Bora developed a new mixed-integer/disjunctive programming model that is composed of scenario linking and non-anticipativity constraints that are similar in spirit to Vikas's model. One importance difference is the time varying uncertainty, which for simplicity Bora considered is revealed over two time periods. Furthermore, he assumed that the time required for a pilot plant study corresponds to one time period, meaning that uncertainty is reduced to only one time period. This scheme is quite restrictive but we adopted it as a simplifying assumption that we intend to relax at a later stage. In order to solve this Bora developed a dual Lagrangean branch and bound method, also similar in spirit to the work by Vikas Goel. The corresponding subproblems are obtained by relaxing the disjunctions and transferring the first period non-anticipativity constraints to the objective function with Lagrange multipliers. The resulting model can be rewritten as independent subproblems for each scenario. The overall objective is to find the minimum upper bound by updating the multipliers. The branch and bound involves branching over both discrete and continuous variables that are involved in the non-anticipativity constraints. Bora has successfully applied this method to a small 3 process network, with one existing process and two with new technologies and for which investment of pilot plants can be considered over a 10 year horizon. Reformulating this problem as a single MILP involves 7,360 0-1 variables, 8,841 continuous variables and 85,139 constraints. Using CPLEX after one week the best solution that could be obtained had a net present value of $61.5 million. With the proposed method a solution of $80.14 was found in 10 hours of CPU time with a gap of 3%. The proposed solution did not select pilot plants to reduce the uncertainty, and proposed expanding Process I up to a capacity of 10 tons/day and making an additional expansion of 4.49 tons/day at time period 1 if the yield turns out to be 69%. If the yield for Process I is found to be 81% then an expansion of 2.98 tons/day is made also at the time period 1. The manuscript on this work has been submitted for publication.

Bora spent last year his internship at ExxonMobil's Upstream Research Center in Houston to get acquainted with planning problems related to deep-water oilfield development. The problem he has considered is the one of an oil field consisting of a number of reservoirs where each contains several possible well sites. Some of these well sites have to be drilled and exploited for oil over a planning horizon. The oil field infrastructure can be composed of Floating Production Storage and Offloading (FPSO) and/or Tension Leg Platform (TLP) facilities. The FPSO facility can be either a small FPSO, converted from a retiring oil tanker, or a large FPSO, newly constructed grassroots facilities. An FPSO facility can produce, store and offload the produced oil to other tankers. Unlike FPSO, a TLP facility cannot produce oil; it possesses only drilling and oil recovering capability. TLP and FPSO facilities can be connected to each other through pipes. There are two options for drilling wells. Each well can be drilled as a sub-sea or a TLP well. Drilling ships are used to drill sub-sea wells, so there is no need to have an FPSO or a TLP facility present to drill a sub-sea well. A sub-sea well has to be connected to an FPSO facility, whereas a TLP well has to be connected to a TLP facility. The problem consists of selecting investment and operation decisions such as selection of the type, location of facilities, time to build them, selection of wells to drill, the time to drill each well, time to connect each well to the facilities and production from the wells. There are uncertainties in

the sand quality, size of the reservoir and breakthrough time. Given the above assumptions, the goal is to maximize the expected net present value of the project. A simplified reservoir model has been considered where the oil rate decreases linearly, and the water-to-oil ratio is follows a nonlinear function with the cumulative oil production.

Bora has developed an MINLP model and solution method that he has largely completed in his second internship at ExxonMobil this summer. He has developed a model in which facilities and wells of the original problem are aggregated. Instead of deciding which well to drill or which facility to build, the decisions are how many wells or facilities to build. In order to account for the fact that uncertainties are not revealed immediately, a number of rules have been incorporated that specify when the uncertainty is revealed, either in terms of number of items (e.g. number of wells) or in terms of time of production. Because of the aggregation, variables for connection of facilities and wells are disregarded, and lengths to wells are underestimated in order to guarantee that the model predict an upper bound on the detailed model. This model is similar to the process networks model with the exception that each scenario is a non-convex MINLP. The steps of the algorithm are the same, except that each subproblem is solved using BARON as the global optimization algorithm. This relaxation yields an upper bound and the lower bound is generated by a simple heuristic. At this point Bora has implemented the method using a special scheme for subgradient optimization to update the Lagrange multipliers. He has recently considered the case of one reservoir. The best feasible solution is obtained on an example had an expected NPV of $\$6.5 \times 10^9$. In the optimal solution, the model predicts start building two small FPSO facilities and drill 9 subsea wells. Depending on the future outcomes trhe investments range from building up to 21 TLPs and 8 additional small FPSOs (best case) to only drilling subse wells (worst case). This solution was shown to have a significantly higher expected NPV compared to the deterministic solution (NPV=$\$4.4 \times 10^9$). Bora is close to completing the manuscript of this work.

Simultaneous Planning and Scheduling of Multiproduct Plants

New developments: Extension to scheduling of reactors with finishing lines

Students: Muge Erdirik [Ph.D. started Jan 2004]

Muge's project has dealt with the simultaneous planning and scheduling of multiproduct plants.

The initial objective in her work has been to consider the case of a single processor on which a number of products must be produced continuously over a given number of time periods. Sequence-dependent changeovers are given and due dates are assumed to take place at the end of each time period. The objective is to determine a production plan and schedule in order to maximize the profit (income minus inventories and changeovers). She has also considered recently the extension to the case of parallel processors, for which she applied ideas of te parallel batch reactors described below. To address the scheduling problem Muge developed a detailed slot-based MILP scheduling model. This model cannot be used to solve planning problems that typically require long time horizons. Therefore, the objective was to develop an iterative scheme that relies on aggregated models is guaranteed to converge to the same solution as if we had solved the detailed scheduling model. To accomplish this objective, Muge developed an aggregated MILP model that underestimates the changeover times and includes 0-1 variables for deciding what products may be produced in a detailed schedule. The iterative scheme consists in solving a sequence of aggregated MILP planning models and detailed scheduling models with fixed assignment of products to be produced at each time period. In addition to using a simple integer cut, Muge developed superset, subset and capacity cuts that eliminate a larger number of alternatives. The results that Muge obtained are quite encouraging. For instance, in a 24 week problem (720 0-1, 5907 continuous, 5526 constraints) the proposed method converged within 6% of the optimum in 3190 secs, while the detailed model did not terminate the search after 4000 secs (18% gap of bounds) and obtained an inferior solution. For the case of parallel units the solution approach is similar except that the aggregate model has two new features: (a) sequencing constraints that provide a more accurate estimation of changeover (see Dow project below); (b) a more effective formulation of changeover constraints that is tighter and requires fewer constraints. Using this model Muge has been able to solve problems with up to 10 products and 5 reactors over 24 weeks.

Based on an internship at Dow Chemical in Midland, Muge addressed the planning and scheduling problem for parallel batch reactors, a case study that was selected by Dow for the Enterprise-wide Optimization project. In this problem we are given a unique set of raw material costs and availability, storage tanks with associated capacity,

reactors with associated materials it can produce and batch sizes and times for each material it can produce, as well as operating costs for each material, and sequence dependent clean out times. We are also given a set of customers, each with a set of demand and prices for desired products. Finally, specified are the materials produced: process intermediates and final products. Dedicated storage tanks are considered. Another issue is that a final product of one process may be used as a raw material for another process. However, once a final product is fed to the dedicated storage tank, it can not be retrieved back to the plant. The problem is then to determine the monthly production quantities for each reactor and the assignment of materials to storage tanks to maximize profit.

Muge proposed a novel continuous time MILP optimization model for scheduling that is based on slot time representation that overcomes some of the major difficulties faced by the STN and RTN discrete and continuous time models. While effective for short-term scheduling, the proposed model becomes computationally very expensive to solve for long planning horizons. Therefore, as in the case of the single continuous processor, Muge has devised a rigorous bi-level decomposition algorithm. The problem is decomposed into an aggregated upper level planning model and a lower level planning/scheduling problem. The upper level determines the products to be produced at each time period as well as number of batches of each product, production levels and product inventories. The upper level is based on a new relaxed STN model where the detailed timing constraints and changeovers are replaced by time balances yielding a tight upper bound on the profit. A major new development here has been the *incorporation in the aggregate planning model of sequencing constraints* similar to the ones in the traveling salesman problem that yield accurate predictions for the changeovers at the planning level. The lower level is solved in the reduced space of binary variables and with number of slots according to the information obtained from the upper level model, yielding a lower bound on the profit. The lower level determines production and inventory levels as well as detailed timing of the sequence of products and associated assignments to processing equipments and storage tanks. The procedure iterates until the difference between the upper and lower bound is less than a specified tolerance. The biggest surprise with the new aggregated planning model is that for small problems (e.g. 5 products, 2 reactors) it usually predicts the exact scheduling solution (i.e. zero gap). For larger problems it predicts much smaller gaps than a relaxed model that simply underestimates the changeover times. A limitation, however, is that the new aggregate planning model leads to a larger MILP model. This, however, can be solved with a rolling horizon approach, with relatively small compromise of the optimality. The largest problem solved by Muge involved 15 products and 6 reactors, over 48 week period. the problem involved 10,092 0-1 variables, 25,798 continuous variables, and 28,171 constraints and was solved in about 11,000 secs using the rolling horizon approach. As for scheduling problems, the two level procedure works very well thanks to the accuracy of the planning model. For example a problem with 4 reactors, 6 products and 1 week, was solved in 4 major iterations, requiring 460 secs. Several papers have emerged from this work and are listed in the references.

In the last part of her Ph.D. Muge has worked with John Wassick on an important extension, the short-term scheduling of a multi-product batch plant which consists of parallel batch reactors that are connected to continuously operating finishing trains to form work groups. Finishing operations are required to convert the outputs from the reactors to trade products for a diverse set of markets and customers. A complication that arises in this type of plant is that each time a product switch occurs, not only the reactors but also the finishing trains need to be cleaned up and made ready for the next product. Since these clean up operations involve sequence-dependent changeovers, determining the optimal sequence of production is of great importance for improving equipment utilization and reducing the costs. The main challenge of modeling this scheduling problem arises from the structure of the plant, where the work groups are not fixed, but are flexible in the sense that subsets of work groups can be selected by manipulating valves that interconnect the reactors with the finishing trains. Therefore, in addition to the challenge of determining the optimal production sequence given the sequence-dependent changeovers with high variance, there is also the challenge of regrouping the units periodically when the demand varies from one period to the next one, or when new products are introduced while maximizing profit. In order to address the aforementioned issues, Muge used as basis long-term planning model and added special constraints to enforce that workgroups have the same assignment and sequence of products. As an example, Muge solved a problem with 10 products, 6 reactors and a horizon of 4 weeks, which gives riser to an MILP with 1992 0-1 variables, 2904 continuous variables and 6183 constraints. The optimal solution was obtained in 644 CPUs. Muge is completing a manuscript on this work.

Design and Planning of Responsive Supply Chains

New Development: Incorporation of probabilistic inventory for safety stocks

Students: Fengqi You [Ph.D. started Jan 2006]

The major goal of this project, which is being performed by Fengqi You in the context of the Enterprise-wide Optimization initiative, is to develop a comprehensive optimization model that allows the effective integration of long term strategic design decisions for multisite process manufacturing facilities, with short term planning for production and distribution that accounts for the time delays across the supply chain. The motivation for this project is that virtually all optimization models assume that material can be transferred instantaneously. In that way lead times, or response times once orders are placed, are not taken into account. It is our major goal to establish the trade-offs between economics and lead times.

As a first step Fengqi has addressed the long term design problem, for which he has developed a model for designing the supply chain of multisite network of processes in a superstructure that involves both dedicated and multiproduct continuous plants. The time horizons considered are of the order of years, and zero-inventory levels are considered, which qualitatively corresponds to the worst case for lead times. The problem is then posed as a bi-criterion optimization problem in which the objectives are to maximize net present value and to minimize lead time. In order to reflect lead times for different choices of topologies Fengqi has considered constraints that measure the duration of the longest time path of chemical flows from a supplier to a customer by way of manufacturing sites. The proposed constraints involve transportation times and residence times in processes. For dedicated times these are simply constants, while for multiproduct plants they correspond to cycle time plus residence time minus its processing time. Note that the cycle time results from a scheduling optimization that has to be accounted. For the case of dedicated plants the problem can be formulated as an MILP, since nonlinear terms defining the lead times can be linearized. For the case of multiproduct plants, the model and leads to a nonconvex MINLP problem. Fenqui has obtained results on a production network for polystyrene resins that involves a dedicated process (styrene), and two multiproduct plants (solid polystyrene and expandable polystyrene). Three potential plant sites are located in PA, TX and AL. the PA site can install all the three types of plants, the TX sites can only install plant I, and the AL site can only install plant 2 & 3. Two suppliers of ethylene are located in TX and OH, and two suppliers of benzene are located in TX and VA. Two customers of SPS resins are located in CA and NY, another two customers of EPS resins are located in GA and MN. For 3 time periods (2, 3 and 5 years) the model involved 133 0-1 variables, 2249 continuous variables and 3041 constraints. To develop the trade-off curve the ε-constraint method was used. DICOPT required 3.5 minutes while BARON required about 100 hours. The solution involving shortest lead time of 8.85 days had an NPV of $158 million, while the longest lead time was 14.42 days at a much higher NPV of $1,261 million.

Fengqi has recently extended the above problem to by using a probabilistic model for stockout. In this way instead of using a deterministic lead time, Fengqi has proposed the expected lead time as the quantitative measure of supply chain responsiveness that represents the expected value of time delays incurred by transportation and production across the supply chains. The probabilistic model can also predict the safety stock levels by integrating stockout probability with demand uncertainty. This model is integrated as a chance constraint for which Fengqi developed analytical expressions for the triangular and the normal distributions. The multi-objective optimization model was also solved with the ε-constraint method, but Fengqi has also developed a hierarchical algorithm for the solution of the resulting large-scale MINLP problem that is based on decoupling of the decision-making levels (strategic and operational). Fengqi has solved two examples related to the styrene problem described above. The results show that small changes in expected lead time can lead to significant changes in the net present value and the network structure, which in turn suggests the importance of integrating responsiveness into the design and operations of process supply chain network. An interesting by-product of the model is a trade-off curve of safety stock versus expected lead time, which provides very useful information. Fengqi is writing a manuscript on this work which should be available in the next newsletter.

Optimal Scheduling of Crude Oil Operations

New development: **New continuous time MILP model**

Student: **Sylvain Mouret [Ph.D. started Jan 2007]**

Sylvain joined the department in January from Ecole Polytechnique in Paris. He is working in a new project funded by Total through the collaboration with Pierre Pestiaux. The specific problem that Sylvain is addressing is a crude oil blending system composed of crude marine vessels, storage tanks, charging tanks and CDUs. Crude vessels unload crude oil into storage tanks during a time window depending on the arrival time to the refinery. These crudes are then mixed kerosene, gas oil and residues. into charging tanks before being distilled by CDUs which separates the charged oil into fractions such as gasoline. Given arrival time of marine vessels, capacity limits of tanks, flow rate limitations, initial key components concentrations in vessels and tanks, components concentration ranges as part of distillation specifications, demands for each mixed oil, and a time horizon, the objective is to determine time and volume variables of all crude-oil transfer operations in order to maximize the gross margins of distilled mixed oil.

Sylvain has developed a continuous time model that in the spirit of constraint programming, relies on the idea of postulating potential assignments of tasks (slots) to operations that include the various transfers in the network. By introducing the appropriate 0-1 variables for assignments, as well as disjunctive constraints that enforce non-overlapping operations (e.g. inlet and outlet of a given tank), the problem can be formulated as an MILP provided the constraints on compositions for blending are relaxed. Once the solution is obtained for this problem, an NLP subproblem is solved with fixed 0-1 variables to enforce the composition constraints. Sylvain has applied this solution approach to several problems obtaining very encouraging results, The largest problem had 3 vessels, 6 storage tanks, 4 charging tanks and 3 CDUs. Postulating 30 tasks (slots) the MILP was solved in 567 sec and the NLP in 31 secs leading to a solution with 0% gap. Sylvain will be presenting this work for his Ph.D. qualifying exam. One of the next major steps will be too investigate how to determine a priori the number of tasks (slots).

Planning of Refinery Operations

New development: **Implementation of swing cuts method**

Student: **Abdulahraman Alattas [PhD, started Jan 2007]**

Abdul has started to work on this project which is a joint collaboration with BP through Ignasi Palou-Rivera in the Enterprise-wide Optimization project. The major objective is to develop refinery planning models that incorporate nonlinear process models, in contrast to the common fixed yield models that lead to robust LP models that are prevalent in industrial practice (eg.g. PIMS).

The specific problem that Abdul is addressing is for complex refinery configurations for processing heavy crudes. The crude is introduced into the crude distillation unit (CDU) that combines the atmospheric distillation column and the vacuum distillation column and produces the first cuts of the crude. These include the overhead fuel gas, straight-run naphtha, straight-run gasoline, straight-run light distillate, straight-run gas oil and the bottom residue. Along with the CDU, the configuration of interest includes the following process units: naphtha reforming unit that produces reformed gasoline and fuel gas from straight-run naphtha, catalytic cracking unit that produces fuel gas, gasoline and fuel oil from straight-run light distillate and straight-run gas oil, residue hydrotreating unit that treats the bottom residue to blending quality, and product blending units that combine different intermediate product streams to produce the desired final products: premium gasoline, regular gasoline, diesel, fuel oil and residue. The objective of the planning model is to determine the types, quantities and mixing strategies for the different crude oils available for purchase, so that the refinery will meet the objectives of maximizing profits while meeting specific demands over a specified time period.

Abdul has implemented both fixed-yield models and swing-cuts models in order to assess their relative benefits. The swing cuts model, which can also be formulated as an LP, can be thought of a model that has the flexibility of transgressing the fixed boundaries of the fixed yields models within certain limits. In a specific instance Abdul found that thee swing cuts model can predict a solution with 10% improvement in the profit, largely due to different

decisions in the purchase of crudes. He has started to investigate the feasibility of incorporating the aggregate distillation models proposed by Jose Cabllero. This requires the CDU to be represented through cascaded columns. Abdul will be presenting his PhD qualifying exam based on this work. After the exam he will concentrate on implementing the aggregated model.

Scheduling of Batch Multiproduct Plants

New Development: **Simultaneous batching and scheduling**

Collaboartors: **Pedro Castro (INETI, Portugal)**

At Carnegie Mellon, Pedro first examined the single stage problem with parallel lines. Pedro found if that he does not use a common time grid for the parallel stages, but that rather uses a multiple time grids for each stage, then the RTN MILP model can be solved almost as fast as the hybrid MILP/Constraint Programming model. He solved problems ranging from 12 orders and 3 units, up to 30 orders and 5 units for the cost minimization case. Another interesting result that emerged was that Pedro solved the discrete time model with up to about 400 time intervals in order to obtain exact or very close approximations. When the objective is minimization of earliness the discrete time model performed the best followed by constraint programming. In the next phase, Pedro investigated the optimal scheduling of multistage plants. In this case he performed a non-trivial extension of the multi-time grid RTN MILP model for a single stage. He also examined in detailed a sequential MILP model that had been proposed previously by Harjunkoski and Grossmann. He performed extensive numerical experiments using as objective functions cost minimization, minimization of makespan, and earliness minimization. The problems ranged from 6 orders, 4 units, 2 stages to 10 orders, 8 units, 4 stages. His results showed that constraint programming tended to be the more effective solution method for makespan minimization. The sequential model proved to be best for earliness minimization, while the proposed model performed best for the cost minimization criterion. On an overall basis, the discrete RTN model was also competitive. Here again the discrete-time formulation showed very good performance, particularly for total earliness minimization, despite generating very large MILPs when considering the exact problem data. The main conclusion was that for the multistage case not a single model proved to be the dominant one. This work also led to a manuscript that has been published.

The extension to handling changeovers in multistage plants Pedro completed by developing two new continuous-time formulations for the short-term scheduling of single/multistage plants. The formulations rely on the use of multiple time grids, one per equipment resource. While one formulation uses binary variables linked to such tasks, giving rise to 4-index binary variables, the other maintains the 3-index binary variables of the previous model and changes one set of constraints to make it possible to handle sequence dependent changeovers. Both formulations were shown to be very efficient in single stage problems with the surprising result coming from the fact that the 4-index binaries formulation was found to be slightly better than its 3-index binaries counterpart, despite featuring a number of binary variables that can be up to one order of magnitude larger. As the number of stages increases, the performance of the multiple time grid formulations decrease steadily and feasibility may even be compromised. The other goal was to provide a critical review of other approaches. These included an RTN-based discrete-time formulation, a continuous-time model with global precedence sequencing variables, a constraint programming model and a hybrid MILP/CP model. A total of 39 examples were solved and the results, together with those of the two previous works. Overall the best model proved to be the continuous-time formulation with global precedence sequencing variables.

More recently Pedro with input from Muge has a new mixed integer linear program (MILP) for the optimal short-term scheduling of single stage batch plants with sequence dependent changeovers and optimal selection of the number of batches to produce. It is a continuous-time formulation employing multiple time grids that is based on the resource-task network (RTN) process representation. The main novelty is that aggregated processing and changeover tasks are considered that account for the time required to produce all batches of the product, plus the changeover time to the next product in the sequence. The performance of the new formulation was studied by Pedro through the solution of 12 example problems for the objective of revenue maximization and 4 for the objective of makespan minimization. The same problems were solved by a multiple time grid implicit batching approach, by a continuous-time model with global precedence sequencing variables, by a model with immediate precedence sequencing variables that does not determine the timing of events, and by a constraint programming model. The new

formulation emerged overall as the best performer for the scenario of maximum plant flexibility, where different batches of the same product can be produced in different units. The model developed by Muge with immediate precedence sequencing variables was the fastest but it is not a general scheduling model in the sense that it assumes a single cyclic schedule in each unit, which can be broken, but two or more cyclic schedules per unit may result. In such cases, subtour elimination constraints can be added and the problem solved iteratively to find a feasible schedule at the likely expense of removing the global optimal solution from the feasible space. When compared to the implicit batching approach, the computational effort of the new formulation was typically one order of magnitude lower, which in practice indicates that the new formulation can tackle larger problems. When compared to the traditional approach of considering a single processing task per batch, fewer event points are needed, which results in significantly lower computational effort as illustrated through the solution of several example problems. A manuscript describing this work has been submitted for publication and is listed in the refrerences.

Simultaneous Scheduling and Control

New development: **Lagrangean decomposition for simultaneous scheduling and control**

Collaborator: **Antonio Flores-Tlahuacac (Professor U. Iberoamericana)**

This is a collaboration with Antonio Flores from the Universidad Iberoamericana (Ignacio's alma mater). Antonio, being a control person, has been motivated by the idea of using dynamic models for control in scheduling problems. Given our interest in the area of scheduling, we decided to join forces in a work in which the basic idea is to combine a scheduling optimization model, with a dynamic model for the optimization and control of the transitions. In this work we have addressed the simultaneous scheduling and control problems for a continuous stirred tank reactor (CSTR) that produces multiple products within a cyclic schedule that involves sequence dependent transitions. In the previous newsletter we reported a formulation where integer variables are used to determine the production sequence and continuous variables take into account production times, cycle time and inventories. The scheduling part of the model is similar to our previous work with Jose Pinto. Because, dynamic profiles of both manipulated and controlled variables are also decision variables, the dynamic part of the model is formulated with DAEs. The resulting problem can then be cast as a Mixed-Integer Dynamic Optimization (MIDO) problem in which the objective function includes income from sales of products, inventory costs and transition costs that takes into account through quadratic deviation terms, the amount of off-specification material produced during product transition. To solve the MIDO problem the MIDO problem is transformed into an MINLP using orthogonal collocation, where initial guesses on the duration of the transitions must be provided. These are then revised in a subsequent optimization.

Antonio and his student Sebastian Terrazas-Moreno have developed a new MINLP formulation to simultaneously solve the scheduling and control problems in polymerization reactors during a cyclic manufacturing operation. In contrast to the previous model, the problem need not be solved sequentially by iteratively assuming fixed lengths for the duration of the transitions. Another interesting feature of the model is that by assuming that the performance of each polymer is only dependent of the initial conditions, the problem can be formulated in terms of 0-1 variables for assigning products to slots. The transitions are then simply computed from the difference in the initial conditions. This leads to a much smaller number of 0-1 variables compared to the case when sequence dependent transitions are explicitly modeled. Two case studies related to the polymerization industry were solved: the isothermal free radical bulk polymerization of styrene, and methyl-methacrylate polymerization. In the latter the production of four grades (A,B,C,D) was considered corresponding to molecular weight distributions of 15000, 25000, 35000 and 45000, together with complex kinetic models. The predicted cycle time was 172,2 hrs with an optimal sequence of D $\rightarrow$ A $\rightarrow$ B $\rightarrow$ C in which the dynamics of the transitions were explicitly accounted. The required CPU with DICOPT for the corresponding MIDO problem using orthogonal collocation was 70 secs.

Recently, Antonio in collaboration with Sebastian Terrazas, addressed the simultaneous scheduling and control (SSC) problem using Lagrangean Decomposition as presented by Guignard and Kim. The model was decomposed into scheduling and control subproblems, and solved using a heuristic approach used before by Sarette Van den Heever in oilfield problems. The method was tested using a Methyl Methacrylate (MMA) polymerization system, and the High Impact Polystyrene (HIPS) polymerization system, with one continuous stirred-tank reactor (CSTR), and with complete HIPS polymerization plant composed of a train of seven CSTRs. In these case studies, different polymer grades are produced using the same equipment in a cyclic schedule. The computational times in the first

two examples were lower for the decomposition heuristic than for the direct solution in full space, and the optimal solutions found were slightly better. The example related to the full scale HIPS plant, which involved 16 0-1 variables and 22,700 variables, was only solvable using the decomposition heuristic. A manuscript describing this work is being completed and will be available in the next newsletter.

Software for MINLP Optimization in Design and Scheduling

Research Assistants: Rosanna Franco (started July 2006)

Rosanna Franco has been working on the web-interfaces that are available in:
http://newton.cheme.cmu.edu/interfaces

She completed the new PC-interface ISO-Synheat for handling isothermal streams that was developed by Jose Maria Ortega and Arturo Jimenez. That interface should be available soon on the web. Rosanna is also completing a new interface for integrated water systems, based on the work of Ramkumar Karuppiah.

The current list of programs that we have available, most of them in our website, are the following:
(description in http://egon.cheme.cmu.edu)

Synthesis:

SYNHEAT	MINLP synthesis heat exchanger networks (Yee) Also includes transshipment model for targeting (Papoulias)
STEAM	MINLP Model for the synthesis of combined cycles for utility plants (Bruno) Model includes correlations for steam, efficiencies and cost data
GLOBESEP	Global NLP optimization for synthesis of separation networks and single feed/mixed products (Quesada)
WATER	Global NLP Model for synthesis of wastewater treatment configuration (Galan)
EXTRACTOR	Disjunctive MINLP for synthesis of liquid-liquid extraction systems (Reyes)
GDP-DISTILL	GDP Model for the optimal selection of number of trays and feed tray location in distillation columns using tray-by-tray model (Barttfeld)

Batch design:

BATCHSPC	MINLP and MILP models for multiproduct batch plants single product campaigns (Kocis, Voudouris)
BATCHMPC	MILP model for multiproduct batch plants mixed-product campaigns (Birewar, Voudouris)

Scheduling:

STN	State-Task-Network MILP formulation for scheduling multipurpose batch plants. Both the the Kondili, Pantelides and Sargent (1993) model and the Maravelias and Grossmann (2003) are implemented.
PARALLEL	MINLP continuous multiproduct scheduling on parallel lines Features feasibility preanalysis (Sahinidis)
MULTISTAGE	MINLP continuous multiproduct in multistage plants (Pinto)
CYCLE	LP/MILP aggregate flowshop scheduling (cycle time/makespan) Includes loop tracing algorithm (Birewar)
STBS	MILP short term multistage scheduling (Pinto, Bolio)
CRUDEOIL	MILP model for refinery scheduling (Lee, Pinto)
DECAY	MINLP model for scheduling of clean-up of parallel furnaces (Jain)
UTILPLAN	MILPmultiperiod model for utility plants (Iyer)
PRODEV	MILP model for scheduling of tests in new product development (Schmidt, Najimas) MILP for resource scheduling in new product development (Jain, Maravelias)

Planning:

PLANNER	MILP multiperiod model for capacity expansion in process networks (conventional and lot sizing model) (Sahinidis, Norton)

MULTISITE MILP model for planning the selection of processes and capacity expansion in different geographical location and accounting for transportation costs (Turkay)
GREENPLAN Bi-criterion MILP model for selection of processes that maximize the net present value and minimize toxicity (Drabbant)
NETCHAIN Multiperiod MILP for supply chain optimization of multisite facilities with flexible processes, intermittent deliveries, changeovers and inventories (Bok/Iyer)

Nick Sahinidis' Group

THRUST 1—OPTIMIZATION ALGORITHMS, THEORY, AND SOFTWARE

Algorithms and Software for Global Optimization of NLPs and MINLPs

Student: Ms. Xiaowei Bao (Ph.D. student in Chemical and Biomolecular Engineering at the University of Illinois)

Collaborator: Mohit Tawarmalani (Associate Professor, Purdue University)

As a result of research that was initiated in 1991, we have developed algorithms and software for global optimization of NLPs and MINLPs. The main results of this work have been:

- A theory of convex extensions that provides a systematic means for developing the functional expression of convex/concave envelopes of nonlinear functions of continuous and integer variables.
- An entirely linear outer-approximation of factorable nonlinear programs. Relying on LP relaxations results in a robust solution approach to global optimization.
- A variety of range-reduction schemes for reducing the search space of integer and nonlinear programs.
- Finite branching schemes for concave minimization and two-stage stochastic integer programs.
- The BARON software for the global optimization of NLPs and MINLPs.

Xiaowei Bao is currently working on the development, computational implementation, and testing of techniques for the automatic exploitation of convexity in global optimization. The convexity detection scheme she has considered has three main parts: a decomposition of the function under consideration in order to facilitate convexity detection, a bounding process to provide useful bounds as an aid for accurate convexity detection, and a convexity detection process that relies on existing tools from convexity analysis. We used this procedure to preprocess GAMS models before they were turned for solution to BARON. Computational results with 32 problems from the globallib collection demonstrated that the proposed convexity identification scheme improves the performance of the BARON global optimization solver significantly by allowing the solver to strengthen its lower bounds and reduce the relaxation gap once convexity has been automatically identified and this information has been provided to the solver through its CONVEX_EQUATIONS construct. The current approach relies on the use of a library of currently known convex/concave functions. As this library grows over time, the convexity identification scheme will be enhanced, thus permitting the construction of even tighter bounding functions in global optimization algorithms.

Nick Sahinidis and **Mohit Tawarmalani** are currently maintaining the BARON software. Over the past year, updates to BARON have included (1) the introduction of a new heuristic for local search and (2) improved range reduction for monomial functions. In addition, an interface to the Xpress LP code and the MOSEL modeling system was completed in summer 2007 and is currently in the final testing stages by Dash Optimization.

Algorithms and Software for Black-box Optimization

Student: Mr. Luis Miguel Rios (Ph.D. student in Industrial Engineering at the University of Illinois)

This project is currently aiming at a systematic testing of existing derivative-free algorithms that are capable of optimizing black-box problems. Derivative-free optimization is an area of recent interest and rapid growth, fueled by a growing number of applications, especially in the oil and gas, and chemical process industries. The major challenge is that the objective function in many problems is expensive to evaluate, while no bounds or Lipchitz

constants are available, and strategies to directly estimate derivative information are impractical or expensive. The most recent systematic testing of derivative-free algorithms for solving problems of this nature was done 9 years ago. **Luis Miguel Rios** has collected 225 test problems from the GAMS globallib and solved them under different conditions using sixteen different black-box solvers. These codes were: Adaptive Simulated Annealing, ASA version 26.23 by Ingber; Solvers APPS, DIRECT, EA, PATTERN, and SOLIS-WETS under Design Analysis Kit for Optimization and Terascale Applications (DAKOTA), Version 4.0, from Sandia National Laboratories; Derivative Free Optimization (DFO), Version 2.0, by Conn, Gould, Toint, and Scheinberg; Multilevel Coordinated Search (MCS), by Huyer and Neumaier; the Nelder-Mead algorithm implemented in MATLAB; Nonlinear Optimization for Mixed vAriables and Derivatives (NOMAD), Cycle 6, by Couture, Audet, Dennis, and Abramson; SID-PSM, Version 0.3, by Custódio and Vicente; and solvers EGO, GLB, GLC, LGO, and RBF under TOMLAB.

The main conclusions from this computational study were that: (a) even obtaining a feasible solution cannot be taken for granted for these problems/solvers, (b) larger problems diminish the chances for obtaining good solutions, (c) LGO and MCS are better, on average, than other solvers, (d) all solvers are 'useful' in the sense that there are at least a few problems for which each solver is best in terms of solution quality.

Current plans in this line of research include the addition of non-smooth problems in the test set collection and the inclusion of additional solvers. Test problems of black-box models from industry are currently sought. In the long run, we plan to develop novel algorithms for this difficult class of optimization problems.

Algorithms and Software for Linear Optimization Problems (LP)

Student: Mr. Joseph Elble (Ph.D. student in Industrial Engineering at the University of Illinois)

Algorithms for solving LPs represent the workhorse of optimization systems for solving large-scale MILPs, NLPs, and MINLPs. While highly successfully commercial software exist for solving LPs, none is guaranteed to provide reliable results in the sense that they are all subject to the effects of floating point arithmetic and round-off errors. The goal of this project is to develop new simplex algorithms and software in order to provide tools that can reliably solve large-scale linear optimization problems even in the presence of round-off errors. Towards this goal, we plan to develop symbolic algorithms for linear programming preprocessing, matrix scaling, and matrix factorization.

Over the past three years, **Joseph Elble** worked simultaneously on two related M.S. theses, one in Industrial Engineering and one in Computer Science, both of which were completed in August 2007.

In his Industrial Engineering thesis, **Joseph Elble** investigated the current state of direct methods for solving sparse linear systems. The data structures for sparse linear systems were studied, and the thesis explored the four stages of direct methods: analysis, numerical factorization, forward and backward elimination, and iterative refinement. This work was exploratory in nature, aiming at understanding conditions under which current methods for linear systems work well and conditions under which such methods are likely to give incorrect results.

In his Computer Science thesis, **Joseph Elble** studied scaling of LPs. Scaling of linear programs, while poorly understood, is definitely not devoid of techniques. Scaling is the most commonly used preconditioning technique utilized in linear programming solvers. The purpose of scaling is to improve the conditioning of the constraint matrix and hopefully decrease the computational effort for solution. Most importantly, scaling provides a relative point of reference for absolute tolerances. Many techniques for obtaining scaling factors for linear systems were investigated in this thesis. With a focus on the impact of these techniques on the performance of the simplex method, over half a billion LP solves were executed in Nick's Linux cluster at Illinois. Some of the scaling techniques studied are, by construction, computationally more expensive than others. Some are more successful in practice than others. There is no current scaling technique that dominates all others.

The long-term goal of this project is to develop novel algorithms for LPs and make them available via distributed implementations on modern FPGAs.

THRUST 2—APPLICATIONS OF OPTIMIZATION IN BIOLOGY, CHEMISTRY, ENGINEERING, AND MEDICINE

Inverse Imaging Problems in X-ray Crystallography

Student: **Mr. Alexander Barton Smith (Ph.D. student in Chemical and Biomolecular Engineering at the University of Illinois)**

A vast majority of 3D structures of compounds are derived using the physics of X-ray diffraction, especially in the case of important biological macromolecules. The computation of a structure from X-ray diffraction data, however, remains a very challenging, nontrivial problem, both experimentally and computationally. A major obstacle, coined, "the phase problem," represents a dilemma in which phase information, critical to computation of the 3D structure of a crystal, is not directly measurable in a traditional X-ray diffraction experiment.

The phase problem has recently been approached via combinatorial optimization techniques and the resulting sieve method has been demonstrated to be effective for phasing centrosymmetric structures (Smith, Xu and Sahinidis, 2007). The purpose of the current work is to (a) develop a more robust enforcement of atomicity constraints in direct space and (b) extend the approach of Smith et al. from the centric to the most challenging non-centric case, thus making the approach directly applicable to proteins and other chiral molecules.

Alexander Smith has recently developed a mixed-integer linear programming model for phasing based on the minimal principle; one which includes the introduction of specific atomicity constraints. Building on the MILP model presented in Smith et al. (2007), atomicity is constrained through sampling of electron density on a grid. First, a set of points is selected, at random, to sample the unit cell. Electron density is calculated at these points in terms of the integer variables, which describe the phases. Physical constraints in direct space are then enforced using the grid of electron density. Computational results demonstrate that the proposed approach can solve many challenging structures that were not solvable with the widely used crystallographic software package Shake-and-Bake.

Protein Side-chain Conformation Problem

Student: **Wei Xie (Ph.D. May 2007, Chemical and Biomolecular Engineering at the University of Illinois; currently at American Airlines Operations Research and Decision Support Group, Fort Worth, Texas)**

The protein side-chain conformation problem is a central problem in proteomics with wide applications in protein structure prediction and design. The problem calls for determining the side-chain orientations for a protein whose backbone structure is already known. Computational complexity results show that the problem is hard to solve. Yet, instances from realistic applications are large and demand fast and reliable algorithms. **Wei Xie** has developed a new global optimization algorithm which for the first time integrates residue reduction and rotamer reduction techniques previously developed for the protein side-chain conformation problem. We showed that the proposed approach simplifies dramatically the topology of the underlining residue graph. Computations show that our algorithm solves problems using only 1 to 10% of the time required by the mixed-integer linear programming approach available in the literature. In addition, on a set of hard side-chain conformation problems, our algorithm runs 2 to 78 times faster than SCWRL 3.0, which is widely used for solving these problems. Our algorithm currently represents the state-of-the-art algorithm for the protein side-chain problem.

Protein Structural Alignment

Student: **Wei Xie (Ph.D. May 2007, Chemical and Biomolecular Engineering at the University of Illinois; currently at American Airlines Operations Research and Decision Support Group, Fort Worth, Texas)**

Aligning proteins based on their structural (3D) similarity is a fundamental problem in molecular biology with applications in many settings, including structure classification, database search, function prediction, and assessment of folding prediction methods. Structural alignment can be done via several methods, including contact map overlap (CMO) maximization that aligns proteins in a way that maximizes the number of common residue contacts. **Wei Xie** has developed a reduction-based exact algorithm for the CMO problem. Our approach solves CMO directly rather than after transformation to other combinatorial optimization problems. We exploit the mathematical structure of the problem in order to develop a number of efficient lower bounding, upper bounding, and reduction schemes. Computational experiments demonstrate that our algorithm runs significantly faster than existing exact algorithms and solves some hard CMO instances that were not solved in the past. In addition, the algorithm produces protein clusters that are in excellent agreement with the SCOP classification. An implementation of our algorithm is accessible as an on-line server at http://eudoxus.scs.uiuc.edu/cmos/cmos.html. This algorithm currently represents the state-of-the-art algorithm for the CMO problem.

Combinatorial Library Design

Student: **Wei Xie (Ph.D. May 2007, Chemical and Biomolecular Engineering at the University of Illinois; currently at American Airlines Operations Research and Decision Support Group, Fort Worth, Texas)**

Designing proteins with novel or improved functions via combinatorial libraries involves first mutating or recombining existing sequences and then exploring the resultant sequences. Compared to the traditional sequence design approaches that require detailed knowledge of protein structure and function, combinatorial library design approaches are more straightforward to implement and prove quite successful in practice. An indispensable component of a successful library design approach is a powerful computational method that reaches balance between diversity and activity. Although quite a few computational studies have been conducted in the past, limited theoretic analysis exists that unveils the inherent difficulty of the proposed models, which would provide important guidelines for the future development of models and algorithms for this problem. **Wei Xie** studied this problem from a computational complexity perspective and reached several interesting results. We showed that existing models for combinatorial library design vary substantially in difficulty: while some models are fairly easy in that they admit low order polynomial-time algorithms, others may demand exponential time to solve. In addition, we propose several new algorithms for combinatorial library design under sequence-independent site-directed chimeragenesis (SISDC) protocol, and the resultant implementation outruns popular RASPP package by a factor of 10 to 100.

Steady State Optimization with Guaranteed Robust Stability under Parametric Uncertainty

Student: **YoungJung Chang (Ph.D. December 2006, Chemical and Biomolecular Engineering at the University of Illinois; currently postdoc with Costas Maranas at Penn State)**

Recently, Chang and Sahinidis (2005) proposed a global optimization method to find robustly stable steady-state solutions to biochemical process optimization problems using analytical necessary and sufficient stability conditions as constraints. This approach aimed to address structural and general model uncertainties and could produce conservative solutions for the case of parametric uncertainties alone. In the current work, we show how to extend the approach developed in Chang and Sahinidis (2005) to handle parametric uncertainties in a way that does not lead to conservative designs. The methodology proposed relies on an analytical approach to enforce robust stability in steady-state optimization problems. The resultant formulation is intuitive and exact, and a global optimization algorithm is developed to solve it. In contrast to prior approaches to this problem, our methodology requires no

bifurcation analysis of the system while providing a deterministic guarantee for the least conservative stable solution.

DNA Sequencing by Hybridization

Student: **YoungJung Chang (Ph.D. December 2006, Chemical and Biomolecular Engineering at the University of Illinois; currently postdoc with Costas Maranas at Penn State)**

DNA sequencing by hybridization (SBH) uses DNA chips to reconstruct a DNA sequence from subsequences. SBH is often used in custom re-sequencing and mutation detection. If errors are present in the experimental data, the reconstruction problem is NP-hard and, thus, computationally challenging. This problem has been studied extensively but no current approaches provide global optima, alternative solutions, or a guarantee for the correctness of solutions. With **YoungJung Chang**, we formulated the DNA SBH problem with errors as an integer linear program with an exponential number of constraints. A row generation solution algorithm was developed to solve this model. The proposed approach solved large SBH problems to global optimality efficiently and was able to locate all the alternative optimal solutions. These alternative solutions exhibited a wide range in terms of their ability to reproduce the target DNA sequence.

Protein Binding Site Identification

Student: **YoungJung Chang (Ph.D. December 2006, Chemical and Biomolecular Engineering at the University of Illinois; currently postdoc with Costas Maranas at Penn State)**

In this work with **YoungJung Chang**, the problem of simultaneous identification of a protein binding pattern and sites has been solved within an integer programming framework. Instead of using a probabilistic model, a difference model was used to make the problem more tractable, and an exact efficient linearization scheme was proposed for the resulting nonlinear model. Depending on the amount of available biological information, we could employ two different formulations. If the pattern shape is known, then we can solve an easier problem, for which the state-of-the-art integer programming solver is very efficient. Even when there is limited prior knowledge on the pattern such as its maximal and minimal lengths, the proposed formulation can solve the problem within a reasonable amount of time..

A Branch-and-Bound Algorithm for the Continuous Facility Layout Problem

Student: **Wei Xie (Ph.D. May 2007, Chemical and Biomolecular Engineering at the University of Illinois; currently at American Airlines Operations Research and Decision Support Group, Fort Worth, Texas)**

Finding optimal facility layouts is a classic problem in Process System Engineering as well as Operations Research. As initial models were unsuitable for instances of unequal facility sizes or unknown potential positions, continuous facility layout (CFL) models were introduced to address these limitations by modeling facilities as geometric entities and searching for an optimal 2-dimensional packing. However, solving these new models becomes dramatically harder: finding optimal layouts for these models is beyond reach of current optimization techniques, except for tiny instances. **Wei Xie** obtained several important theoretical results for this problem. First, we proved that it suffices to enumerate finitely many candidate solutions to secure an optimal solution, despite the fact that CFL admits infinitely many feasible layouts. We then developed a specialized branch-and-bound algorithm to further boost search efficiency by exploiting problem structure to prune large portions of the solution space. Comprehensive computational studies show that this new algorithm substantially outperforms three existing approaches. We also discussed extensions of this algorithm to more general layout instances.

Portfolio Optimization for Wealth-dependent Risk Preferences

Student: **Mr. Luis Miguel Rios (Ph.D. student in Industrial Engineering at the University of Illinois)**

Empirical and theoretical studies of preference structures of investors have long shown that personal and corporate utility is typically multimodal, implying that the same investor can be risk-averse at certain levels of wealth while risk-seeking at others. **Luis Miguel Rios** has studied the problem of optimizing the portfolio of an investor with an indefinite quadratic utility function. The convex and concave segments of this utility reflect the investor's attitude towards risk, which changes based on deviations from a fixed goal. Uncertainty is modeled via a finite set of scenarios for the returns of securities. A global optimization approach based on BARON was developed to solve the proposed nonconvex optimization problem. We performed computations in order to investigate the effect of short sales and demonstrate that the proposed approach systematically produces portfolios with higher values of skewness than the classical expectation-variance approach.

Medical Diagnosis and Prognosis

Collaborator: **Professor Hong Ryoo (Associate Professor, Department of Industrial and Information Engineering, Korea University, Seoul Korea)**

Over the past two decades, diagnostic techniques have grown out of the desire to replace surgical biopsy by breast cancer diagnosis that is based solely on the use of samples obtained through fine needle aspirates (FNA). Once FNA samples are taken from the breast mass, the material is examined for a number of characteristics of each nuclei, including size, shape, and texture. These attributes can then be used to classify the sample as benign or malignant. The fundamental question is how to perform this last step of differentiating between benign and malignant samples. One approach is to use FNA data from hundreds of patients that were surgically diagnosed and learn from these how to diagnose future patients based on FNA samples alone. The underlying mathematical problem calls for the development of a discriminant function that separates two sets of points in a high dimensional space. This is a problem that arises in data analysis and pattern recognition problems in many domains, including financial modeling and investment planning, behavioral modeling, and data-driven managerial decision making. Except for certain special cases that are easily solvable, this problem is known to be challenging. With **Hong Ryoo**, we approached the problem based on the hypotheses that it suffices to develop the best possible pair of hyperplanes for separating the experimental data. We then devised a systematic optimization methodology for solving this problem. On a set of approximately 600 clinical FNA samples from the University of Wisconsin Hospital, our methodology yielded 99% correct breast cancer diagnosis. Compared to the 95% accuracy of the best previous techniques, our developments would imply 24 fewer misdiagnosed patients for this small sample alone. This is an important improvement given that millions of patients undergo breast cancer diagnosis every year. A paper on this subject is nearing completion. We plan to extend our methodology to diagnosis of other types of medical conditions as well as prognosis of the long-term behavior of the disease.

Design of Novel, Environmentally Benign Chemicals

Students: **Currently seeking postdoctoral researcher (synthetic chemist)**

Due to concerns regarding the depletion of the ozone layer by chlorofluorocarbon (CFC) refrigerants, extensive research efforts have been directed towards finding environmentally benign CFC replacements. In the mid 1980s, it was proposed that the search for appropriate Freon and other CFC replacements can be approached computationally by using group contribution techniques to predict properties of potentially new compounds. The main question is then how to efficiently search the astronomically large space of all potential group combinations in order to identify the most promising refrigerants.

In work funded by an NSF/Lucent Technologies Industrial Ecology Fellowship, we developed an optimization model and a systematic solution methodology for the Freon replacement search problem. Methyl chloride and other

CFCs used as refrigerants in the past turned out to be some of the solutions of our model. Furthermore, our model was able to identify several *novel* potential alternative refrigerants (compounds that do not appear in chemical databases as well as some that appear but have never been used as refrigerants.) This is the first theoretical approach to propose novel potential refrigerants after finding the *complete* set of solutions to a Freon replacement problem that was open for the last 20 years.

Recently, we extended our approach to the problem of identifying replacements for refrigerants currently used in retail food refrigeration. With funding from the Environmental Protection Agency and the National Science Foundation, we identified over 3000 potential new secondary refrigerants. A paper on this subject is nearing completion. We currently plan to seek to hire a synthetic chemist as a postdoc in order to synthesize and test a carefully select subset of 12 of these compounds.

In the long term, we plan to develop similar computational and experimental techniques for the design of fire suppressants, industrial solvents, polymers, drilling fluids, and drugs with an emphasis on minimizing the environmental impact over the entire life cycle of the new compounds.

Erik Ydstie's Group

Real Time Optimization and Distributed Adaptive Control

Eduardo J. Dozal-Mejorada (Ph.D.)

Wayo (Eduardo) has developed an online optimization technique for unconstrained optimization based on extremum seeking control. The optimization algorithm behaves as a stand-alone module using existing process models to gather information and adaptively drives the process to its extremum without altering the simulation code. The optimizer uses a second order approximation to a high order system and takes a set of modified equality constraints constructed so that they have the same geometric characteristics of the true steady-state behavior of the process. The module employs a dynamic model to obtain a steady-state model of the system. The steady-state model is then used to find the optimal input to the process. The optimum point obtained by the optimizer is tracked throughout process operation. The advantages of this adaptive algorithm over other traditional optimization approaches include: 1) it uses current process models, 2) it can handle multiple objective functions, 3) it only applies a subset of all process states, 4) it self-learning, and, 5) it is appropriate for steady-state or dynamic models. We have developed theoretical convergence and stability results for the exact-matching case and have started working on the robustness problem. Successful implementation has been applied to two case studies: 1) optimization of biomass production in a bioreactor, and, 2) optimization of silicon production in a reactor.

Passivity Based Control of Multi-Phase Reactor Systems

Student: Yuan Xu (Ph.D.)

The focus of this research is on passivity-based control of multiphase systems with reaction transport (diffusion and convection). To study this type of system, a metallurgic process has been chosen involving the carbothermic reduction of aluminum. This process takes carbon and aluminum oxide feed to produce aluminum. Work thus far has included developing a model using MATLAB to describe a variation of this process, as is being created by ALCOA, the world's largest aluminum producer. Proportional control is currently being used to explore the controllability, stability, and sensitivity of the system. Future work will be directed toward interfacing the FACT thermodynamics program with MATLAB via a MEX Interface. This will allow for the model to handle ranges of temperatures and compositions without extra work needed to determine equilibrium constants, activity coefficients, and extent of reactions. Another future improvement will be to incorporate computational blocks using the SIMULINK tools in MATLAB. Not only will this give the model a more "user-friendly" interface, but it will also allow for the exploration of modular simulation, where numerous monolithic simulation blocks can be combined and individually interchanged or altered without major recoding needed to modify the overall model.

Modeling the Vapor Recovery Reactor in Carbothermic Aluminum Production using Multi-Scale Modeling Methods

Student: Mohit Aggarwal (co-supervised with Prof Lee White) (Ph.D.)

Mohit just joined the group in November. He will start out his PhD by developing a model for the vapor recovery section of the carbothermic aluminum process under development by ALCOA. In this process aluminum is produced in a high temperature (2000C) two stage process. A significant amount of aluminum vaporizes from the aluminum reactor and this aluminum must be recovered in a vapor recovery column in order to maximize the production yield and save energy. We will model the primary reaction in the column, the gas flows as well as solid transport. The focus is to develop efficient methods to represent the thermodynamics and the multiphase behavior of the VRR. This work is a continuation of Vianey's modeling work (PhD/PostDoc 2004). Mohit will develop a three phase (liquid/solid/gas) multi-scale, simulation model which will be used for system design, scale-up, economic evaluation and control studies.

Multi-Scale Modeling of Particulate Processes with Fluid Flow

Student: Juan Du

This research addresses modeling and control of yield and size distribution in particulate processes. We use a novel method for solar-grade silicon production, the thermal decomposition of silane gas in a fluidized bed reactor, as a benchmark. We have developed a model and control scheme for the behavior of particles in a fluidized bed reactor based on silicon production. The model simulates growth of silicon particles with ordinary differential and algebraic equations that track particle movement through discrete size intervals. The model solves quickly and is easily tuned to fit experimental data. The passivity-based inventory controller maintains a constant mass of a specified size of silicon particles. The results from this research will be published in Powder Technology.

Last year we have matched the model to pilot-scale process data obtained from Solar Grade Silicon LLC in Moses Lake, Washington. We developed an observer for on-line estimation of process states and parameters. The method allows for estimation of particle size distribution in real time. We have combined the observer based modeling scheme with inventory control for total mass and seed-mass control for on-line stabilization of the particle size distribution. The model and control scheme is being used for scale-up and control system design for production system under current development at SGS. It expected that that when the new process is in operation that it will provide several competitive advantages relative to the current Siemens process, including higher throughput per process unit, lower capital cost and significantly lower energy usage.

Process Networks

Student: Michael Wartman (PhD)

We have introduced a novel modeling framework for studying dynamics, distributed control, and optimization of complex chemical process networks. We are interested in developing distributed control systems that self-organize so that stability and optimality follows as a consequence of how the networks are put together and how they are connected with boundary conditions or other networks. By considering only the topology of the system, basic conservation principles and the second law of thermodynamics we have developed a multi-component analog to Tellegen's Theorem of electrical circuit theory. This result has been combined with the passivity theory of nonlinear control. It is shown that under certain convexity conditions the network converges to a stationary solution. Under similar conditions, it is shown that the network is self-optimizing in that the entropy production is minimized.

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