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CAST Communications - Winter 2009-10

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Editorial Notes

by Karl Schnelle and Peter Rony

Welcome to the 13th online issue of *CAST Communications*. In this issue, we publish three papers from the recent annual AIChE meeting, a presentation from our new 2010 AIChE President, and the CAST Division Award lecture given at the CAST banquet in Nashville. The CAST Division Award winners were announced at the banquet before the lecture, so we also have several photos in this issue. If you did not make it to the 2009 annual meeting, then hopefully these articles will help you stay in touch.

As a result of the last issue of *CAST Communications*, the very first Chair of CAST sent the Editors copies of all the original Division documents. We have archived them for posterity in...

"**The Vern Sterba Archive**":

1974_MCC_Annual_Report
1975_MCC_Annual_Report
1976_07_23_HO_to_RLM
1976_10_05_CHW_to_RLM
1976_10_08_KDT_to_VJS
1976_10_08_RLM_to_FJvA
1976_10_19_RLM_to_FormationComm
1976_11_04_RLM_to_AIChE_Council
1976_11_24_RLM_to_AIChE_Council
1976_12_07_RLM_to_VJS
1976_MCC_Annual_Report
1977-1979_MCC(CAST)Meetings
1977_01_06_VJS_to_Officers_OPlan
1977_01_13_WDS_to_VJS_Budget
1977_01_25_RLM_to_CCN_etal
1977_01_28_RLM_to_VJS_status_rpt
1977_02_08_VJS_to_FJvA_Objective
1977_02_28_RLM_to_FormComm_Mtg
1977_03_05_VJS_to_RLM
1977_03_17_HSO_to_VJS_survey
1977_03_25_RLM_to_FJvA_June_Agen
1977_03_25_RLM_to_VJS
1977_03_Bylaws
1977_03_Houston_Council_excerpt
1977_04_25_RLM_to_Council
1977_04_28_FJvA_to_RLM
1977_05_RLM_to_MCC(Ballot)
1977_06_03_HSO_to_FJvA
1977_06_05_Council_Minutes(part)
1977_07_14_AVC_Liaison_Letter
1977_09_15_RLM_to_CAST_Exec_Comm
1977_10_11_RJL_to_RLM
1977_10_14_AVC_Liaison_Letter
1977_11_21_RLM_to_ASW
1977_MCC_Annual_Report
1978_03_02_VJS_to_CAST_Exec_Comm
1978_03_02_VJS_to_RH_Membership
1978_CAST_Div_Objectives
1985_12_08_EMR_to_Past_ExecBoard

And the Quote of the Day is attributed to Richard Feynman.

Articles

NOTE: The following three presentations were recently given at the CAST Plenary Session at the 2009 Annual Meeting of AIChE in Nashville.

Smart Manufacturing – Using Automation to Lower Production Costs

by Pete Sharpe, Emerson Process Management, Glen Allen, VA

Smart Manufacturing combines people, technology and processes to optimize performance and anticipate plant problems before they occur. Automation plays an important role as an enabling technology to achieve Smart Manufacturing goals. Intelligent field sensors not only monitor their own health, but can apply sophisticated statistical algorithms to detect changes in the process that indicate impending problems. Advanced process control technology can operate processes at minimum cost, more safely, consistently and reliably than a board operator. This paper will use industrial examples to illustrate how

companies have used automation technology to improve their manufacturing operations and the actual results achieved.
pdf [2MB]

Comparison of Sampling Strategies for Kriging-Based Reduced-Order Models of Nanoparticle Dynamics
by Andres F. Hernandez and Martha Grover, Department of Chemical and Biomolecular Engineering, Georgia Tech

The task of identifying an empirical model is difficult for nonlinear dynamic systems, especially when the sampled data is limited, expensive or noisy. Since an empirical model is based on sampled data, the choice of samples taken plays an important role in the prediction and accuracy of the resulting model. This is particularly true in nonlinear systems when the functional form of the empirical model is not known a priori. Here we consider the effect that sampling strategies have in a regression-based reduced order model to describe a nonlinear system. Here we apply our approach to nanoparticle dynamics. One of the the most challenging problems in nanoparticle synthesis is the control over particle size and distribution, while sustaining a high yield of the process [1]. Platinum nanoparticles are needed for catalysts in fuel cells and for drug delivery, and a monodisperse size distribution is required for these applications. This nanoscale process can be simulated using a kinetic Monte-Carlo (kMC) method, based on a stochastic model that represents the sequence of chemical reactions to synthesize platinum nanoparticles on carbon nanotubes.

Because of the high computational demands of the kMC simulations, an approximated model is needed for engineering tasks like process optimization and control. A new methodology to create approximate models for multivariate stochastic dynamic simulations is employed here, using simulated stochastic data sampled from the kMC simulations. The methodology is based on kriging [2], a statistical technique—coming from geostatistics—that interpolates the value of a random field at an unobserved location, using observations of its value at nearby locations. We combine kriging with model reduction techniques to create a reduced state for the kMC simulation data.

We compare sampling strategies for building and refining an approximated model for stochastic dynamic simulations. Specifically, we compare a sequential design of computer experiments, guided by the mean squared prediction error of the kriging model, to a uniform sampling strategy. This work describes the impact of this additional sampling in the performance of the approximated model, for the local and global prediction of the state variables, and contrasts the results with the original kMC simulation. Optimized selection of new sampled data from the kMC simulation can improve the performance of the approximated model, while minimizing the number of sample points and thus the computational time for building the approximated model.
pdf [1.2MB]

References
[1] Y. Zhang and C. Erkey, “Preparation of supported metallic nanoparticles using supercritical fluids: A review,” Journal of Supercritical Fluids, vol. 38, pp. 252–267, 2006.
[2] N. Cressie, Statistics for Spatial Data. Wiley Interscience, 3 ed., 1993.

Scheduling Algorithm for Large-Scale Multiproduct Plants
by Pedro Castro (INETI, Lisbon, Portugal), Iiro Harjunkoski (ABB, Ladenburg, Germany), and Ignacio Grossmann (Carnegie-Mellon University)

The increasingly large literature in the scheduling field highlights the successful application of optimization approaches to a wide variety of challenging problems (Méndez et al., CCE 2006, 30, 913). This important achievement comes from the remarkable advances in modeling techniques, algorithmic methods and computational technologies that have been made in the last decade or so. However, there is still a significant gap between theory and practice. Academic developments are mostly tested on relatively small problems whereas real-world applications consist of hundreds of batches, dozens of pieces of equipment and long scheduling horizons. In order to make exact methods mode attractive, efforts have been increasingly oriented towards the development of systematic techniques that allow maintaining the number of decisions at a reasonable level. Manageable model sizes may be obtained by applying heuristic model reduction methods, decomposition or aggregation techniques. Once an initial solution is generated, gradual improvement through optimization based methods can be obtained with modest computational effort. Although these can no longer guarantee optimality, this may not be critical in practice due to the following: (i) very short time is available to generate a solution; (ii) theoretical optimality easily gets lost due to the dynamic nature of industrial environments; (iii) implementing the schedule as such is often limited by the real process; (iv) only a subset of the actual scheduling goals are taken into account.

The purpose of this paper is to systematically address the short-term scheduling of multistage batch plants with parallel units following the decision, for each particular product, of the number and size of batches to produce; resulting in a set of orders with fixed processing times and release/due dates. A complex algorithm is proposed that can be parameterized for the fast and efficient solution of problems of varying size. The key idea is essentially the one proposed by Röslof et al. (CCE 2001, 25, 821) and further explored by Méndez and Cerdá (CCE 2003, 27, 1247). The complete set of orders is scheduled sequentially by considering one, or a couple of them, at a time. As we proceed through the iterations, previously scheduled orders can be partly rescheduled to allow for some flexibility while keeping the combinatorial complexity at a manageable level. Once a complete schedule is obtained, the same concept is applied to improve the schedule locally.

The novel aspects are: (i) the use of a multiple time grid continuous-time model instead of one based on sequencing variables; (ii) the decomposition strategy specifies on each iteration the minimum number of time slots in the grid for the unit-specific model, thus removing the uncertainty in the specification of this parameter; (iii) the introduction of an intermediate level of complexity between the full-space problem and the option of fixing both the order-unit assignments and relative ordering of previously scheduled orders.

The results show that the fixed relative ordering strategy is a better option than its free ordering counterpart, which has a high computational cost. It is able to generate good solutions very rapidly and we were able to tackle a real-life 50-order, 17-unit, 6-stage problem in less than a minute. In terms of the tradeoff between solution quality and total computational effort, the best option is to schedule two orders per iteration. Two alternative preordering heuristics were also evaluated leading to the conclusion that is better to use the minimum slack time (MST) rather than the earliest due date (EDD) heuristic for order-iteration assignment.
pdf [1MB]

Plans for the Coming Year
by Henry T (Hank) Kohlbrand, 2010 President

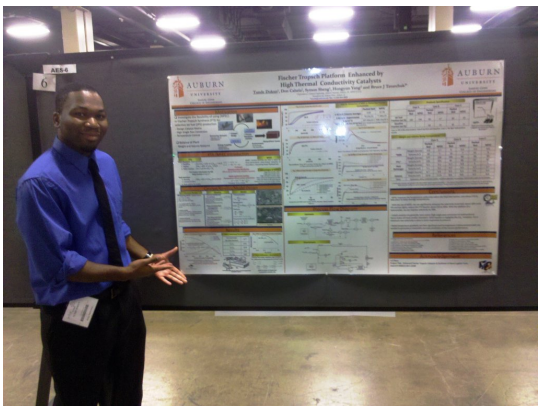
NOTE: The following presentation was given at the 2010 AIChE Annual Business Meeting, Nashville, TN.

Goals for AIChE in 2010 include: increasing professional membership, providing greater value for members, and improving understanding of the value AIChE provides. Read the full presentation here [1MB].

Communications

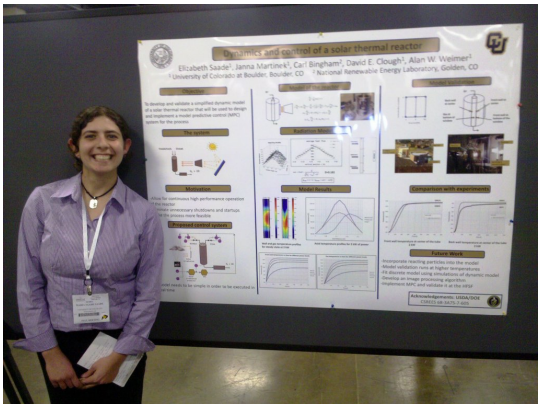
2009 CAST Directors' Award
By Martha Grover

Given for the best poster presentations at the AIChE Annual Meeting. The following are for Work Presented at the 2009 AIChE Annual Meeting in Nashville, TN.



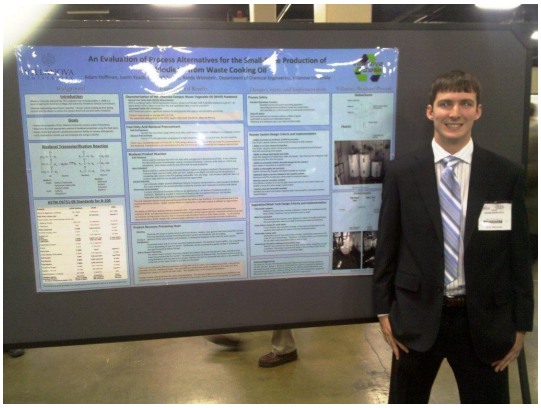
The winner of the Directors' Award is:

Tunde Dokun (with Don Cahela, Symon Sheng, Hongyun Yang, Bruce Tatarchuk), Auburn University, "Fischer Tropsch: Applied Mathematics and Numerical Analysis to Determine Reactor Temperature Profile"



The judges also decided to give two Honorable Mentions:

Elizabeth Saade (with David Clough, Alan Weimer), University of Colorado at Boulder, "Dynamics and Control of a Solar Thermal Reactor"



Adam Hoffman, (with Justin Yeash, Kenneth Muske, Randy Weinstein), Villanova University, "An Evaluation of Process Alternatives for the Small-Scale Production of Biodiesel From Waste Cooking Oil"

2009 CAST Award Winners
by Peter Rony

NOTE: The 2009 CAST Division Awards were announced previously - details are here [].

Venkat Venkatasubramanian is the recipient of the 2009 CAST Computing in Chemical Engineering Award

For his (a) innovative advances in abnormal-events management, (b) automated hazard and operability analysis, (c) rational approaches to molecular product design, and (d) informatics-based systems for pharmaceutical product development, Purdue Professor of Chemical Engineering Venkat Venkatasubramanian has been selected as the recipient of the 2009 CAST Computing in Chemical Engineering Award.

We now provide selected quotes from the supporting letters on behalf of Venkat:

“Venkat has made the use of AI techniques in chemical engineering a main theme of his research. If I were asked who is the leader in AI and its application to chemical engineering, I would put Venkat and George Stephanopoulos (winner of this award already) at the top of that list.”

“I saw and was impressed with his presentation entitled "Computer-aided Molecular Design Using Genetic Algorithms" at FOCAPD the late 1990s. He found an ideal application for genetic algorithms, and, as far as I am aware, was the first to approach the problem in this manner. His example problems convinced me that the method was commercially useful. The subsequent invitations and recognitions he has received for this work strongly support his being a highly recognized leader on this topic.”

“His papers are among the most cited ones in Process Systems Engineering. He has also been a linchpin with Rex Reklaitis and Joe Pekny in the Purdue University research consortium CIPAC (Center for Integrated Process Operations), which is one of the five outstanding research centers in process systems in the world.”

“Automated hazard and operability analysis: Venkat and his co-workers have developed novel knowledge-based systems, called HAZOPExpert, Batch HAZOPExpert, and PHASuite for automating HAZOP analysis. This work has been received with great enthusiasm by leading practitioners of HAZOP analysis in the industry. The Batch HAZOPExpert is regarded as the Irrst, and currently the only. intelligent system that is being used for process hazards analysis in an actual industrial environment. Also in this area, his papers on process safety analysis are among the most frequently cited.”

“Synthesis of operating procedures for batch plants: Venkat and his co-workers have developed an intelligent systems framework in which operating procedures are developed from information about the plant setup, process chemistry and recipe, and product properties and requirements. An intelligent system called iTOPS (Intelligent Tool for Operating Procedures Synthesis) has been success fully tested on industrial case studies and could be regarded as the first intelligent system that was used for operating procedure synthesis in an actual industrial environment. 1udging by the number of publications and invited conference presentationa, it can be stated that Venkat's contributions in the area of process fault diagnosis and safety have been well rccojnized in the process engineering community and he is regarded as one of the experts.”

“Pharmaceutical informatics: This is a new area of research that Venk:at has recently established and currently involved with. The objective is to develop the ontological informatics infrastructure for the modelling, analysis and optimization of the pharmaceutical products discovery-to-delivery pipeline, called Pharmaceutical Informatics. Already from the initial publicationa, the research has attracted a lot of attention as well as funding for several collaboration projects.”

“Rational framework for molecular products design and engineering: Venkat and his research group have pioneered the development of a novel, rational, model-driven framework called Discovery Informatics. This integrated framework enables the management of complexity, accumulation of knowledge, systematic hypotheses testing by interaction with experiments, and efficient search for new materials with desired performance characteristics. Again, his research has made a significant impact and he is recognized as one of the leading international experts in this area.”

“In connection with this research, Venkat has played a leading role in preparing teaching materials and in organizing research conferences. Most notably, he authored a three-volume series on *Knowledge-Based Systems in Process Engineering: Case Studies in Heuristic Classification* and coauthored a monograph on *Advanced Reasoning Architectures for Expert Systems*, all distributed to the universities and industry by the CACHE Corporation. Furthermore, Venkat was one of the three co-chairs of the first Intelligent Systems in Process Engineering (lSPE'95) Conference. Subsequently, in recognition of his leading role, Venkat was elected Vice President of the CACHE (Computer Aids for Chemical Engineering Education) Corporation. He served as president of CACHE in 2003-2004.”

“Two features of his work especially support his receiving the CAST Award:

- His approach and techniques are well grounded in theory, hence his methods are general and can be ported to practical problems;
- He has developed software that is effective for large-scale problems.”

“He was the first to develop educational material to use in teaching AI techniques to undergraduate students.”

"Keep things as simple as possible, but no simpler", believes Brian J. Froisy, the 2009 CAST Computing Practice Award winner

For a career of outstanding project management and technical development of advanced process control computing technology including IDCOM-M, SMCA, and the AspenONE State Space Controller, J. Brian Froisy, retired director of technology at Aspen Technology, Inc., is the recipient of the 2009 CAST Computing Practice award.

Given below are comments from the nominator and one of the supporting letters:

“He made a point of communicating current technology problems to researchers and supported development of solutions. He did this by presenting research talks at numerous conferences including CPC meetings, AIChE meetings, and American Control Conferences. He was an excellent communicator and careful listener, and he encouraged a generation of young academic MPC researchers.”

“Brian's largest impact on control technology is likely the recent SSC advanced control product at Aspentech. This successful development represents many years of hard work and gifted leadership on Brian's part. Brian carefully recruited a small development team and was tireless in maintaining management support for the project. He also contributed technical solutions to problems that arose in the inevitable gap between existing theory and practical application. Many of these contributions are documented in the paper accompanying his invited lecture at the 2006 CPC 7 meeting [1]. As Brian

described the project: A major objective was to develop an MPC environment, not just a controller, to enable engineers without formal control theory training to efficiently build, deploy and maintain control applications. This included the objective that the environment would be suited to a wide range of control problems, especially in industries where the benefits of MPC have not been fully realized."

"Because successful control vendor technology is leveraged across a wide array of companies and industries, Brian's impact in this successful deployment of new technology will be felt for many years to come."

"Brian is, first and foremost, a technical innovator. Time and again, he has taken a promising idea from the process control literature and reduced it to practice. His motto is 'keep things as simple as possible, but no simpler'."

[1] Froisy, J. B. *Model predictive control - building a bridge between theory and practice*, **Comput. Chem. Eng.**, 30: 1426-1435, September 2006.

Daniel R. Lewin is the recipient of the 2009 David Himmelblau Award for Innovations in Computer-Based Engineering Education

For developing a novel multimedia package that teaches the use of computer process simulators (ASPEN, HYSYS, MATLAB) to students and practitioners worldwide – in encyclopedia and tutorial formats, Professor Daniel R. Lewin, of the Department of Chemical Engineering at the Technion, Israel Institute of Technology, received the David Himmelblau Award for Innovations in Computer-Based Chemical Engineering Education at the CAST Division awards banquet in Nashville.

The nomination statement for Professor Lewin includes the following paragraphs:

"Since 1998, Danny has led the development and distribution of the Wiley CD-ROM product, *Using Process Simulators in Chemical Engineering: A Multimedia Guide for the Core Curriculum* (Lewin et al., 2003). This CD-ROM has been distributed as a separate product by Wiley – as well as included with every copy of the second edition of the textbook, *Product and Process Design Principles: Synthesis, Analysis, and Evaluation* (Seider, Seader, Lewin, 2004). Since January 2009, thanks to increased bandwidth, it has become available for downloading from the Wiley web site associated with the third edition of this textbook."

"Using the authorware, MACROMEDIA DIRECTOR, multimedia material was generated for self-paced instruction on the usage of the major process simulators, ASPEN PLUS and HYSYS, and on basic concepts in the usage of MATLAB. Sequences of instructional materials were generated using text frames, animations, and frames displayed by the simulators, often narrated by voice and accompanied by videos of the industrial processing equipment. These were presented in DIRECTOR movies that are easily navigated by the students. Furthermore, to facilitate the usage by inexperienced students, Danny introduced two interconnected formats: (a) an encyclopedia-like source of reference materials on several subjects (e.g., Principles of Process Flow sheet Simulation, Separators, Heat Exchangers, Chemical Reactors, …), delivered on many subtopics in the form of instructional modules, and (b) as a series of tutorials that are used in a self-paced fashion (e.g., under Material and Energy Balances, tutorials on Ammonia/Water Separation and Ethyl chloride Manufacture). Materials under (b) are provided to accompany the core courses in Material and Energy Balances, Thermodynamics, Heat Transfer, Separations, Reactor Design, and Process Design."

"On three occasions, at the ASEE Summer Schools for Chemical Engineering Faculty (2002 and 2007) and at the Austin Meeting of AIChE (Nov. 2004), Danny and Warren Seider conducted hands-on workshops on teaching process design using the multimedia materials. Following his lead at the Technion, he recommended that students be introduced to problem-solving using the process simulators in a one-credit, computer-lab course at the junior level, either following or in parallel with many of the core courses in the chemical engineering curriculum. ..."

"In summary, over the past decade, Professor Daniel Lewin has led the development of a novel multimedia package for teaching the use of the computer simulators. Beginning in the late 1990s, this package was one of the first to use animation, voice, and video – in encyclopedia and tutorial formats – to provide detailed instructions for inexperienced users. Students have used it successfully at their own pace and have required relatively little assistance from their instructors and teaching assistants. In my view, Danny's multimedia package is an excellent example of the use of computers to improve chemical engineering education. In some respects, this package is comparable, to the extensive set of educational modules introduced by Professor David Himmelblau in his CACHE Project in the earlier 1980s. For all of these reasons, in my opinion, Danny is an excellent candidate to receive the first Himmelblau Award."

Yiannis N. Kaznessis is selected as the 2009 CAST Outstanding Young Investigator Award winner

Yiannis N. Kaznessis, Associate Professor at the University of Minnesota, has been selected as the 2009 CAST Outstanding Young Investigator recipient, *for pioneering contributions in computational and mathematical biology aiming at unraveling the connection between living organisms and chemical thermodynamic principles.*

According to the Qualifications statement: "Kaznessis is trying to tackle the biggest question in the biosciences: how does life emerge from a soup of chemicals? Phrased differently, can we develop mathematical models based on physical laws that explain and reduce biological phenotypes to interacting molecules? What distinguishes Kaznessis' efforts from other engineers who successfully employ mathematics to study biological systems is the focus on statistical mechanical interpretations of systems away from the thermodynamic limit. Kaznessis is thus developing mathematical descriptions that span multiple levels of organization from molecules, to their pairwise interactions, to networks of biomolecular dynamics, to cellular phenotypic complexity"

"He has explored the relationship between the sequence, the structure and the function of biomolecules. He is developing novel methods and successfully applying them primarily to antimicrobial peptides. These are small molecules that are potent antibiotic agents. These efforts are supported by a competitive R01 grant from the US National Institutes of Health. What is worth noting here is that Kaznessis always builds the necessary collaborations with wet lab groups. Currently he is on sabbatical spending time at Robert Lehrer's group in the Medical School at UCLA, learning biochemistry techniques."

"A recent example, illustrative of the quality of the work, is the manuscript published in PLoS Computational Biology with the title "Poisson-Nernst-Planck Models of Nonequilibrium Ion Electrodiffusion through a Protegrin Transmembrane Pore" (Open Web Access, 2009). In this work, the first multiscale theoretical treatment is presented of an antimicrobial pore. This model reveals the timeline of molecular phenomena that give rise to the bactericidal

phenotype: it captures the molecular interactions of peptide binding on bacterial membranes, the formation of pores, the resulting diffusion of ions and the final, irreversible collapse of the transmembrane potential. The models thus capture the biophysical events that ultimately result in cell death. This is the type of understanding, not available by experimental techniques alone, required for rational engineering of novel antimicrobial peptides."

"Kaznessis is also exploring the principles that determine the strength of pair-wise interaction between biomolecules. From peptide-lipid to protein-ligand and protein-protein interactions, Kaznessis is pioneering the development of statistical mechanical methods that shed light in the energetics of interactions. Kaznessis and his group have been collaborating with Dr. John Lambris in the Medical School at the University of Pennsylvania."

"Last but not least, Kaznessis is studying the mathematical rules that dictate the behavior of gene regulatory networks. Biological systems are on occasion not at the thermodynamic limit. Stochasticity can take hold then, rendering traditional methods for modeling reaction kinetics false."

Eric Haseltine, winner of the 2009 W. David Smith, Jr. Graduate Publication Award, has made an impact at an early stage in his career

For outstanding contributions in extending the tools of chemical reaction engineering to the molecular level, Eric L. Haseltine, previously a postdoctoral fellow at Caltech, will receive the 2009 W. David Smith Jr. Graduate Publication Award at the CAST Division banquet associated with the 2009 Nashville AIChE meeting.

Because of problems with the PDF pages submitted by the primary sponsor of Dr. Haseltine, we are writing this story based upon the supporting letters.

"It is a real pleasure for me to write this letter enthusiastically supporting the candidacy of Dr. Eric Haseltine (of Vertex Pharmaceuticals) for the CAST W. David Smith, Jr. Graduate Publication Award. The nominated paper, *Approximate Simulation of Coupled Fast and Slow Reactions for Stochastic Chemical Kinetics*, **J. Chem. Phys.** 117(15) pp.6959-6969 (2002), contains a vital contribution to the atomistic modeling of chemical reactions: a real breakthrough in critically extending the "traditional" chemical reaction engineering tools of the partial equilibrium / quasi-steady state approximation assumptions to the realm of molecular level stochastic reactive simulations. This powerful extension of the ideas and tools of separation of time scales and singular perturbation to the realm of atomistic simulation also has a significant impact beyond chemically and biochemically reactive simulations to comparably modeled interdisciplinary problems such as the crystallization example in the paper."

"The nominated paper is (and will continue to be) a very influential one, as its citation record amply demonstrates; it contains a truly lucid discussion of the need for the techniques it develops: the partitioning of the processes involved into fast and slow ones and the approximations involved in dealing with the fast reactions in either a stochastic (Langevin) or a deterministic way. The paper also provides an approximate simulation to master equations subject to time-varying constraints. The critical analysis of the stochastic approximations shows a depth and clarity that makes the paper a real pleasure to read. The work is remarkable in that it contributes to the mathematics and to the development of good approximation algorithms for a large class of models, while at the same time significantly advancing reaction engineering concepts and opening the way for the efficient stochastic simulation of many interesting applications. The viral infection example successfully treated in it is representative of a truly wide class of practically important multiscale biochemical phenomena that the approach makes significantly more tractable."

"... The paper addresses the important situation when the stochastic nature of reactions at small scales cannot be ignored and conventional methods for model reduction are inadequate. Such situations are commonly encountered in fields such as systems biology, where Eric's work has been eliciting significant interest and is highly cited. This work is an excellent example of the types of contribution that process systems engineering and computing technology can make in emerging fields. More importantly, it demonstrates the high quality of Eric's research and his worthiness for this award."

"This paper is well on its way to becoming a classic. I am not aware of many members of our community—young or not-so-young—who have already made such an impact at such an early stage in their careers."

Award Lecture Introduction
by B. Wayne Bequette, 2006 CAST Chair

Computing in Chemical Engineering Award - *Recognizes outstanding contributions in the application of computing and systems technology to chemical engineering*

The introduction [2MB] to the attendees of the 2009 CAST Awards Dinner in Nashville may be downloaded in pdf format.

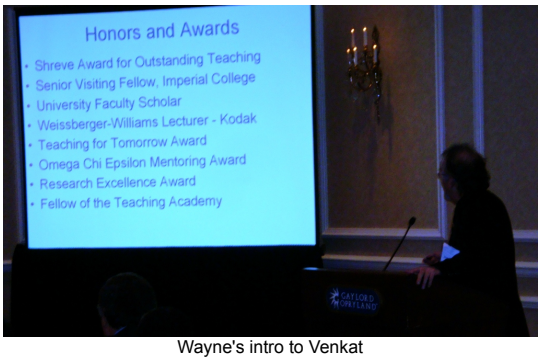
[*www.eng.rpi.edu*]

2009 Computing in Chemical Engineering Award Lecture
by Venkat Venkatasubramanian, Purdue University

In his award talk given at the 2009 CAST Awards Dinner in Nashville, Venkat quoted his favorite poet, Robert Frost. Thus, his presentation was entitled The Road Less Traveled By: Adventures in Process Systems Engineering.
[1.1MB].

Photos from the 2009 CAST Awards Dinner
taken by Mahmoud El-Halwagi, CAST Second Vice-Chair

Venkat receiving award from Mahmoud [Credit: KDS]



Wayne's intro to Venkat

Travel Grant Winners and Ray Adom

Daniel Lewin video clip for the Himmelbalu award

Warren Seider receives award on behalf of Lewin

W. D. Smith best paper award to Eric H

Brian Froisy receives practice award

Yiannis Kaznessis receives young award from Marianthi and Martha

2008 poster award to Chris Rao (pictured) a

Frank receiving plaque of appreciation as outgoing CAST Chair [Credit: KDS]

CAST Election Results

by Karl Schnelle, CAST Secretary

The CAST elections committee is pleased to announce the results of the election of officers for 2010.

Please join us in congratulating our *three* new Directors. Two Directors are normally elected per year to serve a two year term. However, continuing the tradition from last year, we had a dead heat for Director so we are announcing one additional Director for 2011-13. (Last year, we had a tie for Second Chair, so no election for this position was held this year.

2010-2012 DIRECTOR: Thomas A. Badgwell

Thomas A. (Tom) Badgwell Ph.D., P.E., is a Staff Engineer at the ExxonMobil Baytown refinery and an Associate Adjunct Professor at Rice University. He received a BS degree in Chemical Engineering from Rice University and MS and PhD degrees from the University of Texas at Austin. Tom's career has focused on modeling, optimization, and control of chemical processes, with past positions at Setpoint, Fisher/Rosemount, Rice University, and Aspen Technology.

Tom has been an active member of AIChE and the process control community since 1982, serving on the Board of the local South Texas Section, chairing many CAST10b sessions at Annual Meetings, serving as CAST10b Program Coordinator, and more recently, co-chairing the CPC7 meeting with Professor Mike Henson.

[www.isr.umd.edu]

2010-2012 DIRECTOR: Ray Adomaitis

Ray Adomaitis is a professor in the Chemical and Biomolecular Engineering Department of the University of Maryland. He received his BS and PhD in Chemical Engineering, both from the Illinois Institute of Technology. He was a postdoctoral research associate at Princeton University starting in 1988 and in 1990, moved to the University of Maryland as a postdoctoral fellow at the Systems Research Institute. In 1995 he joined the ChE department of Maryland, and has since held a joint appointment in Chemical Engineering and the Institute for Systems Research. He also belongs to the Maryland Nanocenter and the University of Maryland Energy Research Center. His work focuses on developing mathematical models of the chemical reactors used for thin-film manufacturing processes. His research is split between theory and computations, experimental work, and collaboration with industrial partners. The applications include solar energy, microelectronics, and nanomanufacturing processes.

Ray is active in both CAST and the National Capital Section (NCS) of the AIChE. Ray moderates the CAST listserv, is the chair of the graduate travel grant program, and has served as the 10d program chair. He has served as the NCS secretary for the past 10 years and also maintains the NCS listserv.

2011-2013 DIRECTOR: Matt Bassett

I received a BS in Chemical Engineering from Drexel University in 1992 and a PhD in Chemical Engineering from Purdue University in 1996. My thesis was on scheduling of large-scale batch production facilities using math programming-based optimization techniques. I have been a member of the Global Ag Math Modeling and Analysis (GAMMA) group at Dow AgroSciences (DAS) since joining the company after graduate school. Throughout my career, I have developed and applied quantitative decision-making models within numerous functions throughout DAS. Some areas of focus include mixed integer linear programming, discrete event and Monte Carlo simulation, options analysis, as well as Excel and Access development.

I have been very involved in AIChE, CAST, and PSE related activities over the years. I have chaired or co-chaired many CAST-sponsored sessions in addition to serving as the Area 10C Programming Coordinator for the 2006 Annual Meeting. I served on the General Arrangements Committee as well as the Plant Tour Committee for the planning of the 2002 Annual Meeting in Indianapolis. For FOCAPO 2003, I served on the Industrial Advisory Committee, and I was a member of the International Program Committee for ESCAPE-16 / PSE'2006. Most recently, I chaired the successful FOCAPO 2008 conference in Boston.

Although I have not yet held an executive position within CAST, I have performed a number of duties supporting the Division. These include: web-page coordinator for www.castdiv.org, judge for the CAST Director's Award, and regular attendance at executive committee meetings. As a Director of the CAST Division, I plan to continue my current involvement as well as step up my engagement in the areas of growth and fiscal responsibility. For growth, I believe we need to develop a comprehensive strategy for conveying why CAST exists and presenting this in such a way as to grow the membership. There has been a group looking at the "value proposition" for CAST and we need to focus on this at the Executive Committee level. As for fiscal responsibility, one of the first things that I will stress is the need for all CAST Awards to be fully sponsored by 3rd parties. Also, we need to make sure that when we do spend money, we are doing so with an eye to increasing visibility for the Division. WebCASTs and travel grants are great examples of efforts that should be supported by the Division.

Student Travel Grants
by Ray Adomaitis

Please congratulate the following individuals for winning the third annual CAST Travel Grant (for attending the 2009 AIChE Annual Meeting):

Melissa St. Amand, Matthew Colvin, Sebastian Terrazas-Moreno, Charles Solvason, and Zukui Li

Nominations are due August 1st for the 2010 grants.

Announcements

How to Contact AIChE

Publication sales, meeting registration, applications for membership, technical training, and other AIChE products and services may be obtained by visiting AIChE Contacts or using the On-line contact form.

For answers to specific questions, try one of the following AIChE Staff:

Felicia Guglielmi Director, Volunteer and Membership Activities	Bette Lawler Director, Operations
Joseph Cramer Director, Technical Programming	Steve Smith Director, Technical Activities and Publications

CAST10 E-Mail List

The following websites are used to participate in the list:

1. listserv.umd.edu/archives/cast10.html is the link that subscribers can use to read and post emails.
2. www.ench.umd.edu/cast10/ has lots of archived emails.

The address to post messages to the list is CAST10 at LISTSERV.UMD.EDU .

2010 Award Nomination Form

Please use the 2009 Award Nomination Form [52KB, MS Word], which should be completed by April 15, 2010. See CAST Division Awards for submission guidelines. Electronic submissions are encouraged.

Quote of the Day

Philosophy of science is about as useful to scientists as ornithology is to birds. --- attributed to Richard Feynman (1918–1988)

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Deadlines:	December 1 for the Winter issue; July 1 for the Summer issue.
Payment Details:	Prior to publication of advertisement, please submit check payable to CAST Division, AIChE to the CAST Division Secretary/Treasurer
Questions:	Peter R. Rony, Telephone (540) 951-2805

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The Computing and Systems Technology (CAST) Division of AIChE is responsible for the wide range of activities within AIChE that involve the application of computers and mathematics to chemical engineering problems including process design, process control, operations, and applied mathematics. We arrange technical sessions at AIChE Meetings, organize special conferences, and publish this newsletter - *CAST Communications* - twice a year. These activities enable our members to keep abreast of the rapidly changing fields of computing and system technology. The cost is $10 per year, and includes a subscription to this newsletter. Shouldn't you join the CAST Division now?

To join the CAST Division, please contact AIChE.
