

CAST Division Newsletter

Spring 2017

Contents

Student Awards at the 2016 Annual Meeting.....	1
Meet the new CAST officers.....	2
Introducing CAST's first Social Media Chair.....	4
Recap of the 2016 CAST Awards Banquet at the AIChE Annual Meeting	5
2016 CAST Division Awards	6
Tributes to Professor Floudas.....	9

Student Awards at the 2016 Annual Meeting

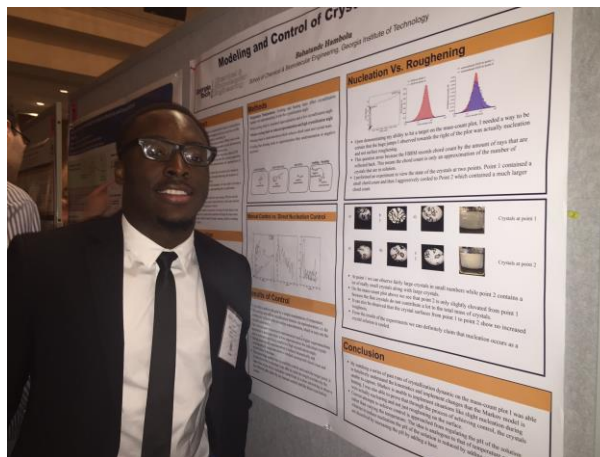
This year CAST participated in the **Undergraduate Student Poster Competition**. The 20 submissions to the “Computing and Process Control” Topical Area were judged by CAST officers. CAST gave awards for the first (\$100) and second (\$50) place posters.

- First place: **Peter Tancini**, University of Pittsburgh, *Understanding Water Effects in Alcohol Dehydration Activity on gamma-Al₂O₃ Using Microkinetic Modeling*
- Second prize: **Babatunde Hambolu**, Georgia Institute of Technology, *Modeling and Control of Crystallization Kinetics*

First prize: **Peter Tancini**



Second prize: **Babatunde Hambolu**



In 2016, for the first time, CAST held a [single session](#) for the eight Graduate Student Presentation Award Finalists on Sunday afternoon at the Annual Meeting. The finalists

were Brandon Corbett, Markus Drouven, Omar Guerra, Nikolaos Lappas, Yu Luo, Richard Pattison, Joel Paulson, and Michael Zachar.

The winner of the **Graduate Student Presentation Award, for the best oral presentation at the 2016 Annual Meeting**, is:

Nikolaos Lappas at Carnegie Mellon University for his presentation “[A Theoretical and Computational Study of Continuous-Time Process Scheduling Models in the Context of Adjustable Robust Optimization](#)”.

The winner of the **2016 CAST Director's Poster Award** is:

Ian Moskowitz at University of Pennsylvania (and currently Air Liquide) for his poster “[Understanding Rare Safety and Reliability Events Using Transition Path Sampling](#)”

CAST worked with the AIChE this year to develop a website showcasing the slides from the 2016 AIChE Rapid Fire Presentations:

<http://www.aiche.org/conferences/aiche-annual-meeting/2016/cast-division-rapid-fire-presentations>

There's a lot of really nice work there, so check it out! We're also thinking to continue this next year, so feedback is very welcome (contact [Ruth Misener](#)).

Congratulations to all the student winners!

Meet the new CAST officers

Our newest CAST officers include the 2019 CAST Programming Coordinators, as well as two new directors and the new Second Vice President. [2019 CAST Programming Coordinators](#)

10a: Faruque Hasan	Texas A&M University
10b: Victor Zavala	University of Wisconsin
10c: Pieter Schmal	Process Systems Enterprise
10d: Yash Puranik	Rockwell Automation
10e: Fani Boukouvala	Georgia Institute of Technology

2017-2019 Directors: Michael Baldea and Benoit Chachuat

Michael Baldea is Assistant Professor and Frank A. Liddell, Jr. Centennial Fellow in the McKetta Department of Chemical Engineering and a core faculty member in the Institute for Computational Engineering and Sciences (ICES) at The University of Texas at Austin. He received his Diploma (2000) and M.Sc. degree (2001) in Chemical Engineering from "Babes-Bolyai" University in Cluj-Napoca, Romania and obtained a Ph.D. in Chemical Engineering from the University of Minnesota in 2006. Prior to joining The University of Texas, he held an industrial research position at Praxair Technology Center in



Tonawanda, NY. He has received several research and service awards, including the NSF CAREER award, the Moncrief Grand Challenges Award, the Model-Based Innovation Prize from Process Systems Enterprise and the Best Referee Award from the Journal of Process Control. His research interests include the design, control and optimal operation of process and energy systems, areas in which he has co-authored one book, four book chapters and over 90 peer-reviewed journal and conference articles.

Benoit Chachuat is a Reader in the Department of Chemical Engineering at Imperial College London and an executive member of the Centre for Process Systems Engineering (CPSE). He has 15-year experience in process simulation and optimization technology. His background includes a PhD in Chemical Engineering from INPL, France (2001), followed by several post-doctoral positions at INRIA Sophia-Antipolis (2002-2003), MIT (2003-2005), and EPFL (2005-2008). He was an Assistant Professor at McMaster University prior to joining Imperial College in 2010. Benoit's research focuses on the development of new methods and tools for the efficient/reliable optimization and control of complex process systems, for which he won the 2014 Outstanding Young Researcher Award from the CAST division. This theoretical and computational work is motivated by problems encountered in process engineering applications, with a particular focus on energy and environmental systems. Benoit is serving as an Associate Editor for the Journal of Process Control and the Journal of Optimization Theory & Applications. He has been a Program Coordinator for Area 10d of CAST for 2016 and he has chaired numerous CAST sessions at AIChE meetings as part of his volunteer leadership.



Second Vice-President: Christos Maravelias

Christos Maravelias obtained his Diploma in Chemical Engineering at the National Technical University of Athens (Greece) and an MSc in Operational Research from the London School of Economics (UK). After completing his military service in Greece, he joined Carnegie Mellon University where he completed his doctoral studies under the supervision of Professor Grossmann in 2004. He is now a Vilas Distinguished Achievement Professor and Executive Officer of the Department of Chemical and Biological Engineering at the University of Wisconsin – Madison. His research interests lie in the areas of a) chemical production planning and scheduling; b) supply chain optimization; c) chemical process synthesis and analysis, with a focus on renewable energy systems;



and d) computational methods for novel material discovery. He received an NSF CAREER award, as well as the 2008 David Smith and the 2013 Outstanding Young Researcher awards from CAST. Also, among others, he is the recipient of the 2012 and 2014 Best Paper Award from Computers and Chemical Engineering, and the 2016 *Production and Operations Management Society* (POMS) Applied Research Challenge.

Introducing CAST's first Social Media Chair

Ashlee N. Ford Versypt is an assistant professor in the School of Chemical Engineering at Oklahoma State University. She has earned three degrees in chemical engineering: a B.S. from the University of Oklahoma and an M.S. and a Ph.D. from the University of Illinois at Urbana-Champaign. As an undergraduate student, Prof. Ford Versypt was named the Outstanding Chemical Engineer Senior in the University of Oklahoma College of Engineering and graduated *summa cum laude*. During graduate school, Prof. Ford Versypt was awarded the Department of Energy Computational Science Graduate Fellowship and the National Science Foundation Graduate Research Fellowship. Prof. Ford Versypt spent a summer as a graduate research intern in the Computational Science Center at Brookhaven National Laboratory. In 2013, Prof. Ford Versypt was recognized as the Frederick A. Howes Scholar in Computational Science, which



is awarded annually to a recent alumnus of the DOE Computational Science Graduate Fellowship for outstanding leadership, character, and technical achievement. In 2012-2014, Prof. Ford Versypt was a postdoctoral research associate with Prof. Richard Braatz in the Department of Chemical Engineering at the Massachusetts Institute of Technology. Currently, in addition to her appointment in chemical engineering, she is a member of the Harold Hamm Diabetes Center at the University of Oklahoma Health Sciences Center and the Oklahoma Center for Respiratory Infectious Diseases at OSU. She is active in the AIChE CAST, Education, and Food, Pharmaceutical, & Bioengineering Divisions.

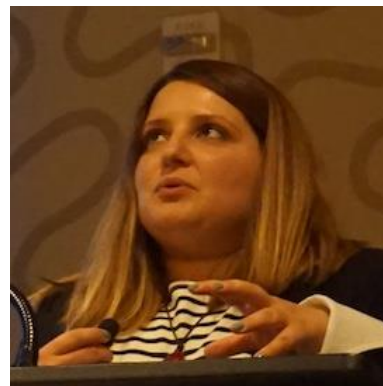
Follow CAST on social media using the handle @AIChECAST10

Twitter: <http://twitter.com/AIChECAST10>

Facebook: <http://www.facebook.com/AIChECAST10/>

Recap of the 2016 CAST Awards Banquet at the AIChE Annual Meeting

The CAST Awards Banquet included a special session remembering Professor Chrisodoulos A. Floudas with remarks by Ruth Misener, Warren Seider, Fani Boukouvala, Yannis Androulakis, Stratos Pistikopoulos, and Ignacio Grossmann.



Professor Floudas passed away of an apparent heart attack on 14 August 2016 while vacationing in Greece with his family. Professor Floudas is survived by his wife, Fotini, and their daughter, Ismini. Born 31 August 1959 in Ioannina, Greece, Professor Floudas earned a Diploma of Chemical Engineering at the Aristotle University of Thessaloniki in 1982, and a PhD in chemical engineering from Carnegie Mellon University in 1986.

Professor Floudas subsequently moved to Princeton University where he served 29 years and, in 2007, was appointed Stephen C. Macaleer '63 Professor in Engineering and Applied Science. In 2015, Professor Floudas moved to Texas A&M University where he was appointed Director of the Texas A&M Energy Institute and Erle Nye '59 Chair Professor for Engineering Excellence at the Artie McFerrin Department of Chemical Engineering.

To name only a few of his accolades, Professor Floudas was a Member of the National Academy of Engineering (2011), a SIAM Fellow (2013), a Thompson Reuters Highly Cited Researcher in two consecutive years (2014, 15), and a Corresponding Member of the Academy of Athens (2015). Professor Floudas was also an outstanding mentor and teacher. In 2007, he became the first recipient of Princeton University's (now annual) Graduate Mentoring Award; recognition for his teaching includes the Princeton University Engineering Council Teaching Award (1995) and the Aspen Tech Excellence in Teaching Award (1999). Professor Floudas supervised 35 PhD students to completion and 20 post-doctoral research associates; many of these are now internationally-leading researchers or professors. Eight further PhD students are working on their degrees. Professor Floudas' academic tree is here: <http://titan.engr.tamu.edu/tree/caf/>

Tributes by Professors Ignacio Grossmann and Warren Seider conclude this newsletter. Other tributes from the [Texas A&M Energy Institute](#), [Princeton University](#), [Bryan-College Station Eagle](#), and [SIAM Activity Group on Optimization](#) are available here: <http://titan.engr.tamu.edu>

2016 CAST Division Awards

CAST recognized past chairs Ray Adomaitis (left) and Karl Schnelle (right) for their service.



Student award winners from the 2015 Annual Meeting were also recognized: (left) **Kristen Severson** for her 2015 CAST Directors' Best Poster Award and (right) **Helen Durand** for her 2015 CAST Graduate Student Presentation Award.



The **2016 CAST Division Awards** were recognized at the CAST Banquet.

CAST President Karl Schnelle presented the six award winners with a plaque and an award check. The winners are listed below.

David Himmelblau Award for
Innovations in Computer-Based
Chemical Engineering Education,
Jeffrey Gray

Computing Practice Award,
Leo Chiang



Sponsored by the CACHE Corporation



Sponsored by Aspen Technology Inc. and the
ExxonMobil Chemical Company

W. David Smith, Jr. Graduate Publication Award, **Rebecca Hanes** and **Joseph Scott**



Sponsored by Process Systems Enterprise, Inc.

CAST Outstanding Young Researcher Award, **Alexander Mitsos**

Computing in Chemical Engineering Award, **Marianathi Ieriapetritou**



Sponsored by Air Products and Chemicals, Inc.

Sponsored by the Dow Chemical Company

Marianthi Ieriapetritou, Computing in Chemical Engineering Award Winner, also gave the award [talk](#) entitled “Twenty years of PSE research: A book with four chapters.”

Congratulations again to all our CAST award winners.

Tributes to Professor Floudas

I. E. Grossmann, former PhD advisor of Chris Floudas

I would like to first offer, on behalf of my wife Blanca and me, our deepest sympathy to Fotini and Ismini. We have been deeply shocked and saddened for the untimely loss of Chris, which has been truly a tragedy.

I consider myself to have been extremely fortunate to have had Chris as a Ph.D. student. As his former Ph.D. advisor, I could not have been prouder of him. He was a truly outstanding student who showed great passion and devotion for his research work. After he graduated from Carnegie Mellon, he had an exceptional career, first at Princeton and then at Texas A&M where he became the director of the Energy Institute. Chris made outstanding contributions to the field of Process Systems Engineering that had a huge impact in the field. He was a highly respected world leader who set very high standards, goals and challenges in research. In recognition to his work, he received many awards, including membership to the National Academy of Engineering.

Chris' death is a huge loss to the Process Systems Engineering community. We have lost a major intellectual leader and a very good friend. His absence will be felt for many years to come. The only consolation is to know that Chris' legacy will without any doubt inspire the new generation of researchers in Process Systems Engineering.

Fotini and Ismini, we would like to offer you our deepest sympathy to you. You can both be proud for having had as a loving husband and father such a prominent and respected intellectual leader. Chris will be sorely missed. May he rest in peace. Our thoughts and prayers are with him.

W. D. Seider February 5, 2017

These comments share my perspectives as a UPenn colleague of Chris, just 60 miles from Princeton.

When Chris arrived at Princeton University in 1987 as a young Assistant Professor, he was global-optimization-oriented, having focused in his Ph.D. research on the optimization of heat exchanger networks with the limited physical model, $Q = UA\Delta T_{LM}$. As we began to interact, I was concentrating on problems involving phase and chemical equilibrium, free- radical reaction systems, and steady-state multiplicity in azeotropic distillation. These often involved trace species, and the need to locate multiple and periodic solutions using homotopy-continuation methods.

Shortly after arriving at Princeton, Chris began organizing Global Optimization Conferences and he edited the new Journal of Global Optimization. My students and I began participating.

Gradually, Chris and his students tackled more complex physical systems including phase and chemical equilibrium; protein folding involving global minimization of free energy; complex energy conversion processes. Invariably, high precision, global optima were needed and displayed in their results. More importantly, in my view, was the high

precision required of their physical models. They didn't seek global optima unless their models were sufficiently accurate to justify the search.

Also, I should mention that in 1995, Chris, Prof. Bill Luyben (Lehigh Univ.), and I obtained a grant from the NSF's Combined Research- Curriculum Development Program. We sought to adopt our most outstanding research results to improve our design courses. Chris focused on global optimization, I focused on process simulator architectures, and Bill focused on plant-wide control. Each of us delivered six lectures at all three schools – while teaching our students, we shared teaching strategies and techniques. Chris had a remarkable skill and precision at the blackboard as, in rapid action, he defined the convexity/non-convexity conditions, the Karush-Kuhn-Tucker conditions, and various solution methods.

Several years later Chris moved to TAMU, which unfortunately meant he could no longer include my graduate students in his optimization course at Princeton. Then, last spring, I invited him to present a seminar at UPenn. More than ever before, the highlights of our close interactions rang clear. I especially appreciated his enthusiasm and precision. He is sorely missed!

One Final Thought – The late Leon Lapidus at Princeton, an excellent tennis player at age 52, and now Chris Floudas at age 56, have died in acute heart attacks. Perhaps this was coincidental – with these two giants in process systems engineering both experiencing such tragic endings.

Please visit the CAST webpage for more information about CAST:

<http://www.castdiv.org/>

and join the CAST listserv for continued updates

<https://listserv.umd.edu/archives/cast10.html>

Follow CAST on social media using the handle @AICHECAST10

Twitter: <http://twitter.com/AICHECAST10>

Facebook: <http://www.facebook.com/AICHECAST10/>