

FOCAPD 2019

Foundations of Computer-Aided Process Design

High Performance Design

July 14 – July 18, 2019 ♦ Copper Mountain Resort ♦ Copper Mountain, Colorado

FINAL PROGRAM

Revised July 4, 2019

*All general sessions Monday – Thursday will be located in the Bighorn Ballroom B
The opening Keynote Address & Welcome Reception will be in the Ptarmigan Ballroom & Foyer*

Sunday, July 14

2:00 p.m. to	8:00 p.m.	Conference Registration (Outside Ptarmigan Ballroom)
6:00 p.m. to	6:45 p.m.	Welcome Reception (Pre-function Foyer – Ptarmigan Ballroom)
6:45 p.m. to	7:00 p.m.	Welcome Address (Ptarmigan Ballroom) Conference Chairs: <i>Matthew J. Realff, Georgia Institute of Technology</i> <i>Carl D. Laird, Sandia National Laboratories & Purdue</i> <i>Salvador García Muñoz, Eli Lilly</i>
7:00 p.m. to	8:00 p.m.	Keynote Address From IoT to Ephemeral Computing: Understanding Cyber-Physical Interactions for Monitoring and Control <i>Julie McCann, Imperial College London</i>

Monday, July 15

7:00 a.m. to	5:00 p.m.	Conference Registration Coffee will be available outside General Session
8:00 a.m. to	12:10 p.m.	ADVANCED MANUFACTURING AND DESIGN <i>Chair: Jason Goepel, Eastman Chemical Company</i> <i>Chair: Kody Powell, University of Utah</i>
8:00 a.m. to	8:15 a.m.	Conference and Session Introduction
8:15 a.m. to	9:05 a.m.	Optimization Opportunities in Product Development: Perspective from a Manufacturing Company <i>Larry Biegler, Carnegie Mellon University</i> <i>Clas Jacobson, United Technologies Corporation</i>
9:05 a.m. to	9:45 a.m.	A New Framework for Process Design and Optimization <i>David Miller, National Energy Technology Laboratory</i>
9:45 a.m. to	10:10 a.m.	Refreshment Break
10:10 a.m. to	10:50 a.m.	Smart Manufacturing and Designing for Data Centricity <i>Jim Davis, University of California – Los Angeles</i>
10:50 a.m. to	11:30 a.m.	Data-Driven Model Development for Design and Manufacturing – Applications in Healthcare <i>Selen Cremaschi, Auburn University</i>
11:30 a.m. to	12:10 p.m.	The Unreasonable Effectiveness of Equations: Advanced Modeling for Biopharmaceutical Process Development <i>Pablo Rolandi, Amgen</i>
12:10 p.m. to	1:30 p.m.	Lunch (Jack's Slopeside Grill)
1:30 p.m. to	5:30 p.m.	MACHINE LEARNING AND DESIGN <i>Chair: Raymond Smith, US Environmental Protection Agency</i> <i>Co-Chair: Alexander Dowling, University of Notre Dame</i>
1:30 p.m. to	1:35 p.m.	Session Introduction
1:35 p.m. to	2:25 p.m.	Learning from Flowsheets <i>Nick Sahinidis, Carnegie Mellon University</i> <i>Jeffrey Sirola, Purdue University</i>
2:25 p.m. to	3:05 p.m.	Global Optimization with Neural Networks Embedded: Theory, Applications and Future Outlook <i>Alexander Mitsos, RWTH Aachen</i>
3:05 p.m. to	3:30 p.m.	Refreshment Break
3:30 p.m. to	4:10 p.m.	Machine Learning and Its Promises: From Molecule Designs to Process Systems Engineering <i>Jay Lee, KAIST</i>
4:10 p.m. to	4:50 p.m.	Reinforcement Learning: Planning and Control through Experience <i>Gavin Taylor, United States Naval Academy</i>

4:50 p.m. to	5:30 p.m.	Machine-Learning Assisted Modeling and Optimization for Process Design Synthesis <i>Fani Boukouvala, Georgia Institute of Technology</i>
5:30 p.m. to	8:00 p.m.	Dinner on own
8:00 p.m. to	10:00 p.m.	POSTER SESSION A (Jack's Slopeside Grill)

Tuesday, July 16

7:00 a.m. to	5:00 p.m.	Conference Registration Coffee will be available outside General Session
8:00 a.m. to	12:00 p.m.	MODULAR DESIGN AND PROCESS INTENSIFICATION <i>Chair: John Sirola, Sandia National Laboratories</i> <i>Chair: Jia Li, Cal Poly Pomona</i>
8:00 a.m. to	8:05 a.m.	Session Introduction
8:05 a.m. to	8:40 a.m.	RAPID Manufacturing Institute – Computer-Aided Process Design Role in MCPI <i>Ignasi Palou-Rivera, RAPID/AIChE</i>
8:40 a.m. to	9:15 a.m.	A Novel Optimization Approach for the Integrated Design and Operation of Flexible Manufacturing Systems <i>Joseph Scott, Clemson University</i>
9:15 a.m. to	9:50 a.m.	Systemic Process Intensification: Challenges, New Perspectives and Future Directions <i>Faruque Hasan, Texas A&M University</i>
9:50 a.m. to	10:15 a.m.	Refreshment Break
10:15 a.m. to	10:50 a.m.	Scaling Relations in Modular Process Design <i>Michael Baldea, University of Texas at Austin</i>
10:50 a.m. to	11:25 a.m.	Operability in Process Intensification and Modular Design <i>Stratos Pistikopoulos, Texas A&M University</i>
11:25 a.m. to	12:00 p.m.	Space-Time Dynamics of Electricity Markets Incentivize Technology Modularization <i>Victor Zavala, University of Wisconsin – Madison</i>
12:00 p.m. to	1:30 p.m.	Lunch (Jack's Slopeside Grill)
1:30 p.m. to	3:45 p.m.	HIGH-PERFORMANCE COMPUTING, DESIGN TOOLS & OPTIMIZATION <i>Chair: Robert Johnson, ExxonMobil Research and Engineering</i> <i>Chair: Qi Zhang, University of Minnesota</i>
1:30 p.m. to	1:35 p.m.	Session Introduction
1:35 p.m. to	2:25 p.m.	High Productivity High Performance Simulation and Optimisation through Code Generation in Firedrake <i>David Ham, Imperial College London</i>
2:25 p.m. to	3:05 p.m.	Surrogate-Based Modeling and Optimization for Advanced Decision Making <i>Marianthi Ierapetritou, Rutgers University</i>
3:05 p.m. to	3:45 p.m.	Nonsmooth Analysis in Process Modeling, Design and Optimization <i>Paul Barton, MIT</i>
3:45 p.m. to	8:00 p.m.	Free time, Dinner on own
8:00 p.m. to	10:00 p.m.	POSTER SESSION B (Jack's Slopeside Grill)

Wednesday, July 17

7:00 a.m. to	5:00 p.m.	Conference Registration Coffee will be available outside General Session
8:00 a.m. to	11:20 a.m.	SUSTAINABLE DESIGN AND ENERGY SYSTEMS <i>Chair: Bruce Vrana, DuPont</i> <i>Chair: Kirti Yenkie, Rowan University</i>
8:00 a.m. to	8:05 a.m.	Session Introduction
8:05 a.m. to	8:55 a.m.	Process Synthesis in the Era of Renewable Energy: New Approaches for New Problems <i>Christos Maravelias, University of Wisconsin – Madison</i>
8:55 a.m. to	9:35 a.m.	Recent Advances in Life Cycle Optimization for Sustainable Process Design <i>Fengqi You, Cornell University</i>
9:35 a.m. to	10:00 a.m.	Refreshment Break
10:00 a.m. to	10:40 a.m.	Maximizing Our Impact: A Call for the Standardization of Techno-economic Analysis for Sustainable Energy Systems Design Research <i>Thomas Adams II, McMaster University</i>
10:40 a.m. to	11:20 a.m.	From Molecules to Sustainable Life Cycles: Integrated Design of CO ₂ Conversion Processes <i>André Bardow, RWTH Aachen</i>
11:20 a.m. to	1:00 p.m.	Lunch (Jack's Slopeside Grill)
1:00 p.m. to	7:00 p.m.	PRODUCT AND MATERIAL DESIGN <i>Chair: Ben Weinstein, Procter & Gamble</i> <i>Chair: Omar Basha, North Carolina A&T State University</i>
1:00 p.m. to	1:05 p.m.	Session Introduction
1:05 p.m. to	1:55 p.m.	Next Generation Software Tools for Chemical Process and Product Design <i>Mario Eden, Auburn University</i>
1:55 p.m. to	2:35 p.m.	Mathematical Optimization for the Design of Nanostructured Materials <i>Chrysanthos Gounaris, Carnegie Mellon University</i>
2:35 p.m. to	3:00 p.m.	Refreshment Break (Coffee & Sodas only)
3:00 p.m. to	4:30 p.m.	Workshop: Institute for the Design of Advanced Energy Systems <i>Jaffer Ghouse & Andrew Lee, National Energy Technology Laboratory</i> <i>Carl Laird & Michael Bynum, Sandia National Laboratories</i>
4:30 p.m. to	5:00 p.m.	Refreshment Break (for workshop participants only)
5:00 p.m. to	7:00 p.m.	Workshop: Institute for the Design of Advanced Energy Systems (Continued) <i>Jaffer Ghouse & Andrew Lee, National Energy Technology Laboratory</i> <i>Carl Laird & Michael Bynum, Sandia National Laboratories</i>
7:00 p.m. to	8:00 p.m.	Dinner on own
8:00 p.m. to	10:00 p.m.	POSTER SESSION C (Jack's Slopeside Grill)

Thursday, July 18

7:00 a.m. to	5:00 p.m.	Conference Registration Coffee will be available outside General Session
8:00 a.m. to	11:45 a.m.	SESSION IN HONOR OF PROFESSOR ROGER SARGENT Sponsored by Process Systems Enterprise, Ltd. <i>Chair: Ignacio Grossmann, Carnegie Mellon University</i>
8:00 a.m. to	8:05 a.m.	Session Introduction
8:05 a.m. to	8:30 a.m.	Roger Sargent: Intellectual Leader and Pioneer of Process Systems Engineering <i>Ignacio Grossmann, Carnegie Mellon University</i>
8:30 a.m. to	9:15 a.m.	Process Modeling: From Sargent's Vision to its Current Directions <i>Costas Pantelides, Imperial College London & Process Systems Enterprise, Ltd.</i>
9:15 a.m. to	9:40 a.m.	Major Contributions by Roger Sargent on Nonlinear Optimization and its Applications to PSE <i>Ignacio Grossmann, Carnegie Mellon University</i>
9:40 a.m. to	10:05 a.m.	Refreshment Break
10:05 a.m. to	10:30 a.m.	Distillation & Hybrid Separation: Modelling, Synthesis, Design & Operation <i>Rafiqul Gani, PSE for SPEED</i>
10:30 a.m. to	10:55 a.m.	Scheduling in PSE: Before and After the State-Task Network <i>Pedro Castro, University of Lisbon</i>
10:55 a.m. to	11:20 a.m.	Impact on Optimization, Control, and MPC <i>Larry Biegler, Carnegie Mellon University</i>
11:20 a.m. to	11:45 a.m.	The Centre for Process Systems Engineering: Interactions and Integration <i>Eva Sorensen, University College London</i>
11:45 a.m. to	1:00 p.m.	Lunch (Jack's Slopeside Grill)
1:00 p.m. to	3:15 p.m.	HIGH-PERFORMANCE COMPUTING, DESIGN TOOLS AND OPTIMIZATION <i>Chair: Anthony Burgard, National Energy Technology Laboratory</i> <i>Chair: Helen Durand, Wayne State University</i>
1:00 p.m. to	1:05 p.m.	Session Introduction
1:05 p.m. to	1:55 p.m.	Multi-scale Simulation of Multiphase Systems: Towards Exa-scale Supercomputing And Virtual Process Engineering <i>Wei Ge, Chinese Academy of Sciences</i>
1:55 p.m. to	2:35 p.m.	Approximation Algorithms for Process Systems Engineering <i>Ruth Misener, Imperial College London</i>
2:35 p.m. to	3:15 p.m.	Asset Optimization Software Suites to Drive Digitalization – From Process Modeling to Optimization to Asset Optimization <i>Ajay Lakshmanan, Aspen Technology</i>
3:15 p.m. to	3:30 p.m.	Refreshment Break

3:30 p.m. to	5:00 p.m.	COMPUTER-AIDED PROCESS DESIGN EDUCATION IN THE 21ST CENTURY – ACADEMIC CHALLENGES IN REALIZING INDUSTRY NEEDS
		Panel Discussion <i>Moderated by Eva Sorensen, University College London</i>
5:00 p.m. to	5:30 p.m.	Free Time
5:30 p.m. to	8:00 p.m.	Reception and Banquet (Grand Hall – Copper Station East Village)
5:30 p.m. to	6:15 p.m.	Reception
6:30 p.m. to	8:00 p.m.	Dinner Buffet
8:00 p.m. to	9:00 p.m.	Closing Plenary Address
		Why Exascale? <i>Doug Kothe, Oak Ridge National Laboratory</i>
		Questions after the remarks are welcome
9:00 p.m. to	10:00 p.m.	Closing Reception