

FOCAPD 2019

Foundations of Computer-Aided Process Design

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

FINAL PROGRAM

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

Sunday, July 14

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|---------------------|------------------|--|
| 2:00 p.m. to | 6:00 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 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 7:00 a.m. to	5:00 p.m. 8:00 a.m.	Conference Registration Continental Breakfast
8:00 a.m. to	12:10 p.m.	ADVANCED MANUFACTURING AND DESIGN <i>Chair:</i> <i>Chair:</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 on own
1:30 p.m. to	5:30 p.m.	MACHINE LEARNING AND DESIGN <i>Chair:</i> <i>Co-Chair:</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 (Jack's Bar)
8:00 p.m. to	10:00 p.m.	POSTER SESSION A (Jack's Bar) <i>Chair:</i> <i>Chair:</i>

Tuesday, July 16

7:00 a.m. to	5:00 p.m.	Conference Registration
7:00 a.m. to	8:00 a.m.	Continental Breakfast
8:00 a.m. to	12:00 p.m.	MODULAR DESIGN AND PROCESS INTENSIFICATION
		<i>Chair:</i>
		<i>Chair:</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 on own
1:30 p.m. to	3:45 p.m.	HIGH-PERFORMANCE COMPUTING, DESIGN TOOLS & OPTIMIZATION
		<i>Chair:</i>
		<i>Chair:</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 Bar)
Chair:
Chair:

Wednesday, July 17

7:00 a.m. to	5:00 p.m.	Conference Registration
7:00 a.m. to	8:00 a.m.	Continental Breakfast
8:00 a.m. to	11:20 a.m.	SUSTAINABLE DESIGN AND ENERGY SYSTEMS <i>Chair:</i> <i>Chair:</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.	From Molecules to Sustainable Life Cycles: Integrated Design of CO ₂ Conversion Processes <i>Andre Bardow, RWTH Aachen</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, McMaster University</i>
10:40 a.m. to	11:20 a.m.	Recent Advances in Life Cycle Optimization for Sustainable Process Design <i>Fengqi You, Cornell University</i>
11:20 a.m. to	1:00 p.m.	Lunch on own
1:00 p.m. to	7:30 p.m.	PRODUCT AND MATERIAL DESIGN <i>Chair:</i> <i>Chair:</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>
3:00 p.m. to	7:00 p.m.	Workshop: Institute for the Design of Advanced Energy Systems
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 Bar) <i>Chair:</i> <i>Co-Chair:</i>

Thursday, July 18

7:00 a.m. to	8:00 a.m.	Continental Breakfast
8:00 a.m. to	11:45 a.m.	SESSION IN HONOR OF PROFESSOR ROGER SARGENT <i>Chair:</i> <i>Chair:</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</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.	Initial Steps into the Field of Machine Learning <i>Erik Ydstie, Carnegie Mellon University</i>
11:20 a.m. to	11:45 a.m.	The Centre for Process Systems Engineering: Interactions and Integration <i>Claire Adjiman, Imperial College London</i>
11:45 a.m. to	1:30 p.m.	Lunch on own
1:30 p.m. to	4:00 p.m.	HIGH-PERFORMANCE COMPUTING, DESIGN TOOLS AND OPTIMIZATION <i>Chair:</i> <i>Chair:</i>
1:30 p.m. to	1:35 p.m.	Session Introduction
1:35 p.m. to	2:25 p.m.	Multi-scale Simulation of Multiphase Systems: Towards Exa-scale Supercomputing And Virtual Process Engineering <i>Wei Ge, Chinese Academy of Sciences</i>
2:25 p.m. to	3:00 p.m.	Approximation Algorithms for Process Systems Engineering <i>Ruth Misener, Imperial College London</i>
3:00 p.m. to	3:35 p.m.	Asset Optimization Software Suites to Drive Digitalization – From Process Modeling to Optimization to Asset Optimization <i>Ajay Lakshmanan, Aspen Technology</i>
3:35 p.m. to	4:00 p.m.	Refreshment Break

**4:00 p.m. to 6:00 p.m. COMPUTER-AIDED PROCESS DESIGN EDUCATION IN THE 21ST CENTURY
– ACADEMIC CHALLENGES IN REALIZING INDUSTRY NEEDS**

Panel Discussion

Moderated by Eva Sorensen, University College London

6:00 p.m. to 6:30 p.m. Free Time

6:30 p.m. to 8:00 p.m. Reception and Banquet (Grand Hall)

8:00 p.m. to 9:00 p.m. Closing Plenary Address

Doug Kothe, Oak Ridge National Laboratory

9:00 p.m. to 10:30 p.m. Closing Reception