ETH zürich

Symposium on

Artificial Intelligence in Chemical and Bioengineering

5 – 6 February 2020

The aim of this symposium is to provide an introduction to artificial intelligence (AI) and machine learning (ML) in chemical and process engineering. In the same way it is revolutionizing several areas of science and technology, artificial intelligence has huge potential to impact also core activities of chemical engineers such as modeling, material design, reaction engineering, process control and intensification. This series of seminars, delivered by world-class leaders in the field, will provide a comprehensive overview of this very exciting and rapidly evolving area, from a historical perspective to the most recent developments, from fundamental scientific questions to examples of concrete applications. The seminars will also provide a critical overview on challenges and opportunities in building hybrid mechanistic/data driven models.

Prof. Dr. Paolo Arosio
Head of ICB Seminar Series

ICB Institute for Chemical and Bioengineering

Wednesday, February 5th

3 pm, HCI J 3

Smart Process Analytics and Machine Learning

Richard D. Braatz, MIT
joint with Weike Sun and Fabian Mohr

Richard D. Braatz, *Edwin R. Gilliand Professor of Chemical Engineering, Massachusetts Institute of Technology (MIT).*

Professor Richard D. Braatz is the Edwin R. Gilliland Professor of Chemical Engineering at the Massachusetts Institute of Technology (MIT) where he does research in advanced manufacturing systems. He received MS and PhD from the California Institute of Technology and was the Millennium Chair at the University of Illinois at Urbana-Champaign and a Visiting Scholar at Harvard University before moving to MIT. He is a Fellow of IEEE, IFAC, and AAAS and a member of the U.S. National Academy of Engineering.

Abstract:
Data analytics can be invaluable for improving manufacturing operations, but selecting the best method requires a high level of expertise. An automated process data analytics approach is presented which empowers users to focus on objectives rather than on methods. Tools are applied to automatically interrogate the data to ascertain characteristics (e.g., nonlinearity, multicollinearity, dynamics), which are used to select among the best-in-class data analytics method.

4 pm, HCI J 3

Global optimization with hybrid models embedded

Alexander Mitsos, RWTH

Alexander Mitsos, *Edwin R. Gilliland Professor of Chemical Engineering, Massachusetts Institute of Technology (MIT).*

Professor Alexander Mitsos is the Director Process Systems Engineering in RWTH (AVT.SVT) and of Energy Systems Engineering at Forschungsentrum Juelich (IEK-10). He received his Dipl-Ing from Karlsruhe and his Ph.D. from MIT, both in Chemical Engineering. Prior appointments include a junior research group leader position in RWTH and the Rockwell International Assistant Professorship at MIT. Mitsos' research focuses on optimization of energy and chemical systems and development of enabling numerical algorithms.

Abstract:
A promising avenue for process design, is to utilize hybrid mechanistic/data-driven models. However, such models result in large-scale nonconvex nonlinear optimization problems. We discuss an efficient solution strategy and apply this strategy to challenging cases in chemical engineering.

Thursday, February 6th

10 am, HCI J 3

Artificial Intelligence in Chemical Engineering: Past, Present, and Future

Venkat Venkatasubramanian,
Columbia University

Venkat Venkatasubramanian, *Samuel Ruben-Peter G. Viele Professor of Engineering at Columbia University*

Professor Venkat Venkatasubramanian is Samuel Ruben-Peter G. Viele Professor of Engineering at Columbia University. He is a complex dynamical systems theorist interested in developing mathematical models of their structure, function, and behavior from fundamental conceptual principles. His research interests are diverse, ranging from AI to systems engineering to theoretical physics to economics. He won the *Computing in Chemical Engineering Award* from AIChE and is a *Fellow of AIChE.*

Abstract:
Artificial intelligence in chemical engineering started off with great promise in the early 1980s, spurred by the success of expert systems. However, AI didn't quite live up to its promise. So, what went wrong? I will offer an explanation and discuss opportunities going forward. The intellectually challenging problems lie in developing hybrid and causal models and domain-specific knowledge discovery engines. These would require an integration of symbolic reasoning with data-driven techniques.

11 am, HCI J 3

Intersections of AI/ML and Chemistry in Catalyst Design and Discovery

Zachary Ulissi,
Carnegie Mellon University

Zachary Ulissi, *Assistant Professor in Chemical Engineering at Carnegie Mellon University in Pittsburgh PA.*

Zachary Ulissi is an Assistant Professor in Chemical Engineering at Carnegie Mellon University in Pittsburgh PA. He did his undergraduate work in Chemical Engineering and Physics at the University of Delaware, a Masters in Applied Mathematics at Churchill College, Cambridge, and his PhD in Chemical Engineering at MIT funded by the DOE CSGF fellowship. His PhD research at MIT focused on the the application of systems engineering methods to understand selective nanoscale carbon nanotube devices and sensors working with Michael Strano and Richard Braatz. Prof. Ulissi did his postdoctoral work at Stanford with Jens Nørskov where he worked on machine learning techniques to simplify complex catalyst reaction networks and discover new catalysts. Current research interests include the design of high-throughput computational systems for surface science and catalysis, as well as the development of machine learning models and design of experiments processes to accelerate the discovery process. Methods include both all-atom classical (MD) and electronic (DFT) simulations techniques.

Abstract:
Increasing computational sophistication and resources can enable a larger and more integrated role of theory in the discovery and understand-

Thursday, February 6th (cont.)

Abstract Z. Ulissi (cont.)

ing of new materials. This process has been slower to infiltrate surface science and catalysis than the field of bulk inorganic materials due to additional scientific complexity of modeling the interface. Most catalyst studies start in a data-poor regime where the material of interest is unrelated to previous to studies (new structure, composition etc.) or the computational methods are incompatible with previous studies (different exchange-correlation functionals, methods, etc.). Efficient methods to quickly define, schedule, and organize necessary simulations are thus important and enable the application of online design of experiments approaches. I will discuss on-going work and software development to enable data science methods in catalysis including open datasets for the community. These large datasets enable the use of graph convolutional models for surface properties and the uncertainty in these methods can be carefully calibrated. Finally, I will describe applications of our approach to ordered bimetallic alloy catalysts, with applications to several electrochemical catalyst discovery efforts including CO2 reduction, oxygen reduction, and water splitting chemistry.

ICB Institute for Chemical and Bioengineering

ETH Zurich
ICB Institute for Chemical and Bioengineering
Vladimir-Prelog-Weg 1
CH-8093 Zürich

www.icb.ethz.ch
info-icb@chem.ethz.ch

2 pm, HCI J 3

Learning the language of organic chemistry: developing artificial intelligence models using existing knowledge

Teodoro Laino,
IBM Research Zurich

Teodoro Laino, *Principal Research Staff Member, IBM Resarch Zurich.*

Teodoro Laino is Principal Research Staff Member and technical leader for Chemistry/Materials at IBM Research-Zurich. He graduated in theoretical chemistry in 2001 from University of Pisa and Scuola Normale Superiore (SNS) di Pisa, and received the doctorate in chemistry in 2006 from SNS. The focus of his research is on materials simulations for industrial-related problems and on the application of machine learning/artificial intelligence technologies to chemistry and materials science problems.

Abstract:
Reaction prediction is a fundamental task in organic chemistry. What if one could learn from all reactions published in articles and patents? What if this knowledge could be used to build a system that would assist researchers in the synthesis route design process? The use of data-based models combined with Artificial Intelligence (AI) strategies is emerging as a valuable and robust solution to address these fundamental questions. In this presentation, I will introduce few AI models to treat forward reaction prediction, retrosynthesis and the processing of action sequences. All models are freely accessible world-wide as cloud applications: https://www.research.ibm.com/ai4chemistry