SPECIAL SEMINAR

“Methods for Nonlinear and Stochastic Optimization”

Dr. Raghu Bollapragada

Tuesday, January 15, 2019
3:00 PM – 4:00 PM
JEC 3117

Abstract:

Nonlinear stochastic optimization problems arise in a wide range of applications, from acoustic/geophysical inversion to deep learning. The scale, computational cost, and difficulty of these models make classical optimization techniques impractical. To address these challenges, we have developed new optimization methods that, in addition, are well suited for distributed computing implementations. Our techniques employ adaptive sampling strategies that gradually increase the accuracy in the step computation in order to achieve efficiency and scalability, and incorporate second-order information by exploiting the stochastic nature of the problem. We provide some interesting (and perhaps surprising) complexity results for our methods. The performance of our algorithm is illustrated on large-scale machine learning models, both convex and non-convex. We conclude by highlighting some open questions that arise when training deep neural networks.

Bio: Raghu Bollapragada is a PhD candidate in the Industrial Engineering and Management Sciences department at Northwestern University under the supervision of Professor Jorge Nocedal. During his graduate study, he was a visiting researcher at INRIA, Paris, hosted by Professor Alexandre d’Aspremont. He received his Bachelor’s and Master’s Dual Degree in Mechanical Engineering with minor in Operations Research from the Indian Institute of Technology (IIT) Madras, India. His current research interests are in nonlinear optimization and its applications in machine learning. He has received the IEMS Arthur P. Hurter Award for outstanding academic excellence, the McCormick terminal year fellowship for outstanding terminal-year PhD candidate, and the Walter P. Murphy Fellowship at Northwestern University.
When will artificial intelligence be able to reason like a chemist?

A perspective will be presented on the “three waves” of artificial intelligence and their impacts. From E. J. Corey’s first attempts at an expert system with the Logic of Total synthesis to the remarkable achievements of statistical learning in cheminformatics and the exciting prospects of context aware AI systems in chemistry, artificial intelligence techniques have found fertile ground for application in chemistry. This story will be told from the perspective of my career. We will discuss computational descriptors and robotic screening for discovering lignin depolymerization reactions and novel catalytic C-O bond activation catalysts. We will then move on to state-of-the-art machine learning methods for inferring the health of the microbiological systems in wastewater treatment plants. Finally, the future of AI in chemistry is automated reasoning systems that can reason over various structure, reactivity, and property contexts to hypothesize and test new chemistry. A novel proposal will be presented for an autonomous agent that can reason over structure property relationships to generate novel structures and synthesize these novel compounds without human intervention.
Abstract

Bacterial biofilms are a major cause of chronic infections in humans and biofouling in industrial settings. However, controlling biofilm formation remains challenging due to the high-level tolerance of biofilm cells to antibiotics and disinfectants. To overcome this grand challenge, we investigated how material properties affect bacterial adhesion using polymers with varying stiffness and specific topographic patterns. Based on the obtained results, we proposed a set of principles for rational design of antifouling surfaces and validated the design using protruding hexagonal patterns, which were found reduce biofilm formation of *Escherichia coli* by around 90%. Inspired by these findings, we further developed a new strategy to remove established biofilms using biocompatible shape memory polymers with micron-scale topographies. These surfaces can both prevent bacterial adhesion and remove established biofilms through rapid change in surface topography triggered by moderate shift in temperature, thereby offering more prolonged antifouling properties. We demonstrate that this strategy can achieve a total reduction of *Pseudomonas aeruginosa* biofilms by 99.9% compared to the static flat control. It was also found effective against biofilms of *Staphylococcus aureus* and an uropathogenic strain of *Escherichia coli*. The detached cells were found to be more sensitive to antibiotics than the original biofilm cells. The underlying mechanism and possible applications will be discussed.
Dr. Ren received his Ph.D. in Chemical Engineering from University of Connecticut in 2003. After finishing postdoctoral training at Cornell University, he joined Syracuse University in 2006. Currently, he is Stevenson Endowed Professor in the Department of Biomedical and Chemical Engineering, and the director of Syracuse Biomaterials Institute.

Dr. Ren received an Early Career Translational Research Award in Biomedical Engineering from the Wallace H. Coulter Foundation in 2009 and a NSF CAREER award in 2011. He was named the College Technology Educator of the Year by the Technology Alliance of Central New York in 2010. Dr. Ren is also a recipient of the Faculty Excellence Award from the School of Engineering and Computer Science at Syracuse University in 2014, and Chancellor’s Citation for Faculty Excellence and Scholarly Distinction in 2018. Dr. Ren currently has 60 journal publications with over 3,700 citations and an h-index of 31, 10 issued/pending patents, and more than 30 invited talks. Dr. Ren has broad research interests in biotechnology and biofilm control. His research has been supported by NSF, NIH, EPA, Wallace H. Coulter Foundation, Alfred P. Sloan Foundation, and industrial sponsors.

**Refreshments: 9:00 a.m., Coonley Lounge**

For more information, please contact Lisa Martin – swishl@rpi.edu
“Radioxenon Nuclear Forensics”

Wed., January 16, 2019
10:30 AM – 11:30 AM
DCC 318

Steven Biegalski

Professor and Chair of Nuclear and Radiological Engineering and Medical Physics Program
Georgia Institute of Technology

About the presentation: Since the Partial Test Ban Treaty in 1963, nuclear explosion tests have largely been conducted in underground locations. To monitor the emissions from underground nuclear tests, the world community relies upon atmospheric monitoring for radioxenon among other technologies. The Comprehensive Nuclear Test-Ban Treaty (CTBT) incorporates radioxenon monitoring within International Monitoring System (IMS) with a focus on $^{131m}$Xe, $^{132m}$Xe, $^{133}$Xe, and $^{135}$Xe. It is expected that radioxenon monitoring will also be incorporated into the On-Site Inspection (OSI) protocols along with radioargon monitoring.

When an atmospheric radioxenon signal is observed, the isotopic ratios are examined to see if they match the expected values for nuclear explosions. These isotopic ratios are utilized to distinguish between nuclear explosion sources of radioxenon and other anthropogenic sources such as the commercial nuclear industry and the radiopharmaceutical industry. Current methods to predict the various isotopic ratio signatures have largely focused on modeling the production source. While this is a good first order approximation, it does not account for the chemical and isotopic fractionation that occurs during environmental transport of radioxenon and its parent radionuclides. This fractionation causes a significant change in the isotopic ratios from their point of creation to the point where they are collected in the atmosphere.

This seminar will focus on developments that advance the field of noble gas nuclear forensics. Analysis will be shown for both natural and anthropogenic signals and forensic methods for distinguishing between radioxenon sources will be discussed. A forensic assessment of radioxenon emissions from the Fukushima nuclear accident will be presented and results showing the variability induced by underground radionuclide transport will be detailed.

Bio: Steven Biegalski is the Chair of Nuclear and Radiological Engineering and Medical Physics Program. He has held many leadership positions and brings these experiences to the leadership. Prior to becoming a faculty member, Dr. Biegalski was the Director of Radionuclide Operations at the Center for Monitoring Research. In this position Dr. Biegalski led international efforts to develop and implement radionuclide effluent monitoring technologies. This work supported both US national capabilities and international treaties. Dr. Biegalski held the position of Reactor Director for The University of Texas at Austin TRIGA reactor for over a decade. In this capacity he led a multi-disciplinary team of faculty and staff to manage reactor operations. He has advised 25 Ph.D. students to graduation. He is an Associate Editor for the Journal of Radioanalytical and Nuclear and holds a Professional Engineering license in the states of Texas and Virginia.
Abstract Halide Perovskites have shown great potential for high-performance cost-effective photovoltaics. Previous work in this field was primarily focused on pristine perovskites. We discovered that perovskites in form of composites can exhibit more desirable optical properties with improved material stability. In this colloquium, I will discuss the correlation between material morphology and physical properties in composite halide perovskites, and their performance as optoelectronic building blocks.

Biosketch: Dr. Hanwei Gao received his B.S. in Physics from the University of Science and Technology of China in 2004 and Ph.D. in Materials Science from Northwestern University in 2009. Since 2010, he had worked at the University of California-Berkeley as a Postdoctoral Researcher where he studied plasmonic enhanced solar energy devices, both solid state photovoltaics and photoelectrochemical water splitting. Dr. Gao joined the Florida State University as an Assistant Professor in Physics in the Fall 2013. His research since then has been focussing on the photoresponse and charge transport behaviors of photoactive materials with potential for optoelectronic applications.