Department of Biological Sciences
Seminar Series

Dr. Hanna Irie
Icahn School of Medicine at Mount Sinai

“Personalizing Treatment for Triple Negative Breast Cancer.”

Monday, October 30, 2017
12:00 pm
CBIS, Bruggeman Room

Refreshments served at 11:45
Large-Scale Simulations Of Solid-Liquid Interfaces Under Realistic Electrochemical Conditions For Energy Conversion and Storage

Ismaila Dabo, PhD
Assistant Professor, Department of Materials Sciences and Engineering
Pennsylvania State University

ABSTRACT
Solid-liquid interfaces are at the heart of a wide array of electrochemical technologies such as batteries, supercapacitors, fuel cells, electroactuators, and dye-sensitized solar cells. To optimize these technologies, the interactions of the charged electrodes and the ions from the surrounding electrolyte need to be understood at the molecular level. While existing quantum-mechanical models are applicable to either the electrolyte or the electrode in isolation, their combination is challenging using available computational approaches. This presentation will highlight progress in the quantum-continuum modeling of solid-liquid interfaces. The focus will be on the storage of energy in electrochemical capacitors and the production of chemical fuels in photoelectrochemical reactors. We will describe the use of newly developed, embedded quantum-mechanical techniques and large-scale finite-temperature sampling methods to elucidate pseudocapacitive storage at ruthenia electrodes and to predict the electrification of silicon photoelectrodes in realistic aqueous media.

BIO
Ismaila Dabo graduated with a Ph.D. in Materials Science and Engineering from the Massachusetts Institute of Technology (MIT) in 2008. His doctoral research under the supervision of Dr. Marzari was dedicated to predicting the electrical response of quantum systems embedded in electrochemical environments and to studying chemical poisoning in low-temperature fuel cells. After graduation, Ismaila Dabo became a postdoctoral researcher and then a permanent researcher at Ecole des Ponts, University of Paris-Est (France). He joined the Department of Materials Science and Engineering at Penn State in 2013. He is a recipient of the ORAU Ralph E. Powe Junior Faculty Award and of the NSF Faculty Early Career Award (CAREER).
“Design as a Sequential Decision Process with Applications in Structural Engineering”

Wednesday, November 01, 2017
JEC 3117
1:00 – 2:00

Dr. Gordon Warn
Associate Professor
Dept. of Civil & Environmental Engineering
The Pennsylvania State University

ABSTRACT:
The engineering design community is being tasked with generating designs that must satisfy ever more criteria, such as purchase cost, various performance metrics, life-cycle costs, and others. Integrating these broad, often conflicting, criteria into the design causes the design process to become more complex, the decisions more difficult, and a need for higher fidelity (and more computationally demanding) modeling efforts to gain insight to resolve tradeoffs and find satisficing design alternatives. For such complex systems, a diverse set of design solutions exists that the designer must broadly explore to select the ideal design alternative.

This seminar presents an emerging design concept that closely couples set-based design with model-based simulation treating the design process formally as a sequential decision process (SDP). In this paradigm, mathematical models of increasing fidelity, $M_j$, are used in a sequence to successively provide tighter bounds on the decision criteria, facilitating the systematic contraction of the set of design alternatives, $X_i$, through a sequence of discrete decision states (see left of Fig. 1), until a choice set is obtained from which a design can be selected. The SDP using models to bound objectives is introduced, formally defined, and applied to the system-level design of seismic-resisting structural frames with deterministic decision criteria using the capacity spectrum method. In spite of its desirable features, the SDP using models to bound objectives has an important limitation. The multiple model fidelities and multiple discrete decision states result in a multitude of model sequences (see Fig. 1 right) that can be used to arrive at a choice set, some sequences requiring significantly fewer model evaluations than others. It is desirable to select the most efficient sequence possible. However, the optimal sequence of model fidelities can only be determined, using for example dynamic programming, after constructing a complete dataset of the computational cost of executing each model fidelity on each design alternative and the associated bounds on the decision criteria, thus requiring an excessive number of model evaluations and limiting the practical application of the SDP. Recent efforts to overcome this limitation will be presented, whereby the SPD is reformulated as a finite Markov Decision Process that is solved using reinforcement learning (RL) to identify approximately optimal sequences of model fidelities on the fly using actual experienced transitions in place of knowledge of expected transitions. The efficiency
Physics, Applied Physics & Astronomy

Colloquium

Wednesday, November 1, 2017
4:00 p.m.
Low Center for Industrial Innovation (CII) Room 3051
Lite refreshments 3:30 p.m.

Pearl Sandick, Ph.D.
University of Utah

“Mixing It Up: A New Take on WIMP Dark Matter”

Abstract:

The question of the identity of dark matter remains one of the most important outstanding puzzles in modern physics. Weakly Interacting Massive Particles (WIMPs) have long been the frontrunner dark matter candidate, with the supersymmetric neutralino serving as the canonical WIMP. In this talk, I’ll discuss recent results relevant to the search for dark matter, supersymmetric and otherwise, and highlight the spectrum of theoretical and phenomenological approaches to its study. As I’ll demonstrate, even canonical WIMPs may reveal themselves in surprising ways!
DEPARTMENT OF INDUSTRIAL AND SYSTEMS ENGINEERING SEMINAR

Data Analytics for IBM's IT Service Deals’ Solutioning: Methodologies and Practical Implications
Analytics and OR Applications in Cloud Computing, IoT, & Blockchain Technologies

Dr. Aly Megahed
IBM’s Almaden Research Center

Thursday, November 2, 2017
10am – 11am
CII 5003
(The public is invited to attend. Refreshment will be served)

Abstract:
IBM competes in a tender-like process to win highly valued IT service contracts as part of its $20B outsourcing business. Focusing on deals that are $10M and above, the typical negotiation lifecycle is anywhere between 3 to 12 months. Each deal contains IT services like cloud computing, service desk, and databases. The average number of total components/services in such opportunities is 10k. Given this complexity and high value, pricing these deals is a challenging problem. In the first two-thirds of this talk, we present the data analytical approaches that we successfully developed for the business, leading to “revenue increases in the range of millions of dollars each quarter and enabling the pricing of solutions in a tiny fraction of the time that this task used to take us, and in a more accurate and efficient manner”, as quoted by our business VP of global solutions. The approach relies on data mining of historical and market data to produce some pricing points that are then fed into a predictive analytics model that outputs the chances of winning a deal at different pricing points. Lastly, we also briefly discuss other data analytics problems in the same framework of IT service deals, such as deal progress monitoring and revenue prediction.

In the last third of this presentation, we will go over multiple interesting problems in Cloud Computing, Internet of Things (IoT), and Blockchain technologies that use operations research and analytics to solve them. We will show some of our developments in these areas and illustrate potential research collaborations as well.

Bio:
Dr. Aly Megahed is a research staff member at IBM’s Almaden Research Center in San Jose, CA. In his current job, he develops and advances research in analytics, statistics, machine learning, and operations research to address different service science, cloud computing, Internet of Things (IoT), and blockchain technology problems. Dr. Megahed got his Ph.D. in Industrial Engineering from Georgia Tech with a focus on the development of operations research and analytics tools for solving problems in supply chains and logistics systems. He has two master’s degrees in Industrial and Production Engineering from Georgia Tech and Alexandria University, respectively, and a B.S. in Production Engineering from Alexandria University. He has done multiple analytical research/consultancy projects for over 6 companies in the past, has given both invited and submitted talks at several conferences, companies, and institutions/universities, and has his work published in several academic journals and conferences in addition to filing 25 patent disclosures. He has taught university level courses at 7 different academic institutions. Dr. Megahed has also won several internal IBM awards and external ones, including being a finalist for the INFORMS Innovative Applications in Analytics Award. Being an active INFORMS member for the past few years, he organized and gave talks at multiple sessions in the analytics and service science sections, got elected as the secretary of the service science section, participated as a panelist in industrial job search panels, served as an organizer for Ph.D. colloquia, reviewed multiple papers for different journals, judged best student paper awards, and mentored several students.
Osteoarthritis (OA) is a debilitating disease that afflicts nearly 20% of people in the US, costing more than $185.5 billion a year (in 2007 dollars), and its prevalence is projected to increase by about 40% in the next 25 years. We understand neither the cause nor progression of the disease, and treatment remains primarily symptomatic, as no cure yet exists. Furthermore, despite an enormous body of literature on cartilage mechanics, a great need remains to understand the in vivo mechanobiology of human cartilage, particularly regarding how mechanical stimuli influence chondrocyte (cell) function and regulate matrix synthesis. We discuss experimental and computational advances toward the development of a multidisciplinary analysis framework for cartilage: a virtual cartilage. Patient-specific computational analysis of virtual human joints and cartilage enables a unique opportunity to couple the in vivo solid and fluid biomechanics of cartilage at the joint and tissue levels with cell-mediated changes in cartilage structure, properties, and geometry. In the future, evolving virtual cartilage will help clarify relationships between the biology and physics of cartilage function in health and disease. Virtual cartilage could also advance understanding of patient-specific pathological changes due to biomechanical factors, improve clinical diagnostics and therapies, and enable new methods for non-invasive diagnosis and pre-/post-operative decision making.

Dr. Pierce received the B.S. degree from the University of Minnesota, Minneapolis, and the M.S. and Ph.D. degrees (with S.D. Sheppard) from Stanford University, CA, all in mechanical engineering. Additionally, he received a Ph.D.-Minor degree in mathematics from Stanford University and completed his Habilitation (Venia Legendi) in experimental and computational biomechanics (with G.A. Holzapfel) at the Graz University of Technology in Austria. The driving interest of Dr. Pierce's research is to understand and predict the mechanics of soft tissues and...
engineering materials. His current work employs theoretical, computational, and experimental tools to explore the interplay of form and function in cartilage, specifically the multiscale and multi-phase mechanics and how these evolve in health, damage, and disease. Working at the intersection of imaging, image analysis, biology, physiology, and experimental and computational mechanics, his lab's overarching aim is to establish a virtual human cartilage—a patient-specific analysis framework—to integrate diverse data, facilitate interdisciplinary collaborations, and accelerate testing of hypotheses, including those previously unapproachable. To this end, Dr. Pierce's Interdisciplinary Mechanics Laboratory (imLAB) establishes novel experimental protocols and builds validated simulation tools that inform our understanding of the mechanics of cartilage, the complex progression of osteoarthritis, and clinical perspectives on causes, treatments, and possible preventions. His other work encompasses characterization and modeling of arteries and intraluminal thrombi and failure prediction and design tools for Si-based MEMS devices.