Khorana Bose Research Opportunities in the United States and India

Brenda Rubenstein (Faculty/Lab can provide matching support, up to $1000)
Brown University
brenda_rubenstein@brown.edu

Department
Chemistry

For Student: Concentration should be in Chemistry, Physics, Computer Science, Applied Mathematics, or Biophysics

Project Title:
Computational Chemical Physics and Biophysics in the Rubenstein Group (Brown)

Project:
The Rubenstein Group at Brown is interested in a diverse array of theoretical/computational Chemical Physics and Biophysics problems. Key topics include: 1) developing new stochastic electronic structure methods; 2) modeling how small molecules can be used to read/write/compute data; 3) exploring how noise arising from molecular adsorbates in quantum computers may be minimized; and 4) understanding how mutations in beta-lactamases contribute to their evolution. Students interested in the group should be familiar with quantum mechanics and/or statistical mechanics, and willing to learn how to code in high performance languages. For more information, please visit: https://www.brown.edu/research/labs/rubenstein/.

Iris Bahar (Faculty/Lab cannot provide matching support)
Brown University
iris_bahar@brown.edu

Department
Engineering

For Student: Minimum age is 20 with knowledge of C/C++, basic digital design. Knowledge of computer architecture and data structures also helpful

Project Title:
Exploiting Application Error Tolerance in Multicore Computing Systems for Performance and Energy Efficiency

Project:
This proposal aims to exploit bounded approximate computation with the goal of increased runtime performance and reduced energy consumption of embedded multicore systems. We focus on approximations resulting from runtime computation errors that are intentionally allowed to be left uncorrected.

We consider two main types of runtime errors: errors resulting from timing violations and memory synchronization conflicts. Timing errors are introduced by relaxing guardbands, that is, reducing the voltage and/or corresponding clock frequency below the minimum level that guarantees correct functionality, with the goal of achieving significant energy savings. Memory synchronization conflicts result from intentionally skipping portions of code required for synchronization, or by allowing for data conflicts that were detected to remain uncorrected.

This project proposes new architectural level techniques to allow for inexact computation, utilizing a novel lightweight error recovery mechanism adapted from hardware transactional memory (HTM). Our framework is capable of correcting runtime errors by rollback and re-execution. We will determine the tolerance of different portions of a range of applications to errors both statically via profiling, and dynamically via performance counters, and then allow for approximation within those acceptable bounds. The key is to trade-off exact computation for increased energy-efficiency and runtime performance. Furthermore, we will examine the error behavior of various functional units, such as floating point units versus integer units. This will allow us to create new error models to capture the delay behavior of different functional units more accurately than existing error models, in order to more reliably exploit error tolerance.

Vicki Colvin (Faculty/Lab can provide matching support, up to $1000)
Brown University
colvin@brown.edu

Department
Chemistry and Engineering

For Student: Concentration should be in Chemistry or Chemical Engineering or Environmental Engineering

Project Title:
Creating Super-Small Solids: Towards Understanding How Magnetic Nanocrystals Form

Project:
This laboratory applies magnetic nanocrystals formed from iron, manganese and cobalt oxides to diverse problems including clean water, imaging disease and the reducing of carbon emissions. However, forming these materials is based on very new chemistry that while effective is not well understood. This precludes scale-up of nanocrystal synthesis to manufacturing, and also limits rational design of the material size and composition. In this project, a student will focus on one of the most iconic nanocrystal reactions: the formation of metal/mixed metal oxide nanocrystals through the thermal decomposition of metal salts in non-polar solvents. The products are highly uniform, and have a surprising lack of Ostwald ripening at long reaction times. We hypothesize that the fatty acid surfactant thermally decomposes during the particle nucleation and growth. This decomposition may be catalyzed by the iron oxide surfaces leading to a disproportionation reaction that releases carbon dioxide (CO2) and carbon monoxide (CO). CO would subsequently generate reduced forms of iron oxide that subsequently catalyze the disproportionation of other CO molecules. The student will investigate the thickness and type of graphitic carbon that deposits from this process, and will evaluate under what conditions this

carbon deposition may occur. Additionally, the student will have the opportunity to study how the graphite-coated nanocrystals perform in water treatment applications focused on the magnetic removal of viruses and arsenic from water.

Professor Venkat Viswanathan
Carnegie Melon University
venkatv@andrew.cmu.edu

Department
Mechanical Engineering

Project Title
Electric Flight

Project Description
There is a general consensus emerging regarding the overall feasibility of electric aircraft. One of the key distinctions of the electric propulsion with conventional propulsion is the fact that electric motors can be combined in several ways to achieve the same overall power, but the distribution improves other parameters like lift coefficients. The goal of this project is to study such strategies to exploit the advantages of electric propulsion and minimize the energy consumption characteristics of aircraft and thereby lower demands on battery packs.

Professor Venkat Viswanathan
Carnegie Melon University
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Department
Mechanical Engineering

Project Title
Machine Learning for Materials Design

Project Description
The aim of the proposed project is to enable a rational design approach for electrolytes for Li-ion batteries via a combination of physics-driven models that are coupled with large datasets and machine learning. The design of an electrolyte for properties such as conductivity, voltage stability depends on a large number of properties. While physics-driven models can identify simple descriptors, these tend to be inadequate for actual material selection. The advent of big data and machine learning allows the opportunity to couple physics-driven descriptor selection for machine learning. This effort will leverage our current capabilities around SEED, System for Electrolyte Exploration and Discovery, which contains an exhaustive dataset on liquid electrolytes. In partnership with Citrine Informatics, we aim to leverage the Citrination platform to carry out advanced electrolyte discovery.

Professor Rakesh Tiwari
Chapman University
tiwari@chapman.edu

Department
Life Sciences

Project Title
Developing Neurotherapeutic Agents:

Project Description
We are interested in developing a potent compound that will modulate the brain derived neurotrophic factor (BDNF)/Tropomyosin receptor kinase B (TrkB) receptor signaling pathways to treat Angelman Syndrome (AS), Parkinson's, and ALS. AS is a severe neurogenetic disorder that occurs in one in 15,000 live births with no available drug therapy. This project originates based on developed peptidomimetic CN2097 using rational drug design approaches for AS and neuroprotective agents in the lab of collaborator Dr. John Marshall at Brown University. We as a medicinal chemist in this interdisciplinary team of the investigators are interested in designing and synthesizing various analogs of the potent CN2097 compound to tune physicochemical property without changing potency. This proposal harnesses medicinal chemistry-centered strategies to modulate properties of CN2097 and develop libraries of potent analogs. Detailed information about Dr. Tiwari laboratory can be found at link below
https://sites.chapman.edu/tiwari/

Professor Shaun Brinsmade
Georgetown University
shaun.Brinsmade@georgetown.edu

Department
Biology

Project
Microbiology

Project Description
As for the description: "The scholar will contribute to our efforts to understand how specific regulatory factors control virulence gene expression in Staphylococcus aureus and other Gram-positive bacteria relevant to human health. In doing so, the scholar will learn to apply biochemical, molecular genetics, and cutting-edge imaging techniques to solve biological questions at the intersection of metabolism and pathogenesis. For more information, please see https://brinsmadelab.com/"

Professor Siva Theja
Georgia Institute of Technology
siva.theja@gatech.edu

Department
Industrial & Systems Engineering

Project Description
I work at the intersection of optimization and applied probability, with a focus on resource allocation, scheduling, load balancing and pricing problems in Data centers, Cloud computing, wired and wireless networks, cyber-physical systems and transportation systems.

Professor Pierre F.J Lermusiaux
Massachusetts Institute of Technology
pierrel@mit.edu

Department
Mechanical Engineering

Project Description
Our research vision is to develop and transform ocean modeling and data assimilation and to quantify regional ocean dynamics on multiple scales. Our group creates and utilizes new models and methods for multiscale modeling, uncertainty quantification, data assimilation and the guidance of autonomous vehicles. We then apply these advances to better understand physical, acoustical and biological interactions. Our environment is collaborative within a lively group of students and researchers. We seek both fundamental and applied contributions to build knowledge and benefit society. Many of our present projects are available here http://mseas.mit.edu/?page_id=26 and recent papers here http://mseas.mit.edu/?page_id=526

Professor Nirbhay Kumar
Tulane University
nkumar@tulane.edu

Department
Tropical Medicine

Project Title
Malaria Vaccine Development

Project Description
We are working toward development of an effective malaria vaccines. We use recombinant DNA and immunology techniques to develop and evaluate functional outcome, including parasite transmission through mosquitoes. In other projects, we are also studying DNA damage response

and epigenetic modifications in the parasites exposed to anti-malaria drugs. The students will be involved in ongoing research projects and have the opportunity to learn relevant techniques and scientific approaches.

Professor Yih-Kuen Jan
University of Illinois at Urbana-Champaign
mailto:yjan@illinois.edu

Department
Kinesiology and Community Health

Project Title
Biomedical Engineering

Project Description
The purpose of this project is to develop an algorithm to accommodate the motor impairments of children with cerebral palsy for maneuvering the power wheelchair. The project will involve the analysis of electromyographic signals of the upper extremity and the assessment of wheelchair trajectories.

Professor Philip Kaaret
University of Iowa
philip-kaaret@uiowa.edu

Department
Physics and Astronomy

Project Title
Astrophysics

Project Description
Work to determine whether X-ray binaries, consisting of a neutron star or black hole orbiting a normal star, were important in reionizing the early universe by enabling ionizing photons to escape their host galaxies. Scholars will learn to analyze data from the Chandra X-ray Observatory and likely coauthor a publication on the results

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Professor: Vinod Srinivasan
University of Minnesota
vinods@umn.edu

Department
Mechanical Engineering

Project Title
Characterization of Biodiesel Sprays From a Counter-flow Nozzle

Project Description
We are currently studying the spray energetics and formation of viscous liquids emerging from a novel counter-flow nozzle developed in our lab. This nozzle is able to produce very fine droplets from extremely viscous liquids at very low energy cost, potentially enabling the use of viscous biofuels/vegetable oils as combustion fuels. The student's responsibilities would be to run the facility, assist in data acquisition and analysis of images, and collate and present data on the droplet size distribution as a function of operating parameters such as liquid properties, air and liquid supply pressures and flow rates, and nozzle geometries.

Professor: Vinod Srinivasan
University of Minnesota
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Department
Mechanical Engineering

Project Title
Sand-like Particle Heat Exchanger for Renewable Energy (SPHERE)

Project Description
The next generation of solar-thermal plants will operate at temperatures greater than 700 oC, for which conventional heat transfer fluids are required to be replaced by high temperature ceramic-based fluids (i.e. engineered sand) Researchers in our lab are performing fundamental experiments on heat transfer from cylinders to flowing ceramic particulate media. The understanding of the flow and heat transfer behavior will lead to the design, for the very first time, of a particle heat exchanger for solar-thermal applications. The Khorana scholar would participate in experimental runs, understand principles of automated data acquisition for high temperature systems, and collate and present data on the physics of granular flows.

Professor Robert Landick
University of Wisconsin- Madison
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Department
Biochemistry & Bacteriology

Project Description
An opportunity exists in Summer 2018 for a Khorana Scholar to conduct research in the Landick Lab engineering new synthetic biology tools to control gene expression and metabolism in microbes. Possible foci include biosensors to screen RNA polymerase from pathogens for antibiotic leads and optimizing alpha-proteobacteria for chemical or fuel synthesis from lignocellulose.

Professor Manish Patankar
University of Wisconsin- Madison
patankar@wisc.edu

Department
Obstetrics and Gynecology

Project Title
Disease Specific Diagnostic Tests

Project Description
We are investigating the immunome of circulating B cells, T cells, NK cells and monocytes to identify biomarkers for ovarian cancer and preeclampsia (a pregnancy disorder). The project involves RNASeq analysis in combination with multi-parameter flow cytometry analysis to develop multidimensional datasets. Analysis of the flow cytometry results using t-SNE and other computational algorithms will be pursued to identify a panel of disease-specific biomarkers. Students will work with a team of cancer biologists, reproductive biologists, immunologists and computational biologists.

Khorana Bose Research Opportunities in India

Professor: G. K. Ananthasuresh
Indian Institute of Science
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Department
Mechanical Engineering

Project Title
Multimodal mechanical characterization of biological cells

Project Description
Using techniques we have developed to probe mechanical properties of single biological cells, we are investigating how different cell types behave in different disease conditions as against healthy control cells. This work involves a study on a particular type of cells in a disease condition along with a therapeutic condition to figure out the efficacy of a drug. The student would learn about mechanical testing of biological cells vis-a-vis mechanobiology. A student with bioengineering or biotechnology background is preferred for this project."