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Sunil Badal¹, Jacob Shelley¹, Shawn Michalak², Jessica Hellinger¹
¹Rensselaer Polytechnic Institute, ²Stark State College, North Canton, OH 47720

Effects of Molecular Gas Addition on a Helium-based Flowing Atmospheric-Pressure Afterglow (FAPA) Ambient Desorption/Ionization Source

Mass spectrometry (MS) is very sensitive and selective analytical technique, but often requires extensive sample preparation and/or time-consuming chromatographic methods to purify analytes. This problem has been partly addressed through the development of ambient desorption/ionization (ADI) methods, where chemical species are rapidly desorbed and ionized from their native environment through the use of specially designed ionization sources. Plasma based ADI sources, which employ a low-energy plasma as a means to desorb and ionize molecular species, have attracted considerable attention in the field, but their analytical capabilities are not fully explored. Here, we demonstrate the effects of different operating parameters, such as discharge current, gas flow rate, and gas composition, on plasma processes and ionization chemistries of a flowing atmospheric-pressure afterglow (FAPA) ADI source. Improved ionization capabilities were observed for non-polar analytes when FAPA was operated at higher discharge currents and lower helium gas flow rates. The addition of small fractions of oxygen led to signal enhancement of up to 25 times for small polar analytes such as methanol, and acetone, whereas, aromatic compounds undergo an unusual chemical reaction to form pyrylium. In another case, He:N2 FAPA improved the ion signal for RDX and different ionization pathways of analytes were observed with He:H2 FAPA.
Ashwin Bahulkar\textsuperscript{1}
\textsuperscript{1}Rensselaer Polytechnic Institute

Coevolution of Multiple Social Networks

We present an analysis of a dataset called NetSense, which captures the dynamics of individuals and their co-evolution within two coupled social networks. The first network is cognitive network defined from repeated surveys of students while the second is built from the behavioral network representing actual interactions between these individuals based on records of their mobile calls, text messages and bluetooth collocations. We address several related questions pertaining to the co-evolution of various dynamics among the individuals.
3D bioprinting of vascularized human skin

Poor vascularization after implantation often compromises the survival of skin grafts. Providing a vascular network to promote survival of cells for full-thickness wounds is crucial for proper perfusion and survival of the grafted tissue, especially when the tissue is thick and its survival cannot be supported by local diffusion of oxygen and nutrients. Here, using a 3D bioprinting platform, we show the fabrication of a dermal/epidermal skin equivalent and a vascularized 3D construct, constituted entirely of primary cells (keratinocytes, endothelial cells and dermal fibroblasts). Histology characterization demonstrated that 3D printed skin tissue is morphologically representative of in vivo human skin tissue. In addition, we demonstrate that printed endothelial networks are able to generate interconnected tubular structures with stable lumens within a 3D collagen matrix that persist beyond 50 days. We anticipate that our new strategy for tissue vascularization via 3D cell printing technology will dramatically improve skin graft survival in vivo and shorten the time of graft incorporation with the host skin. Furthermore, printed vascularized skin can also serve as a valuable in vitro platform to evaluate the permeability and toxicity responses of topical and transdermal agents in a high-throughput manner during the preliminary stages of drug discovery and formulation development.
Kaylyn Bell\textsuperscript{1}, William A. Kronert\textsuperscript{1}, Yimming Guo\textsuperscript{2}, Deepti Rao\textsuperscript{2}, Sanford I. Bernstein\textsuperscript{1}, Douglas M. Swank\textsuperscript{1}
\textsuperscript{1}Rensselaer Polytechnic Institute, \textsuperscript{2}San Diego State University

The Muscle Mechanical Basis of Freeman Sheldon Syndrome

We have generated the first animal models for Distal Arthrogryposis type 2A, commonly known as Freeman-Sheldon Syndrome (FSS). FSS is characterized by congenital contractures resulting from point mutations in skeletal muscle contractile proteins, yet how these mutations alter muscle contractile properties is not known. We created two myosin heavy chain transgenes containing point mutations Y583S and T178I, each known to cause dominant FSS. We expressed them in Drosophila muscles, isolated the indirect flight muscles from heterozygous mutant flies, and performed skinned muscle fiber mechanics. The most striking mechanical alteration was a dramatic increase in muscle stiffness. Y583S and T178I fibers’ elastic moduli increased 40\% and 30\%, respectively, under relaxed conditions and 70\% and 46\% when activated. The increased stiffness contributed to decreased work and power generation. Maximum power decreased by 45\% and 62\% because elevated stiffness increased work absorbed values during the lengthening portion of work-loop power measurements. A contributing factor to both decreased power and increased active stiffness was a reduction in rate for at least one strongly-bound cross-bridge cycle transition. This was inferred from 17\% and 31\% decreases in optimal frequency for power generation, and 27\% and 39\% decreases in apparent muscle rate constant $2\pi b$. We conclude that Freeman-Sheldon Syndrome likely results from highly elevated muscle fiber stiffness and decreased ability of the muscles to power limb movement.
Quantifying Synergy in a Model System for Multimodal Ligand Design

Multimodal chromatography represents an important tool in downstream bioprocessing. By using ligands that combine multiple weakly interacting moieties, for example charged, hydrophobic, or hydrogen bonding moieties, multimodal ligands can achieve unique selectivities and complex separations. Here, we present two methods aimed at understanding, predicting, and designing multimodal chromatographic systems.

The first method focuses on developing a theoretical framework for quantifying the total water-mediated interaction between a protein and a multimodal ligand using a PMF-expansion (potentials of mean force expansion) statistical mechanical framework. Such an expansion attempts to estimate the overall free energy of interaction between two complex objects based on contributions from constituent pairs, triplets, etc. of moieties. This method can facilitate multimodal ligand design by enabling the rapid in silico screening of large numbers of ligand designs as well as by generating mechanistic insights into why different multimodal ligands result in different selectivities. The second method employs all-atom Molecular Dynamics (MD) simulations and free energy calculations to identify regions on the protein surface involved in binding and to predict overall binding affinity. We use short all-atom MD simulations to obtain the equilibrated bound structures of the protein of interest in 100 different orientations, and use coarse-grained free energy calculations to estimate binding affinity for each orientation. This method is powerful in that it can predict selectivity and elution behavior as well as generate mechanistic insights for a known protein or set of proteins on a known chromatographic surface.
An Explanation for Acoustic Intensity Patterns from a Mud Propagation Experiment

A classical experiment [Wood and Weston, Acustica 14 (1964)], conducted in Emsworth Harbor at low tide, examined propagation in a 1 m mud layer overlying gravel. Hydrophones on the mud bottom transmitted six source frequencies between 4 and 72 kHz and received signals at ranges up to 50 m. Signal levels show modal fluctuations at lower frequencies but not at higher frequencies, even though the authors did not perform data smoothing. This behavior is hypothesized to arise from a frequency-dependent spread of transmitted frequencies. A Pekeris two-layer model of mud and gravel with a pressure release mud surface is used to idealize the waveguide. Transmission loss is calculated using a weighted frequency average of time-averaged intensity, with a Lorentzian function (Cauchy distribution) modeling the frequency spread. Appropriate values for the Q-factor of the distribution are examined. Compressional wave attenuation values from a recent inversion of the data [Pierce, et al., POMA, accepted (2015)] are incorporated into the calculations. Computational results demonstrate the same behavior in intensity fluctuations as in the data with identifiable modal interference at the three lower frequencies and smoothed patterns at the three higher. [Work supported by the ONR.]
Neutron Spectroscopy for the isotope Mo-96

As global leaders put greater priority on reducing carbon emissions the demand for clean sources of energy becomes greater. Harnessing energy from the sun, whether it is direct conversion from solar radiation or from the macroscopic pressure differences that drive wind farms, is a good clean way to produce energy, but it is not a steady source of energy. Power harnessed from nuclear fission doesn’t emit carbon and provides a steady source of energy that can stabilize a power grid. Developing modern reactors requires accurate computer simulations that rely heavily on data that describe how neutrons interact with the reactor fuel and structural materials. Newly revisited U-Mo fuels have high thermal conductivity and high uranium density, yielding an efficient option for low-enrichment fuels. Neutron interaction cross-sections are experimentally measured and recorded in carefully maintained libraries. This work is part of an effort to increase the accuracy of existing cross-section libraries and to reduce the uncertainty in computer simulations. Neutron transmission measurements were performed at the RPI LINAC using the time-of-flight method with a metallic enriched $^{96}$Mo sample from 0.113-20 keV. Four resonances were assigned an s-wave spin rather than the p-wave assignment in ENDF/B-VII.1. Energies of all fitted resonances were shifted relative to ENDF/B-VII.1, and neutron widths were fitted using the R-matrix Bayesian code SAMMY 8.0. The s-wave strength function $S_0 = 0.87 \pm 0.39$, and the capture resonance integral $R_{Ic} = 17.519 \pm 0.003$ b. These results agree with the values published in the Atlas of Neutron Resonances by Brookhaven National Laboratory.
Kayla Coldsnow¹, Brian Mattes¹, Bill Hintz¹, Jennifer Hurley¹, Rick Relyea¹
¹Rensselaer Polytechnic Institute

Evolved tolerance to road salt disrupts the circadian rhythm of Daphnia pulex

The salinization of freshwater ecosystems is a growing concern, especially for zooplankton (Daphnia pulex), which are essential members of aquatic food webs that help determine water quality. We investigated the potential for Daphnia pulex to adapt to increased road salt (NaCl) and the subsequent consequences of this adaptation on circadian rhythms.

Daphnia were exposed to varying levels of NaCl in a 2.5-month mesocosm experiment and then cultured in the lab. When we subsequently exposed these populations to high concentrations of road salt, populations previously exposed to increased concentrations had higher survival than the control population, confirming they had evolved increased tolerance.

To test their circadian rhythms, we used qRT-PCR to analyze the expression of per, a core clock gene. Daphnia populations adapted to moderate NaCl concentrations showed little difference in their circadian cycle compared to the control population. However, adaptation to high NaCl concentrations ablated the expression of per. Thus, the rapid evolution of tolerance to NaCl has dramatic impacts on the expression of clock genes. Given Daphnia’s importance in aquatic ecosystems, evolved tolerance could buffer ecosystems from salinization. However, ablated circadian rhythms, which may control Daphnia migration in lakes, may have far-reaching effects on biological processes and food-web interactions.
Andrew Cupo¹, Vincent Meunier¹, Neerav Kharche¹
¹Rensselaer Polytechnic Institute

Tunable Band Gap in Phosphorene Antidot Lattices
We used first-principles density functional theory (DFT) calculations to investigate the properties of phosphorene antidot lattices. It was found that the stability (quantified by the edge energy) decreases when the density of edges increases. This trend can be broken for H-passivated systems, where in some cases incrementing to a larger radius can increase stability. Most importantly, the band gap can be widely tuned through variation of the perforation spacing and radius. Moreover, deviations from the expected quantum confinement trends are due to edge effects in general. Spatial distributions of the band gap are roughly bimodal with larger band gap atoms emanating from the zigzag edge, which can be explained by the presence of stronger quantum confinement effects in phosphorene nanoribbons with zigzag termination as compared to armchair termination. Transport will be favored along the armchair direction, which contains a continuous path of the lowest band gap atoms. A system with an electronic signature for metals has bands near the Fermi level that are localized to a new self-passivating 4x1 reconstruction of the zigzag edge and are flat (large effective mass), which suggest transport is not supported. The ability to tune phosphorene's band gap extends its applicability in optoelectronics.
Matthew Dellehunt

\textsuperscript{1}Rensselaer Polytechnic Institute

PLY-Shroud

Art Exhibit
Rahul Divekar¹, Zev Battad¹, Craig Carlson¹, Jieming Ji¹, Qingyun Wang¹, Mei Si¹
¹Rensselaer Polytechnic Institute

Wise Macaw: A social chat-bot built on Amazon Echo
RPI’s team has been selected to compete for Amazon’s Alexa Prize Competition. Towards this effort, we aim to build a chat-bot that converses through voice and runs on Amazon’s Echo device. Our motivation stems from companionship being a fundamental human desire. Our goal is to build a virtual companion -- an emotionally intelligent bot that can converse with a human. The bot will use its personality, humor, and information obtained from online knowledge resources to engage its human partner on both the emotional and practical levels. Our companion bot will bond with its users and make the user-experience as life-like as possible. In our work, we demonstrate how several existing research initiatives at RPI such as story-telling, analogy, etc. are being put together leading to a novel approach in building this companion
Quantification of Nutrient Dependence of SBF/MBF Transcription Factors Controlling Start In Budding Yeast

In all organisms, cells must balance growth and division to maintain cell size homeostasis. Cells commit to division at the end of G1 phase, termed Start in the budding yeast model eukaryote. Start is controlled through the timely activation of the constitutive kinase Cdc28 via G1 cyclins (Cln1-3) which initiates a positive feedback loop allowing for robust activation of Start transcription factors, Swi4/Swi6 (SBF) and Mbp1/Swi6 complex (MBF) responsible for the transcription of over 200 genes involved in cell budding and DNA replication, respectively. However, it remains unknown how nutrients modulate these events. We used two-photon laser scanning Number and Brightness experiments to localize and quantify GFP fusions of Whi5 and the SBF and MBF components. These constructs were expressed from their natural loci at the single cell level in live budding yeast cells grown on rich (glucose) and poor (glycerol) nutrients. All transcription factor components were found to oligomerize in the nucleus and were upregulated in poor nutrient growth. The concentration of Swi6 was found to be limiting compared to the combined concentrations of Swi4 and Mbp1 suggesting competition for binding. These measurements were integrated to a mathematical model of the competition between Swi4 and Mbp1 for Swi6 binding, which predicts that upregulated SBF/MBF components should increase the MBF to SBF expression ratio in lower nutrients.
Colin Garvey¹
¹Rensselaer Polytechnic Institute

On the Democratization of AI R&D

What would it mean to take seriously the democratization of AI? Rather than offering developer tools online for free, I argue that addressing governance of the research and development process itself is the first step to democratization. Drawing on Woodhouse’s framework for democratic decision making through intelligent trial and error (ITE), a design-based approach to the governance of technological R&D that synthesizes the insights of critical technology scholars with democratic political decision theory, I evaluate AI R&D broadly to consider how it could be governed more democratically.

Considerable barriers to the democratization of AI exist. (1) Public deliberation is impaired by deterministic framings of AI’s developmental trajectory, prohibiting partisan disagreement and restricting discussion to a narrow set of concerns. (2) Decision making processes are opaque, exclude most stakeholders, and allocate authority to technical experts and business executives. (3) The rapid pace of AI R&D mitigates against stringent initial precautions and disallows time for social organizations to learn and respond.

Adequately addressing these issues may require significant, unprecedented changes to the R&D process itself—but I would like to believe that the pioneers at the forefront of the field are capable of social innovations in addition to technological breakthroughs.
Viscosity Model For High Index Polymer Nanocomposites

Polymer nanocomposite materials have applications as high index secondary optics for color mixing or graded refractive index (GRIN) materials for microlenses. Processing of these materials is challenging as the effects of grafted polymer nanoparticles on viscosity are hard to predict. There are several models such as the Einstein model or Krieger-Dougherty model that work well for microparticle suspensions but fail to accurately predict the viscosity behavior of nanoparticle suspensions. Previous studies have identified matrix molecular weight, grafted brush molecular weight and particle concentration as key variables. To examine these variables a model system consisting of ZrO2 nanoparticles in PDMS matrix will be used. Oscillatory rheology was done on this system to measure viscosity. Experimental data from rheology experiments was used to generate an empirical equation to predict the viscosity of these materials. This equation can be used in processing of advanced composite materials.
Xiaorui Han¹
¹Rensselaer Polytechnic Institute

Ultrasensitive Detection of Glycosaminoglycans by Rolling Circle Amplification

Glycosaminoglycans (GAGs) are complex polysaccharides that are expressed ubiquitously and abundantly on the cell surface and in the extracellular matrix where they interact with hundreds of proteins and perform a variety of critical roles. Studies during the last several decades have indicated that the changes of GAGs levels are involved in various disease pathologies. Thus, simple and highly sensitive GAG detection methods are needed for the future pathology researches. Rolling circle amplification (RCA) is a DNA replication technique, which can generate a long single DNA strand with multiple repeat units. Since the detection signal of GAGs can be amplified through nucleic amplification, the RCA technique has a good potential to lower the limit of detection of GAGs.
Victoria Hepworth¹, Kelly Jenkins¹, Catherine Royer¹
¹Rensselaer Polytechnic Institute

High Pressure Unfolding of Acyl-CoA-Binding Protein

For over fifty years scientists have been trying to develop well supported theories that explain how proteins are able fold freely into its unique native shape. Folding is studied by perturbing a protein from its native state. The utilization of hydrostatic pressure minimizes the volume of the protein, causing it to unfold, as the unfolded state usually takes up less space than that of the folded. Pressure disrupts the cavities that are located inhomogenously throughout the protein due to improper packing, leading to a local unfolding effect. This makes pressure denaturation a more favorable option compared to chemical or thermal denaturation because it is a more gentle denaturant, allowing for more intermediates to be populated and higher reversibility. Acyl-Coenzyme A binding protein (ACBP) folding has been studied by thermal, urea, and force denaturation to observe different folding pathways when different techniques are used. High pressure fluorescence experiments are used to obtain equilibrium parameters (ΔGo and ΔVo). We wish is to determine a “high pressure m-value” by completing the experiment with two different concentrations of urea. Through the analysis we should be able to understand the manner by which this protein unfolds by pressure in comparison to other unfolding techniques.
Kelly Jenkins\textsuperscript{1}, Martin Fossat\textsuperscript{1,2}, Thuy Dao\textsuperscript{3}, Yi Zhang\textsuperscript{1}, Zackery White\textsuperscript{1}, Doug Barrick\textsuperscript{4} and Catherine A. Royer\textsuperscript{1}

\textsuperscript{1}Rensselaer Polytechnic Institute, \textsuperscript{2}CBS CNRS Montpellier France, \textsuperscript{3}Syracuse University, Syracuse NY, \textsuperscript{4}The Johns Hopkins University, Baltimore MD

Using high pressure to determine the effect of cavities on folding cooperativity in the Leucine rich repeat protein PP32

Proteins are among the important building blocks for life. They are made up of a primary sequence of amino acids which encode their folding pathway as well as their 3D structure. How this primary sequence determines the folding pathway has yet to be fully explained. To study protein folding, a protein is perturbed from its folded or native state, and this is usually accomplished by changing temperature or adding chemical denaturants, whose efficacy depends only upon protein size. Pressure denaturation provides an alternative technique to destabilize folded proteins, as it mainly works to decrease volume by eliminating cavities present in the folded state, thereby leading to a more local unfolding effect. We studied a leucine rich repeat protein called pp32 which has been found with urea denaturation to fold highly cooperatively (where each repeat works together to fold) and has increasing stability from the N- to C-terminus. Cavity forming variants (where one amino acid in the core of the protein is change to a smaller amino acid, leaving a void) were constructed to test how cavities in different parts of the protein would affect folding cooperativity. Our results show that sequence context alters the impact of cavity creation on both stability and cooperativity of folding.
Konstantin Kuzmin\textsuperscript{1}, Xiaoyan Lu\textsuperscript{1}, Partha Sarathi Mukherjee\textsuperscript{1}, Juntao Zhuang\textsuperscript{1}, Chris Gaiteri\textsuperscript{2}, Boleslaw K Szymanski\textsuperscript{1}

\textsuperscript{1}Rensselaer Polytechnic Institute, \textsuperscript{2}Rush University Medical Center, Rush University

Using multilayer networks to promote innovative biological research

Traditionally, the emphasis in biological research was on developing highly specific knowledge about particular diseases and molecules associated with them. However, the growing number of different omics fields is calling for an increase in the breadth of knowledge about massive pools of biological molecules. This demand requires exploring a wide range of potential collaborations which is often limited by institutional, domain, geographic, and other boundaries. Established research programs tend to encourage "safe" incremental research rather than innovative but less predictable transformative approaches. We propose a tool that allows researchers to survey the collaboration landscape associated with their research interests and identify non trivial overlapping interest around novel molecular research topics. Since these collaborations are associated with the researcher's current interests, they can be easy to initiate and therefore low risk. At the same time, these collaborations have the potential for sparking research in novel disease applications. The core component of our solution is a multilayer network populated with different types of data, like molecular interactions, publications, etc. We demonstrate how the tool is used to identify scientists who could contribute to understanding the cellular role of genes with novel associations with Alzheimer's disease, which previously have not been thoroughly characterized.
Contested Meaning at the Feet of the New Colossus

The Statue of Liberty, a widely recognized personification of American values, has served as a symbol of refuge in our popular memories for much of its existence. However, recently, the role of the United States as champion of asylum seekers has been challenged by those fearful of refugees from countries that are also known for extremism. This project seeks to explore the shifting meaning of The Statue of Liberty from “Mother of Exiles” to our old “New Colossus”. Sensory ethnography is utilized to unearth how tourists come to experience The Statue of Liberty in our current historical moment. This phenomenological attempt to understand shifting interpretations of the statue reveals that a reduced emphasis on refuge in the museum and on the narrated boat tour allows for multiple interpretations depending on the values held by tourists.
Benno Lee¹, Peter Fox¹
¹Rensselaer Polytechnic Institute

Modeling Data Versioning Operations

Data sets do not remain stagnant after collection. They must often be corrected and grown to ensure data quality and coverage. Popular version naming methods do not capture the magnitude of change a data set undergoes. We propose a model to capture change information and encode them in a machine-readable fashion into digital change logs.
Fast Event Identification through Subspace Characterization of PMU Data in Power Systems

This paper proposes a data-driven real-time event identification method based on the measurements of Phasor Measurement Units (PMUs). The central idea is to characterize an event by the low-dimensional subspace spanned by the dominant singular vectors of a data matrix that contains spatial-temporal blocks of PMU data. The subspace representation is robust to system initial conditions and characterizes the system dynamics. A dictionary of subspaces that correspond to different events are established off-line, and an event is identified online with the most similar event in the dictionary through subspace comparison. The compact subspace representation reduces the dictionary size and the computational time of the event identification method. Numerical experiments on both simulated events in an IEEE 68-bus power system and record data in New England validate the proposed method.
Variable Annuities based on Structured Product

As the life expectancy has been increasing steadily since the last decade, a large number of population across the world are facing a growing risk of outliving their retirement savings. Granted, annuities, in particular variable annuities, have been advocated to provide a reliable source of life guarantee. However, Financial Crisis in 2007/08 threatened the banking system and gave rise to new challenges of risk management, in which insurance companies inevitably suffered a nightmare due to their variable annuity sectors’ exposure to credit risk and equity market. This paper proposed to investigate an optimal routine to create the optimal asset-liability structures by proposing new financial product design ideas that match the defined individual risk profile with sustained income, along with appropriate hedging strategies to ensure a reliable income level through the extended post-retirement period. In this paper, unlike the traditional investment portfolio consisting of bonds and stocks, derivatives like index options and VIX options are introduced to form a new type of risk structure.
Detection of Metal Ions by Flowing Atmospheric-Pressure Afterglow Mass Spectrometry (FAPA-MS)

Ambient desorption/ionization mass spectrometry (ADI-MS) enables the direct detection of analytes from the surface of objects in open air with minimal or no sample pretreatment. Plasma-based ADI sources, such as the flowing atmospheric-pressure afterglow (FAPA), are usually used for the detection of small organic molecules. In fact, only a few examples of elemental analysis with ADI-MS have been presented in the literature. Atomic ions have negligible vapor pressures, which makes desorption of these species from solid and liquid samples difficult. Here, we explore the ability to directly detect metal ions from complex samples with a FAPA ionization source coupled to a high-resolution mass spectrometer. The desorption efficiency of atomic ions was improved through the aid of chelating ligands, like acetylacetone, to yield volatile complexes. With the aid of chelating ligands, 22 elements, spanning transition metals to actinides, have been detected by FAPA-MS. Detection limits for a number of these analytes were found to be in the tens of parts-per-billion (ppb) and as low as 2 ppb for the uranyl cation complex.
Berardo Matalucci\textsuperscript{1}, Anna Dyson\textsuperscript{1}, Theodorian Borca-Tasciuc\textsuperscript{1}
\textsuperscript{1}Rensselaer Polytechnic Institute

**Investigation of Building Indoor Micro-Climates: Solid-State Heating and Cooling for a Sustainable Personalization of the Thermal Environment**

The conventional approach followed by Heating, Air Conditioning and Ventilation (HVAC) systems is based on an idealized, uniform, and energy-intensive indoor thermal zone, in which conflicting occupant’s preferences often remain unresolved. While previous studies have indicated new strategies for reducing operative energy expenditures through the relaxation of heating and cooling set-points and the use of personal devices, here, I aim to radically improve the way buildings provide comfort and metabolize energy flows. In response, this doctoral study proposes that buildings are repositories of indoor microclimates that can be realized to provide personalized comfort through localized, low-energy heating and cooling, and facilitate on-site net-zero-energy adoptions. This doctoral research aims to: 1) design, test and validate a modular, stand-alone, solid-state system that delivers localized heating and cooling; 2) assess occupants’ responses under diversified thermal environments and inform novel strategies for space heating and cooling. The design of such building systems for personalized thermal comfort will have the broader impact of integrating individuals’ metabolism with building thermodynamics. It will make valuable contributions by offering new technical solutions, through solid-state technologies, allowing novel design strategies and empower occupant experiences.
Clifford Morrison\textsuperscript{1}, Dr. William Armiger\textsuperscript{2}, Dr. David Dodds\textsuperscript{2}  
\textsuperscript{1}Rensselaer Polytechnic Institute, \textsuperscript{2}BioChemInsights, Inc.

Utilizing Electrochemical Bioreactors for Efficient Chemical and Biochemical Applications  
I will investigate the development of electrochemical bioreactors as tools for industrial fermentations and biocatalysis applications. Understanding how electrons and reducing equivalents are transported into cells is critical to engineer microorganisms to optimize carbon efficiencies and product yields. Additionally, understanding how electrochemical NAD(P)H regeneration can be efficiently achieved will allow for the development of technology that allows researchers to utilize biocatalytic processes not easily accessible because of their dependence on stoichiometric amounts of redox cofactor.
Kathleen Morrissey¹
¹Rensselaer Polytechnic Institute

**Discovery of G-quadruplex Aptamers Using a Genome-Inspired Reverse Selection Approach**

Over the last few decades aptamers have become an alternative to antibodies as affinity reagents to a large variety of molecules including proteins. Aptamers were first discovered using the process SELEX. This process is widely used to find new aptamers but it does have certain limitations that can hinder the process of aptamer discovery, particularly for potential aptamers that form multi-tier, G-quadruplex (G4) structures. Such sequences are widespread throughout the human genome and warrant investigation as potential aptamers. We have developed a new genome–inspired, reverse selection approach that allows us to explore these and other challenging sequence spaces. In the reverse selection approach, a specific DNA sequence from the human genome is used for affinity capture of proteins from natural pools such as nuclear protein extracts. The nuclear extracts are incubated with streptavidinated magnetic beads coated with biotinylated G4 oligonucleotides or control oligonucleotides. Rapid screening for affinity captured proteins specific to the G4 DNA is done using MALDI MS. If affinity capture is established, we separate the proteins using gel electrophoresis. Bands that are specific for G4 capture and not the control are analyzed by mass spectroscopy to identify the proteins and the identities are confirmed using Western blotting. Here we will present results of our studies of genomic G4 forming sequences from the promoter region of breast-cancer human genes as potential aptamers for proteins extracted from cell nuclei of breast cancer cell lines.
Alexander New¹, Kristin Bennett¹
¹Rensselaer Polytechnic Institute

Supervised Learning of Predictive Cadres

We consider regression problems in which the population under study may be softly partitioned into a set of clusters such that the behavior of the target variable is more easily understood within any given cluster than it is on the population as a whole. We introduce a discriminative model for a population that, when trained on a set of observations, simultaneously learns clustering and target prediction rules. Our formulation allows priors to be put on the model parameters. These priors allows for independent feature selection processes to be performed during both the clustering and target prediction processes, resulting in simple and interpretable models. An algorithm for parameter learning is developed that reduces the computational infeasibility of the learning optimization problem. We present simulated results showing that, under certain conditions, our method significantly exceeds the performance of simpler methods that learn clustering and target prediction rules separately. Further experimental results show that our method is generally competitive with powerful nonlinear models such as regression forests.
Xiang Niu\textsuperscript{1}, Casey Doyle\textsuperscript{1}, Gyorgy Korniss\textsuperscript{1}, Boleslaw Szymanski\textsuperscript{1}
\textsuperscript{1}Rensselaer Polytechnic Institute

The impact of variable commitment in the Naming Game on consensus formation

One of the crucial questions in evolution of a society is how new ideas are accepted as majority opinion. Computational social systems allow us to study this question via computer simulation of idealized models. Here we study one of such models, the Naming Game that has proven to be an important model of opinion dynamics in complex networks. It is significantly enriched by the introduction of nodes committed to a single opinion. The resulting model is still simple but captures core concepts of opinion dynamics in networks. This model limitation is rigid commitment which never changes. Here we study the effect that making commitment variable has on the dynamics of the system. Committed nodes are assigned a commitment strength, $w$, defining their willingness to lose (in waning), gain (for increasing) or both (in variable) commitment to a single opinion. Such model has committed nodes that can stick to a single opinion for some time without losing their flexibility to change it in the long run. The traditional Naming Game corresponds to setting $w$ at infinity. A change in commitment strength impacts the critical fraction of population necessary for a minority consensus. Increasing $w$ lowers critical fraction for waning commitment but increases this fraction for increasing commitment. Further, we show that if different nodes have different values of $w$, higher standard deviation of $w$ increases the critical fraction for waning commitment and decrease this fraction for increasing commitment.
Step By Step: Dissecting How Heterodimerization Modulates the Catalytic Properties of Heterodimeric Kinesin-2 Motor Domains

Heterodimeric KIF3AC and KIF3AB generate force for microtubule plus-end directed intracellular transport. While the functions of these kinesins are generally known, the significance of heterodimeric motors and advantages they confer to cells are unknown. Previously it was shown that KIF3AC microtubule association and ADP release was intermediate of that of KIF3AA and KIF3CC. In addition, KIF3AB microtubule association and ADP release was significantly slower than that of KIF3AA and KIF3BB. We aimed to determine whether heterodimerization modulates the intrinsic catalytic properties of the motor domains by using stopped-flow and computational methodologies. Mixtures of KIF3AA and KIF3CC or KIF3AA and KIF3BB were rapidly mixed with microtubules plus mantATP. Neither a 1:1 mixture of KIF3AA to KIF3CC nor KIF3AA to KIF3BB could recapitulate the kinetics of ADP release for KIF3AC or KIF3AB, respectively. To determine whether the intrinsic catalytic properties of the motor domains are retained in KIF3AC and KIF3AB, nonlinear ODE modeling of KIF3AC and KIF3AB entry into the processive run was pursued. Simulations showed that heterodimerization modulates the microtubule association of both motor domains, whereas downstream catalytic properties are retained. These results confirm that heterodimerization alters the catalytic properties of each head to establish the mechanochemistry of KIF3AC and KIF3AB.
Chirality, or left-right (LR) asymmetry, is a conserved cell property essential for the proper shaping and positioning of visceral organs during embryonic development. Exposure to teratogens during pregnancy has been shown to disrupt the LR axis resulting in malformations. Due to ethical concerns about using in vitro humanized models, limited investigations have been performed to understand the role of teratogens during pregnancy. Our goal is to identify important signaling pathways involved in stem cell functioning and morphogenesis in order to understand the connection with cell chirality during development. Single human embryonic stem cells (hESCs) were embedded in a 3D bilayer system and treated with different doses of small molecules, such as ROCK and GSK3 regulators. Bright field time-lapse imaging was used to track hESCs rotation. The chiral-based rotation of single hESCs was determined using ImageJ. Data was presented as clockwise (CW) and counterclockwise (CCW) rotation. A large number of hESCs rotated with CCW directionality when treated with different ROCK regulators, and there was a statistically significant difference from controls with a $p$-value $<0.05$. hESCs treated with GSK3 regulators displayed a preference for CW directionality at higher doses. These results suggest that the rotation was significantly switched from CW to CCW directionality at high doses of ROCK and GSK3 regulators as compared to the control groups. Single hESCs strongly rotated with a CCW directionality after treatment with ROCK and GSK3 regulators in a dose-dependent manner. These results may suggest that these signaling pathways play an important role in the establishment of stem cell chirality at early developmental stages.
Andrew Sinkoe\textsuperscript{1} Juergen Hahn\textsuperscript{1}
\textsuperscript{1}Rensselaer Polytechnic Institute

Maximizing the Accuracy of a Mathematical Model for Biological Signaling

In order to understand how biological systems function, it is necessary to study the biochemical mechanisms operating at the cellular level. To facilitate this, mathematical models for biological systems are developed and analyzed, generating new hypotheses of cell function that can be tested experimentally. In addition, these models can be utilized for development of biomedical therapeutics if the model predictions are accurate enough to predict true cellular behavior. The presented work implements a mathematical methodology called optimal experimental design to maximize the accuracy of a model for liver cells and their response to inflammation. The model represents a signaling pathway that carries molecular messages from the cell's exterior to its nucleus so that the cell can respond to the inflammation in its external environment. Simulation results indicate that the optimal experimental design implementation was effective in increasing the accuracy of the model; experiments which replicate the conditions of the simulations may confirm the methodology's effectiveness.
Andres Vargas¹, Kristin Bennett¹
¹Rensselaer Polytechnic Institute

Fault Detection in Smartphone Computer Chip Manufacturing

For my research, I am working on a probabilistic model to detect anomalies in the manufacture of computer chips. For my presentation, I intend to combine mathematical rigor (to explain my approach) with colorful and informative data visualizations (to explain my results).
Effect of Surface Wettability on Thin Film Evaporation Using Spray Cooling

The purpose of this study is to enhance spray cooling multiphase heat transfer through determination and selection of surface wettability and geometry which maximizes evaporation rate. By altering 99.9% aluminum and aluminum 5052 substrates, the surface wettability was altered from hydrophobic to hydrophilic, with micropores, nanopores, and hierarchical pores (nanopores on micropores). An aim of this research is to characterize the relationship between the evaporation rate and substrate contact angle, thereby quantifying the effect of wettability on evaporation heat transfer. It has been shown that hydrophilic samples show the fastest rates of evaporation and that hydrophilic hierarchically-porous substrates yield the lowest contact angle when compared to microporous and nanoporous substrates. Given that the procedures carried out to produce these porous substrates is relatively cheap and the pores are durable, this surface processing technique could be used to enhance evaporation performance in heat exchangers.
Microbial fuel cell (MFC) technology is developed for wastewater treatment and energy generation. Here we evaluate ultrafiltration (UF) membrane filtration as an approach to purify MFC treated effluent for power plant cooling tower water reuse. UF has been widely used in water and wastewater treatment to remove particles and colloids in the nanometer size range. To mitigate UF fouling, we employed photo-induced graft polymerization (PGP) to graft hydrophilic monomers; two candidates identified were a sulfonated betaine, BET SO$_3^-$, and a quaternary amine, N(CH$_3$)$_3^+$. Natural organic matter (NOM), bovine serum albumin (BSA), and sodium alginate (SA) were used as membrane model foulants. Membranes modified with BET SO$_3^-$ and N(CH$_3$)$_3^+$ did not exhibit significantly slower flux decline for the MFC feed, but did show a lower rate of resistance, and lower energy consumption. Membranes modified with 0.6 M BET SO$_3^-$ exhibited significantly slower flux decline for NOM feed, and excellent flux recovery with hydraulic cleaning, but at the expense of higher energy consumption as a result of a higher initial resistance. Modified membranes did not offer significantly improved performance of BSA feed, and consumed more energy, but were easier to clean. For sodium alginate feed, modified membranes exhibited slower flux decline, and excellent flux recovery, but higher energy consumption. The combined pore blockage/cake formation model was able to describe the data quite well, and shows promise as an approach to diagnose fouling mechanisms.
Wei Xing¹, Yoav Peles², Amos Ullmann³, Neima Brauner³, Joel Plawsky¹
¹Rensselaer Polytechnic Institute, ²University of Central Florida, ³Tel Aviv University

Liquid/liquid phase separation heat transfer - a new approach to thermal management?
The potential for applying partially miscible fluid mixture to micro cooling applications
is investigated. Physical evidence of enhanced thermal transport were obtained when the system
undergoes phase separation. Flow visualizations of liquid/liquid phase separation were obtained
and categorized into different flow regimes. The flow patterns affect the heat transfer behavior
of the system. Two effects are responsible for the enhanced thermal transport: latent heat of
mixing and self-induced flow mixing. Reduced pressure drop was observed during experiments
due to the reduction of system viscosity after phase change.
Recognizing human action using computer vision

Robust recognition of human action and activity remains a challenging task partially due to the large volume of intra-class variation. In particular, subject-dependent variation brings uncertainty to the spatial scope and temporal pace of action execution. Such intra-class spatial and temporal variations impose the needs for methods which not only capture the underlying dynamic pattern that is homogeneous within the same action category but also flexible enough to adapt across different trials and subjects. To fulfill such needs, we propose a probabilistic dynamic model called Hierarchical Hidden semi-Markov Model (HHSMM). Leveraging on the Bayesian framework, the model parameters are allowed to vary across different sequences of data which increase the capacity of the model to adapt to intra-class variations including both physical and temporal extent variations in performing the same actions. Meanwhile, the generative learning process allows the model preserving distinctive dynamic pattern for each action class at the population level. Experiments on benchmark human action datasets show our model not only has competitive recognition performance within individual dataset but also has better generalization capability across different datasets."