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PROCEEDINGS

Research Symposium

July 30 – July 31, 2020

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Day 1 | Morning Presentations

July 30, 10:00 am - 11:30 am EDT

AM1

SESSION A: MEDICAL SCIENCE AND TECHNOLOGY

Click here to join this session

Assessing Preference Of Temperature Or Light In Laboratory Mice

Presentation ID: 30-M1
10:05 am - 10:20 am EDT

Haley Davis, Amanda Barabas, and Brianna Gaskill*
*PI: Department of Animal Sciences
Purdue University

Keywords: *Animal Welfare, Temperature Preference, Light Preference, Nesting Material, Mice*

Mice experience several stressors in the laboratory, which reduces welfare and data quality. First, they are typically kept in temperatures between 20-24°C; however, this is lower than their preferred temperature of 30°C. When given the option, mice will locomote to get to their preferred temperature or use nesting material as insulation. Second, it has been shown that rodents spend more time in the colored-tinted enrichments compared to clear. This is likely because they cannot see red wavelengths. Consequently red cages appear dark to them, which is likely preferable for them as nocturnal species. This study investigated lighting environment and surface temperature preference in laboratory mice by giving them free access between two linked cages: a heated cage and a red cage. Seven pairs of female mice were randomly allocated to two linked cages for eight days. Every other day, the temperature in the heated cage was randomly changed between 20, 24, 28, and 32°C and the weight of nesting material and nest complexity score was observed in each cage. This indicates the nest site where the mice preferred to sleep. The difference between the red and heated cage were analyzed as a repeated measures GLM. Temperature did not have a significant effect on nest weights ($F_{3,\ 13.81}=1.03$; $p=0.41$) or nest scores ($F_{3,\ 14.29}=1.77$; $p=0.19$). Indicating mice did not have a temperature preference for nest building but did prefer to build in the dark cages. This allows researchers to better understand the needs and preferences of mice; thus, improving overall welfare.

Investigation Of A Common Canine Factor VII Deficiency Variant In Dogs With Unexplained, Excessive Bleeding On Necropsy

Presentation ID: 30-M2
10:20 am - 10:35 am EDT

Jessica A. Clark, Stephen Hooser, Dayna L. Dreger, and Kari J. Ekenstedt*
*PI: Department of Basic Medical Sciences
Purdue University

Keywords: *FVII, Hemophilia, Dog, Bleeding Disorder, Mutation*

Factor VII (FVII) protein is an integral component of the extrinsic coagulation pathway. Deleterious variants in the gene encoding this protein can result in factor VII deficiency (FVIID), a bleeding disorder characterized by abnormal (slowed) clotting that presents in a wide range of severity, from asymptomatic to life-threatening. In canids, a single FVIID-associated variant, first described in Beagles, has been observed in nearly two dozen breeds and mixed-breed dogs. Because this variant is widespread among dogs, it was hypothesized that it could be a contributing factor to unexplained excessive bleeding observed in some canine necropsy cases. DNA was extracted from tissue samples from 41 cases, and each dog was genotyped for the c.407G>A variant. Forty cases were homozygous for the wild type allele. One case was homozygous for a novel mutation at the same locus (c.407G>T, p.Gly136Val); this variant is predicted to be pathogenic. These results indicate that, while it is unlikely the common FVIID variant is responsible for most cases of unexplained bleeding at necropsy, the locus does appear to be susceptible to change, as we have now documented a second nucleotide substitution at the same position.

Behavioral Comparison Of Comodulation Masking Release Between Chinchillas And Humans

Presentation ID: 30-M3
10:35 am - 10:50 am EDT

Fernando Aguilera De Alba[1], Vibha Viswanathan[2], Andrew Sivaprakasam[2,3], and Michael Heinz*[2]
*PI: Weldon School of Biomedical Engineering
Arizona State University[1], Purdue University[2], and Indiana University[3]

Keywords: *Comodulation Masking Release, CMR, Chinchilla, Human, Cocktail Party Listening, Hearing Loss*

The auditory system is essential to human survival and communication. Moderate noise-induced damage to inner hair cells (IHCs) and outer hair cells (OHCs) within the cochlea leads to noise-induced hearing loss (NIHL) making it difficult to hear in noise (i.e. cocktail-party effect). Currently, the severity of NIHL in humans is challenging to quantify due to the inability to use the highly invasive neural assays performed in animals, and the overly simplified

testing paradigms available for behavioral assays. Pure tone discrimination behavioral tasks fail to quantify the effects of NIHL in speech perception, which tend to involve background noise and multiple speakers. Comodulation masking release (CMR), known to occur in humans, has shown potential to non-invasively estimate sound detection thresholds in the presence of noise. This study examined CMR effects in normal-hearing chinchillas (a common pre-clinical animal model of human hearing) and human subjects using several paradigms to measure detection of a tone in different flanking-band conditions. Moreover, effects of task repetition and task complexity were studied for humans only. Tone-in-noise stimuli were comodulated for three masking conditions: reference (REF)1, correlated (CORR)2, and anti-correlated (ACORR)3. Experimental stimuli confirmed CMR effect in humans. In humans, CORR thresholds were significantly reduced compared to REF and ACORR thresholds. No task training effect was observed. Although no significant CMR effects were observed in chinchillas, ACORR thresholds were the lowest across all three masking conditions.

SESSION B: ENVIRONMENTAL CHARACTERIZATION

[Click here to join this session]

Development Of Open-Source Beehive Monitoring Systems

Presentation ID: 30-M4
10:05 am - 10:20 am EDT

Nathan C. Sprague, Eric Kong, Brock Harpur, and John Evans*
*PI: Department of Agricultural & Biological Engineering
Purdue University

Keywords: *Beehive, Continuous Measurement, Scales, Bees, Computer Vision*

Honeybees are a key part of agriculture and are necessary for the pollination of numerous crops, including the most common fruit trees. Continuous monitoring of beehive temperature, humidity, weight, and bee count can provide beekeepers with data to assess the health of their hives. Currently, beekeepers must manually inspect their hives and have little idea of their health until the next inspection, sometimes resulting in preventable actions such as swarming, where a large portion of the hive leaves. An entomologist needed a cost-effective and simple way to continuously record key data points for multiple beehives. Commercial hive monitoring systems are expensive for large scale operations. The 50 kilogram (kg) load cells meant to be used as bathroom scales were tested for accuracy by regularly recording weights between 0 to 55 kg indoors and outdoors. The temperature and humidity were measured with DHT22 sensors. Three controllers (Arduino, Raspberry Pi and ESP32) were tested to record data from the sensors and relay data to an app created for the project. The components were tested to note and correct failures and accuracy issues as necessary. Using OpenCV, an open-source computer vision library, a Haar Cascade was trained to detect bees by searching for features that are unique to honeybees. The Haar Cascade was trained with 2,000 images of bees to detect and count bees on a hive frame. Depending on the settings, the bee detection algorithm could correctly locate around half of all bees shown. The scales varied less than 0.5 kg when loaded to their maximum, over the course of two months in an indoor environment and 2 kg outdoors. Hardware failures were almost exclusively from unreliable SD card readers and incorrect scale setup, which is correctable. Indoors, the cost effective microcontrollers gave accurate continuous measurement of beehive weight, along with environmental characteristics such as temperature and humidity. Outdoors, the effects of temperature and humidity were greater than the daily changes of the hive's true weight, so the scale is only suitable for recording seasonal trends in the hive's weight.

Improving Biomass Prediction Of Soybean Using Multispectral Imagery

Presentation ID: 30-M5
10:20 am - 10:35 am EDT

Siddhant Singh[1], Bilal Abughali[2], and Keith Cherkauer*[2]
*PI: Department of Agricultural & Biological Engineering
Macalester College[1], and Purdue University[2]

Keywords: *Soybean, Remote Sensing, UAS, Vegetation Indices*

Erratic weather patterns due to climate change and a burgeoning population have necessitated a better understanding of crop management and resource utilization in agriculture. We investigate the growth of soybean using Unmanned Aerial Systems (UAS) in order to build better models for biomass and leaf area index prediction. We calibrate reflectance values obtained from panels placed in the field using ground measurements in order to calculate the various vegetation indices and subsequently used them in empirical models for predicting biomass and leaf area index using python programs. In this project, we sought to determine the efficacy of using individual images over aggregating those images into a single orthophotomosaic for calibrating the reflectance values. Boxplots indicated different median values and greater spread of digital numbers (which quantify intensity of a pixel) for individual images than in the case of the resulting orthophotomosaics. This study further compares the vegetation indices and subsequent biomass predictions obtained from these separate calibration methods and compares them with laboratory measurements to see if calibration using individual images gives more accurate results. The results of this study can provide crucial insight on improving biomass models for UAS applications and understanding soybean growth.

Modeling Spatial And Temporal Emissions For Animal Farming Using Mechanistic Models

Martina L. Macaggi[1], Gargeya Vunnava[1], Yunru Chen[2], and Shweta Singh*[1]
*PI: Department of Agricultural & Biological Engineering
Purdue University[1], and Johns Hopkins University[2]

Presentation ID: 30-M6
10:35 am - 10:50 am EDT

Keywords: *Sustainability, Modelling, Animal Farming, Hog Farming, Environment*

Modeling the production technique of any live animal-based industry is often challenging as the mass transformation process from feed intake to biological body mass growth is very complex. The body mass of animals can vary based on several factors such as quantity and type of nutrient feed, water intake, age, gender, climate and living conditions, etc. In this study, we use a computational model developed in MATLAB to model the hog farming industry in Illinois. The model uses different biomass growth equations for different hog age groups. The nutrient and water intake data were obtained from the United States Department of Agriculture (USDA) databases. The environmental impacts of the hog farming in Illinois were also quantified by integrating environmental impact assessment equations to capture emissions such as CO_2 and methane.
Information regarding characteristics of the hogs and hog feed was gathered here: https://www.nationalhogfarmer.com/nutrition/gestation-diet-s-impact-pig-birth-weights
Formulas derived by the LEAP program of the United Nation's FAO are being used to calculate the methane emissions of the farm. Certain assumptions were made regarding the environmental impact assessment: (1) Assume the hog farm uses a deep pit manure management system, (2) The deep pit system collects 100% of the manure, therefore 100% of manure produced is treated by the system.

NAPRA+: Development Of An Updated Version Of The National Agricultural Pesticide Risk Analysis (NAPRA) WWW System Using Open Source Tools

Julia Schneider, Benjamin Hancock, Ian Zimmer, and Dharmendra Saraswat*
*PI: Department of Agricultural & Biological Engineering
Purdue University

Presentation ID: 30-M7
10:50 am - 11:05 am EDT

Keywords: *NAPRA, Javascript, GLEAMS, SDSS, Open source tools*

The National Agricultural Pesticide Risk Analysis (NAPRA) model, used to provide farmers with agricultural management practices to prevent hazardous chemicals in ground and surface water, was integrated with Groundwater Loading Effects of Agricultural Management Systems (GLEAMS) model in 2003 to help develop a spatial decision support system (SDSS). The SDSS allowed numerous stakeholders such as researchers, consultants, and non-governmental organization (NGO) personnel to assess the impact of agricultural management practices on nutrient loss and pesticide runoff from individual fields. Due to advancement in web technologies and lack of maintenance, the SDSS became outdated and was taken off the internet in 2018. In addition, lack of source code documentation and rotation of personnel, made it difficult to implement revisions later on. In this project, open source tools were used to create an updated version of NAPRA named NAPRA+, with source code fully commented to make it easy to revise and maintain. The process entailed revising old source code written in Perl into Javascript. Another outcome of this project is the development of a user manual based on test data from the original project to help potential users learn to use NAPRA+ in a proper manner. The results showcase the effectiveness of using open-source tools for developing web-based environmental models and good software development practices for help any future enhancement and updates.

The Impact Of Extended Stagnation On Building Water Quality

Danielle M. Angert, Kyungyeon Ra, Caitlin Proctor, and Andrew Whelton*
*PI: Lyles School of Civil Engineering
Purdue University

Presentation ID: 30-M8
11:05 am - 11:20 am EDT

Keywords: *Building Water System, Stagnation, Water Quality, Chlorine Decay*

Water quality can change drastically within a building during periods of stagnation. This study aimed to better understand the change in water quality within a 10,000 sqft residential building over 5 months of stagnation. Building water stagnation is a public health concern: residual disinfectant agents such as chlorine can decay, leading to microbial growth, and metals can leach into the water over time. Hot and cold water quality was monitored within a large residential building over five months of little to no occupancy, with the long-term stagnation driven by the COVID-19 pandemic. Sampling events occurred once every month between April and July 2020, ranging from approximately 1 month to 5 months total stagnation time. Water samples were taken at ten locations within the building, including bathroom sinks, a kitchen sink, and showers on the basement, second, and third floors of the building. A total of 40 samples were collected. Samples were analyzed on-site for pH, temperature, dissolved oxygen (DO), and total chlorine, then transported to lab for analysis of metal content, total organic carbon (TOC), total cell count (TCC), quantitative polymerase chain reaction (qPCR), and *Legionella pneumophila*. Chlorine residual was not legally detectable (>0.2 mg/L) at any sampling location throughout the five month stagnation period. Lead was detected at seven locations, in concentrations ranging from 1.92 ppb to 8.2 ppb. Apparent but unconfirmed *Legionella pneumophila* was present at 2 locations. These results suggest that building water may need to be refreshed after extended building closures prior to re-entry.

SESSION C: THERMAL TECHNOLOGY

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Design Optimization Of 3D Printed Micro-channel Heat Sinks

Presentation ID: 30-M9
10:05 am - 10:20 am EDT

Rafael L. Estrella[1], Serdar Ozguc[2], Liang Pan[2], and Justin A. Weibel*[2]
*PI: School of Mechanical Engineering
University of Arkansas[1], and Purdue University[2]

Keywords: *Thermal Management, Additive Manufacturing, Topology Optimization*

There is a need for more efficient thermal management solutions to keep the next generation of electronic devices within the operational temperatures. Additively manufactured liquid-cooled microchannel heat sink designs with complex geometric features in particular have been demonstrated to achieve high cooling performance. Topology optimization shows potential in effectively leveraging the design freedom brought by 3D printing as a means to generate high performance designs. This study focuses on generating high performance designs with complex geometries using topology optimization which can be easily 3D printed. Effects of different hyperparameters and operating conditions such as design resolution, flow rate, hot spot geometry on topologically optimized microchannel heat sink thermal resistance and pressure drop were investigated. The performance of topologically optimized designs was evaluated against conventional microchannel heat sink designs at different hot spot geometries. It was shown that optimum grid and unit cell resolutions exist for a given set of operating conditions that minimizes thermal resistance and pressure drop, beyond which returns are reduced. The relative performance enhancement achieved by topology optimization was found to highly depend on the hot spot size and geometry.

Design And Manufacturing Of Bio-Inspired Nanocomposites For Radiative Cooling

Presentation ID: 30-M10
10:20 am - 10:35 am EDT

Fernando J. Barrios, Richard Smith, Andrea Felicelli, Joseph Peoples, George Chiu, and Xiulin Ruan*
*PI: School of Mechanical Engineering
Purdue University

Keywords: *Nanotechnology, Bio-Inspiration, Bio Mimicry, Radiative Cooling, Heat Transfer, Energy Saving, Nanostructure*

Cooling buildings correspond to 10 percent of energy consumption or 380 billion kWh. Furthermore, conventional cooling systems transport heat from inside to outside the building, creating the heat island effect and worsening global warming .In recent years, radiative cooling has emerged as a better technique to dissipate heat by dumping it into deep space, providing cooling without power consumption and addressing the global warming challenge. In this work, our objective is to understand how radiative cooling properties appear in animal shells and aim to mimic these structures and test the properties. We used two MATLAB codes, based on Monte Carlo and transfer matrix methods, to compare optical properties of two nanoporous shells with different morphologies. Variables based on measurements were needed to perform the simulations. Therefore ImageJ, an image processing program, was used to analyze SEM images of the two shells and obtain them. The main results of the current research are a graph that contains reflectivity of both structures over the solar spectra. It was found that both morphologies show promise as radiative cooling materials, while the new bio-inspired shell had a better reflectivity than its predecessor with same thickness. Nanocomposites are being manufactured to mimic the identified optimum shell structures, and their properties will be characterized with optical spectroscopies. To conclude, our research provides insights on which structures give the better radiative cooling performance. Moreover, the new bio-inspired structure can give good reflectivity with lower thickness, meaning it can be used in various situations to cool down objects.

Design And Analysis Of A Novel Membrane Heat Exchanger

Presentation ID: 30-M11
10:35 am - 10:50 am EDT

Bryan Pamintuan, Andrew Fix, David Warsinger, and James Braun*
*PI: School of Mechanical Engineering
Purdue University

Keywords: *HVAC, Dehumidification, Membranes, Energy Efficient Buildings, Thermodynamic Analysis*

Traditional heating, ventilation, and air conditioning (HVAC) systems utilize the vapor compression cycle to dehumidify air through condensation at very low temperatures. Operation of this cycle at low temperatures and the phase change involved in condensing a vapor to a liquid are associated with significant energy usage. Thus, this conventional method of air treatment suffers from energy penalties in hot, humid climates where large amounts of dehumidification are required. Membrane dehumidification has recently been studied as an alternative method of dehumidification that utilizes a pressure gradient across a semipermeable membrane to mechanically separate water vapor from air, avoiding condensation altogether. An HVAC system that integrates and optimizes membrane dehumidification and cooling could result in substantial energy savings. In this study, thermodynamic modeling is used to analyze the overall air treatment performance of the existing vapor compression, adsorption dehumidification, and membrane HVAC systems for a range of outdoor conditions. Then, a novel membrane system configuration of simultaneous cooling and dehumidification (the membrane heat exchanger) is proposed and similarly analyzed. The performance of the membrane heat exchanger is simulated in a variety of climates using EnergyPlus (modeling software developed by the US DOE). Modeling of the system demonstrates the potential

improvements in air treatment efficiency. An experimental testing apparatus is designed and modeled for future small-scale validation of the proposed configuration. The results demonstrate the viability of the proposed membrane heat exchanger and the possible electrical energy savings in different areas of the world.

SESSION D: MACHINE LEARNING I: BIG DATA

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Income Inequality Effect On Travel Pattern During COVID-19

Chengyuan Yang, Takahiro Yabe, and Satish Ukkusuri*
*PI: Lyles School of Civil Engineering
Purdue University

Presentation ID: 30-M12
10:05 am - 10:20 am EDT

COVID-19 is the largest catastrophe people encountered in the year 2020. The situation is severe for the people who stay in the United States, with the total number of cases reaching 4 million. Studies on the behavior of people during the COVID-19 crisis are necessary to inform government decisions on non-pharmaceutical interventions. Using large scale mobility data collected from mobile phones and open census data, we unravel human mobility patterns during the COVID-19 pandemic. More specifically, we understand travel behavior and exiting inequality across income groups. To achieve these goals, we apply time series analysis methods and statistical analysis techniques. In this study, we have focused on the states of New York and Indiana. In New York state, the higher-income class intended to travel further, while Indiana people had an opposite trend. Further analysis of the New York residents showed that New Jersey, Florida, and Connecticut were among the three most popular destinations for the high income group population in New York.

Keywords: *Large Scale Mobility Data, Time Series Analysis, COVID-19*

Analyzing Social Distancing Using Large Scale Computer Vision

Isha Ghodgaonkar[1], Abhinav Goel[1], Subhankar Chakraborty[2], Fischer Bordwell[1], Kohsuke Kimura[1], Shane Allcroft[1], Mohammed Metwaly[1], Vishnu Banna[1], Akhil Chinnakotla[1], Ellen Zhao[1], Caleb Tung[1], George K. Thiruvathukal[3], Wei Zakharov[1], and Yung-Hsaing Lu*[1]
*PI: School of Electrical and Computer Engineering
Purdue University[1], IIT Madras[2], and Loyola University Chicago[3]

Presentation ID: 30-M13
10:20 am - 10:35 am EDT

With the development of the COVID-19 pandemic, countries around the world have published social distancing guidelines to constrain the spread of the disease. However, monitoring the efficacy of these guidelines is difficult without knowing whether social distancing is being practiced. Lack of traditional observational methods, such as in-person reporting, make it difficult to collect visual data in order to confirm that persons are following social distancing guidelines. An existing network camera database developed by Purdue University researchers provides a unique opportunity to investigate social distancing around the world without putting researchers at risk. In this work, we investigate crowd sizes in public areas over time. We also analyze whether citizens are observing a distance of 6 feet between one another. To perform these analyses, we narrow down over 8 TB of video and images to about 4 TB. We run person detection to detect people in the images and video. We then plot these data in a time-series fashion and observe changes over time. To detect physical distancing of 6 feet, we develop a camera perspective-independent, automatic algorithm to determine whether 2 detected people are 6 feet apart. We find that in the United States, there is no change in crowd sizes over time, but in European countries such as France and Germany, there is an increase in crowd sizes following lifting of lockdown policies. Our work will inform future pandemic policies by elucidating which policies are better at controlling the spread of the virus.

Keywords: *Social Distancing, COVID-19, Computer Vision, Deep Learning, Object Detection, Big Data*

Impact Of State HCBS Waiver Policies On Patient Outcomes

Makayla Roma[1], Jennifer Leising[2], Ping Huang[2], and Paul Griffin*[2]
*PI: School of Industrial Engineering
University at Buffalo[1], and Purdue University[2]

Presentation ID: 30-M14
10:35 am - 10:50 am EDT

With long term care costs on the rise, states have begun to expand home and community based services (HCBS) using 1915c waivers in hopes of lowering institutional and long term care costs. The use of these waivers varies greatly among states making it difficult to assess patient outcomes. The objective of this study is to determine the impact of different state waiver policies on patient outcomes. Two separate stepwise ordinal logistic regression models were used to determine HCBS policy impacts on patient outcomes of cost and quality. The results of our study indicate that use of cost controls, geographic controls, and stricter financial eligibility are associated with increased inpatient services spending, while the use of self-direction, and 1115 waivers are associated with less spending on inpatient services. The use of service controls and cost controls were associated with higher level of readmissions as well while, the use of self-direction is associated with lower levels of readmissions. From these results we can conclude that there is an association between poorer patient outcomes and the following policies:

Keywords: *Long Term Care, 1915c Waivers, State Policy, Medicaid, Patient Outcomes*

cost controls, service controls, and geographic controls. It is possible these policies are limiting HCBS waiver usage providing inadequate care resulting in higher spending on patients and higher readmission levels. While these policies try to limit waiver expenditures, the results of our study indicate these policies may actually be increasing patient costs and decreasing quality.

Effects Of Lifting Task On Heart Rate

Presentation ID: 30-M15
10:50 am - 11:05 am EDT

Nan Chen, Guoyang Zhou, and Denny Yu*
*PI: School of Industrial Engineering
Purdue University

Keywords: *Lifting Index, Heart Rate, NIOSH*

In the working field, work injuries can be easily caused by overload and repetitive lifting. Experts have developed numerous task-factors based guidelines to evaluate lifting risks, such as the National Institute for Occupational Safety and Health (NIOSH) lifting equation. However, most of the existing guidelines require task factors that are hard to attain in real life, for example, the object's weight. Previous works have also been focused on measuring muscle activity or body movements to evaluate lifting risks. However, sensors that can measure muscle activity (e.g., sEMg) or body motion (e.g.,IMUs) are highly intrusive and expensive. Wearable devices that can measure heart rate are becoming more and more popular in the market these days. In this study, we purposed using wearable heartrate sensors to evaluate people's risk in lifting. In the experiment, we have designed three different lifting tasks with different lifting indexes for subjects to perform. While the subjects are performing the lifting tasks, we record their heart rate data and provide conclusions and recommendations based on our observation of the changes in the subjects' heart rate.

SESSION E: MATERIAL MODELING AND SIMULATION

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Three-Dimensional Structural Real-Time Hybrid Simulations Applied To Extra-Terrestrial Habitats

Presentation ID: 30-M16
10:05 am - 10:20 am EDT

Sterling Reynolds[1], Yuguang Fu[2], Arturo Montoya[1], Amin Maghareh[2], Davide Ziviani[2], Arsalan Majlesi[1], Adnan Shahriar[1], Mehdi Najarian[1], Jordan Soberg[2], and Shirley Dyke*[2]
*PI: School of Mechanical Engineering
University of Texas at San Antonio[1], and Purdue University[2]

Keywords: *Real-Time Hybrid Simulation, Structural Dynamics, OpenSees Modeling, Geodesic Dome, Extra-Terrestrial Habitats*

Extra-terrestrial habitats must be resilient with capabilities in adapting, absorbing and rapidly recovering from expected and unexpected disruptions without fundamental changes in function or sacrifices in safety. Multi-physics cyber physical testing is crucial in understanding the resiliency of extra-terrestrial habitats where physical loading conditions are applied, and structural software is evaluated. The novel test-bed being constructed at Purdue University serves partially to validate and assist development of structural software methods using computational mechanics under nominal and hazardous operational or dormant states. Emulating emergent behaviors of deep space habitats on Earth is physically limited and pure numerical models need validation, thus the authors propose using real-time hybrid simulations (RTHS). RTHS joins physical structures and computational models, where numerical models are updated with physical measurement data to obtain structural system responses in real time. The authors implement RTHS methods with three-dimensional computational mechanics using OpenSees open-source finite element (FE) software. The OpenSees model is reduced from 276 to 138DOF by neglecting nodal rotations, resulting in real-time capabilities under ground acceleration loading using truss elements. The mass matrix of the reduced model is updated to resemble the addition of shell panels while neglecting their stiffness contribution to the structure and is verified using Abaqus commercial FE software with a natural frequency analysis. By using OpenSees software with many FE methods, materials, and solvers available, researchers can accelerate evaluating resiliency of extra-terrestrial habitats by altering geometries and configurations for real time hybrid simulation application.

Finite Element Modeling Of Transmembrane Potential Under Applied Electric Fields

Presentation ID: 30-M17
10:20 am - 10:35 am EDT

Lorin Breen and Allen Garner*
*PI: School of Nuclear Engineering
Purdue University

Keywords: *Electroporation, Cell Inactivation, Finite Element Method*

Pulsed electric fields (PEFs) are well known for disrupting cells by inducing a transmembrane potential on the order of 1 V to cause electroporation, which is a process in which the cell membrane begins to produce pores. PEFs of sufficient electric field strength and duration can create sufficiently large pores that cannot reseal after exposure, leading to cell death. While many studies have modeled PEF exposure, most have focused on simple models, such as spherical cells representing mammalian cells (with or without a nucleus) with the electrodes in direct contact with the suspension. While these models have been extended in one or more ways (for instance, using non-spherical

cells or incorporating a dielectric between the electrodes and the suspension), a more generalized model that can guide experiments with non-spherical cells with cell walls could provide valuable information for applications in agriculture and decontamination. Examples include microorganisms, such as algae and bacteria, in Petri dishes where one cannot leverage the standard planar geometry used in simpler experiments. Initial calculations using Maxwell 3D have reproduced transmembrane potential for spherical mammalian cells with and without a nucleus for a PEF and an alternating current (AC) field. Next, Maxwell 3D will be used to model the transmembrane potential and the potential drop across the cell wall for spherical and non-spherical cells under various conditions. These results will eventually be compared to experimental results for various conditions to assess the feasibility of using Maxwell 3D simulations to guide parameter selection for optimizing biological response to PEFs and other electric waveforms, such as AC fields.

Automatic Machining Feature Generation

Presentation ID: 30-M18
10:35 am - 10:50 am EDT

Siying Chen, Xingyu Fu, and Martin Jun*
*PI: School of Mechanical Engineering
Purdue University

Keywords: *Modeling and Simulation, Computer and Web Based Application, Manufacturing*

In the era of fourth industrial revolution, a high level of automation in manufacturing is required. Automatic machining feature generation is needed for training the Convolution-Neural-Network-based automated feature identification. The objective of the research is to develop an automatic machining feature generation system that can demonstrate and save massive CAD models with machining features spontaneously. In this research, a feature generation algorithm was built based on FreeCAD geometrical calculation library. About 200 of CAD models were collected to learn about machinability and machining processes. Basic CAD functions include building geometries, setting view, importing and exporting files, extrusion, and operating Boolean. Compiling code for these CAD functions set up a database of functions for further machining feature generation. Machining features like slot were generated by using Boolean operation. The size of the cubic base was set as 50x50x50. When generating the features, tolerance of 1 was set to avoid the appearance of thin walls that cannot be manufactured or small features that cannot be identified. The sizes of the features were set as random by using uniform random parameter with the consideration of the sizes and other parameters of actual cutting tools. Four types of slot features were generated, which included T-slot, V-slot, ball end slot and dovetail slot. Folders for the features were created automatically. 100 CAD models for each of the slot features were displayed in the window of FreeCAD and saved in these folders spontaneously by iteration. Automatic feature generation developed in the research provides the foundation for developing the automated identification of machinability and the processes of machining.

Optimization Of Centrifugally Tensioned Metastable Fluid Detectors (CTMFD) For Alpha And Neutron Detection

Presentation ID: 30-M19
10:50 am - 11:05 am EDT

Jacob Minnette, Nathan Boyle, and Rusi Taleyarkhan*
*PI: School of Nuclear Engineering
Purdue University

Keywords: *Metastable Fluids, Radiation Detection, Degassing, Spectroscopy*

Tensioned metastable fluid detectors (TMFDs) boast the ability to detect neutron, alpha, and fission fragment particles with high intrinsic efficiencies approaching 95%+ while remaining blind to background gamma-beta radiation. Consequently, TMFDs are able to differentiate, with great accuracy, the decay signatures form specific radioisotopes that may either pose a health or national security hazard, e.g. Actinides (like Pu, and U) and Radon and its related progeny isotopes. In TMFDs, the detection fluid is placed under tension or in other words sub-vacuum (negative) pressure (Pneg) states, whereby it can become selectively sensitive to various types of radiation and neutron-alpha type particles can be detected via transient cavitation bubble formation – a process that can be seen, heard and recorded electronically. Desired Pneg states can be induced via tailored acoustics, or use of centrifugal force. For the purposes of this project the centrifugally tensioned detector (CTMFD) design was utilized. Of importance involves ensuring absence of false bubble detection events caused due to pre-dissolved gases in the CTMFD fluid – a time consuming process. Optimizing (reducing) the time for such degassing was the focus of this project. This was accomplished via acoustic agitation, vacuum pulling, and further accelerated gas removal induced via external neutron source. All such methodologies make use of Fick's Laws of Diffusion in expediting the process of removing non-condensable gases from the liquid media (mainly via creating of large concentration gradients between liquid-vapor phases). The results of this research enabled ~60-80% functionality improvement.

Automated Fitting Of Freeform Surfaces To Point Cloud Datasets For Comparison Of Manufactured Components

Presentation ID: 30-M20

11:05 am - 11:20 am EDT

Ryoma A. Kawakami[1], Saikiran Gopalakrishnan[2], and Michael Sangid*[2]
*PI: School of Aeronautics and Astronautics
The Ohio State University[1], and Purdue University[2]

Keywords: *Point Cloud, Surface Fitting, Computer-Aided Design (CAD), Materials Review Board (MRB), Manufacturing, Coordinate Measurement Machine (CMM)*

During manufacturing, the produced components often possess variations in their geometries due to manufacturing variability, potentially resulting in components with features that exceed allowable tolerances. Before eliminating these components as scrap, their structural integrity can be analyzed within a materials review board (MRB) process, to make more informed decisions to use as-is, repair and use, or eliminate the component. However, to perform the structural analysis for disposition of these components, creating models replicating the manufactured geometries is necessary. Currently, this process would involve physically measuring each component, followed by interpreting and utilizing the data for manual creation of CAD models, which is error-prone and time-consuming. To improve this process, we present a framework which enables an automated approach of creating CAD models of individual manufactured components, starting from their nominal CAD models. Firstly, the framework facilitates integration of point cloud measurement data from a manufactured component obtained using a coordinate measurement machine (CMM) to measured surface features within the nominal CAD model. Secondly, it enables retrieval of these datasets and applying a suitable surface fitting algorithm, to update the surfaces in nominal CAD model to create an as-manufactured CAD model of the component. A specific use case has been demonstrated for components with a machined surface with varying geometries, wherein the as-manufactured surfaces have been generated by fitting the scanned point cloud dataset using freeform spline surfaces to generate as-manufactured instances of CAD models of individual components. The demonstrated framework presents opportunities to create digital twins of serialized physical components.

Day 1 | Afternoon Presentations

July 30, 2:00 pm - 3:30 pm EDT

PM1

SESSION A: BIOLOGICAL CHARACTERIZATION AND IMAGING

[Click here to join this session]

Abdominal Aortic Aneurysm Progression And Thrombus Formation Displayed Using Various Murine Models

Presentation ID: 30-A1

2:05 pm - 2:20 pm EDT

Blake J. Tanski, Alycia Berman, Jennifer Anderson, and Craig Goergen*
*PI: Weldon School of Biomedical Engineering
Purdue University

Keywords: *Abdominal Aortic Aneurysm, Lumen, Murine, Thrombus, Ultrasound Imaging*

An abdominal aortic aneurysm (AAA) is defined as the pathological expansion of the abdominal aorta. This vascular disease is often asymptomatic, which can leave patients at high risk of rupture if left undetected. Even when diagnosed, the current metrics that define rupture risk are vessel diameter and growth rate, which are not always accurate. Further research is needed to fully understand the progression that leads to the rupture of an aneurysm. This study uses four different murine aneurysm models to display the progression of aneurysms over time. The four models include elastase, calcium chloride ($CaCl_2$), BAPN-elastase, and Angiotensin-II-BAPN. Ultrasound imaging allows us to view and analyze aneurysm progression. These images can be used to obtain various metrics that can define the state of the vessel. First, images can be used to define strain, vessel area, and diameter. When three-dimensional ultrasound images are processed, they can be used to produce 3D segmentations of the lumen and wall. The segmentations can also show thrombus formation within the lumen. Using these 3D segmentations, aneurysm progression can be displayed, and various measurements can be taken throughout the vessel. Through this study, three models were compared by their 3D segmentations, and the last was analyzed through quantitative data taken from ultrasound images. The BAPN-elastase model showed the greatest growth of the four models. With further analysis of these murine models, we hope to provide insight to aneurysm progression and thrombus formation.

Characterization Of In Vivo Aortic Valve Dynamics Using Four-Dimensional Ultrasound

Presentation ID: 30-A2

2:20 pm - 2:35 pm EDT

Daniel P. Gramling, Frederick Damen, and Craig Goergen*
*PI: Weldon School of Biomedical Engineering
Purdue University

Keywords: *Aortic Valve, Ultrasound, Echocardiography, Small Animal Models, Small Animal Imaging*

The aortic valve (AoV) is a structure that aims to maintain unidirectional flow of newly oxygenated blood from the heart to the rest of the body. Unfortunately, the AoV frequently becomes diseased through progressive calcification and stiffening that, when severe, can be detrimental to a person's quality of life. Aortic valve disease affects 2-5 percent of Americans over the age of 65; a prevalence that is expected to double by 2050. While three-dimensional in vivo imaging is used clinically to monitor AoV function in humans, similar methods are not currently available to study preclinical small animal models. This hinders the ability of researchers to better understand disease mechanisms in vivo and explore new potential treatments through these models, which allow systematic control of disease inducing factors. We demonstrate a technique that overcomes this limitation through a novel implementation of high-frequency ultrasound that provides four-dimensional imaging data of the murine AoV. Volumetric data are digitally reconstructed and stabilized against spatial AoV translation to isolate leaflet motion. Enabled by the high temporal and spatial resolutions, 2D and 3D measurements are extracted from the imaging data to characterize AoV structure and function over the full cardiac cycle, such as tracking individual leaflet motion in 3D space to quantify valve kinematics. Our work provides a previously unavailable research tool to both better characterize, and study progression of, valvular heart disease in mice.

Localization Imaging Of Neuronal Signaling With Spatiotemporal Fluorescent Reporter Data

Presentation ID: 30-A3

2:35 pm - 2:50 pm EDT

David M Czerwonky, Justin Patel, Paula Ivey, and Kevin Webb*
*PI: School of Electrical and Computer Engineering
Purdue University

Keywords: *Biomedical Engineering, Sensing And*

Many inner workings of the brain remain unknown. Calcium is a crucial component in brain cell communication, and it would provide tremendous insights into neural networks, the inner workings of the brain, and

neurodegenerative disease if the calcium interactions could be imaged. We have previously developed an imaging technique allowing us to localize fluorescent markers of calcium known as calcium fluorophores in brain tissue using computational tools such as cost functions, temporal scanning, and multiresolution analysis. A remaining question is how the properties of certain calcium fluorophores can be an asset or a hindrance to our imaging technique. We simulate the imaging process of nine types of calcium fluorophores in a tissue-like medium with a calcium concentration typical of a neuronal region. The localization accuracy of eight calcium fluorophore variants show no significant difference in localization accuracy. However, Rhod-2 performed at a significantly lower level than the other choices. In terms of greatest intensity, Cal-520 and Oregon Green 488 BAPTA-1 are the leaders with Cal-590 falling close behind. The intensity results provide an important insight into the fluorescent source response model used in this research. The low-affinity choice Mag-Fluor-4 nearly outperforms its high-affinity derivative in terms of fluorescence intensity. Indicating that the fluorescent source response derived from solely optical properties is insufficient for modeling a variety of fluorophores. We propose that a fluorescent source model needs to be constructed to represent the optical-chemical duality of fluorophores to yield better results by working in the dissociation constant.

Measurement, Modeling And Simulation, Neuroimaging, Diffuse Optical Imaging

Using Automated Image Processing To Characterize The Osteocyte Lacunar-Canalicular System

Rachel Wang Zhang[1], Brennan Flannery[2], Melanie B. Venderley[2], Roy Lycke[2], Eric A. Nauman[2], and Russell P. Main*[2]
*PI: Weldon School of Biomedical Engineering
University of Michigan[1], and Purdue University[2]

Presentation ID: 30-A4
2:50 pm - 3:05 pm EDT

Osteocytes, cells that regulate bone remodeling, reside in a large network of lacunae and canaliculi within the bone matrix of most vertebrates. This osteocyte lacunar-canalicular system (OLCS) plays an important role in regulating the biological and mechanical properties of bone. Despite having extensive knowledge on the qualitative structure and function of the mineralized matrix, there is a lack of quantitative data on how the OLCS is organized. Quantitative data will help us better understand how the OLCS adapts to new stress regimes and provides insight for diagnosis and treatment of diseases. An automated image analysis algorithm was previously developed to produce these results from confocal microscopy volumes of bone. The focus of this study is to validate and optimize this processing algorithm. Simple computer-generated geometries were used to verify the algorithm's results and performing Cotter's sensitivity analysis optimized the parameters for confidence in the program outputs. Completing the analysis revealed select input parameters to be more impactful on the resulting measurements. This knowledge allows future researchers to better understand which inputs require more consideration to accurately retrieve their output variables. The validated algorithm can be used to reveal the effects of various mechanical stresses and biological changes on the OLCS organization.

Keywords: *Osteocytes, Mechanobiology, Image Processing, Confocal Microscopy, Lacunae*

SESSION B: ECOLOGY AND SUSTAINABILITY

Click here to join this session

Salinity In Arid Landscapes: A Case Study From Arequipa, Peru

Xochilth Saldana[1], Abigail Tomasek[2], Alejandro Rodriguez Sanchez[2], Lori Hoagland[2], and Sara McMillan*[2]
*PI: Department of Agricultural & Biological Engineering
University of California, San Diego[1], and Purdue University[2]

Presentation ID: 30-A5
2:05 pm - 2:20 pm EDT

Soil salinization occurs in many arid climates around the world and leads to decreases in agricultural productivity. This is detrimental for citizens in developing countries where local agriculture is typically their main source of income and food. Soil salinization is caused by both natural processes, such as the weathering of surrounding geology, and anthropogenic processes, such as agricultural irrigation and poor drainage systems. The goals of this project were to characterize patterns in salinity and potential drivers of salinization in the region of Arequipa, Peru. Arequipa has an arid climate, receiving 100 mm of precipitation per year, and water for the city is provided by the Chili River, which runs through the middle of Arequipa. Soil samples from 50 agricultural fields in Arequipa were analyzed for soil texture, cation exchange capacity (CEC), pH, organic matter (OM), and electrical conductivity (EC), which we used as a proxy for quantifying salinity. Linear regression correlations were computed to characterize salinity patterns and potential drivers. To analyze how location plays a role in salinity, ArcGIS was used to calculate the distances of field sites from the Chili River and to categorize whether the sites were floodplain (in the floodplain of the Chili River) or terrace (uplands). The age of agriculture and the irrigation network density of the sites were also explored to see their effect on the soil's retention of soluble salts. Through linear regression, the only significant correlation to EC was CEC. Floodplain areas tended to a have higher EC as well as higher CEC.

Keywords: *Agriculture, Soil Salinization, Data Trends and Analysis*

The oldest agricultural area in Arequipa had one of the highest average EC and CEC, and it was also located closest to the river. The relationship between CEC and EC suggests that due to the higher CEC, the soil is more capable of retaining ions that lead to increased salinity. It was also found that sites irrigated with saline water tended to have higher soil salinity, suggesting that irrigation with saline water may be leading to soil salinization in Arequipa fields.

Fragmentation And Carbon Storage In Forest Ecosystems

Presentation ID: 30-A6
2:20 pm - 2:35 pm EDT

Breanna E. Motsenbocker, Benjamin McCallister, and Brady Hardiman*
*PI: Environmental & Ecological Engineering
Purdue University

Storage of atmospheric carbon by forests is an essential method of mitigating climate change. As urban areas expand, fragmentation of forest ecosystems is a growing concern. Forest fragmentation causes an increase in unconnected forest patches that consist mostly of edge, which is defined as areas where trees experience a loss of protection on one side. The edge of a forest experiences a unique microenvironment which may have implications for its ability to store carbon. This study examines the relationship between forest fragmentation and carbon storage capacity of forests. We used publicly available data on land cover, tree canopy cover, and carbon storage from ten counties around the greater Chicago region. We analyzed landscape patterns between these data to quantify the effect of fragmentation on carbon storage in and around the Chicago area. Our results show that while forests store 40% more carbon than non-forests, forest edges store 18% less carbon on average compared to forest interiors. These results suggest that global patterns of urbanization and the resulting fragmentation of adjacent forest ecosystems may impair forest's capacity to take up and store carbon, exacerbating anthropogenic climate change effects.

Keywords: *Forest Fragmentation, Carbon Storage, Forest Edge, Land Cover, Land Use, Edge Effect*

Recent Lake Michigan Shoreline Changes Along Indiana's Coast

Presentation ID: 30-A7
2:35 pm - 2:50 pm EDT

Ben T. Nelson-Mercer, and Cary Troy*
*PI: Lyles School of Civil Engineering
Purdue University

Near-record Lake Michigan water levels are rapidly changing Indiana's shoreline. Understanding how the shoreline responds to water level changes will help predict the future shoreline of Indiana to better prepare for risks posed by shoreline recession. The comparison between the current shoreline state with historical shoreline positions can provide important insights to further this understanding. This research hypothesizes that in spite of the widespread shoreline changes currently being experienced along Indiana's coast, the current shoreline condition is consistent with historical shoreline responses to similar high water levels. To quantify how Indiana's shoreline has changed, orthorectified aerial images were analyzed with the Digital Shoreline Analysis System (DSAS) software, an add-in for ArcGIS. This system allowed for the delineation of the shoreline position, and the temporal tracking of this position along discrete shore-perpendicular transects. Imagery was analyzed from two high water years, 1997 and 2019, and one low water year, 2013. Indiana's 2019 shoreline has receded due to high water levels, but it still hasn't receded to its 1997 position. This study theorizes that the period of low wave and low water conditions preceding the recent increasing water levels contributed to this difference. While the shoreline generally grew during decreases in water level and eroded during increases in water level, the amount of growth or erosion was highly variable throughout Indiana's coastline. These findings indicate that variables like human-caused sediment transport and shoreline structures need to also be considered when analyzing Indiana's shoreline changes.

Keywords: *Shoreline Change, ArcGIS Modeling, Indiana's Coastline, Sediment Transport*

Results Of A Nearshore Lake Michigan Mixing Experiment

Presentation ID: 30-A8
2:50 pm - 3:05 pm EDT

Kira M. McCorry, and Cary Troy*
*PI: Lyles School of Civil Engineering
Purdue University

In order to better understand the role of invasive quagga mussels in the Lake Michigan food web, it is essential to examine the motion and mixing of the lake's waters. While factors that impact lake turbulence such as wind stress, inertial waves and radiative convection have been studied extensively at deep regions of the lake, the shallower regions remain largely unanalyzed. This study aims to quantify the mixing of the typically unstratified Lake Michigan water column nearer to the lakeshore. Velocity, temperature, and microstructure data taken from a 10m depth site in Lake Michigan near Milwaukee, WI are analyzed in order to characterize lake mixing. Strong correlation between the winds and near-surface currents is observed while examining the experiment's conditions. Vertical structure of the currents is evaluated through the law of the wall, which predicts velocities near boundaries. The law of the wall model is found to occur at a range of .159-.299 m and is used to calculate several directly related

Keywords: *Flow Analysis And Processing, Great Lakes, Data Trends And Analysis, Environment*

values: hydrodynamic roughness is estimated as .021741 m, friction velocity as .0030468 m/s, and the drag coefficient as .01142. Spectral analysis also demonstrates heavy wave influence on the currents. Despite the shallow range of this study, through in-depth analysis, the 10m depth is observed to be an extremely dynamic and layered region. The observations made in this study of Lake Michigan may be applied to the shallower waters of the Great Lakes and used to contribute to the full understanding of the health of Lake Michigan.

Computer Simulations Of Polar Ice Calving

Jacques Barsimantov Mandel, Akshay Dandekar, and Marisol Koslowski*
*PI: School of Mechanical Engineering
Purdue University

Presentation ID: 30-A9
3:05 pm - 3:20 pm EDT

Keywords: *Computer Simulation, Ice Calving, Cracks, Fracture, Phase Field Model, Viscoelastic Material*

The objective of this work is to generate a predictive model for ice calving in polar regions. Over the past decade, several new cracks have nucleated in the Antarctic ice sheets due to the global warming and the motion of glacial ice. These cracks could lead to huge masses of ice floating in oceans, eventually melting and increasing the global sea level which can lead to catastrophic scenarios around the world. Previous studies showed simulations on ice calving process in relatively short periods of time such as 9000 hours whereas such processes can take more than 10 years. Ice is modeled as a viscoelastic material. The hydrostatic and gravitational forces acting on floating tips of glaciers may generate bending moments large enough to cause fracture. A parametric study is performed using a representative ice structure to see the effect on the crack nucleation and propagation. The purpose of this parametric study is to better understand how the geometry will behave and where to expect crack nucleation. Results suggest that the time required, and location of the crack nucleation is very sensitive to the geometry. The model would also help to understand the effects of basal boundary condition angle and earthquakes effect on the crack propagation.

SESSION C: MATERIAL PROCESSING AND CHARACTERIZATION

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Sputter Deposition With Transparent Conducting Oxide

Xingyu Wang, and Sunghwan Lee*
*PI: School of Engineering Technology
Purdue University

Presentation ID: 30-A10
2:05 pm - 2:20 pm EDT

Keywords: *Transparent Conducting Oxide, Thin Films, Semiconductor, Magnetron Sputtering Deposition, Tin Oxide*

Discovered last century, there have been tremendous progress in transparent conducting oxides (TCO) due to their unique combined properties of high transparency in the visible regime and high conductivity. Major applications of transparent conducting oxide thin films include circuitries and opto-electronic devices such as touch screens and solar panels. Nowadays, with the increase in the demand of these products, TCO materials have been widely applied, so there is no doubt that the great potential of such TCO material will lead to further study, in order to maximize the efficiency and stability of the products. The objective is to study for thin films that are made out of Tin oxide, with other doping materials, and find out the effect of deposition condition and after-deposition treatment on the properties of thin films such as transparency and sheet resistance. The method used in the lab for thin film production is a DC/RF magnetron sputtering system. Resulting properties of sputter-deposited TCO thin films depend on process parameters such as power applied to target material, substrate temperature and working pressure in the chamber. Due to the very special characteristics of this Tin oxide material, sheet resistance may not be measured for pure Tin oxide from equipment in the lab, and therefore it will need further doping process to have a decreased sheet resistance. Compared to previous works found in the literature, higher transparency and lower sheet resistance have been achieved with better stability, which is promising for next generation electronic and optoelectronic devices that require high conductivity and high visible regime transparency.

3D Simulation Of Shrinkage During Femtosecond Two-Photon Polymerization

Yijie Chen, Paul Somers, and Xianfan Xu*
*PI: School of Mechanical Engineering
Purdue University

Presentation ID: 30-A11
2:20 pm - 2:35 pm EDT

Keywords: *Two-Photon Polymerization, Polymerization Shrinkage, Structural Deformation*

3D microstructures fabricated by femtosecond two-photon polymerization (TPP) face the problem of polymetric shrinkage, resulting in reduced sizes and structural deformation. Despite the vast research concerning stability and printing accuracy, little is known about material shrinkage from the perspective of polymerization dynamics. In this work, a mathematical model is presented to simulate the photochemical processes during TPP, including initiation by laser irradiance to generate free radicals, polymer chain propagation, and termination as well as inhibition, which end up with dead polymer chains. Molecular diffusion and non-local polymer chain growth are incorporated in this model. The partial differential equations are solved using forward time centered space (FTCS) method to obtain the spatial distribution of monomer conversion during and after laser exposure, with which the volumetric strain development in the sample is predicted. Using this simulation approach, the contraction of simple structures such as a suspended line is estimated. Comparisons between different scanning parameters are present, showing that an increased laser power causes larger chemical shrinkage at a certain scanning speed. This study also provides a method to qualitatively reflect the locations prone to shrinkage-induced deformation near a fixed boundary.

Stress And Failure Analysis Of Thin Film Electrodes Induced By The Volumetric Strain

Gary Li, Xiaokang Wang, and Kejie Zhao*
*PI: School of Mechanical Engineering
Purdue University

Presentation ID: 30-A12
2:35 pm - 2:50 pm EDT

Keywords: *Mechanical Breathing, Stress, Deformation, Failure*

Nowadays, Organic Electrochromic Devices play an important role in our daily life. Organic conductor becomes a popular choice to build the electrode since it is cheap, soft, and flexible. Meanwhile, the lifetime of the organic conductor becomes an important factor to be considered. The transportation of ions makes the electrodes inflate and shrink cyclically which makes itself deform. This phenomenon is called mechanical breathing. The cyclic deformation will lead to failure. We sought to simulate and understand the stress distribution of the film electrode when the mechanical deformation is presented. We built a thin film-substrate model in the cylindrical coordinate system since the bubble on thin film is circular shape. By using the constitutive law, we applied a volumetric strain to the thin film. With the help of the COMSOL, we were able to solve three sets of governing equations which were the constitutive law, the momentum balance, and the strain-displacement relation. We analyzed the stress and deformation of the model with respect to the number of cycles. While the volumetric strain was applied, the center part of thin film inflated upward, the bubble tended to expand horizontally outward, and the magnitude of stress increased. With the number of cycles increased, the unrecoverable deformation became obvious, the crack between the thin film and substrate started to grow, and finally resulted in a failure. This simulation shows that the deformation makes the crack between the thin film and substrate bigger so that more efforts can be made to alleviate the effect brought by the volumetric strain to elongate the lifetime of the electrode.

Single Crystal HMX Under Quasi-Static Loading

Kristyna Hyblova[1], Christian Blum-Sorensen[2], and Steven Son*[2]
*PI: School of Mechanical Engineering
Walla Walla University[1], and Purdue University[2]

Presentation ID: 30-A13
2:50 pm - 3:05 pm EDT

Keywords: *HMX Quasi-Steady Loading, HMX, Single Crystal HMX,Octahydro-1,2,5,7-Tetranitro-1,3,5,7-Tetrazocine, HMX Low Strain Rate, Birefringent Properties Of HMX, HMX Photoelastic Method, Photoelastic Method, Explosives*

Models of Octahydro-1,2,5,7-tetranitro-1,3,5,7-tetrazocine(HMX) that accurately predict its response under various levels of insult (e.g., impact) are paramount to safety and effectivity. In recent years the models of HMX behavior have been improved and verified by experiments at different loading conditions. However, few experiments have been conducted with single HMX crystals at a quasi-static loading. It is thought that the initiation of chemical reactions leading to detonation begin at small regions of high temperature near defects in the crystal. Therefore, studies of single crystal HMX with engineered defects have been conducted to improve understanding of this high temperature region formation. This study seeks to investigate the stress gradients near engineered defects in single crystal HMX with quasi-static loading in compression. Engineered defects are machined into single crystals of HMX by mechanical means (microscale drilling) or via laser ablation. These crystals are loaded in compression until fracture. During the test, the fringe patterns in the crystal are captured using circular polarizers and a 520-540nm LED. The fringe patterns are analyzed to determine the stress gradients caused by the engineered defects. Additionally, a PVDF (thin film piezoelectric) gauge is used to record the changes in stress on the crystals. Because of the fast response of this gauge to changes in pressure, a high-speed camera records the progression of strain relief

through cracking in the crystal. This study draws conclusions about how various engineered defects in single crystal HMX effect the stress gradients and nucleation of crack formation under quasi-static loading.

High Pressure Burning Characteristics Of Additively Manufactured Gun Propellants

Presentation ID: 30-A14
3:05 pm - 3:20 pm EDT

Chase W. Wernex[1], Aaron Afriat[2], Timothy Manship[2], and Steven Son*[2]
*PI: School of Mechanical Engineering
Mississippi State University[1], and Purdue University[2]

Keywords: *Gun Propellants, Combustion and Propulsion, Additive Manufacturing, Sustainability*

Vibration Assisted printing (VAP) has been demonstrated as a manufacturing technology for printing extremely viscous materials. VAP has been shown to have high printing speed and precision allowing for the creation of novel internal geometry. This project investigated extending VAP to two well-studied gun propellant formulations with little to no change to their original formulation. Manufacturing gun propellants using this approach also allows for a minimization of solvent which can reduce the environmental impact of manufacturing. Multiple cross sections were manufactured including thin strands, perforated cylinders, and gyroidally infilled cylinders. Testing was performed by burning the thin strand samples in a high-pressure strand burner at up to 13.8 MPa. VAP consistently had enhanced flow rates when compared to direct write printing of the gun propellant. This is due to a decrease in wall friction for the flowing propellant when subjected to the ultrasonic vibrations. Additionally, VAP allowed for the printing of several formulations that were too viscous for direct write alone. Data from burning tests was compared to other published results in order to make recommendations on how to best leverage the advantages of additive manufacturing using VAP.

SESSION D: MACHINE LEARNING II: DEEP LEARNING

Click here to join this session

Applications Of Deep Reinforcement Learning

Presentation ID: 30-A15
2:05 pm - 2:20 pm EDT

Anurag L. Shah, Abishek Umrawal, Phu Pham, and Vaneet Aggarwal*
*PI: School of Industrial Engineering
Purdue University

When compared to conventional vehicles, electric vehicles are not only environmentally friendly but also more cost-effective, as their fuel costs are lower than a conventional vehicle. They bring their own problems to the situation of ride-sharing taxis, however, as they have much longer charge times and a low maximum distance on a full charge, which require modifications to the model to incorporate them in. We sought to eliminate the concern of long charge times from the model, and find a replacement, to make this competitive for a ride sharing based system. We simulated mobile, replaceable batteries to charge the main car battery, and set up a system within the model to simulate this. We set up simulated “depots” across the city model which charge these mobile batteries and exchange them with cars driving to them. We also ensured that the car does not get stranded by making sure it can always access a depot and discouraging trips when at low charge in the main battery. This model is competitive with the original model with handling requests, not requiring any additional cars and only adding short detours to accommodate switching the batteries. Hence this is a more cost-effective solution to the problem of ridesharing.

Keywords: *Reinforcement Learning, Deep Learning, Ride Sharing, Dynamic Fleet Management, Electric Vehicles*

Sparsity Aware Core Extension Benchmarking In Resource-Limited Microcontroller

Presentation ID: 30-A16
2:20 pm - 2:35 pm EDT

Ruoyi Chen, Jacob R. Stevens, and Mark C. Johnson*
*PI: School of Electrical and Computer Engineering
Purdue University

With the introduction of wearable devices and the 5G network, the demand for machine learning workload for edge computing has been increased. The biggest issue for machine learning to be adapted to those devices is high resource usage. This issue attracted many researchers to focus on optimizing from both software and hardware aspect to pack the workload into lower performance devices. The accelerator is a widely accepted hardware optimization method is not applicable to edge node applications due to size constraints and the lack of development of the internal IP component. This led us to implement a sparsity architecture modification for which the improvement has not been proved on a power limited device. Therefore, to prove the viability of the sparsity ISA extension, benchmarking of the proposed sparsity ISA extension is needed. To assess the performance gain achieved, the Bonsai and ProtoNN model is translated using SeeDot quantization tools and the compiled codes are implemented into the simulated chip on the DE1-SOC FPGA. The overall performance is determined by the execution time of processing USPS10 testing datasets. The result is expected to demonstrate the reduced execution time of the sparsity ISA extension on a microcontroller device compared to an equivalent device without the sparsity ISA extension. It would further increase the variety of chip can be chosen for edge computing devices.

Keywords: *Microcontroller, Sparsity, Deep Neural Network, Benchmark, Machine Learning*

A Query Processing Engine for Vehicle Re-Identification: A Clustering Approach

Presentation ID: 30-A17
2:35 pm - 2:50 pm EDT

Kaiwen Shen, Tiantu Xu, Xiaozhu Lin, and Felix Lin*
*PI: School of Electrical and Computer Engineering
Purdue University

The increasing effort in the development of smart cities is leading to a drastic increase in the number of cameras. This calls for a need of automated video analysis in tasks such as matching target vehicle in a system of cameras, or vehicle re-identification, for traffic flow analysis or crime investigation. Previous methods on vehicle re-identification have shown to have good accuracy, but also resulted in high computational cost because of the use of complex neural networks and over analyzing videos due to redundancy in cameras deployment and between camera frames. We hereby propose a query processing engine that identifies specific vehicle by efficiently retrieving the camera (location) and frames (time) that contains the vehicle using a clustering technique with only a small portion of video data. We make the assumption that there exist certain prior knowledge camera locations, or clusters of cameras based on location, and user will provide image of desired vehicle in order to perform the search. We select representative cameras from each location cluster and perform object detection on sampled frames. We then perform clustering algorithm, rank the result from representative cameras, and retrieve the camera and frame information of the desired vehicle. Experiments have been carried out using the CityFlow Dataset, a public surveillance camera dataset, and our approach resulted in fast computing with high re-identification rate.

Keywords: *Vehicle Re-identification, Computer Vision and Pattern Recognition, Cluster Computing*

Modeling Light Transport In Fog For Computational Imaging

Presentation ID: 30-A18
2:50 pm - 3:05 pm EDT

Emi Mondragon[1], Brian Bentz[3], and Kevin Webb*[2]
*PI: School of Electrical and Computer Engineering
Trinity University[1], Purdue University[2], and Sandia National Laboratories[3]

Fog is a common degraded visual environment that restricts vital processes and hinders perception of the surroundings. Likewise, absorption and light scatter from the randomly distributed water aerosol can hinder or interfere with optical recording devices that are essential for obtaining sensory or image information. By coupling scattered light measurements with a model for the fog, computational imaging becomes possible. A refinement of the photon diffusion approximation to the Boltzmann equation is investigated to describe the intensity of the scattered light for the important regime where the level of scatter is moderate. To describe the interface between free space and the scattering medium, boundary conditions that incorporate a weak angular dependence approximation is implemented. With this new diffusion representation, analytical results for reflectance and transmittance are compared with published data. This model is shown to capture the measured data accurately for a scattering domain that is less than the transport length, where a standard diffusion model is inaccurate, and the full transport model is computationally burdensome. Beyond application to imaging in fog, this result should prove valuable in biophotonics applications and for other environmental sensing situations where use of light is essential, and scatter is significant.

Keywords: *Light Transport, Degraded Visual Environment, Diffusion Theory, Scattering Media, Inverse Problem, Fog*

Day 2 | Morning Presentations

July 31, 10:00 am - 11:30 am EDT

AM2

SESSION A: CELLULAR BIOLOGY

Click here to join this session

Multi-Fidelity Analysis To Study The Emergence Of Drug Resistance In Multiple Tuberculosis Granulomas

Presentation ID: 31-M1

10:05 am - 10:20 am EDT

Shaurya Gaur, Alexis Hoerter, and Elsje Pienaar*
*PI: Weldon School of Biomedical Engineering
Purdue University

Keywords: *Monte Carlo, Markov Chain, Rare Events*

Tuberculosis is caused by Myobacterium tuberculosis and is characterized by the formation of granulomas in patients' lungs. Granulomas are the sites of infection and consist of host cells, dead cell debris and bacteria. Myobacterium tuberculosis can mutate to acquire resistance against several antibiotics such as rifampicin and isoniazid. However, these events are relatively rare and very hard to study experimentally at the single host level. Yet, resistance mutations have major impacts at the population level. Our objective is to quantify these rare events by performing Markov Chain and Monte Carlo analysis on multiple granulomas to predict the probability of emergence of drug resistance in our virtual hosts. We extend the scope of previous research which performed such an analysis on a single granuloma. For our study, we begin with only two granulomas as our base case. We obtain information regarding bacterial population growth trajectories, bacterial deaths, and divisions over time from an existing simulation of granuloma progression (GranSim). GranSim is a hybrid, multiscale, agent-based model describing bacterial growth, division and death during granuloma formation. We then apply Markov Chain and Monte Carlo methods to the two individual granulomas as well as a single combined granuloma formed by the fusion of these two granulomas to predict the probability of drug resistance over time. To address the challenge of understanding the emergence of drug resistance in multiple granulomas, we will apply Markov Chain and Monte Carlo analysis to more than two granulomas and compare the results.

Computational Investigation Of Mechanical Interactions Between Cells And Extracellular Matrix

Presentation ID: 31-M2

10:20 am - 10:35 am EDT

Brandon Slater, Jing Li, and Taeyoon Kim*
*PI: Weldon School of Biomedical Engineering
Purdue University

Keywords: *Cell, Extracellular Matrix, Contraction, Matrix Remodeling, Mechanotransduction*

Living cells require mechanical forces for many of their physiological functions. Using these forces, cells keep remodeling and interacting with extracellular environments. Such mechanical interactions between the cell and the extracellular environment are critical for many biological processes, such as cell migration, morphogenesis, and wound healing. The actomyosin cortex underlying a cell membrane is one of the main force generators in cells. Via physical links between the cortex and an extracellular matrix (ECM) called focal adhesions, forces generated from the cortex can be transmitted to the ECM, resulting in structural remodeling of the ECM. Due to the importance, matrix remodeling and force transmission induced by force-generating cells have been investigated in several studies. In those previous studies, the ECM was assumed to be an elastic material. However, the ECM is highly viscoelastic and henceforth exhibits a time-dependent response to applied stress and forces. To overcome limits of the previous studies and thus provide more physiological insights, we employed a two-dimensional computational model for investigating how mechanical interactions take place in the ECM with realistic rheological properties. We found that the transient nature of cross-links between matrix fibers and the structural properties of the ECM cooperatively regulate the degree of remodeling and force transmission.

The Application Of Single Cell Genomics In Viral Infectious Disease

Zonghao Zhang, Bingyu Yan, and Majid Kazemian*
*PI: Department of Biochemistry
Purdue University

Presentation ID: 31-M3
10:35 am - 10:50 am EDT

Epstein-Barr virus(EBV), this very virus founded in 1964 infects 95% of adults worldwide. Since EBV could alter the host DNA and DNA structure, those infected might suffer from a series of diseases induced by EBV. The list of disease is getting longer thanks to the virus itself and diligent works done by scientists and medical doctor. This list of disease includes several types of cancer, EBV-associated lymphoproliferative diseases(Rezk et al, 2018), gastric cancer and nasopharyngeal carcinoma. And more than 200,000 cancer cases per year are thought to be the result of EBV(Cancer Research UK, 2014). Moreover, several evidences showed that EBV is responsible for several childhood disorder (Mastria et al, 2016) and autoimmune disease(Toussirot et al, 2008). The vaccine is the ultimate weapon for us to defeat virus, but unfortunately none EBV vaccine has been came out and commercialized. Thus, it is important for us to discover every aspect of EBV and illustrate the regulation of EBV replication in host cells and cellular response to EBV. Single cell RNA sequencingoffers the ability to discover rare features at single cell level and uncover the heterogeneity of the bulk cell population. Moreover, a newly developed genomic method called single cell ATAC sequencing can also offer the ability to detect the chromatin accessibility at single cell level. Here, by building virus-human chimeric reference genomes and mapping the scRNA-seq reads and scATAC-seq reads to the corresponding reference genome, we identified pervasive single cells that are harboring virus fragment in EBV transformed human B-Lymphocyte. This pipeline can be used to dissect the cells with virus load at single-cell level and enables the detailed investigation into the host cell response to virus infection.

Keywords: *Next Generation High Throughout Sequencing(NGS), Single Cell RNA Sequencing(Scrna-Seq), Single Cell ATAC Sequencing(Scatac-Seq), Cancer Inducing Virus, Human Papillomarius Infection (HPV), Epstein-Barr Virus (EBV), SARS-Cov-2*

Effects Of Cell-Cell Contact During Multicellular Migration

Anuhya Edupuganti, Hye-ran Moon, and Bumsoo Han*
*PI: School of Mechanical Engineering
Purdue University

Presentation ID: 31-M4
10:50 am - 11:05 am EDT

Cell migration is essential in the development and maintenance of a multicellular organism and plays a vital role in wound healing, tumor progression and metastasis, and immune response. Understanding the characteristics and mechanisms of cell migration could advance the development of effective therapeutics and innovative biotechnologies. In addition to experimental research, physical and mathematical models have provided valuable insights into cell migration characteristics. However, mechanical interactions among cells and between cells and matrix, especially in collective cell migration, are difficult to quantitatively measure and predict. In this study, collective cell migration in fibroblasts and epithelial cells has been simulated by the Cellular Potts Model using a python/XML-based software package CompuCell3D. Specifically, the effects of cell-cell contact are investigated in the interactions between fibroblasts and between epithelial cells. Fibroblasts and epithelial cells were chosen by virtue of their role in wound healing and cancer metastasis, and the difference in migration pattern demonstrated by them: fibroblasts tend to migrate individually, whereas epithelial cells migrate as collective sheets. The model in this study represents the simplified mechanics of cells' response in migration dependent on the interplay between the strength of cell-cell adhesions and cell-matrix adhesions, and magnitude of protrusion force exerted by the cell. Cell migration is quantified primarily in terms of cell speed, deviation from straight path and number of cells that migrate into the outer matrix past the population baseline, and distance of migration. This model can be adapted to explore the behavior of fibroblasts and epithelial cells in response to external environmental cues and other cell types in the population.

Keywords: *Collective Cell Migration, Cellular Potts Model, CompuCell3D*

Noninvasive Measurement And Visualization Of Vagus Nerve Activity To Improve The Efficacy Of Gastric Electrical Stimulation In Human Subjects With Gastroparesis

Rama G. Coimbatore, and Matthew Ward*
*PI: Weldon School of Biomedical Engineering
Purdue University

Presentation ID: 31-M5

11:05 am - 11:20 am EDT

Gastroparesis is a stomach condition that results in abnormal processing of food and delayed gastric emptying without a mechanical obstruction. Symptoms may include nausea, vomiting, early satiety, and bloating. To treat this condition, gastric electrical stimulation (GES) is proposed as an option for patients who do not respond to medication. A GES device is implanted and used to electrically stimulate the stomach wall, which is innervated by the vagus nerve. There is evidence that GES activates the vagus nerve, which is the primary nerve that the stomach uses to communicate sensory information to the brain, including signals that may contribute to nausea and vomiting via the area postrema ("vomiting center of brain"). We hypothesize that GES relieves nausea and vomiting by

Keywords: *Data Visualization, Modeling, Gastroparesis, Vagus Nerve*

stimulating the vagus nerve. Vagal nerve recordings were obtained in human subjects receiving GES for gastroparesis using a novel, noninvasive method, consisting of placing a 5x6 multi-electrode array (MEA) on the skin surface overlying the left and right cervical vagus nerves. Demographical data and neck measurements were also collected. A graphical user interface was created as a tool to visualize placement of the MEA and vagal nerve activity. We are determining the limitations of detecting vagal nerve activity through the skin surface, including body mass index and the parameters of the GES device used to stimulate the stomach wall. Visualizing and analyzing the data traveling across the electrodes may provide insight into the typical anatomic course of the vagus nerve. The data will be represented on a virtual person whose neck anatomy is defined by the measurements collected from the subjects. We aim to visually display the vagus nerve activity to decode and analyze its involvement in GES and the treatment of gastroparesis. Another aim of the visualization is to simplify the interpretation of the complex datasets that we collect so that these NIH-funded research studies can be made more accessible to a broad audience with different backgrounds and interests.

SESSION B: LEARNING AND EVALUATION

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Novel Ethnographic Investigations Of Engineering Workplaces To Advance Theory And Research Methods For Preparing The Future Workforce

Paige Kadavy[1], Swetha Nittala[2], Tasha Zephirin[2], and Brent Jesiek*[2]
*PI: School of Engineering Education
Colorado School of Mines[1], and Purdue University[2]

Presentation ID: 31-M6
10:05 am - 10:20 am EDT

Virtual teaming is becoming a more common professional practice used around the world to create more flexible and multifaceted teams and optimize group output. While becoming more commonplace, there remains considerable room for discovery in terms of how team structure, processes, tools, and other factors may contribute differently to virtual team performance, including as compared to more traditional team configurations. In this paper, we review a corpus of literature that analyzes virtual teams and then compare those findings to insights drawn from interviews with technical professionals who engage in virtual work. Our goal is to discover common structures and practices used in virtual teaming within engineering and allied fields. Literature was gathered and chosen systematically from the Engineering Village database based on criteria related to team performance and satisfaction. We additionally conducted semi-structured interviews that explored participants' current and previous experiences working on virtual teams. Based on the literature review and interviews, we compare the findings from each and identify best practices for virtual teaming in engineering disciplines and provide associated guidance moving forward. These findings will guide further research, inform the creation of more effective virtual teams, and help identify avenues in the discipline that are under investigated or require more research. This work will be useful to both members and managers of virtual teams in technical fields, as well as engineering education teachers and researchers who are engaged in preparing students for a rapidly evolving workplace.

Keywords: *Virtual Team, Interview, Literature Review, Engineering, Technical Professionals*

Auto-Grading Workflow For College Programming Assignment

Swapnil M. Kelkar, Brandon Xu, Xiao Hu, Yung-Hsiang Lu, and Milind Kulkarni*
*PI: School of Electrical and Computer Engineering
Purdue University

Presentation ID: 31-M7
10:20 am - 10:35 am EDT

With the recent increase in popularity of Computer Science and programming-based courses at universities, comes the demand for an efficient framework to grade the homework programming assignments which are an integral part of these courses. Currently, the grading systems used at Purdue are time consuming and require significant manual intervention from the teaching assistants. We sought to optimize this by developing a framework which will facilitate not just the submission of the assignment but also the grading and feedback for these assignments. We first interviewed several professors and teaching assistants who had been using auto- graders in the past and listed down their various needs and requirements. Taking these needs into consideration, we made use of one of the most popular online code hosting platforms, GitHub and posted all the assignments on GitHub Classroom, one of GitHub's features tailored specifically for classes with a large enrollment. We then integrated this with another tool called CodePost to receive the code from GitHub and run the necessary tests on it. Through this project, we aim to create an easy to use grading framework for both the students and the teaching assistants. In the past, students would have to wait a minimum of 2 to 3 days to obtain their results, however, with our system, students can get instant feedback on their submissions. We believe that our workflow will not only benefit the students but would definitely help save TA's and professors' time.

Keywords: *Workflow, Education, Auto-grader*

Automated Grading Of Programming Assignments

Presentation ID: 31-M8
10:35 am - 10:50 am EDT

Brandon Xu, Swapnil Kelkar, Xiao Hu, Yung-Hsiang Lu, and Milind Kulkarni*
*PI: School of Electrical and Computer Engineering
Purdue University

Keywords: *Computing Education, Automatic Grading, Learning Tools*

With the increasing prevalence of online learning platforms and growing sizes of university programming classes, efficient automated grading systems are becoming more and more necessary. Currently, the grading methodologies of programming classes at Purdue University are varied and require time-consuming manual work by teaching assistants. Through various discussions with faculty and past teaching assistants within the Electrical and Computer Engineering Department at Purdue, we formed a list of essential features necessary to create a foundation for our autograding system. In general, an ideal autograder would be easy to set up, provide immediate feedback to students, and grade each assignment automatically. Instead of developing such a system from scratch, we discovered that our needs would be best met by integrating two existing platforms: GitHub Classroom and CodePost. GitHub Classroom is a service that allows class instructors to easily create and distribute individual code repositories for students, and CodePost is a learning platform with autograding capabilities. Utilizing the two services' APIs (Application Programming Interface), we created an intermediate server that allows GitHub to interact with CodePost. By doing so, code that is submitted to GitHub by students will also be sent to CodePost automatically, where test cases will be run to determine grades. This workflow not only saves time during the setup and grading process for instructors and teaching assistants, but also allows students to receive their grades for assignments more quickly.

Predicting Subsequent Memory From Cognitive States During Learning

Presentation ID: 31-M9
10:50 am - 11:05 am EDT

Gloria Dietz, and Yu-Chin Chiu*
*PI: Department of Psychological Sciences
Purdue University

Keywords: *Cognitive State, Attentional State, Conflict Resolution, Motor Inhibition, Response Times, Stroop Task*

Learning and memory are such an integral part of life that we often take their relationship for granted: we remember what we have learned. However, this relationship may not be as simple as it seems. This is especially the case when the learning is incidental, rather than the main focus, as we go about fulfilling other behavioral goals. Cognitive control, which is required to produce goal-directed behavior, entails a set of functions that affect learning differently. Some functions (e.g., conflict resolution) appear to help, while others (e.g., motor inhibition, fluctuating attentional states) appear to hurt, resulting in opposite subsequent memory effects (SME). However, the effects of these different aspects of cognitive control have not been assessed jointly to reveal how they interact with each other during learning. It is, therefore, difficult to predict the mnemonic fate of information that is learned under a combination of cognitive controls. In this study, we utilized a cognitive control task that requires both conflict resolution and motor inhibition, along with a surprise memory task to assess the SME of these control functions. We also estimated each trial's attentional state by considering the fluctuation of response times on previous trials. We then built a novel model that combines all three aspects of cognitive control to predict the subsequent memory on a trial-by-trial basis for each of the participants. We found that our model can predict each subject's trial-wise memory, suggesting that different aspects of cognitive control do jointly contribute to how well information is learned.

SESSION C: BIOTECHNOLOGY DATA INSIGHTS

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Automation In Drug Approval Process Information

Presentation ID: 31-M10
10:05 am - 10:20 am EDT

Bobby Putra Santoso, Andrew Strongrich, and Alina Alexeenko*
*PI: Davidson School of Chemical Engineering
Purdue University

Keywords: *Lyophilization, Automation, Algorithm, Drug Trends*

Lyophilization has been around since the Incan civilization. In terms of pharmaceuticals, widespread use started in the 1940's. Lyophilization is needed for certain drugs to keep them stable, meant for prolonged use. The lyophilization process involves freezing the drug, then lowering the atmospheric pressure to get sublimation to remove excess water. After the water is removed, the final product can be stored as a preserved drug. The Food and Drug Administration is an organization that approves and regulates lyophilized and non-lyophilized drugs in the United States. Often, information regarding these drugs are kept in a website, and are updated regularly. However, up until now, obtaining information of newly approved drugs requires arduous manual search. This study is to help researchers and health officials better understand drug trends. For instance, researcher can better analyze the trends of lyophilized drugs within the years. We used Python programming language to create an automation algorithm that gather data from the Food and Drug Administration website. Since the drugs information was displayed based on the first letter of the name, the algorithm would loop repeatedly until it reached through every drug. The algorithm would go through every link and save drug labels presented. These drug labels would determine if a drug is lyophilized or not. Supposedly, this automation algorithm should be used every time the FDA approve new drug. We tested this automation algorithm against manual (human checking) in a single drug run. The human individual spends 25.85 seconds to check for a single drug and its label, while the automation algorithm only spends 13.15 seconds. The whole database contains 89 pages, each with around 100 main drugs. An estimate to the run time for the algorithm to run through a page is one hour. A human individual can take up to weeks of data gathering in comparison to just tens of hours using automation. Furthermore, the automation algorithm was evidently more consistent in checking for keywords and saving the drug labels. A possible reason for non-consistency for manual checking factors affecting the human individual, such as fatigue. It was an arduous task for a human to go through pages, all of which have 100 drugs. Based on the findings, we recommend that automation is the key to data mining drug information for analyzing trends. Automation will be needed for researchers and health officials for data gathering regarding new approved drugs.

Bioinformatic Analyses And Synthesis Of Natural Product Inspired Cyclic Peptides

Presentation ID: 31-M11
10:20 am - 10:35 am EDT

Chloe Smith, Matthew Hostetler, and Elizabeth Parkinson*
*PI: Department of Chemistry
Purdue University

Keywords: *Natural Products, Antibiotic Resistance, Cyclic Peptides*

Antibiotic resistance has created an urgent need for novel therapeutics. Natural products, especially cyclic peptides, have been a fantastic source of antibiotics, including the FDA-approved vancomycin and daptomycin. However, there is great need to find additional molecules with activity against antibiotic resistant infections. Bioinformatics analysis of the natural product biosynthetic gene clusters combined with chemical synthesis of the predicted cyclic peptides will likely allow us to find new non-ribosomal cyclic peptides that could potentially combat antibiotic resistant bacteria. Using BLASTp, we identified 500 biosynthetic gene clusters containing the enzyme responsible for peptide cyclization. Further analysis of the gene clusters using antiSMASH and PRISM allowed us to identify 130 unique cyclic peptides. Cheminformatics combined with gene cluster comparisons have allowed us to prioritize the 50 most diverse compounds. These peptides are currently being synthesized and tested for purity and bioactivity. High pressure liquid chromatography and mass spectrometry are used to determine purity and identity of the synthesized cyclic peptides while standard bioactivity assays are used to determine their antibiotic effects. Bioinformatics combined with chemical synthesis of predicted natural product cyclic peptides will allow us to identify novel antibiotic molecules that will likely help to fill the antibiotic pipeline for the challenging to treat antibiotic-resistant bacteria.

Expanding A Lipid Fragmentation Database And LIQUID Functionality

Presentation ID: 31-M12
10:35 am - 10:50 am EDT

Chisa Zensho, Daniela Sanchez, Manxi Yang, Miranda Weigand, and Julia Laskin*
*PI: Department of Chemistry
Purdue University

Keywords: *Lipids, Lipidomics, Lipid Annotation, Mass Spectrometry, Software, Tandem Mass Spectrometry*

Accurate identification of lipids is key to a better understanding of biological functions as well as the roles of lipids in diseases and drug studies. Lipid Quantification and Identification (LIQUID) is a lipid identification tool that annotates tandem mass spectrometry (MS/MS) data with a customizable target database and scoring function that allows users to distinguish the accuracy of identification. However, since this software was originally developed to analyze samples that were desalted by chromatographic separation, it is limited in its application to samples in which metal adducts are not present. This presents a challenge to mass spectrometry imaging applications, in which lipids are typically observed as alkali metal adducts. We have expanded the target database of LIQUID by adding potassium and sodium adducts for the existing database entries recorded by LIPID MAPS. Furthermore, we have incorporated new fragmentation rules for those adducts to improve the accuracy of lipid identification and scores calculated by the software. The identification ability of the software with the expanded target database and fragmentation rules was compared to the original database with the previous set of fragmentation rules and was found to have a higher rate of detecting and accurately annotating fragments with a higher accuracy of score assignments for data without chromatographic separation. The enhanced LIQUID enables accurate large-scale analysis of a larger variety of lipid species for a broader type of experiments than the previous LIQUID. This work shows the improved annotation capabilities of LIQUID for direct infusion tandem mass spectrometry data.

Applications Of Biotechnology In Phage Discovery, Lipidomics, & Proteomics

Presentation ID: 31-M13
10:50 am - 11:05 am EDT

Emma Lietzke, Gillian Smith, and Kari Clase*
*PI: Department of Agricultural & Biological Engineering
Purdue University

Keywords: *Bacteriophages, Phages, Proteomics, Lipidomics, Mass Spectrometry*

Bacteriophages, or viruses that infect specific bacterial hosts, are essential in understanding evolutionary mechanisms and viral diversity, especially in modeling interactions of phage infection. The application of molecular genetics on phages provides a means to understand their specific gene functions through investigating their proteome and lipidome profiles. Current phage genomic annotation software has many limitations in expanding the understanding of unknown gene functions, as well as structural protein and lipid expressions. Mass spectrometry (MS) in tandem with analysis software, such as MetaboAnalyst, can be used to identify relevant lipids and proteins in phages. Experiments were designed to compare ion intensity outputs from MS from different phages in exponential and stationary phases, and varied time infected by *M. smeg*, with those from a negative control. Statistical and biomarker analyses were utilized to examine the expressions of varying lipids within these samples; the results were then analyzed to determine which lipids were significant and how often. This study compares the results between phages FrenchFry and MrGordo. These phages were chosen to provide the widest range of comparison, as FrenchFry was the most prolific lytic phage and MrGordo, a prolific temperate phage. 509 lipids were identified in MS. From the 9 test variations in MetaboAnalyst, 64 lipids were identified as significant. 11 of these, which appeared 3 or more times across volcano plots and ROC tests, were investigated in metabolite databases and literature. Many came back as toxins or related to inflammatory and anti-viral responses, their potencies dependent on specific chemical structures.

SESSION D: NANOTECHNOLOGY

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Modeling Ferroelectric Domain Switching Kinetics

Presentation ID: 31-M14
10:05 am - 10:20 am EDT

Minh Tran, Jackson Anderson, and Dana Weinstein*
*PI: School of Electrical and Computer Engineering
Purdue University

In recent years, ferroelectric materials are a rising research topic due to the discovery of a scalable, CMOS compatible ferroelectric phase in thin film HfO2. This study presents an open-source implementation of the Du-Chen model of ferroelectric switching, using Python, that has been verified against previously published results. Using experimental data which includes polarization changes with regards to electric field with multiple variations of temperature and signal input, the model computes relevant parameters such as number of domains, time switching, and shortest nucleation time possible as a function of bias voltage and film temperature. This new capability will enable future studies at Purdue of the impact of processing conditions and film composition on the switching kinetics of ferroelectric films, furthering the understanding of this important class of materials.

Keywords: *Ferroelectric, Non-Volatile, Memory System, Power Efficiency, Memory Devices, Applications, Polarization, Switching Behaviors, Hysteresis, Electric Field, Models, Du-Chen, Temperature, Time Switching, Domains, Nucleation*

Optimization Of Focused Ultrasound Output From Piezoelectric Micromachined Ultrasound Transducers For Neural Stimulation

Presentation ID: 31-M15
10:20 am - 10:35 am EDT

Daria A. Shkel[1], Imtiaz Ahmed[2], and Dana Weinstein*[2]
*PI: School of Electrical and Computer Engineering
University of California, Irvine[1], and Purdue University[2]

The search for neural stimulation methods that do not require direct contact between the stimulation device and biological structure (e.g. brain) is of great scientific and practical interest. Pulsed focused ultrasound is one of such non-invasive techniques, in which low-intensity ultrasound is delivered to targeted deep localized regions, resulting in neural activity. Multi-element arrays of hundreds to thousands of ultrasound transducers may enable direction of the outputted ultrasound waves to effectively focus within deep target regions in the brain. We explore the possibility of using custom designed, microfabricated, Piezoelectric Micromachined Ultrasound Transducers (PMUT) and Fresnel Lenses with tuning capabilities, to accomplish this task. The objective of this research was to optimize the design and geometry of PMUT devices. The research aimed to understand how geometric and electrical parameters of devices will affect characteristics of the outputted ultrasound, including the focal point, spot size, and acoustic pressure. For our study, we modeled the device using the COMSOL Multiphysics Finite Element Analysis software and built in Acoustic Module. Our parametric study included variations in geometry of the PMUT device, material layers, material properties, and input actuation voltages. We also investigated the effect of driving different combinations of actuation electrodes on the focal point size and maximum acoustic pressure of the ultrasound. Understanding the effects of these parameters on the generated ultrasound is essential for guiding design and manufacturing of our future PMUT devices.

Keywords: *Piezoelectric Micromachined Ultrasound Transducers, Fresnel Lenses, COMSOL, Focal Spot Size, Finite Element Analysis, Acoustic Pressure*

Finite Element Implementation Of Strain Gradient Plasticity For Microscale Amorphous Polymer Structures

Presentation ID: 31-M16
10:35 am - 10:50 am EDT

Fredrik Arentz, Paul Somers, and Xianfan Xu*
*PI: School of Mechanical Engineering
Purdue University

Finite Element Analysis (FEA) has proven to be invaluable in the design of metamaterials – engineered materials with properties not found in nature. Nanomanufacturing techniques such as Two Photon Polymerization have the capability of producing polymer metamaterials, but the classical mechanics approach used in commercially available FEA tools do not accurately predict deformation in polymers on the micro scale. This can make it difficult to predict the precise deformation observed in mechanical metamaterials. It has been shown that strain gradient plasticity models can describe the size-dependent deviations from classical mechanics in microstructures, but the FEA implementations that have been created so far are specialized for metals, whose inelastic deformation differs from polymer structures. In this paper, the mathematical basis for an FEA implementation of strain gradient plasticity for amorphous polymers will be presented. The FEA solver will be based on existing mathematical models and will be implemented in FEniCS, a partial differential equation solver in C++. The study will give the framework for building an FEA solver that can be used to characterize the deformation of metamaterials with a higher level of precision than that offered by current models.

Keywords: *Strain Gradient Plasticity, Finite Element Analysis, Micro-Scale Amorphous Polymer Structures, 3D Printing*

Design And Simulation Of An On-Chip LC Filter For Superconducting Quantum Circuits

Gozde Iloglu, Jeremy Cadiente, Botao Du, Alex Ma, and Ruichao Ma*
*PI: Department of Physics and Astronomy
Purdue University

Presentation ID: 31-M17
10:50 am - 11:05 am EDT

Keywords: *Superconducting Circuits, Quantum Information Science, Transmon Qubit, Microwave Design*

Our motivation behind this study is the search for new and better quantum bits (qubits). In our circuit, the performance will be enhanced with the use of an on-chip low pass filter. An LC low pass filter will be designed and added to our circuit design to prevent qubit excitation by outside sources. The filter will allow the low frequencies to pass but block the high frequencies. This filter will improve the circuit design by protecting the qubit and producing more reliable results. The filter design is constructed in Klayout software using Python. After verifying the design, the filter is simulated in HFSS using ANSYS Electronic Desktop to analyze the performance. Once the design is finalized, it is incorporated into the circuit. From the performance analysis, we saw that the filter does a successful job filtering frequencies until 9 GHz. The filter is most effective at the range of 5-6 GHz. In future work, we will be increasing the frequency range in which the filter is effective.

Simulation, Identification, And Application Of CMOS Inverters Using OFETs

Walter Kruger, Mohammad Javad Mirshojaeian Hosseini, Robert Nawrocki*
*PI: School of Engineering Technology
Purdue University

Presentation ID: 31-M18
11:05 am - 11:20 am EDT

Keywords: *Electronics Simulation, Organic Electronics, Emerging Technologies*

Organic Field-Effect Transistors (OFETs) have been fabricated and characterized in laboratories with increasing success. OFETs have been identified as an emerging technology with great potential in the biosensor and bioinspired neuromorphic areas of study. Comprehensive mathematical models of these types of electrical components have also been developed successfully, but as their intrinsic characteristics greatly differ inorganic counterparts, there has been a lack of computational tools that allow for these models to be simulated in complex electrical networks. The goal of this research project is to create the tools necessary for OFET simulation in the Simulink and Simscape platforms. Custom code blocks developed using Marinov and Universal Model and Extraction Method (UMEM) mathematical models for OFET characterization are used to simulate single OFET components and construct a fully functioning virtual Organic Complementary Metal–Oxide–Semiconductor (CMOS) inverter for signal amplification and neuromorphic applications. Through the simulated OFETs and CMOS inverters' I-V output and transfer characteristics, we seek to provide data on the accuracy of the simulated components to those used in a laboratory environment. Additionally, by amplifying low-power signals, we aim to demonstrate the usability of these systems in real world applications. This project seeks to provide researchers with a method for simulating OFETs on a virtual platform capable of integrated network simulation to verify their performance and the feasibility of fabrication and construction for these networks.

SESSION E: BIOLOGICAL SIMULATION AND TECHNOLOGY

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Modeling Of Mass And Fluid Transfer In Hemodialysis To Maximize Treatment Efficiency

Presentation ID: 31-M19
10:05 am - 10:20 am EDT

Dunya Al Al Marzooqi, Farzad Mohajerani, and Vivek Narsimhan*
*PI: Davidson School of Chemical Engineering
Purdue University

Keywords: *Hemodialysis, Solute Clearance, Modeling, Optimum Treatment Conditions*

Hemodialysis is a highly regulated and customizable medical treatment used to remove toxins and waste products from the blood stream to a low and safe concentration. This treatment is utilized for patients suffering from advanced kidney disease or end-stage renal disease who have lost the functionality of their kidneys. Over the years, several experimental and modeling efforts have been made in order to find the optimal treatment conditions and newer, more efficient dialyzer designs. This is motivated by the mortality and morbidity rates of these patients, which still remain high. In this study, we will be modeling the hemodialysis process to investigate the ways in which different experimental conditions affect the solute clearance and thus, to increase the efficiency of hemodialysis. MATLAB is used in order to model the hemodialysis system and the command, bvp5c, is used to solve its governing differential equations over the length of the dialyzer. This command requires boundary conditions to be set that mimic the treatment conditions. The toxin clearance efficiency of the dialyzer is then calculated at varying treatment conditions. We observe that larger toxins are harder to be filtered out and therefore, cleared from the patient. With this model, we will be able to validate its accuracy by comparing our simulation results to previous experimental data, specifically by comparing the clearance level of toxins achieved to the modeling results. From the results, we can suggest strategies to increase the clearance level of large toxins. Consequently, this study will guide us to the optimum treatment condition which will be tested experimentally in the future.

Computational Modeling Of Fluid Flow Through Porous Media In A Cholera Enrichment Device

Presentation ID: 31-M20
10:20 am - 10:35 am EDT

Julio Rivera[1], Melinda Lake[2], and Jacqueline Linnes*[2]
*PI: Weldon School of Biomedical Engineering
University of Puerto Rico, Mayagüez[1], and Purdue University[2]

Keywords: *Enrichment Device, Vibrio Cholera, Simulation*

Cholera is an infectious disease that can be contracted by ingesting a substance that contains the bacterium Vibrio cholera. Studies have shown that each year there are 1.3 million to 4.0 million cases of cholera and 21,000 to 143,000 deaths worldwide due to this disease1. It is most commonly found in the tropics particularly Asia, Africa, Latin America, India, and the Middle East. We propose a cholera filtering device to enrich cholera from one liter of water from an environmental source. Furthermore, we aim to detect cholera at very low concentrations of 1-1000 cells/mL. To understand the pumping mechanism to drive this device, we develop a COMSOL fluid flow model through porous membranes in a cholera enrichment device". This model demonstrates the device functions with the use of different pressure-driven flows through nylon membranes; providing a parametric study that predicts the filtration system's velocity with respect to time providing us with an expected behavior for further design improvements. The model predictions indicate that we can design a device to filter 1L of water to enrich cholera in a time span below 15 minutes, thus making this device suitable for point-of-care applications, particularly in places where cholera is endemic.

Mechanobiology Computational Modeling Of Healing Following Breast Conserving Surgery

Presentation ID: 31-M21
10:35 am - 10:50 am EDT

Muira Fontaine, Zachary Harbin, David Sohutskay, Adrian Buganza Tepole, and Sherry Harbin*
*PI: Weldon School of Biomedical Engineering
Purdue University

Keywords: *Computational model, Lumpectomy, Wound Healing, Breast Reconstruction, Collagen, Tissue Engineering*

Breast conserving surgery (BCS; otherwise known as lumpectomy), in conjunction with radiation therapy, has replaced mastectomy as the standard of care for eradicating breast carcinoma because of its preservation of surrounding tissue. Following lumpectomy, the tissue void heals by wound contraction and scar formation, making it challenging for surgeons to predict cosmetic outcomes. This is further exacerbated by the significant patient-to-patient variation in breast size, composition, and tumor geometry and location. Based on these considerations, surgeons would benefit from new options to optimize oncologic and cosmetic outcomes of BCS. Few computational models of wound healing following lumpectomy have been developed, and there is still a gap in current computational models due the lack of mechano-biological coupling. This project adapts an existing three-

dimensional computational mechanobiological model of cutaneous wound healing to the lumpectomy scenario. Breast tissue parameters and properties are modulated to simulate patient-specific conditions and therapeutic interventions, including soft tissue fillers. Preliminary results derived from the coupled mechanobiological model correlated to normal wound closure trends in cell migration and proliferation, causing wound contraction and extracellular matrix (ECM) remodeling. These were consistent with results obtained from the independent biochemical and mechanical models. Studies are ongoing to i) verify model predictability, ii) determine effects of critical parameter modulation (e.g., surgical wound geometry), and iii) simulate applications of collagen-based soft tissue fillers. Computational models quickly inform researchers of new surgical reconstruction strategies or tissue-engineered product design and help clinicians personalize therapies, improving breast wound healing and cosmetic outcomes.

Coarse-Grained Model Of Proteins

Presentation ID: 31-M22
10:50 am - 11:05 am EDT

Kata Alilovic[1], Rajat Dandekar[2], and Arezoo Ardekani*[2]
*PI: School of Mechanical Engineering
University of Florida[1], and Purdue University[2]

Proteins play an important role in metabolism of living organisms. Proteins are built from amino acids that fold into unique 3D structure that determinates its function. Modeling of proteins is used to understand its physical properties and structure. They are large molecules that are hard to study in simulations with all atom models when large number of proteins are involved. Therefore, we are looking to develop a coarse-grained model that will be applicable to various proteins and used in simulations to study physical properties like viscosity and diffusivity in a crowded environment. Coarse-grained models are built in open source molecular visualization program VMD using the all atom coordinates file from Protein Data Bank. Martini force field is applied to create residue-based coarse-grained models while shape-based coarse-grained models are created using CHARMM force field. Chosen coarse-grained model will be studied using LAMMPS, open source simulation software.

Keywords: *Proteins, simulation, Martini model, Bioinformatics, VMD, LAMMPS*

Day 2 | Afternoon Presentations

July 31, 2:00 pm - 3:30 pm EDT

PM2

SESSION A: GENETICS

Click here to join this session

Analysis Of The Indenoisoquinoline Compound Library For Myc G-Quadruplex Targeting

Joshua Kosnoff, Jonathan Dickerhoff, Kaibo Wang, Guanhui Wu, and Danzhou Yang*
*PI: Department of Medicinal Chemistry and Molecular Pharmacology
Purdue University

Presentation ID: 31-A1
2:05 pm - 2:20 pm EDT

Keywords: *Myc, Promoter, G-Quadruplex, Indenoisoquinoline, Cancer Therapeutics, Structure-Activity Relationships*

The Myc protein is known as a master regulator of cancer cells, and its suppression greatly diminishes the viability of these cells. Unfortunately, the Myc protein is considered "undruggable." However, G-quadruplexes (G4) are non-canonical globular DNA structures that can form in the Myc promoter region and downregulate Myc expression. As such, stabilizing the Myc G4 has become a key strategy in cancer therapy. The indenoisoquinoline has previously been identified as a promising scaffold for this purpose, and optimization of this scaffold's side chains can lead to the achievement of desired activity. With access to over 1000 different indenoisoquinoline-based molecules, we establish a first-of-its-kind compound library and explore the chemical space of indenoisoquinolines to determine the positive Myc G4 hit compounds. The molecules are tested with biophysical and cell-based assays to determine G4 inducing ability, G4 thermal stability, and cytotoxicity. Data from all experiments are compiled into a singular database and filtered bioinformatically. The compiled orthogonal data sets are analyzed together to identify positive hit compounds and provide insights into the side chain structure-activity relationships (SAR). The combined analysis successfully filters the library to identify the top compounds in the library and allows for further hit identification and SAR activity.

The Role Of BMAL1 And CLOCK In The Formation Of Alveolar Structures In 3D Cultures

Jacob T. Larsen, Aridany Suarez-Trujillo, Kelsey Teeple, Karen Plaut, and Theresa Casey*
*PI: Department of Animal Sciences
Purdue University

Presentation ID: 31-A2
2:20 pm - 2:35 pm EDT

Keywords: *Mammary Gland, Circadian Timing System, Alveoli, 3D Cultures, BMAL1, CLOCK*

Circadian clock disruption during pregnancy is related to impaired lactation in humans and cows. Transcriptional targets of the circadian clock genes, BMAL1 and CLOCK, include epithelial cell junction proteins. The formation of milk-producing alveolar structures is dependent on these cell-cell junctional proteins. We hypothesized that if BMAL1 and CLOCK genes are disrupted, mammary epithelial cells (HC11) will have a reduced ability to form alveoli and produce milk. Our objective was to measure the effect of BMAL1 gene deletion (BMAL1-KO) and CLOCK protein reduction (shCLOCK) in HC11 cells on the formation of alveoli and expression of the cell-cell junction proteins zona-occludins 1 (ZO-1) and e-cadherin (CDH1) in 3D cultures. Cells were plated (13,000 cells/well) on Matrigel and cultured in the presence of lactogenic hormones. On day 7, phase-contrast microscopy was used to capture images of all alveolar structures (n=3 wells/treatment). ImageJ software was used to count the number of alveoli and measure alveolar area, perimeter, minimum diameter, maximum diameter, and circularity. General linear model and post-hoc Tukey analysis indicated that shCLOCK and BMAL1-KO were significantly different in all parameters from HC11 ($p < 0.05$). The total number of alveoli was also reduced in shCLOCK and BMAL1-KO lines relative to HC11 ($p < 0.05$). These results indicate that the BMAL1-KO and shCLOCK cells have a reduced ability to form alveoli in culture, which supports our hypothesis. Evaluation of ZO-1 and CDH1 expression is ongoing, initial staining patterns are consistent with cell-cell junction proteins.

Structural Studies Of Phospholipase C Epsilon

Presentation ID: 31-A3
2:35 pm - 2:50 pm EDT

Amanda J. Everly, Elisabeth Garland-Kuntz, Isaac Fisher, and Angeline Lyon*
*PI: Department of Chemistry
Purdue University

Phospholipase Cs (PLCs) are an enzyme family responsible for hydrolyzing phosphatidylinositol lipids at the membrane to produce second messengers, which in turn activate other cellular signaling pathways. This study focuses on PLC epsilon, a subfamily differentiated by several unique regulatory domains. Understanding PLC epsilon's regulation via its structure is important due to its roles in cellular signaling and involvement in heart disease. Our research aims to produce high-resolution structures of truncated PLC epsilon variants to better understand how the structure dictates regulation and activity. Experimental procedures begin with a variety of molecular biology techniques to produce a virus that contains the DNA encoding the target protein, which is then used to infect other cells, allowing them to produce the protein. The target protein is then purified by extracting it from the cells based on the presence of affinity tags on PLC epsilon, along with its charge and size. The purified PLC epsilon can then be imaged by utilizing single-particle cryo-electron microscopy (EM), which uses electron detectors to determine a two-dimensional picture of the protein frozen in non-crystalline ice. Software is then used to process these images and eventually produce a three-dimensional structure from the two-dimensional protein images. This will result in an intermediate to a higher resolution structure (8-15 Å resolution) for the protein compared to what has been determined in the past (20-40 Å). These outcomes will allow for a better understanding of the structure of PLC epsilon and its regulation, which improves understanding of its role in cellular signaling.

Keywords: *Cellular Signaling, Protein Biochemistry, Cryo-Electron Microscopy, Phospholipase Cs (PLCs), Structural Biology*

The Characterization Of The Formation Of SAGA And CHAT In Drosophila

Presentation ID: 31-A4
2:50 pm - 3:05 pm EDT

Hannah R. Blum, Eliana Torres-Zelada, and Vikki M. Weake*
*PI: Department of Biochemistry
Purdue University

Regulation of genes in eukaryotes often involves large multi-subunit complexes to carry out histone modifications, in order to make chromatin more accessible to the transcriptional machinery. One key histone modification is histone acetylation, and one of the most well-known histone acetyltransferases (HAT) is Gcn5, which works as part of multisubunit complexes. While yeast contains the Spt-Ada-Gcn5 acetyltransferase (SAGA) and Ada2/Gcn5/Ada3 transcription activator (ADA) complexes, metazoans have a third complex: Ada2a-containing (ATAC). It was recently discovered that *Drosophila melanogaster* have two isoforms of Ada2b, a subunit of Gcn5 complexes, and that the Ada2b-PB isoform is in SAGA, while the Ada2b-PA isoform associates with Chiffon, forming a novel complex: the chiffon histone acetyltransferase (CHAT). Unlike their yeast counterpart, metazoan SAGA complexes have not been illustrated to show how each part functions as a whole and neither has CHAT. To expand on the characterization of the formation of these complexes in *Drosophila*, the interactions between different proteins that comprise each complex were tested. A Yeast 2-Hybrid (Y2H) assay was used to test the interactions between the different domains of Spt7 with other SAGA-specific subunits: Spt3, Taf10b, Sf3b3 and Sf3b5, as well as the interactions between the regions of the Ada2b isoforms with Spt7. The results from these two Y2H assays will provide a better understanding of the interactions that drive the separate formations and aid in the eventual illustration of these two complexes.

Keywords: *SAGA, CHAT, Gcn5, Histone Acetylation*

R-Loops And DNA Damage In Aging Photoreceptor Neurons

Presentation ID: 31-A5
3:05 pm - 3:20 pm EDT

Alyssa N. Easston, Hana Hall, and Vikki M. Weake*
*PI: Department of Biochemistry
Purdue University

While it is established that aging increases susceptibility to ocular disease, the biological mechanisms are not fully understood. This study explores the possibility that harmful R-loop (DNA:RNA hybrid structure) accumulation as a result of aging predisposes cells to DNA damage, epigenetic dysregulation, and neurodegeneration. Unscheduled R-loops can have detrimental effects on genome stability and cell survival, as they can block transcription and cause double-stranded breaks (DSBs). Here, we examined R-loop levels and DNA damage levels in aged *Drosophila Melanogaster* using DNA dot blots and histone western blots, respectively. Preliminary data suggest that there may be a correlation between age and global R-loop levels, but not global DSB levels in *Drosophila* heads. Now that we have identified a strong signal for R-loops in photoreceptor nuclei, we will repeat the previous experiment with photoreceptor nuclei rather than heads. Beyond this global analysis, genome-wide mapping may reveal trends in R-loop and DNA damage levels and location that are not visible on a global scale. To map localization of R-loops in aged *Drosophila* genome, we will use enzymatically dead human RNase H1 (D210N) mutant expressed specifically in photoreceptor cells using the QF-QUAS systems. We expect that old *Drosophila* photoreceptor nuclei will have higher levels of R-loops and DNA damage than young; this would suggest that unscheduled R-loop formation plays a significant role in neuronal aging.

Keywords: *R-Loop, DNA Damage, Aging, Gene Expression, Photoreceptor Cells, Drosophila*

SESSION B: ENERGY AND ENVIRONMENT

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Marine Renewable Energy: Aligning The Technology, Geography, And Markets

Presentation ID: 31-A6
2:05 pm - 2:20 pm EDT

Sean P. Murphy, Abhishek Ajmani, Ananya B. Sheth, and Joseph V. Sinfield*
*PI: Lyles School of Civil Engineering
Purdue University

The U.S. Department of Energy (DoE) has long recognized the potential for the oceans to provide a sustainable source of energy for society at great scale. However, progress toward this energy ideal has waned due to the technical challenges of effectively harnessing the power of the seas, the community engagement needed to place systems in use, and the financial risks of this endeavor. In this work, through partnerships with the National Renewable Energy Laboratory (NREL), Pacific Northwest National Laboratory (PNNL), and the DoE's Water Power Technologies Office (WPTO), methods of innovation science have been applied to help highlight paths to the development of a sustainable Blue Economy. Specifically, a pattern associated with the successful development of high-impact innovations – termed enabling innovation – has been applied to highlight intersections of purpose and context that may be particularly amenable to adopt marine renewable energy (MRE). Identification of these opportunities has been pursued by combining existing perspectives on ocean conditions along U.S. coastlines, with geo-spatial views of MRE commercial activity, potential application markets, and community amenability to renewable energy projects, yielding a visualization of zones along the coast that likely offer the highest opportunity for marine development. Preliminary findings suggest significant potential for MRE development along the north-west coast, southern Georgia, and North Carolina, with additional, albeit smaller scale opportunity, along the coasts of Maine and Texas.

Keywords: *Marine Renewable Energy, Ocean Renewable Energy, Blue Economy, Renewable Energy, Energy, Maritime Market, Ocean Power, Hydropower, Hydroelectric, Power*

Development Of A Riverine Energy Harvesting Device: Characterization Of Wabash River In Lafayette As A Test Site

Presentation ID: 31-A7
2:20 pm - 2:35 pm EDT

Jingzhe (Zack) Zhang, Yijie Wang, and Jun Chen*
*PI: School of Mechanical Engineering
Purdue University

In recent years, there has been a large focus on improving and innovating methods to harness renewable energy. The widespread nature of rivers across the U.S. provides an opportunity to utilize the fast-flowing water current for hydrokinetic electricity generation. The minimal environmental impact and user maintenance regarding hydropower are highly preferable to conventional energy sources. Our research team is partnered with the U.S. Department of Energy (DOE) with the task to design, build, and implement a modular river current energy converter. Before the prototype phase of the device, extensive bathymetric surveying and research on the proposed region of deployment

Keywords: *Renewable Energy, River, Wabash, Turbine, Survey*

were conducted. The local Wabash River was surveyed remotely using data collected from prior research in the region. Various software allowed visualization of the findings, with primary results including meshgrid surfaces of the riverbed and heat maps indicating average water velocity and water depth. A notable location on the river with exceptional characteristics to house a test-turbine was found. The results of this study highly suggest the suitability of the Wabash River as a test site for our device. Moreover, the recommended location derived from this study has a high probability of being selected as the prototype test site.

Wind Energy Production And Resource Optimization

Presentation ID: 31-A8
2:35 pm - 2:50 pm EDT

Abigayle Elaine Moser[1], Diego Siguenza[2], Ali Doosttalab[2], and Luciano Castillo*[2]
*PI: School of Mechanical Engineering
Iowa State University[1], and Purdue University[2]

Keywords: *Atmospheric Dynamics, Renewable Energy Systems, Sustainability, Wake Effects, Wind Energy Systems*

Power transmission across vast expanses remains a major barrier in providing energy security to underserved regions. Energy isolation remains a challenge for underserved communities. The renewable energy sector has grown substantially in the past decades in terms of industrial expansion and natural resource utilization. Microgrid systems integrating wind, solar, and water are a unique solution to solving imbalances and connectivity in hard to reach areas. This study seeks to outline a framework for resource characterization and subsequent wind farm implementation in isolated regions through meteorological assessment coupled with experimental data, in Peru and Ecuador. Data from meteorological stations were used to sssess the wind resource availability coupled with the economic viability of future implementation. In order to examine the effect of the complex terrains, wind tunnel experiments were performed with a 1:950 scaled-down model wind farm. Computational fluid dynamics (CFD) simulations were performed in OpenFOAM software to validate the wind tunnel experimental data with large-scale simulations. The results from the modeled wind farm over the complex terrains indicate greater wind power resources in the mountainous regions than in more flat regions.

Development Of A More Environmentally Sustainable Machine Tool Through Innovative Design

Presentation ID: 31-A9
2:50 pm - 3:05 pm EDT

Adriana M. Muñoz-Soto[1], Matthew Triebe[2], and John Sutherland*[2]
*PI: Environmental & Ecological Engineering
University of Puerto Rico, Mayaguez Campus[1], and Purdue University[2]

Keywords: *Machine Tool Cost, Milling Machines, Lightweighting, Machine Tools*

Machine tools are an essential asset in the infrastructure of the businesses, making it essential to monitor their entire Life Cycle. These machines generate an environmental impact that negatively affects the living creatures nearby emitting large amounts of CO_2 through their energy consumption. There are various ways to redesign the machine to reduce the energy needed, such as light weighting, which consists of reducing the material of certain features of the machine to reduce their energy consumption. However, these design changes may increase their cost due to the greater complexity. In order to implement any design changes, we must primarily understand the features that drive the cost. By strategically researching and redesigning those key components, we will be able to accurately reduce the carbon footprint without increasing the cost dramatically. To better understand the cost drivers, a data sheet is being created with all the key features and prices of various machines, specifically milling machines. This data sheet will be analyzed using a regression model to highlight the features with greater impact. We are able to estimate that features relating to the main table, such as travel and how much weight the table is able to withhold, have the greatest influence in terms of pricing. Having most of our components direct us to the main table, light weighting such component will, in theory, not only reduce the operational cost of the machine, but also reduce carbon footprint since it requires less energy in order to run.

An Online Behavioral Experiment On Users-Agency Interactions In The Provision Of A Public Service

Presentation ID: 31-A10
3:05 pm - 3:20 pm EDT

Mauneel M. Amin, Samuel Park, Peyman Yousefi, and David Yu*
*PI: Lyles School of Civil Engineering
Purdue University

Keywords: *Exit-Voice, Behavioral, Public Service, Human-Subject, Infrastructure*

Infrastructure is an important facility that serves people in a specific area or region. These facilities can either be public or private based on exclusivity and competitiveness. Moreover, these resources are often underinvested, exploited, or overused based on its accessibility by the provider or user. A critical challenge of this situation is to evaluate adequate service provision in the face of potential underinvestment to infrastructure by the provider. To solve problems, behavioral experiments on human subjects are performed to understand the real-life crisis. Behavioral experiments can be administered in several ways, including laboratory testing using a paper-pen experiment (in classrooms) or using online testing via various platforms like Amazon mechanical Turk (Mturk), VCWeb, etc. For the Exit-Voice experiment, we will be deploying an online human-subject experimental game on a crowdsourcing platform (e.g. Mturk) to generate a practical insight in the field. Previous studies have shown

significant similarities between results collected from lab testing and online platform testing. Using the data collected, we will be testing hypotheses to gain empirical evidence about what kind of policy change is required in terms of infrastructure improvement so that both the user and provider make the best use of the resource.

SESSION C: ENGINEERING THE BUILT ENVIRONMENT

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Exploration Of Trust In Automation In Complex, Safety-Critical Systems

Presentation ID: 31-A11
2:05 pm - 2:20 pm EDT

Jacob W. Evans[1], Murali Krishnan Rajasekharan Pillai[2], Ali Baigelenov[2], Paul Parsons[2], Ilias Bilionis[2], and Shirley Dyke*[2]
*PI: School of Mechanical Engineering
Georgia Institute of Technology[1], and Purdue University[2]

In 2000 the International Space Station (ISS) began housing astronauts in low-earth orbit for extended periods of time, creating a previously unfathomed sandbox for scientific exploration and discovery. The logical next step beyond earth's orbit is a habitat on an extraterrestrial body (e.g. the moon or Mars). The Resilient Extra-Terrestrial Habitats (RETH) Institute is creating a framework based on resilience to be used in future habitat designs. Any deep-space habitat would require a significant contribution from autonomous systems to assist and aid human decision-making and ensure continued habitation and mission success. These systems would not act independently, but rather would need to interact with trained human agents. Previous autonomy failures across industries highlight the need to explore an explainable relationship between the human agent and the autonomous system. By examining these failures and the literature in human factors and autonomy domains, this work will derive generalizations and identify areas for future study for RETH.

Keywords: *Automation, Trust, Health Management, Human-Computer Interaction, Artificial Intelligence, Explainable AI, Human Factors*

Investigating Membrane Material Alternatives For Carbon Dioxide Removal In Space

Presentation ID: 31-A12
2:20 pm - 2:35 pm EDT

Gabriela Cesar[1], Debraliz Isaac Aragones[1], Justin Wiebel[1], Maximillian Cobos[2], and David Warsinger*[1]
*PI: School of Mechanical Engineering
Purdue University[1], and Wabash College[2]

Recently, NASA's ultimate goal has been to launch a crewed Mars mission. However, the current system used for carbon dioxide (CO_2) removal in air revitalization on the International Space Station (ISS) is not equipped to handle missions beyond low-earth-orbit. The Carbon Dioxide Removal Assembly (CDRA) is a complex system that relies heavily on sorbent materials and faces challenges in reliability, energy, efficiency, and material degradation. Although the CDRA has operated well on the ISS for the past two decades, health effects from high CO_2 levels are amongst the most common complaints and challenges from astronauts. Recent developments in membrane technology prove to be a promising alternative to sorbent-based systems for CO_2, since they can easily separate gases while being energy efficient. Maintaining high selectivity for CO_2 with a reasonable permeability, at such low partial pressures and in the presence of water, is among the main challenges of using membranes in this application. In this work, we have created a membrane-based model to identify, and optimize, membrane material for effective CO_2 separation in this application. We expect to determine a working range of critical parameters such as permeability, selectivity, membrane area and thickness for successful CO_2 separation. We will also be comparing thermodynamic efficiency of a membrane-based process to that of the CDRA to pinpoint areas of improvement.

Keywords: *Membranes, Carbon Dioxide Removal, Modeling, Gas Separation*

Thermal Transfer System Development Of Cyber-Physical Testbed For Resilient Extra-Terrestrial Habitats

Presentation ID: 31-A13
2:35 pm - 2:50 pm EDT

Jordan Soberg, Yuguang Fu, Davide Ziviani, Amin Maghareh, and Shirley Dyke*
*PI: School of Aeronautics and Astronautics
Purdue University

The future of human spaceflight relies on the development of habitats to house astronauts. Developing and designing these habitats will require a level of resilience that is not currently well understood. To advance knowledge in the field the Resilient Extra-Terrestrial Habitat Institute (RETHi) is taking steps to develop the technology that will enable resilient habitats outside of Earth's atmosphere. To study, demonstrate, and evaluate the technologies developed in pursuit of this mission, a multi-physics cyber-physical test-bed built upon a dome-like structure is being founded at Purdue University. The test-bed must reflect the hazardous conditions of space one of which being

Keywords: *Space Habitats, Thermal Modeling, Physical Systems, Thermal Design*

extreme temperatures, which is being modeled via a cooling loop on the test-bed exterior. To accurately reflect the cooling loop and its controls computationally, a model is being developed in the Simulink software using the Simscape add-on. The methods of creating this model as well as the effectiveness and accuracy of this software's modeling and controls capabilities will be highlighted in this study. This information will allow for the development of other similar physical models in the Simulink software for further space analogs.

Real Time Occupancy Sensing With A Low-Cost Seat Based Temperature Array

Aayush Mathur, Danielle Wagner, and Brandon Boor*
*PI: Lyles School of Civil Engineering
Purdue University

Presentation ID: 31-A14
2:50 pm - 3:05 pm EDT

Keywords: *Real Time Detection, Seated Occupancy, Spatial Tracking, Building Sensors, Thermocouples, Indoor Environmental Quality*

Humans are active emission sources of carbon dioxide, volatile organic compounds, and bioaerosols. Human-associated emissions can alter the composition of air inside enclosed spaces. Thus, a real-time means of detecting occupancy can be used to determine the quality of air in these spaces, and the corresponding ventilation required to maintain conditions at a safe and comfortable level. Current occupancy detection methods are both inaccurate and wholly unable to determine spatial distributions of occupants. This study aims to develop and evaluate a new means of detecting spatiotemporal seated occupancy patterns in an open-plan office in real time using low-cost Arduino-based temperature sensors. Arduino microcontrollers were coupled with nRF24l01 radio transmitters and K-type thermocouples to develop a low-cost temperature sensor array. These sensors were mounted to chairs, and each chair's surface temperature was transmitted to a receiver microcontroller in real time. The seated occupancy was calculated using two different algorithms, the Peak Temperature Algorithm, and the Delayed Occupancy Algorithm. The Peak Temperature Algorithm calculated occupancy in real time but suffered a delays ranging from 5-15 seconds. The Delayed Occupancy Algorithm calculated occupancy with a 1-minute delay and had errors of 3-5 seconds. This study aims to expand the sensor array, and use it to develop a apical map of seated occupants. This will then be integrated in the Living Laboratories at Purdue University's Herrick Laboratories. The effectiveness of the sensor array will be evaluated against a manual count of actual seated occupancy.

SESSION D: CHEMICAL UNIT OPERATIONS

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More Olefins: Oxidative Dehydrogenation Of Ethane In Shale Gas To Ethylene

Cristian Oviedo[1], Zewei Chen[2], and Rakesh Agrawal*[2]
*PI: Davidson School of Chemical Engineering
University of Houston[1], and Purdue University[2]

Presentation ID: 31-A15
2:05 pm - 2:20 pm EDT

Keywords: *Shale Gas, Olefins, Ethylene, Process Simulation, Oxidative Dehydrogenation*

In the U.S. the shale gas revolution has resulted in large amounts of shale gas, primarily composed of methane and ethane, to enter the market. Shale gas in remote areas of the U.S. are currently being handled in low value ways such as being flared, re-injected into drilling-wells, and being sold at fuel value prices when it could be used to produce high value olefins such as ethylene and propylene. The demand for these products continues to grow. However the current technology for producing these products is steam cracking, an energy intensive, equipment heavy, and high CO_2 emitting process. To address the growing demand for high olefins and limitations of steam cracking, this study investigates and incorporates existing oxidative dehydrogenation technology into process flow diagrams on a systems level to present a viable alternative to steam cracking. Aspen Plus will be used to create these process flow diagrams, and experimental oxidative dehydrogenation catalytic data will be used to design the chemical reactor. The oligomerization reactor, used to convert compounds like ethylene and propylene to higher weight olefins will be specified downstream. Furthermore, heat integration will be incorporated to maximize energy efficiency and recycle streams will be used to minimize product losses. The results of this study will be used to propose a viable alternative to steam cracking in order to address the growing the demand for high value olefins.

Consequences Of Brønsted Acid Site Proximity And Location In H-MFI Zeolites For Propene Dimerization

Presentation ID: 31-A16
2:20 pm - 2:35 pm EDT

Lauren Kilburn[1], Elizabeth Bickel[2], Mykela Deluca[1], David Hibbitts[1], and Rajamani Gounder*[2]
*PI: Davidson School of Chemical Engineering
University of Florida[1], and Purdue University[2]

Keywords: *Catalysis, Zeolites, DFT*

Shale gas feedstocks contain propane, which can be dehydrogenated to propene and subsequently oligomerized to form transportation fuel-range molecules. Brønsted acidic zeolites can be synthesized with different active site and structural properties, which affects oligomerization rates and product distributions. Zeolite frameworks are composed of silicon tetrahedrally coordinated to oxygen; substitution of Al for framework Si generates a negative lattice charge, which compensates an acid site (H+). Al can be substituted in MFI frameworks at 12 crystallographically unique lattice positions (T-sites) with corresponding acid sites oriented in straight and sinusoidal channels (~0.5 nm diameter) or intersections (~0.7 nm diameter). Propene oligomerization rates on MFI have been previously reported to increase with proximal Al content, attributed to steric constraints imposed by proximal adsorbates that facilitate product desorption by destabilizing adsorbed alkyls. This study uses density functional theory (DFT) to calculate relative energies for surface-bound propyl at each T-site in MFI, and activation barriers for propene dimerization at representative isolated and proximal sites. Differences in local Al coordination have a smaller influence on the range of 1-propyl and 2-propyl adsorbate energies (19 kJ/mol and 27 kJ/mol), than differences among O-sites (158 kJ/mol and 136 kJ/mol), because adsorbates bound to different O atoms are confined within different voids. The presence of proximal 2-propyl adsorbates and physisorbed propene increases intrinsic dimerization barriers by 40 kJ/mol and 23 kJ/mol, respectively, suggesting that the extent to which proximal sites influence oligomerization rates depends on the identity of the proximal adsorbate.

Shale Gas To Oil: Kinetic Model For Oligomerization Reactor

Presentation ID: 31-A17
2:35 pm - 2:50 pm EDT

Dorinda Y. Ntim[1], Zewei Chen[2], and Rakesh Agrawal*[2]
*PI: Davidson School of Chemical Engineering
Prairie View A&M University[1], and Purdue University[2]

Keywords: *Oligomerization, Shale Gas, Fossil Fuel, Kinetic Models, Renewable Energy, Bridge Fuels*

Looking at the current state of the energy industry, there seems to be a gradual shift from the use of coal, oil shale and other fossil fuels to the use of renewable sources of energy such as wind and solar energy. In order to bridge the gap between the present dependence on fossil fuels and the transitioning to the future, the energy sector has resorted to using bridge fuels (shale gas). Converting shale gas to usable oil involves the use of several processes. Since shale gas is mostly composed of lower count alkanes like methane, ethane and propane, the best way to reach the goal of producing these liquid fuels with higher carbon numbers is to produce it by repeating the lower count hydrocarbon chains units through a process called oligomerization which is the heart of the process. This process aids in producing higher carbon number liquid fuels and to reach this goal, kinetic models are being investigated to determine the product distribution from the oligomerization process. After the feed is obtained from a dehydrogenation process, the main component that is oligomerized is ethylene and through the process, heavier carbon chains are formed. These heavier chains are the liquid fuels used in everyday life such as diesel, gasoline and lubricating oils. The Anderson-Flory-Schulz distribution is analyzed. Using this kinetic model, the product distribution was then determined. It was observed by the end that, the higher the chain growth probability factor which is dependent on the chosen catalyst, the better the yield for the heavier hydrocarbon liquids.

Sensing And Measurement For Controlled Nucleation In Lyophilization

Presentation ID: 31-A18
2:50 pm - 3:05 pm EDT

Siyue Shen, Andrew Strongrich, and Alina Alexeenko*
*PI: Davidson School of Chemical Engineering
Purdue University

Keywords: *Lyophilization, Freeze-drying, Controlled Nucleation, Sensing and Measurement, Computer and Web Based Applications, Biotechnology*

Lyophilization is a technique used for the stabilization of otherwise unstable productions by removing the water from them at low temperatures and pressures. Lyophilization is advantageous in extending shelf lives of pharmaceuticals and foods without damage their active contents, while the prolonged process is the major disadvantage. In modern aseptic cGMP manufacturing environments the nucleation event is homogeneous in nature, often taking hours or days for the entire batch to freeze. The reason why controlled nucleation has gained so much attention is that the whole batch of vials would nucleate. Thus, freezing time for entire batch would reduce remarkably. One of the methods for controlled nucleation is called rapid depressurization, but performing such control need accurate real-time pressure and temperature data inside vials. Developing a sensor, which can take temperature and pressure measurements inside the vials during the process, helps us to analyze the relationship between temperature/pressure and the nucleation time. Also, it is important to have a control portal for the sensor so that it is possible to visualize and record the real-time data easily during lyophilization. Thus, a web application for data visualization would be favorable. On the developed web page, users can visualize the temperature and

pressure data as well as performing data recording for selected and enabled devices. The web application runs without crashing. By using the specialized sensor, it is possible to read and record real-time temperature and ambient pressure data in the individual vials. Nucleation is induced uniformly corresponding to the measured pressure drop within the vial headspace due to the adiabatic depressurization.

SESSION E: COMPOSITE MATERIALS AND ALLOYS

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Progress Towards 20% Efficient Flexible Perovskite Solar Cells

Presentation ID: 31-A19
2:05 pm - 2:20 pm EDT

Yiyuan (Melody) Zhang, Blake Finkenauer, and Letian Dou*
*PI: Davidson School of Chemical Engineering
Purdue University

Keywords: *Perovskites, Flexible Solar Cells, Thin Films, Semiconducting Material, Solution Processing*

Halide perovskites have been considered excellent materials for solar cells because of their long charge carrier lifetimes, high absorption coefficient, defect tolerance, and low-cost fabrications. These properties further allow the fabrication of thin flexible solar cells, which are portable, easier to install, and lower in the fabrication cost compared to the rigid devices. However, traditionally high-performance perovskite solar cells require the use of rigid transition metal oxide. In addition, these materials have different thermal expansion coefficients, which lead to large stresses in the perovskite thin film. Meanwhile, the substrate must be kept flat during fabrication to coat uniform films. To increase the device flexibility, semiconducting polymers and small organic molecules can be used as electrodes and transport layers. However, these materials require sensitive processing and doping to achieve uniform electronic properties. In this work, we use a PET/ITO/PTAA/perovskite/PC61BM/BCP/Ag architecture as a starting point towards an ultra-flexible high-performance perovskite solar cell. We investigate modifying layer thickness, layer interfaces, doping of PTAA, and annealing time for each layer. To assist the analysis of data output from the solar simulator, we developed a code that inputs raw solar simulator data and outputs current-voltage plots with key device parameters for each measurement all together. With these advancements, we expect to quickly improve the flexible device performances and develop a 20% efficient flexible perovskite solar cell. This project provides valuable insight to the study of flexible solar cells.

Examining Fatigue Damage Mechanisms In Carbon Fiber Reinforced Composite Laminates Through High Resolution X-Ray Micro Computed Tomography

Presentation ID: 31-A20
2:20 pm - 2:35 pm EDT

Javi Solano[1], Alejandra Ortiz-Morales[2], Imad Hanhan[2], and Michael Sangid*[2]
*PI: School of Aeronautics and Astronautics
University of Houston[1], and Purdue University[2]

Keywords: *Carbon Fiber / Epoxy Composites, Damage Analysis, In-situ Tomography*

In aircraft load bearing structures, carbon fiber reinforced polymer (CFRPs) composites have seen increased use due to their lightweight and high strength as compared to traditional titanium and aluminum alloys. The usage of laminate composites into aircraft structures solicits the introduction of new damage mechanisms. Crack growth in such laminate composites is comprised of a complex interaction between microstructural damage mechanisms, which are events that are observed as inter-laminar matrix cracking (delamination), intralaminar matrix cracking, fiber breakage, and fiber-matrix debonding. Although the presence of specific mechanisms has been established, an understanding of the interaction between mechanisms throughout crack growth in CFRPs is necessary to produce optimal damage tolerant designs and reliable predictions for the slow crack growth behavior of structures. Therefore, towards a better understanding of this interaction, a T650/5320 laminate composite with two distinct lay-ups ([+45]6 and [+45/-45/+45]s) was studied under cyclic loading. The local microstructure and the progression of damage was tracked via in-situ synchrotron X-ray micro-computed tomography (μ-CT) in order to identify the individual contributions of delamination and intralaminar matrix cracking to the overall crack profile.

Mathematical Modeling of the Anionic Diffusion In Halide Perovskites

Presentation ID: 31-A21
2:35 pm - 2:50 pm EDT

Alan Pistone, Akriti Akriti, and Letian Dou*
*PI: Davidson School of Chemical Engineering
Purdue University

Keywords: *Semiconductor, Perovskite, Energy, Solar, Materials, Modeling*

Halide perovskites are novel semiconductor materials that have been shown to have great potential applications in solar panels. Perovskite based solar panels can be made at a much lower cost compared to traditional solar panels while boasting a high efficiency. As an emerging technology, a lot can be explored with the unique properties of these halide perovskites, beyond their solar applications. A halide perovskite crystal structure is generally of the form ABX_3, where A is an organic or inorganic cation, B is a heavy metal cation, and X is a halogen. Though perovskites have great potential in optoelectronic applications, their commercialization is held back in part due to

their inherent instability. Part of this instability stems from the tendency of the halogen anions to diffuse and move around the soft lattice crystal structure of the perovskite. Researchers have designed heterostructure platform to study the halide diffusion process in perovskites. However, the calculations required to mathematically model this phenomenon are cumbersome and can take up hours of research time. In order to streamline the calculation process, we have written several user defined functions in MATLAB to calculate the diffusion coefficient in a few minutes. The codes require minimal user input and is planned to be extended for use in different types of heterostructure platforms. Here, I have successfully utilized the code for calculating bromide-iodide diffusion coefficient in two-dimensional halide perovskite vertical heterostructure.

Thermodynamic Modeling Of Oxidation In Refractory Complex Concentrated Alloys

Presentation ID: 31-A22
2:50 pm - 3:05 pm EDT

Haydn E. Schroader, Pilsun Yoo, Saswat Mishra, Alejandro Strachan, and Michael Titus*
*PI: School of Materials Engineering
Purdue University

Keywords: *High Temperature Oxidation, Modeling and Simulation, Materials Science, First Principles Calculations*

Traditional refractory alloys, which comprise a mixture of metals exhibiting melting temperatures above 2000 ºC, are often used in state-of-the-art, high temperature technologies such as rocket engines. However, their use is severely limited due to their poor resistance to environmental degradation resulting from reactions with oxygen and nitrogen at elevated temperatures. Recent work has suggested that an emerging class of alloys, denoted as refractory complex concentrated alloys (RCCAs), may exhibit significant improvement in environmental degradation resistance. RCCAs are encompassed by complex concentrated alloys (CCAs), a novel class of materials that lack a single principal component. Due to the nearly limitless combinations of elements and compositions possible in RCCAs, properties of such compounds remain largely unexplored. Thus, this research project aims to provide a method of rapid modeling for the layering of oxides in RCCAs using thermodynamic principles. The model utilizes the Materials Project density functional theory database to calculate grand potentials, which will in turn be used to determine equilibrium phases and compositions. The user-interface is a Jupyter notebook, which calls methods from Python scripts. The model has been validated against phase diagrams in the Materials Project database and verified against experimental results from pure metals, and predictions of oxide formation in select alloys agree well with elevated temperature oxidation testing results. This model provides a novel and rapid method of predicting oxide layering in RCCAs and can be used to guide future RCCA design and development.