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Abstracts – Morning Session
AEP: Applied Electromagnetics and Plasma Science
A Novel Integrated Scalable Phased Array with a Reduced Number of Phase Shifters

Fatemeh Akbar, Amir Mortazawi

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A phased array is an ensemble of antennas capable of beam forming and steering by adjusting the relative phase and amplitude of signals received or transmitted by each antenna element. Due to the spatial selectivity offered by phased arrays, they can reduce co-channel interference, multipath fading, and the required transmit power in telecommunication systems. Phased arrays can also enhance cross range resolution and SNR in radar systems. Therefore, phased arrays are very attractive in commercial applications.

In phased arrays, phase shifters are the key components responsible for adjusting the signal phase across the array. In conventional phased arrays, one phase shifter is used for each array element. Phase shifters and their associated control circuitry are responsible for a large portion of complexity, size, and cost of phased arrays.

This research presents a new technique (based on incorporating vector summation method into a new RF feed network) for designing a scalable phased array such that distribution of the signal phase along the array can be controlled by a single phase shifter. Therefore, the size, and complexity of phased arrays will be reduced. As a proof of concept, a Ku band 8-element phased array has been designed and fabricated based on the proposed method.

The phased array is being integrated to be applied to automotive radar applications. So far, two different phase shifters are integrated using the IBM 130nm CMOS process. These phase shifters are being utilized in the phased array system supposed to operate at 24GHz (as required by automotive industry).
Magnetospheric Multiscale Mission Examination of Stress Balance in FTE-Type Flux Ropes at the Earth’s Magnetopause

Mojtaba Akhavan-Tafti¹, James A. Slavin¹, Guan Le², Jonathan P. Eastwood³, Robert J. Strangeway⁴, Christopher T. Russell⁴, Rumi Nakamura⁵, Wolfgang Baumjohann⁶, Roy B. Torbert⁷, Barbara L. Giles², Dan J. Gershman², and James L. Burch⁷

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Determining the magnetic field structure, electric currents, and plasma distribution within flux transfer event (FTE)-type flux ropes is critical to the understanding of their origin, evolution, and dynamics. We analyze FTEs observed by the Magnetospheric Multiscale (MMS) mission in the vicinity of the sub-solar magnetopause, i.e. 12 ± 22.5° Local Time and $X_{\text{GSM}} > 7 R_E$. High-resolution data from the Fluxgate Magnetometer (FGM) and Fast Plasma Investigation (FPI) are used to determine and compare the extent to which large (> 1 $R_E$) and small (ion scale) diameter FTEs are force-free, i.e. $J \times B = 0$, or non-force-free, i.e. $J \times B = \nabla P$. Three independent methods are used: i) current density parallel and perpendicular to the magnetic field derived from the plasma measurements or magnetic field using the curlometer technique; ii) direct measurement of the plasma pressure gradient by FPI; and iii) fitting magnetic field to force-free ($J = aB$) flux rope models. Our initial results indicate that the plasma content of the ion-scale FTEs often exceeds that of larger FTEs. This results in higher plasma pressure gradients inside smaller FTEs and a magnetic field that is less force-free than the larger flux ropes.
A Broadband, Bessel Beam Radiator

Nikolaos Chiotellis\textsuperscript{1}, Anthony Grbic\textsuperscript{1}

\textsuperscript{1}Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan

Here, a broadband Bessel Beam launcher is presented, capable of radiating short, localized (X-Wave) pulses into free space. The antenna/launcher is formed by flaring a coaxial cable that is partially filled with a dielectric. The design exhibits a low reflection coefficient and high radiation efficiency from 18 to 30 GHz. The fields in the antenna’s radiative near-field remain relatively constant within this bandwidth. As a result, short X-Wave pulses can be generated within this region. Such a device could find use in medical or military applications.
A Phase-tunable, Liquid Crystal-based Metasurface

Amanda Couch¹, Anthony Grbic¹

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Recent advances in the development of low-loss liquid crystals has enabled the design of tunable devices for millimeter-wave applications. The device presented in this work will use the inherent dielectric anisotropy of liquid crystals to create a phase-tunable metasurface. An iterative design procedure for the device has been developed that models the device as an L-C circuit and compares the circuit element values to those taken from an Ansys HFSS simulation.

The metasurface consists of a multi-layer structure with a central cavity that is filled with liquid crystals. The top layer of the structure is a quartz wafer with an array of metallic patches. The metallic patches are connected by bias lines. The bottom layer consists of a glass-in-silicon wafer with another array of metallic patches. Each metallic patch on the bottom layer is placed atop a silicon pillar in the glass-in-silicon wafer. The liquid crystal cavity is made out of SU-8 2000, a negative photoresist often used in MEMS and microfluidic applications. The cavity is made atop the glass-in-silicon wafer. The two wafers are bonded together using a UV-curable adhesive. The fabricated metasurface was tested and demonstrated over 180° phase shift. Losses in the device were higher than anticipated due to fabrication errors. A new device design and fabrication process has been developed to create a device that is more robust to fabrication errors.
Influence of Magnetic Field Variations on a Nested Hall Thruster

Sarah E. Cusson¹, Scott J. Hall¹, and Alec D. Gallimore¹

¹Department of Aerospace Engineering, University of Michigan, Ann Arbor, MI

Nested Hall thrusters, which concentrically nest multiple discharge channels together, are an attractive option for scaling the technology to high power. This is due to their ability to maintain a small mass and footprint at high power and their ability to throttle over a large range of powers. However, much of the underlying physics of how these complex devices work is not understood. One of the most critical parts of these thrusters is their magnetic fields. The fields on a nested Hall thruster are inherently more complicated due to shared magnetics and the interacting fields of multiple channels. The goal of this work was to better understand the optimum magnetic field for each thruster operating condition. A retarding potential analyzer was used to measure ion energy distribution functions (IVDF) on the X3, a three channel 200-kW nested Hall thruster developed at the University of Michigan in conjunction with NASA and the Air Force Research Laboratory. IVDF’s were then used to determine the voltage utilization of the thruster which is a defining characteristic of how well the thruster operates. Additionally, performance measurement were taken while the magnetic field was varied in order to determine optimal performance. The results of this work are critical in determining whether nested Hall thrusters are a viable technology for deep space exploration.

References
Time-Resolved Hall Thruster Plasma Measurements Using a High-Speed Langmuir Probe with Sheath Capacitance Corrections

Ethan T. Dale¹, J.P. Sheehan¹, Alec Gallimore¹

¹Department of Aerospace Engineering, University of Michigan, Ann Arbor, MI

The Langmuir probe is a standard plasma diagnostic tool that has been researched and applied extensively since its invention in the early twentieth century. Although it is usually used for slow measurements (<100 Hz), techniques exist for operating them up to 200 kHz [1]. One area of application for the high-speed Langmuir probe (HSLP) is in the diagnosis of Hall effect thruster plumes. Hall thrusters are electrostatic plasma propulsion devices with crossed electric and magnetic fields. These thrusters exhibit ~10 kHz oscillations that are correlated with performance, and it has been demonstrated that a HSLP can be used to measure these oscillations in the thruster plume [2].

In this work, the HSLP method has been modified to account for capacitance due to the Langmuir probe sheath, the interaction layer between the physical probe and the bulk thruster plasma. Additionally, this correction has yielded a new method for determining certain plasma parameters that are otherwise difficult to extract using the classical Langmuir probe analysis. A comparison between this new method and the standard technique is made, and it is found that the plasma parameters yielded by both agree within error.

The results of time-resolved HSLP measurements in the very-near-field of a Hall thruster are also presented. Transition between different oscillation modes is observed as the probe travels through the very-near-field and inside the thruster discharge channel. The perturbation of the thruster due to the presence of the probe can be characterized with the thruster discharge current, and in this way the meaningfulness of the HSLP measurements can be evaluated.
Investigation of Channel Interactions in a Nested Hall Thruster*

Marcel P Georgin\(^1\), Sarah E. Cusson\(^2\), Ethan T. Dale\(^2\), Vira Dhaliwal\(^2\), and Alec D. Gallimore\(^2\)

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Nested Hall thrusters, which concentrically nest multiple discharge channels together, are an attractive option for scaling Hall thrusters to high power. Their ability to maintain high thrust to power ratios, reduce mass to power ratios and throttle over large ranges makes them ideal for high power missions such as cargo missions to Mars. However, the underlying physics of how having multiple discharges in such proximity affects the device is not well understood.

Previous studies on nested Hall thrusters [1], have shown discrepancies between predicted multi-channel operation based on single-channel operation and actual multi-channel operation. These results suggest that the channels of nested Hall thrusters are interacting to affect the performance of these devices, probably due to increased neutral pressure near the thruster. The mechanism by which this is occurring is the subject of this study. Background neutral ingestion from the facility, neutral ingestion from the adjacent channel, and movement of the acceleration region leading to changes in divergence angle are the plausible candidates.

Thrust, beam current, divergence angle, and laser-induced fluorescence measurements were taken in order to investigate this phenomena. Chamber pressure was kept constant throughout the experiment to eliminate background neutral ingestion as a source of increased efficiency. Results indicate the thrust and efficiency increases in multi-channel operation versus the superposition of single channel operation. The beam current increases indicating neutral ingestion from the other channel is occurring. Additionally, divergence angle decreases suggest acceleration region movement. Laser-induced fluorescence confirms that in multi-channel operation the acceleration region is pushed inwards resulting in a decreased divergence angle.

* This work was partially funded by NASA Space Technology Research Fellowship grant numbers NNX15AQ43H, NNX15AQ37H, and NNX14AL65H

References

A Novel Sub-Millimeterwave Radar System for Autonomous Vehicle and Collision Avoidance Applications

Armin Jam¹, Jack East¹, Kamal Sarabandi¹
¹Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI

Ever since the invention of cars innovation within the automotive industry has continuously improved transportation in many different ways, examples of it being cleaner, safer and perhaps more affordable vehicles. As the next frontier in automotive industry, we are now facing a substantial change engendered by autonomous vehicles. This technology offers significant benefits to our welfare-saving lives; reducing crashes, congestion, fuel consumption, and pollution; increasing mobility for the disabled; and improving land use being some of possible instances of the benefits that this technology offers. However, to enable realization of autonomous vehicles, a number of challenges need to addressed, one of which being development of advanced navigation and collision avoidance sensors. The state of the art sensors used for autonomous applications are often bulky, heavy and power hungry which makes them not suitable for vehicular applications. To overcome this problem, our research team has focused on development of a high technological radar system with minimal size, weight and power consumption. The radar system is designed to have a size of less than 4cm by 5cm by 1.5mm and weighs only 5 grams. The radar also has the advantage of operating on fraction of 1W while having superior detection resolutions, all of which makes it very suitable for autonomous applications. In this work we present a summary of our research on design, microfabrication and measurement of the proposed radar system.
An Accurate Circuit Model for Input Impedance and Radiation Pattern of Two-port Loop Antennas as E- and H-probe

Mani Kashanianfard, Kamal Sarabandi

EECS Department, University of Michigan, Ann Arbor, MI

In this paper a simple but very accurate circuit model for two-port (split) loop antennas typically used for direction finding in the HF band is presented. The circuit model consists of lumped elements and can be used to accurately estimate the input impedances and received voltages of two-port loop antennas in receive mode. It is shown that the same circuit model can be reduced to predict the input impedance behavior of a single-port loop antenna with much more accuracy than the existing transmission line and lumped element models over a wide frequency range. The model is shown to be valid for frequencies up to a point where the loop circumference is about a wavelength. The same circuit model in receiving mode can provide the 3-D radiation pattern of the antenna.
Schlieren High Speed Imaging of Fluid Flow in Liquid Induced by Plasma-driven Interfacial Forces

Janis Lai¹, John E. Foster¹

¹Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, MI

Effective plasma-based water purification depends heavily on the transport of plasma-derived reactive species from the plasma into the liquid. Plasma interactions at the liquid-gas boundary are known to drive circulation in the bulk liquid. This forced circulation is not well understood. A 2-D plasma-in-liquid water apparatus is currently being investigated as a means to study the plasma-liquid interface to understand not only reactive species flows but to also understand plasma-driven fluid dynamic effects in the bulk fluid. Using Schlieren high speed imaging, plasma-induced density gradients near the interfacial region and into the bulk solution are measured to investigate the nature of these interfacial forces. Plasma-induced flow was also measured using particle imaging velocimetry.
Elevation Angular Dependence of Wideband Autocorrelation Radiometric (WiBAR) Remote Sensing of Dry Snowpack and Lake Icepack

Mohammad Mousavi\textsuperscript{1}, Roger De Roo\textsuperscript{2}, Kamal Sarabandi\textsuperscript{1}, Anthony W. England\textsuperscript{3}

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In most remote sensing applications, the gross parameter of the target, such as snow depth and snow water equivalent (SWE), are often the parameters of interest. A novel and recently developed microwave radiometric technique, known as wideband autocorrelation radiometry (WiBAR), offers a deterministic method to remotely sense the microwave propagation time of multi-path microwave emission of low loss terrain covers and other layered surfaces such as dry snowpack and freshwater lake icepack. The microwave propagation time through the pack yields a measure of its vertical extent; thus, this technique is a direct measurement of depth. This technique is inherently low-power since there is no transmitter as opposed to active remote sensing techniques. It also works at angles away from nadir.

We have confirmed the expected simple dependence of the microwave propagation time on the elevation angle with ground-based WiBAR measurements of the icepack on Douglas Lake in Michigan in early March 2016. The observations are done in the X-band for the icepack. At these frequencies, the volume and surface scattering are small in the pack. The system design parameters and physics of operation of the WiBAR is discussed and it is shown that the microwave propagation time can be readily measured for dry snowpack and lake icepack for observation angles away from nadir to at least 70°.
Modal Representation of Broadband Green’s Function with Applications in Periodic Structures

Shurun Tan¹, and Leung Tsang¹

¹Radiation Laboratory, Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan

Waves in periodic structures are important in physics and engineering in the design of photonic, electronic, acoustic, microwave and millimeter devices such as photonic crystals and metamaterials. The common approaches to study periodic structures are to calculate band diagrams.

In this paper, we report our recent progress in characterizing the Green’s function and in integral equation based methods that can be used for broadband simulation of periodic structures. Set upon modal representation of the periodic Green’s function, we have developed the method of broadband Green’s function with low wavenumber extraction (BBGFL), where a low wavenumber component is extracted from the Green’s function, resulting a non-singular and fast-converging remaining part that has separable wavenumber dependence. We’ve applied the approach to simulate band diagrams of periodic structures, applicable to both PEC and dielectric scatterers with arbitrary shapes and volume fractions. Using BBGFL to formulate surface integral equations, the determination of modal solution becomes a linear eigenvalue problem, producing all the modes simultaneously. The modal field solutions are wavenumber independent.

The modal analysis of the band structure is further utilized to construct the broadband Green’s function including periodic scatterers. The methodology of modal expansion with low wavenumber extractions can be used to construct Green’s function that satisfies all the prescribed boundary conditions, greatly reducing the number of unknowns in the surface integral equations when applied to perturbations to the original problem. The method of BBGFL is a new and effective approach to study broadband wave behaviors in periodic wave functional materials.
A Low Profile Wideband Circularly Polarized Omnidirectional Antenna Using an Array of Sectorial Loop Antennas

Behzad Yektakah 
and Kamal Sarabandi

Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI

Circularly polarized (CP) antennas are capable of reducing multipath fading and alleviating the need for precise alignment of the transmitting and receiving antennas in wireless systems. To provide the larger signal coverage and support different wireless standards, CP antennas with omnidirectional radiation pattern and wide bandwidth are more attractive in wireless systems. Several designs have been proposed for omnidirectional CP antennas. However, a few designs have achieved the operation bandwidth more than 50%.

A novel low profile CP antenna with omnidirectional pattern and 53% bandwidth is presented. The antenna operates based on excitation of two cylindrical TE21 modes in a wide bandwidth. One mode is excited such that it is spatially rotated by the rotation angle of 45 deg with respect to the other mode. The two modes are excited with the absolute phase difference of 90 deg. Each mode is generated by eight half sectorial loop antennas radially placed over a circular ground plane.

At each frequency within the operation bandwidth (center frequency at 1.6 GHz), the gain variation in the horizontal plane is less than 0.2 dB. Over the operation bandwidth, the maximum gain in the horizontal plane is in the range -0.5–1.2 dBi and VSWR is less than 1.9. Total height of the antenna is 48 mm.
Intrinsically Switchable FBARs Based on Ferroelectric BST for Switchable BAW Filter Application

Milad Zolfagharloo Koohi¹, and Amir Mortazawi¹

¹Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI.

This work presents optimal design of switchable BST-on-Si composite film bulk acoustic resonators (FBARs) for bulk acoustic wave (BAW) filter applications. To design BAW filters with lower insertion losses and wider bandwidth, resonators' Q×Kt² is maximized. Furthermore, lateral wave spurious resonances that can significantly degrade the composite FBARs performance, are eliminated by designing a frame at the border of ferroelectric-on-Si FBARs. Using COMSOL simulations, a raised frame is designed at the border of BST-on-Si composite FBAR, which is dispersion type I resonator. Designed structure has been validated by fabrication and measurement and it is compared to typical composite FBAR structures without frame. Besides, a switchable filter is designed and fabricated based on BST and its figures of merits are investigated and discussed.
CDR: Control, Dynamics, and Robotics
Model-less Forecasting of Bifurcations: Forecasting the Post-bifurcation Dynamics of Large Dimensional Complex Oscillatory Systems

Amin Ghadami¹ and Bogdan I. Epureanu¹

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Bifurcations are observed in dynamics of complex systems. Such phenomena lead to various types of stability issues and can cause dramatic changes in the dynamics. Therefore, forecasting bifurcations, i.e. predicting bifurcations with measurements only from the pre-bifurcation regime is a significant challenge and an important need. This is especially important for complex large-dimensional systems when an accurate model of the system is not easily available or when the system properties/parameters are unknown.

This work presents a unique approach to forecast Hopf bifurcations and the post-bifurcation limit cycle amplitudes in large dimensional oscillatory systems. The forecasting method does not require a model of the system, and is based only on time series measurements of the way system response to perturbations in pre-bifurcation regime. Hopf bifurcations are very common in a variety of systems, especially fluid-structural systems. To demonstrate the method and highlight its advantages, the method is employed to forecast bifurcation diagrams of a nonlinear aeroelastic system which can experience different operating conditions and bifurcations.

Numerical simulations show that the method accurately predicts the bifurcation point and also the post-bifurcation dynamics in both supercritical and subcritical cases despite the fact that it uses only pre-bifurcation regime data and it does not use a model of the system. Since bifurcations can cause dramatic changes in system dynamics, this type of forecasting which does not require exploring the post-bifurcation regime opens the door to a variety of applications where knowledge of nearby bifurcations is important for safety and maximum system performance.
Fast and accurate modeling of a physical system is useful for estimation and control. We propose an architecture of a deep neural network (DNN) for modeling dynamics of a physical system. Our key ideas are that we utilize a convolutional neural network (CNN) across time domain to extract time-invariant features of model inputs and handle observations and control inputs of the system separately as architectures of Oh’s 2015 work did. Furthermore, we present a theoretical comparison of our model with classical theory in this paper.

We also evaluate the performance of the architecture using data from an actual physical system, and compare its performance to baseline models: Locally Weighted Projection Regression (LWPR), Gaussian Process Regression (GPR), Feedforward Neural Network (FFNN) with Rectified Linear Unit (ReLu) activation for a hidden layer, and Physics-based model. Our experimental results show that our model surpasses other baselines in accuracy.
Combustion Shaping Using Multivariable Feedback Control

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As high exhaust gas recirculation (EGR) is introduced for efficiency, the combustion duration and combustion delay is elongated due to slow fuel burn rates requiring flexible and robust management of both the combustion initiation and duration (what we call combustion shaping). Combustion shaping through cylinder pressure sensing and feedback control of spark advance (SA) and EGR-valve position can be used for spark ignited (SI) engines operating within highly dilute, high efficiency regimes even where the combustion variability (CV) limits controller bandwidth. Although EGR is directly related with combustion duration, spark advance affects the start and duration of combustion simultaneously. This input/output coupling suggests a multivariable controller that coordinates the actuators. Control of SA and EGR is investigated with a coupled linear quadratic Gaussian (LQG) controller and compared with a decoupled proportional-integral (PI) controller. Simulation of the closed-loop system uses a simple engine model derived from system identification. Gain tuning was performed aiming for fast response without overshoot and considering cyclic variability reduction through a Kalman filter. Comparison of the simulated controllers shows that the key advantage of the LQG controller endured the CV.
Hydraulic Transmissions for Wearable Cobots

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A cobot is a passive robot that creates guiding surfaces within a workspace shared with a human operator by controlling transmission ratios to enforce motion direction while the operator controls motion timing. Traditional cobots use Continuously Variable Transmissions (CVTs) based on rolling contacts to create the guiding surfaces. Accommodating motion directions chosen by the operator (rendering free space) requires modulating transmission ratios according to sensed operator forces. Cobots have clear appeal as rehabilitation devices: they guide motions, but dispense with the heavy, unsafe actuators required in most exoskeletons. A wearable cobot would couple joints on the body to enforce desired motions. However, the ability to support loads without slip in rolling-contact CVTs is directly related to the forces transmitted across the rolling contacts, making mechanical design of wearable cobots virtually untenable.

In contrast to a rolling contact transmission, a Digital Fluid Transmission using valves to select from a set of available transmission ratios can support large loads without slip. We have evaluated the potential of a hydraulic transmission for wearable cobots experimentally using a planar elbow-shoulder prototype. As a stepping stone to the digital hydraulic transmission, we implemented and evaluated two hydraulic transmissions: first, a fixed-ratio physical transmission between cylinders spanning each joint, and second, a motorized Continuous Virtual Hydraulic Transmission tethered to the exoskeleton by flexible tubing. By assessing the stiffness of the resulting guiding surfaces and the “free-ness” of free-space motion with the physical and virtual transmissions, we demonstrate the promise of fluid transmissions for implementing wearable cobots.
Exploring the Role of Natural Dynamics in Gait

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While it is largely accepted that energetics plays a fundamental role in causing humans to walk at low speeds and run at high speeds, it is still unclear what makes walking and running the most energetically economical gait choices. In this work, we hypothesize that, analogous to the resonant motion of an oscillator, these gaits represent an optimal usage of the underlying natural dynamics of a legged system. To investigate this hypothesis, we start with an entirely passive legged robotic model, where the gaits that emerge inherently represent the natural dynamics of the system. We then add realistic components to this passive model, such as actuation, feet with mass, and damping in the springs. We optimize for energetics and analyze how these gaits evolve and change to see the role of natural dynamics in a full robotic system. We find that the gaits on the full robotic system closely match the underlying passive model, suggesting that gait choice is in fact driven by the legged system’s underlying passive natural modes.
CEE: Civil & Environmental Engineering
Monitoring a Research Scale Wind Turbine for Damage Detection in the Tower
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This poster presents the efforts for damage detection in wind turbine towers by analyzing the results of an experiment performed on a 3-kW research scale wind turbine. Turbine tower was supported by two pin connections, one located at the lower end of the tower and the other one located approximately at one third of the full height of tower. To simulate loss of stiffness in the tower, the damage scenario consisted of replacing the bottom support pin with a spring. Tower response was measured by recording acceleration in two orthogonal directions at six different locations along the length of the tower. The environmental and operational conditions (EOCs) were retrieved from a meteorological tower located near the turbine in the form of averages over 15 minute intervals. Analysis of acceleration spectrograms revealed strong peaks at high frequency portions of the spectrum. Additionally, since the damaged data sets were collected in a relatively small time interval the variation in EOCs was not substantial enough for efficient data normalizations. In order to explain the high frequency peaks as well as an attempt for extraction of operational conditions including angular velocity of the rotor, two mechanical models were developed: the first one was an analytical model using the Newtonian approach and the other one was a model in FAST, a software developed by the National Renewable Energy Lab for modeling wind turbines. The FAST model was used to model the wind-blade interactions and also to validate the analytical model.
Understanding the Effects of Socio-Cognitive Process on Construction Workers’ Unsafe Behavior

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Construction is one of the most dangerous industries in the U.S. Accident investigations have revealed that workers’ unsafe behavior accounts for the majority of construction accidents. Construction safety practices have been based on prescriptive approaches, which emphasize regulations, incentives, and punishments to reduce unsafe behaviors. However, because of highly complicated work conditions and loosely defined work procedures, workers’ behaviors largely rely on discretionary decisions rather than external regulations. Despite the crucial relationship between unsafe behavior and an individual’s decision making process, there is a noticeable lack of studies exploring a socio-cognitive process which helps to clarify the mechanisms of unsafe behaviors. Hence, this study aims to explore the effects of socio-cognitive processes on construction workers’ unsafe behavior. To achieve the objective, empirical studies are conducted to identify the current status of construction safety, and to examine the associations between social norms, social identities, and safety behaviors. In addition, an agent-based model that incorporates social psychology theories and empirical findings is developed, and simulation experiments are conducted to investigate the effects of the socio-cognitive process. The results indicate that strict safety rules have a positive but limited influence on workers’ safety behavior, which demonstrates the limited impact of prescriptive approaches. In addition, it is found that workers’ safety behavior can be further improved by increasing the frequency of managers’ safety feedbacks and strengthening workers’ project-based identification. From the result, it is suggested that managerial efforts to foster favorable social influence would be an effective means to reduce workers’ unsafe behaviors.
Construction and Operation of Novel Anaerobic Membrane Bioreactor Design Utilizing Rotating Discs for Domestic Wastewater Treatment

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Anaerobic Membrane Bioreactors (AnMBRs) provide a promising alternative to conventional wastewater treatment as they generate substantially less residuals and produce methane which allows for energy recovery. The combination of anaerobic treatment with membrane filtration furthermore guarantees a high quality effluent that is rich in nutrients and can be re-used for irrigation. However, membrane fouling (i.e., clogging of membrane pores) is generally recognized as one of the greatest challenges in MBR operation as it causes a rapid increase in (pumping) power requirements and thus energy consumption. This research project involves the construction and subsequent operation of an AnMBR with a novel membrane filtration system that aims to treat domestic wastewater in temperate climates while putting energy back into the grid.

The AnMBR presented here utilizes rotating membranes to induce shear at the membrane surface and consequently reduce fouling in an energy-friendly manner. This system was custom-made through an iterative design process using computer models and eventually constructed at the University of Michigan. To allow for comparison with other, more conventional AnMBR studies, synthetic domestic wastewater is used for the initial evaluation of the system. The AnMBR is operated at 20°C during this first benchmarking experimental run to evaluate its treatment potential when operated at ambient conditions. This treatment potential is characterized by reactor performance (e.g., pollutant removal) as well as membrane operation parameters (e.g., achieved flux). By demonstrating that this project achieves effective fouling control, anaerobic technologies have a strong potential to push wastewater treatment towards net positive energy operation.
Diverting urine from wastewater streams can provide many environmental benefits. The majority of nutrients in municipal wastewater is found in urine, yet urine accounts for 1% of the wastewater volume. Recycling nutrients from urine is particularly attractive due to the projected depletion of Earth’s phosphate reserves within 50-100 years. Urine diversion can also save costs and reduce pollution associated with wastewater treatment. Recovering nutrients at the source will reduce the required nutrient removal at the treatment plant and may reduce the mass of nutrients released to surface waters. Finally, urine diversion can reduce water use as urine-diverting toilets and waterless urinals require minimal flushing.

Before urine-derived fertilizers can be widely applied, effective processes are needed to remove contaminants present in urine. Unprocessed urine, while it may be high in nutrient content, has microorganisms and pharmaceuticals that could be harmful to ecosystems and to humans. Urine can be transformed to fertilizer with long-term storage (>3 months), heating, or by precipitating the nutrients out of the urine as minerals (e.g. struvite). Previous research has focused on the fate of common enteric pathogens through these processes, but little work has focused on the fate of viruses excreted in urine. Polyomaviruses have received relatively little attention in source-separated urine research, despite the fact that they infect the urinary tract and can be excreted in urine at very high levels. This study aims to determine the fate of the pathogenic human polyomavirus that is found in urine at high levels through treatment for fertilizer use.
Field Construction Workers’ Stress Measurement Applying a Wearable and Affordable Electroencephalogram (EEG) Sensor

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Construction workers are exposed to high mental work load and stress because of their involvement with physiologically and psychologically demanding tasks performed in a hazardous work environment. Working under stress significantly influence workers performance and awareness, which could lead to serious health and safety problems. Recently, a electroencephalogram (EEG) sensor has drawn significant attention to measure the stress level of human subjects in the clinical domain. However, using EEG at the field is challenging since the recorded EEG signals can be easily contaminated from diverse artefact sources in construction fields. To address this issue, we propose an effective and comprehensive signal processing framework for; 1) acquiring high quality EEG signals by using signal processing methods such as filtering methods (e.g., band pass filter and notch filter) and an independent component analysis method to remove prevalent artefacts at a jobsite (e.g., eye blinking, vertical eye movements, and muscular movements); and 2) monitoring construction workers’ stress level at the field. We applied the proposed framework to real world construction projects analyzing the data from eight workers from the field. The results demonstrated that the EEG signal processed based on the proposed framework are quality enough to capture brain activation. Also, significant differences in the stress levels are captured while subjects are working in different levels of hazardous. Results confirm the potential of a wearable EEG device to capture high quality EEG signals and measure workers’ stress at the field, which opens a door to assess workers’ stress level at construction sites.
An Optimization Framework and Case Studies for Design Lightweight Multilayer Plates with High Blastworthiness

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Assessing the dynamic performance of multilayer plates subjected to impulsive loading is of interest for identifying configurations that either absorb energy or transmit the energy in the transverse directions, thereby mitigating the through-thickness energy propagation. The development of a reduced-order modeling approach is presented in last chapter for rapidly evaluating the structural dynamic performance of multilayer plates. To identify the multilayer plate that has the highest levels of blast worthiness and lightest structural weight among a large number of alternative configurations, a design optimization process is also developed and integrated with the reduced-order model.

The framework of design optimization is introduced and a set of numerical case studies are provided for identifying the optimal configuration with different number of sublayers. First, an effective screening metric is developed based on the concepts of the DRI model. This screening metric will help to rank candidate configurations according to their capacity of blast worthiness. The information generated from the design optimization will help designers to select an optimal multilayer plate configuration as a proper armor in an early design stage, in order to reduce the occupant’s injury probability and the structural weight simultaneously. Then the identified optimal configurations can be used in a more complex and computational consuming finite element analysis without performing tedious parametric studies.
Comparison and Validation of Statistical Methods for Predicting the Failure Probability of Urban Trees

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The failure of trees during storms imposes strong economic and societal costs. Being able to predict the probability of a tree failing during storms has the potential to help improve tree risk management. The purpose of this study is to examine disparate statistical learning techniques and compare their accuracies in estimating tree failure probabilities for one case study storm in Massachusetts. The data used in this study consists of four categorical covariates, including location of trees, species, pruned/not pruned and whether nearby trees removed were recorded on trees. There are also two continuous variables, which are diameter at breast height (DBH) and height. We encourage the collection of more data on other variables influencing the failure probability allowing the development of predictive models. The data mining methods we used to predict the failure probability of trees include logistic regression, random forest regression, classification and regression trees (CART), multivariate adaptive regression splines (MARS), Artificial neural network (ANN), naïve-Bayes regression and an ensemble model. These predictive models are built based on all the variables as well as the most important subset of these variables in terms of predictive accuracy. As demonstrated by our computational results, the best model is the ensemble of logistic regression and random forest.
Isogeometric Multi-Layered Shell Formulation Using the Layerwise Theory

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A multi-layered shell formulation is developed based on the layerwise theory [1] within the framework of isogeometric analysis (IGA). IGA utilizes Non-Uniform Rational B-splines (NURBS) to represent the geometry as well as to describe the field variables [2], thus it offers the great opportunity of directly importing CAD designs into finite element analysis without converting the geometry. In this way, the gap between design and analysis is bridged. The derivation also follows a layerwise theory, which assumes a separate displacement field expansion within each layer, and considers transverse displacement component as $C^0$-continuous at layer interfaces, thus resulting in a layerwise continuous transverse strain states. Since the in-plane and through-thickness integrations are carried out individually, this approach is capable of capturing the complete three-dimensional stress states in a two-dimensional setting, which improves the computational efficiency. A knot insertion technique is utilized for the discretization in the through-thickness direction and $C^0$-continuity is enforced by means of knot repetition at dissimilar material interfaces. The performance of the proposed model is demonstrated using multiple laminated composite examples. Numerical results prove the accuracy of the proposed formulation and show that the isogeometric layerwise shell is superior to its finite element counterpart.

Reference
Seawalls and Tsunamis: Quantifying the Risks

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Seawalls are commonly used to defend against tsunamis, making it is essential we understand whether they truly mitigate damage. The north-east of Japan has been stuck by four tsunamis in the past 110 years. A model combining a cellular automaton and hydrodynamic models simulates how land development hypothetically changes with time and under different seawall height options. The insights will indicate which scenarios they provide physical protections and which scenarios require alternative action.
Global Structural Behavior of Steel-Concrete Composite Floor Systems under Traveling Fire Exposures

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Preliminary research has shown that the structural response of a building can be significantly influenced by the size and spread rate of a traveling fire. However, prior works have only focused on 2D structural frames, without taking into account the floor system. To address this limitation, this presentation highlights a computational investigation that was undertaken to better understand the global behavior of a 3D steel-concrete composite (SCC) floor system under a traveling fire exposure. Using the Traveling Fires Methodology, a range of spatially and time-varying fire exposures were applied to a 3D finite element model of a SCC floor system. The sequentially coupled thermal-mechanical simulations were carried out using ABAQUS, where the modeling approach was verified against existing test data on full-scale fire tests. Essential factors influencing the fire resistance of SCC floor systems, namely the passive fire protection scheme, and the burning size of the fire, were varied to investigate the global structural response. Simulation results indicate that structural response during a traveling fire is not only dominated by material stiffness and strength reduction during heating, but also by large axial forces in the beam-to-column connections during the heating and cooling phase of the fire, structurally-significant displacements of the floor slab, and load redistribution between exterior and interior columns occurring as the fire progresses across the floor plan. Additionally, useful trends were observed, in particular the dependency of the slab displacement rate and the maximum displacement to both the distance from the fire origin and fire burning size.
The Sensitivity of Metallic Materials to Non-proportional Multi-axial Fatigue Loading and its Connection with Material Ductility

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This paper presents a comprehensive investigation into non-proportional multi-axial fatigue of various types of metallic materials including structural steels, aluminum alloys, magnesium alloys and titanium alloys using a recently developed Moment of Load Path (MLP) based equivalent stress/strain range as a multi-axial fatigue damage parameter. By comparing with proportional fatigue loading, it is found that there is a significant increase of fatigue damage under non-proportional loading for some materials while others tend to be less sensitive to non-proportional loading. A generalized procedure for extracting material sensitivity parameter from stress-life or strain-life test data under simple multi-axial loading conditions is presented based on MLP based equivalent stress/strain. After obtaining material sensitivity parameters for various types of metallic materials examined in this study, a linear relationship between material sensitivities to non-proportional loading and material ductilities (characterized by e.g. elongation) is observed for different types of materials for the first time. With the linear relationship between material sensitivity and its ductility proposed and the newly developed MLP based fatigue damage parameter, the fatigue life of various types of materials under non-proportional loading can be calculated reliably without having to carrying out separate non-proportional fatigue test for material sensitivity parameter determination.  

Keywords: Multi-axial fatigue, material sensitivity, material ductility, non-proportional loading, fatigue damage parameter.
Estimation of Crossing Conflict at Signalized Intersection Using High-Resolution Traffic Data

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This paper aims to explore the possibility of using high-resolution traffic signal data to evaluate intersection safety. Traditional methods using historical crash data collected from infrequently and randomly occurred vehicle collisions cannot provide an accurate and timely evaluation of intersection safety. By contrast, the proposed method estimates potential traffic conflicts using high-resolution traffic signal data collected from the SMART-Signal system, which has been deployed at over 100 intersections in the Twin Cities area. The potential conflicts estimated in this research include both red-light running events, when stop-bar detectors are available and crossing (i.e. right-angle) conflicts. Using the estimated traffic conflicts and the field collected crash occurrence data, a crash prediction model will be built and calibrated. The proposed work will provide a low-cost and easy-to-use toolbox for traffic engineers to evaluate traffic safety performance at signalized intersections, without relying on vehicle crash event data, which usually have a long data collection period.
Performance-based Multi-hazard Topology Optimization of Structural Systems

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The integration of topology optimization procedures into structural design frameworks is gaining interest as an innovative approach for delivering more efficient designs. To this end, methodologies that incorporate the principles of performance-based design within a probabilistic setting have recently been developed for stochastic dynamic systems subject to natural hazards. This has led to the development of probabilistic performance-based topology optimization frameworks for the identification of optimal structural systems subject to extreme wind or seismic events considered in isolation. However, there are large areas that are subject to both wind and seismic hazards. Therefore, the development of methods that can ensure that target performance metrics are met within a multi-hazard setting is a crucial step towards improving the reliability of the structural systems.

This paper is focused on proposing a simulation-centered performance-based topology optimization framework for the identification of optimal structural systems for multi-hazard wind and seismic environments. A probabilistic performance assessment framework is firstly proposed based on synergistically describing the performance of wind or seismically excited systems. Based on this framework, an augmented multi-hazard simulation strategy is proposed. In particular, the methodology is centered on the definition of an approximate optimization sub-problem that not only decouples the simulation-based performance assessment from the optimization loop, but can also be solved efficiently using any gradient-based optimizer. Optimal lateral load resisting systems, that rigorously meet the first excursion constraints set within the multi-hazard environment, are therefore identified. Case studies are presented demonstrating the potential of the proposed framework.
Airborne Inactivation of Enveloped and Non-enveloped Viruses by a Packed Bed Non-thermal Plasma

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Transmitted diseases are one of the greatest threats to modern agriculture and food security. While much research has been conducted focused on waterborne pathogen inactivation, the same does not hold true for airborne pathogens, particularly for conditions where the objective is a technology capable of airstream disinfection. For the purpose of developing a novel airstream disinfection technology and contributing to the scientific understanding of spontaneous inactivation of airborne pathogens in a plasma environment, a dielectric barrier discharge (DBD) non-thermal plasma reactor was designed and constructed in this study and its airstream disinfection efficiency was examined. Two virus species, MS2 and Phi6, were aerosolized by a nebulizer and suspended in an air flow that passed through the reactor. Two impingers sampled the virus-loaded air flow at both upstream and downstream positions in the reactor, and the samples were analyzed by plaque assay and quantitative Polymerase Chain Reaction (qPCR) to determine the active virus number concentration and total virus genome copies. A commercial power meter was used to measure the power consumption of the system. An ozone filter was installed downstream of the reactor and ozone concentration was measured both upstream and downstream of the filter. The results indicate that this preliminary reactor design can achieve up to three-log reduction in infective virus by inactivation and filtration, with volumetric energy consumption (J/L) significantly lower than that of HEPA filtration only. Unfiltered downstream ozone concentrations were not substantially higher than ambient concentrations and the ozone filter effectively counteracted such increases.
MTR: Medicine and Translational Research
Non-invasive Quantification of Murine Vasculature Biomechanical Properties under a Cardiovascular Challenge

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Exercise tests are used clinically to evaluate: cardiovascular (CV) function, the presence of disease, and treatment plans.¹ A challenge to the vascular system is necessary because, amazingly, while at rest many CV pathologies remain quiescent. It is only upon challenging the CV system that functional deficits are revealed due to lack of adequate blood supply and the accompanying oxygen and nutrients. Clinically, if a patient is unable to perform exercise, pharmacological stimulation with dobutamine is used instead. Biomechanical forces play a primary role in the location, initiation, and progression of CV disease. Non-invasively quantifying alterations in biomechanical forces during exercise using MRI and computational fluid dynamics has been developed in humans² but not in the preclinical models so often used as surrogates to better understand health and disease. One parameter of interest is cyclic strain, measured by lumen expansion over the cardiac cycle. Measurements of cyclic strain give insight into vessel wall properties and offer a better understanding of the progression and pathogenesis of atherosclerosis and cardiovascular disease. These metrics are used in quantifying loss of vessel compliance and are a large component in the rupture of aneurysms. The purpose of this work is to develop methods to quantify lumen expansion along the arterial tree in murine models with and without a vascular challenge to understand the effects of acute and chronic exercise on CV disease pathology.

Recognition of Mood in Bipolar Speech: Controlling for Variations in Audio Quality and Participants

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Individuals with bipolar disorder often exhibit speech that is acoustically different when experiencing manic or depressed mood episodes. Recent research has aimed to model these deviations from the typical speech of an individual to objectively identify the onset of mood episodes. In particular, the PRIORI (Predicting Individual Outcomes for Rapid Intervention) project uses the acoustics of speech collected from smartphone conversations as a biomarker. Much of the previous work in bipolar mood detection has used high quality recordings of speech collected in laboratory settings, which do not necessarily reflect the acoustics of everyday speech. This work investigates variations in audio quality, including clipping, loudness, and noise, that must be controlled for when using real-world smartphone recordings. We describe methods during preprocessing, feature extraction, and data modeling to correct these issues. Additionally, this work explores variations in speech patterns across different participants and how to augment information gathered from a cohort with knowledge on the individual level. We extract i-vectors using the unlabeled everyday calls of a participant in order to learn typical speech characteristics. We then fuse this information with a model trained using all participant data. Both of these techniques have shown significant improvement in performance when classifying bipolar mood, demonstrating the promise of using speech for mood monitoring.
Prostate Cancer Circulating Tumor Cell Isolation and Analysis using a Graphene Oxide (GO) Chip

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One in seven men in the United States will be diagnosed with prostate cancer in his lifetime. While testing for blood levels of the prostate specific antigen (PSA) has increased disease detection, it raises further questions as to how to manage a disease that may take drastically different trajectories, with stark contrasts between the localized and metastatic survival rates. The cancer cells on the path to metastasis, or circulating tumor cells (CTCs), may hold answers to questions about why a disease progresses and what is the best way to address it. Our advanced nanomaterial-based microfluidic technology, the graphene oxide (GO) Chip, facilitates investigation through the sensitive isolation of CTCs from surrounding normal blood cells, enabling subsequent analysis.

Whole blood samples from prostate cancer patients was processed on two parallel GO Chips for CTC isolation based on antibody capture targeting expression of the epithelial cellular adhesion molecule (EpCAM). One chip was used for immunofluorescence staining to quantify CTCs based on staining positive for DAPI (DNA stain) and cytokeratin (epithelial marker) and negative for CD45 (white blood cell maker). CTCs captured on the other chip underwent cell lysis and RNA extraction for qRT-PCR to determine expression levels of 96 genes of interest, including housekeeping genes; epithelial and mesenchymal genes; oncogenes and tumor suppressor genes; prostate specific genes; extracellular matrix and inflammatory genes; and others. The results of this study show the potential of CTCs to answer questions that might help guide therapeutic management, allowing a more strategic approach to prostate cancer care.
Noninvasive, Rapid Ablation of Large Tissue Volume Using Histotripsy

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Current tumor ablation techniques are typically thermal-based, including radiofrequency (RF), microwave, and high intensity focused ultrasound (HIFU). RF and microwave ablation methods are limited to treating tumors < 3 cm in diameter and at a rate < ~2 cm³/minute. While HIFU is capable of treating larger volumes, the treatment duration is excessively long. Perfusion-mediated convection (commonly referred to as the “heat sink effect”) presents a major challenge for these and other thermal ablation modalities in highly vascularized tissues like the liver. Histotripsy is a noninvasive, non-thermal, ultrasound ablation method that uses high-amplitude, very low-duty cycle focused ultrasound pulses to generate precisely controlled cavitation and thereby mechanically homogenize target tissues into liquid-appearing acellular debris. Our previous in vivo studies have shown that histotripsy is not affected by the heat sink effect and can produce homogeneous tissue disruption in the highly vascular liver and kidneys noninvasively through the ribcage and other overlying tissues. Because histotripsy uses microsecond-duration pulses separated by up to seconds of off-time for a given focus, it is possible to electronically steer the focus of a phased array transducer to excite cavitation events throughout a large volume consisting of many overlapping foci during the off-time period for a given focus. We hypothesize that histotripsy combined with electronic focal steering can achieve rapid ablation of a large target volume. As such, histotripsy can be used to treat tumors that cannot be treated by current clinical methods. This study presents the first investigation of this hypothesis.
Isolation and Characterization of Pancreatic Circulating Tumor Cells by Graphene Oxide Based Microfluidic device (GO chip)

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Pancreatic cancer is the fourth leading cause of cancer death in the United States. The overall 5-year survival rate among patients with pancreatic cancer is only 6%. To improve treatment outcome, there is a pressing need to develop biomarkers to monitor tumor progression. Circulating tumor cells (CTCs) hold the potential to be a biomarker to noninvasively monitor disease progression and treatment response. The clinical utility of CTCs, however, is limited due to the inability of current technologies to detect CTCs in pancreatic cancer patients. Here, we developed graphene oxide based microfluidic device (GO Chip) for CTC isolation. GO Chip incorporates graphene oxide (GO) as the basis of an immunocapture system within a microfluidic device to achieve sensitive capture of CTCs. We processed 24 samples from 8 pancreatic cancer patients at different time points throughout the treatment. CTCs were discovered in all patient samples with a median number of 9.6 CTCs per ml, while no CTCs were detected in samples of healthy donors. CTC number decreased in 7 out of 8 patients after chemotherapy, while CTC number increased in 4 out of 8 patients during radiation therapy. This pilot data demonstrated that GO chip is capable of capture CTCs in pancreatic cancer patients with high sensitivity. In future study, we will evaluate the correlation between tumor progression status of patients and the changes in CTC enumeration to evaluate the clinical utility of CTCs.
Scalable Multiplexed Drug-combination Screening Platform Using 3D Microtumor Model

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Drug combinations have been widely accepted in cancer treatment for better therapeutic efficacy as compared to single compound [1]. The chance of finding appropriate drug combination increases with more target compounds under investigation. However, experimental complexity and cost grow exponentially as the number of drug candidates increases. Although several systems have been presented for drug combination studies, they are limited to low throughput of 2 drugs [2-3], requiring complicated operation systems [4], or time-consuming serial processes [5]. Here, we report a scalable, easy-to-handle, high-throughput drug combination screening platform, which enables screening of all possible dual-drug combinations from N different drugs with five different mixing ratios in each combination. As a proof of concept, we implemented an 8-drug combination chip, which is capable of screening 140 different treatment conditions over 1,400 spheroids with single-step pipetting. Using both cancer cell lines and patient-derived-xenograft (PDX), we demonstrated effective drug combination screening for precision medicine.

References
Hydrogel Based 3-Dimensional (3D) System for Toxicity and High-Throughput (HTP) Analysis for Cultured Murine Ovarian Follicles

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Various toxicants, drugs and their metabolites carry potential ovarian toxicity. Ovarian follicles, the functional unit of the ovary, are susceptible to this type of damage at all stages of their development. However, despite of the large scale of potential negative impacts, assays that study ovarian toxicity are limited. Exposure of cultured ovarian follicles to toxicants of interest served as an important tool for evaluation of toxic effects for decades. We hereby demonstrate a hydrogel based 3-dimensional (3D) mouse ovarian follicle culture as a tool to study ovarian toxicity in a different setup. The 3D in vitro culture, based on fibrin alginate interpenetrating network (FA-IPN), preserves the architecture of the ovarian follicle and physiological structure-function relationship. We applied the novel 3D high-throughput (HTP) in vitro ovarian follicle culture system to study the ovotoxic effects of an anticancer drug, Doxorubicin (DXR). The fibrin component in the system is degraded by plasmin and appears as a clear circle around the encapsulated follicle. The degradation area of the follicle is strongly correlated with follicle survival and growth. To analyze fibrin degradation in a high throughput manner, we created a custom MATLAB1 code that converts brightfield micrographs of follicles encapsulated in FA-IPN to binary images, followed by image analysis. The cultured follicles were treated with DXR at concentrations ranging from 0.005 nM to 200 nM, corresponding to the therapeutic plasma levels of DXR in patients. Follicles demonstrated decreased survival rate in greater DXR concentrations. We observed partial follicle survival of 35% ± 3% (n = 80) in 0.01nM treatment and 48% ± 2% (n = 92) in 0.005nM, which we identified as the IC50 for secondary follicles.
Miniature Gas Chromatography based Breath Analyzer for Non-Invasive Point-of-Care Diagnostics of Acute Lung Injury

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The recognition, diagnosis and management of acute lung injury from infection or trauma is very challenging due to its dependence on century old use of radiographs, bacterial cultures and other crude techniques. In recent years there is increasing research on breath analysis, which describes the relation between volatile organic/inorganic compounds (VOC/VIC) biomarkers and lung diseases like lung cancer, COPD and ARDS. The non-invasive nature of breath analysis makes it suitable for early diagnosis of respiratory disease.

Due to the complex composition of exhaled breath, gas chromatography coupled with mass spectrometry (GC-MS) is the most established method for breath analysis [5-7]. However, clinical implementation of GC-MS is quite challenging because of its low mobility, high cost and requirement of experienced personnel.

We have developed a rapid, sensitive and fully automated breath analyzer based on miniature gas chromatography to discriminate patients with acute lung injury and healthy controls. The breath analyzer collects the exhaled breath from a mechanical ventilator for 15 mins from intubated patients. The collected breath undergoes analysis for another 15mins to identify and quantify target VOC/VIC biomarkers. The VOCs in the breath are pre-concentrated in a pre-concentrator that is packed with Carboxen\textsuperscript{TM}-1000 and Carbopack\textsuperscript{TM}-B adsorbent during sampling, then injected to Rtx-1 column for separation, and detected by 10.6 eV photoionization detector (PID) at the end of the Rtx-1 column. The VICs are stored in a sampling loop and then injected to porous layer open tubular (PLOT) column for separation and detected by helium discharged photoionization detector (HD-PID) at the end of the PLOT column.
Photoacoustic In Vivo Imaging of Hepatocellular Carcinoma with Glypican-3-Targeting Nanoshell

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Background: Glypican-3 (GPC3) is a promising cell surface target for in vivo imaging that is highly overexpressed in HBV-derived hepatocellular carcinoma (HCC), the second most lethal cancer worldwide. Plasmonic gold nanoshell (AuNS) probe penetrates into tumors for deep imaging, enables superior photoacoustic contrast. The use of a GPC3 specific peptide conjugated gold nanoshell to detect HCC xenograft tumors in mice with photoacoustic imaging was demonstrated.

Methods: 12-mer peptide binding to GPC3 was selected through direct panning of target glycoprotein by phage display technology. Subcutaneous (n = 10) xenograft tumors from HCC cell line Hep3B were implanted in female nude athymic mice (nu/nu) and monitored weekly with ultrasound and MRI. In vivo imaging via 3D photoacoustic tomography (PAT) was performed to assess tumor growth and GPC3 expression. In vivo probe uptake characteristics were assessed in a time course study (at 0, 1, 2, 4, 8 and 12 hour time points) after intravenous administration of the targeting and control peptides conjugated with AuNS.

Results: A 12-mer peptide demonstrated high affinity (Kd = 71 nM) for GPC3 binding in vitro. HCC xenograft tumor size reached 5.2±1.1mm in diameter after two weeks of implantation, when of 200 uL 1X10¹¹/mL targeting and control peptides conjugated AuNS were intravenously administered respectively. The targeting probe demonstrated tumor uptake after 1 hour and cleared in 12 hours. Images from 0 to 2.1 cm beneath the skin revealed increased PA signal from tumors. PA imaging showed highest tumor uptake and tumor to normal tissue ratio ~two hours post injection (T/B = 4.45±0.22, n = 8). Injection of control peptide showed non-specific binding (T/B = 1.16±0.15, n = 8). The T/B difference between targeting and control peptides were statistically significant, p<0.01 by paired t-test.

Conclusions: In vivo imaging via photoacoustic tomography with molecular probe conjugated AuNS offers a simple, effective and rapid technique for noninvasive in vivo monitoring and semi-quantitative analysis of HCC tumor growth and GPC3 expression.
NRS: Nuclear Engineering and Radiological Sciences
One-Pot Synthesis Method for the Development of Lead Chalcogenide Nanocrystals

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To develop lower-cost, high-performance semiconductor materials, one-pot methods for PbSe and PbS nano- microstructures were successfully developed to grow nanocrystallines (NCs). The molar ratios for each synthesis played a key role throughout the processes, influencing the growth in the formations of PbSe and PbS nuclei, which results in the final morphology of the NCs. Colloidal PbSe NCs were synthesized through a high-temperature process for production of spheres, while the low-temperature process for single-crystalline PbS nano- microstructures included both cube- and star-shaped nanoparticles. Transmission electron microscopy images show size distributions of as-synthesized PbSe and PbS nanocrystals. The photoluminescence properties of these nano- microstructures were also investigated. These results show the possibility for controlling the morphology of semiconductor NCs using solution chemistry, which has important implications for both fundamental scientific studies and future technological applications.
CFD-grade Experiments Addressing Thermal Fatigue in Nuclear Reactor Branch Lines

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Thermal fatigue has been identified as a principle degradation mechanism contributing to loss of coolant accident frequencies in Light Water Reactors (LWRs). At least eight such events involving branch lines have occurred at US plants over the past two years. As a result, interest in the thermal fatigue of stagnant branch lines departing from coolant legs of LWRs has risen.

Thermal cycling in a branch line occurs at the fluctuating boundary created by the penetration of hot fluid from the main flow into the cold stagnant fluid of the branch line. Initial turbulent flow dissipates to a disturbed flow further into the branch line and then to a laminar spiral flow. At the extent of the spiral flow, hot and cold fluids stratify to create a fatigue inducing boundary.

Qualitative experimental techniques, such as visualization of tracer particles, have been employed in past research efforts to capture the large scale evolution from cavity flow to the formation of the stratified layer. However, this qualitative information is insufficient for improving the current methods of predicting such thermal fatigue.

High resolution quantitative measurements of the flow, capturing the small scale motions that affect thermal cycling at the pipe wall, are essential for making further progress to understand the involved phenomena and improve industry fatigue management. Current measurement efforts utilizing particle image velocimetry yield results in agreement with large scale motion observed previously. Time resolved data currently being analyzed from the same studies are opening doors to the new desired insight.
A New Framework for Tomotherapy Treatment, Planning, and Delivery

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The goal of tomotherapy is to deliver a prescribed dose of radiation to malignant tumors while trying to avoid the delivery of toxic doses to healthy organs. A binary multi-leaf collimator sits on a gantry fan and rotates around the patient’s body shuttering a row of binary leaves; it lets radiation through when a leaf is open and blocks radiation when a leaf is closed. Conventional treatment calculates dynamic gantry speeds and dose rates to be delivered at discrete stages of the rotational path of the gantry. We call these discrete stages “projections.” Dose rates are determined by the time the leaves remain open at each of these projections. Because of this, leaves have to open and close at every stage at which any dose is delivered. Doses are calculated using Fluence Map Optimization and in practice the speed of the pneumatic leaf drive is slow and causes inaccuracies in actual dose deliveries. We propose a treatment model that explicitly controls the number of leaf events by requiring leaves to stay completely open or closed at each projection. The model employs a finer discretization along the gantry path, the result is a treatment plan that represents dose effects more realistically, but which results in a large-scale combinatorial problem. We therefore implement a column generation methodology that attains high-quality solutions. The new framework reduces the number of leaf events, diminishes inaccuracies in dose delivery, and achieves faster treatment times since the gantry is not anchored at the slowest speed.
Properties Influencing Plasma Discharges in Packed Bed Reactors

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Atmospheric pressure dielectric barrier discharges (DBDs) sustained in packed bed reactors (PBRs) are being investigated for remediation of toxic gases, CO\textsubscript{2} removal and conversion of waste gases into higher value compounds. Though investigated extensively in experiments, few computational studies of PBRs have been performed to date. For applications involving chemical reprocessing which require a high degree of reactant selectivity, the ability to control plasma properties is particularly important. In this paper, we report on the results of a computational investigation of PBR-DBD properties using the multi-fluid plasma hydrodynamics simulator nonPDPSIM. These results are compared to experimental measurements.

The simulations were performed in 2-dimensions. Seven dielectric beads (rods or circles in 2D) were inserted between two coplanar electrodes, 1 cm apart. Humid air (N\textsubscript{2}/O\textsubscript{2}/H\textsubscript{2}O = 78/21/1) was the fill gas. A step-pulse of -30 kV was applied to the top electrode. Material properties of the beads (dielectric constant, secondary emission probability), gas properties (photoionization and photo-absorption cross-sections, gas temperature), and pulse frequency were varied.

We found that dielectric constant and photo-absorption cross-section have the greatest impact on discharge formation and intensity. Increased frequency led to greater density of inter-pulse pre-ionization which led to easier breakdown, and more uniform plasma density.
OPS: Optics, Photonics, and Solid-State Devices
Localized Room-Temperature Structural and Electronic Modifications of SiC via Ultrafast Laser Irradiation

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Wide bandgap materials such as SiC highly attractive for electronics operating in harsh environments. However, it is difficult to process the material and to accommodate intentional defect formation including electronic doping, where temperatures of 1600 degrees Celsius or higher are typically required. Ultrafast (femtosecond) laser pulses are capable of producing a high-density electron-hole plasma resulting in a dramatic and nearly instantaneous reduction in the covalent bonding allowing for atomic drift and possibly even non-thermal (or cold) melting. In this work, the structural and electronic properties of SiC subjected to subbandgap irradiation with ultrafast laser pulses are studied. Crystalline light-doped n-type 4H-SiC substrates were irradiated with a Ti:Sapphire ultrafast laser (750 nm, 150 fs pulse width) with a 105µm Gaussian beam radius. Rectangular areas were illuminated with variable pulse fluence, separation distance of the laser focal point, and ambient gas (vacuum, nitrogen, and air). High spatial frequency periodic surface structures were observed for laser fluence of 0.25J/cm² and higher. Ni metal contacts were deposited to study electrical conductivity and contact resistance of the irradiated SiC using the transmission line method. Irradiated regions exhibiting periodic surface structures demonstrate a conductivity increase of four orders of magnitude in comparison to irradiation under low fluence where SiC surface modifications are not apparent. Moreover, irradiation in a nitrogen environment demonstrates an additional conductivity increase of two orders of magnitude. The observed increases in electrical conductivity are attributed to the generation of point defects and nitrogen doping.
Sparse Coding with Memristor Networks

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We report experimental demonstration of sparse coding using 32x32 analog memristor crossbar arrays. The memristor array enables efficient implementation of pattern matching and lateral neuron inhibition, and allows input images to be sparsely encoded using neuron activities and stored dictionary elements. Different dictionary sets can be used in the same system depending on the nature of the input signals, allowing more efficient feature extraction and data representation. Using the sparse coding algorithm, we further performed natural image reconstruction using the memristor array and an offline learned dictionary. The ability to sparsely encode complex data in a bio-inspired approach offers the opportunity to develop efficient memristor-based neuromorphic computing systems.
Regioisomeric Effects of Donor-Acceptor-Acceptor Small Molecule Donors on Open Circuit Voltage of Organic Photovoltaics

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We synthesize and characterize donor molecules bearing both an electron donating (d) and two accepting (a, a’) functional groups configured in a d-a-a’ structure. The donor molecules are mixed with the acceptor, C\textsubscript{70}, in vacuum deposited organic photovoltaic (OPV) cells to clarify the mechanisms leading to their high open circuit voltages (\(V_{\text{OC}}\)) and power conversion efficiencies (PCE). Specifically, the donor 2-((7-(N-(2-ethylhexyl)-benzothieno[3,2-b]thieno[2,3-d]pyrrol-2-yl)benzo[c][1,2,5]thiadiazol-4-yl)methylene)malononitrile (antiBTDC) and its isomer 2-((7-(N-(2-ethylhexyl)-benzothieno[3,2-b]thieno[3,2-d]pyrrol-2-yl)benzo[c][1,2,5]thiadiazol-4-yl)methylene)malononitrile (synBTDC) are used to compare regioisomeric effects on their structural, optoelectronic and photovoltaic properties. The OPV comprising antiBTDC donor mixed with C\textsubscript{70} achieves \(V_{\text{OC}} = 0.91 \pm 0.01\) V and \(PCE = 7.2 \pm 0.3\%\) under 1 sun intensity AM 1.5G simulated solar illumination. The cross-conjugation in synBTDC stabilizes its highest occupied molecular orbital (HOMO), leading to an increased \(V_{\text{OC}} = 1.01 \pm 0.01\) V with \(PCE = 6.1 \pm 0.3\%\). Further modification of the d-a-a’ molecule from a quinoidal benzothiadiazole unit to a heteroaromatic pyrimidine unit achieves an even higher \(V_{\text{OC}} = 1.06 \pm 0.01\) V. Finally, together with the previously reported DTP-based d-a-a’ donors, we conclude that a shorter molecular conjugation length results in a deeper HOMO level and hence a higher device \(V_{\text{OC}}\).
GaN Nanostructures by Top-Down Fabrication

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Top-Down fabrication of GaN nanostructures allows for controllable dimensions and shapes, with no restrictions on barrier or wetting layer materials. Taking advantage of the benefits of standard thin-film epitaxy, the resulting structures are only limited by the standard thin-film epitaxial variation. The optoelectronic properties of GaN can be controlled by the geometry of the GaN nanostructures due to the shape's effect on the piezoelectric and strain fields. InGaN/GaN heterostructures etched into nanopillars can be engineered to control emission wavelength, emission intensity, emitter decay lifetime, single photon emission, and photon polarization. In this work, several devices are showcased, including, multi-color pixels, single photon electrically pumped LEDs, Plasmon-cavity coupled single photon emitters, and polarized single photon emitters, demonstrating the control from Top-down GaN nanostructures. Lastly, an approach for improving the single photon out-coupling efficiency from high refractive index semiconductor QDs by an order of magnitude is discussed.
Metal Oxide Memristor Array Based Neuromorphic System for Temporal Information Processing: The Liquid State Machine

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Metal oxide memristors are two terminal semiconductor devices intensively investigated recently as the next generation memory and for neuromorphic applications, due to their abilities to show multi-level, gradual and historical input related resistance change, similar to synaptic weight change in neural network which is inspired by human brain and proposed as a new computing architecture. Some memristors, especially WOx (tungsten oxide) memristor, show unique resistive switching dynamics, thus enabling the encoding of temporal information through internal ion movement.

A special type of neural network, called liquid state machine (also unified as reservoir computing with some other similar systems), is proposed for temporal information processing. It takes input in time series, settle down to certain internal states within the reservoir (or liquid) according to not only the current input but also previous inputs in a certain period, then generate desired output through simple readout function. The difference from previous neural network is that only the readout function (i.e., the connection weight from internal state to the output) needs to be train rather than the whole network, and the system has short-term memory which enables it to do temporal information processing.

WOx memristor array has been utilized to implement the reservoir part of the liquid state machine. Both simulation and experiment on real device show it can implement several tasks including handwriting written digits recognition, high order non-linear system implementation.
Variable-Field Hall Effect Analysis of HgCdTe Epilayers with Very Low Doping Density

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HgCdTe is the most important material used in the production of high performance infrared detectors, due to its versatility across a wide range of wavelengths, high quantum efficiency and dark current that approaches theoretical. Further improvements in detector performance may be achieved by lowering the HgCdTe doping concentration in the absorber layer of a conventional p-n heterojunction detector, or by incorporating low doping regions into new device architectures. Characterizing HgCdTe materials with very low doping concentrations, however, poses a challenge. Typical 4-point Hall effect measurements yield an average carrier concentration, making detection of low doped HgCdTe layers very difficult.

Multi-layered HgCdTe samples were analyzed using a novel technique: the Variable Magnetic Field Hall Effect, and the Multi-Carrier Fitting (MCF). The Hall coefficient, \(R_H\), and the resistivity, \(\rho\), are measured while sweeping the magnetic field from 0-14T. These values are used to compute the conductivity tensor components, \(\sigma_{xx}\) and \(\sigma_{xy}\) and fit to provide numerical values for the carrier density and mobility. Traditional 4-point Hall measurements at 77K give carrier concentration and mobility values of \(n = 2.0 \times 10^{15} \text{ cm}^{-3}\) and \(\mu = 23,500 \text{ cm}^2/\text{Vs}\). Our data indicates two distinct values, including a lower doped layer with \(n = 6.5 \times 10^{13} \text{ cm}^{-3}\) and \(\mu = 275,000 \text{ cm}^2/\text{Vs}\). This technique shows promise as a way to analyze layers with significantly lower doping layers, and a starting point to understand and advance the development of HgCdTe epilayers with very low doping concentration.
Electron-Phonon Coupling in thin TiN Films

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Pump-probe experiments using a femtosecond laser capture the thermal dynamics, and have been used to study the thermal relaxation of metals. This is measured through differential transmission and from this electron scattering times and other material parameters maybe calculated.

TiN is a new material that shows many of the same plasmonic properties as gold, but is a refractory material. As such it can withstand high temperatures and may be suitable for some applications in CMOS. This material parameter is not only useful from an engineering perspective, but it will also help inform the developing theory behind the band structure of TiN. 10nm films were tested at varying temperatures and wavelengths.
III-Nitride Monolithic Nanowire Array Edge-Emitting 1.3 µm Diode Laser on (001) Silicon Substrate

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A monolithic diode laser with emission wavelength beyond 1.1 µm on (001)Si is significantly useful for silicon photonics applications. Catalyst-free Ga (Al, In)N nanowires can be grown on silicon and other substrates and InGaN disks can be inserted in such nanowires. The alloy composition of such disks can be varied to tune the luminescence from visible to near infrared. Some of the most important advantages of such nanowires are very low density of extended defects and minimal strain. In this work such favorable attributes have been exploited to design, epitaxially grow and characterize the first edge-emitting electrically pumped GaN/In(Ga)N disk-in-nanowire lasers with the peak of the coherent emission at ~1.3µm. It is important to note that, due to high piezoelectric fields InGaN/GaN quantum wells cannot emit beyond 590nm. We have described epitaxy and characteristics of the nanowire heterostructures and also measured characteristics of these lasers. Plasma assisted MBE was employed to grow these GaN/InN/InGaN heterostructure nanowire arrays on (001)Si substrates. Multiple InN disks with In₀.₄Ga₀.₆N barriers in between are used as the active gain region. n- and p-doped graded cladding layers from GaN to In₀.₄Ga₀.₆N on both sides surrounds the gain region. From photoluminescence studies the emission peak of the nanowire laser heterostructure with the InN disks is found to have a peak at ~1.6µm. From steady-state L-I characteristics output powers up to ~ 10mW are measured without any heat sinking or facet cooling. The output spectrum confirms ~1.3µm peak emission. A low value of $I_\text{th} = 341$mA is measured.
Using Two-Dimensional Spectroscopy to Map the Excited State Landscape of Fluorescent Proteins

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Fluorescent proteins have become an indispensable tool in biological imaging due to the fact they can be introduced into virtually any species with a known genome and still maintain their fluorescent properties. Since the initial discovery and purification of the green fluorescent protein (GFP), dozens of mutants offering an extensive range of fluorescent colors have been developed from the GFP and DsRed parent proteins \([1],[2]\). Interestingly, several mutants, like mPlum and mCherry which differ only in point amino acid mutations around the chromophore, exhibit nearly identical absorption maxima, but vastly different emissions, suggesting mutations to amino acids around the chromophore are responsible for the Stokes shift. However, the exact nature of the Stokes shift, whether it arises from dynamic solvation or static Stark effects, has yet to be determined \([3],[4]\). In addition, fluorescent proteins exhibit distinct differences in their absorption spectra depending upon the use of one- or two-photon excitation, and the respective excitations initiate different relaxation pathways \([5]\). Unfortunately, not all the available proteins offer the high quantum yield and low photobleaching properties desired for optimal imaging. The reason for this could be uncovered with a detailed understanding of the excited state dynamics following one- or two-photon excitation. We propose three experiments using two-dimensional spectroscopy to map the excited state dynamics of the GFP mutant EGFP and the DsRed mutants mCherry and mPlum under both one- and two-photon excitation. It is our hope that this knowledge will aid in the design of improved fluorescent proteins for biological imaging.

References:
Small-area Photovoltaics for Low-Flux Infrared Energy Harvesting

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Human microchip implants are a promising technology for a variety of applications including identification, biomedical sensors for monitoring neuron pulses, biomarkers and tracking positions. Recently developed low power systems have made implantable systems a feasible approach. Energy harvesting from vibration and RF sources has been tested and evaluated, but the stability of the energy source and miniaturization are challenging. Alternatively, infrared photovoltaic energy harvesting has been considered, utilizing the near-infrared (NIR) transparency window of tissue between 700 nm and 900 nm from natural ambient sunlight or intentional low-intensity LED illumination through tissue. These applications require excellent performance for small-area cells under low-flux illumination condition, which is not commonly achieved for silicon cells due to shunt leakage and recombination losses. Small area (1-10 mm\textsuperscript{2}) GaAs and Silicon photovoltaic cells are studied in this work, where performance improvements are demonstrated using optimized device structures and passivation studies. A power conversion efficiency of more than 17\% for Silicon and 30\% for GaAs is achieved for 660 nW/mm\textsuperscript{2} illumination at 850 nm. Both cells demonstrate improved power conversion efficiency and reduced degradation under low illumination conditions in comparison to conventional crystalline silicon photovoltaic cells available commercially.
Controlling Properties of Hybrid Charge Transfer Excitons at Organic-Inorganic Semiconductor Heterojunctions

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The hybrid charge transfer exciton (HCTE) is at the heart of exciton-to-charge conversion and charge recombination processes at the organic-inorganic (OI) heterojunction analogous to the polaron pair state at an excitonic (organic-organic) HJ. We study the temperature dependent electrical and optical properties of HCTEs at nitride/4,4′-bis(N-carbazolyl)-1,1′-biphenyl (CBP) organic/inorganic semiconductor heterojunctions (OI-HJ) using external quantum efficiency (EQE), photoluminescence (PL) and electroluminescence (EL). We observe that the EL spectrum of the HCTE formed by recombination of injected charge carriers at the OI-HJ blue-shifts with decreasing temperature from $T = 300$ K to 25 K at a constant current density and with increasing current density at fixed temperature, while the full width at half maximum of the spectrum does not systematically change. We describe these phenomena by modelling the change in Fermi level on the inorganic side of the HJ. We develop a first-principles quantum mechanical (QM) model to describe properties of the HCTE. Using the QM model we predict the HCTE EL is due to trapped electrons at the nitride surface recombining with free holes in the CBP. Finally, the inorganic semiconductor is engineered to manipulate properties of the HCTE such as its binding energy and oscillator strength.
Optimal Control of Polarization with All-dielectric Metasurfaces

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A systematic design approach for realization of bianisotropic responses with all-dielectric metasurfaces is presented. The possibility of realizing bianisotropic response by cascading of anisotropic layers is demonstrated. By exploiting the anisotropy inherent in structures such as subwavelength gratings, we propose our structure to control the polarization of impinging waves. The simplicity of the design and the significant improvement in performance make the reported structures an ideal substitute to their plasmonic counterparts.
Here we present a novel in situ chemical modification process to form vertical Schottky diodes using palladium (Pd) rectifying bottom contacts, amorphous zinc tin oxide (Zn-Sn-O) semiconductor made via acetate-based solution-process, and molybdenum top ohmic contacts. Using x-ray photoelectron spectroscopy depth profiling, we show that oxygen plasma treatment of Pd creates a PdO$_x$ interface layer, which is then reduced back to metallic Pd by in situ reactions during Zn-Sn-O film annealing. The plasma treatment ensures an oxygen-rich environment in the semiconductor near the Schottky barrier, reducing the level of oxygen deficiency-related defects and improving the rectifying contact. Using this process we achieve diodes with high forward current density exceeding $10^3$ A/cm$^2$ at 1V, rectification ratios of $>10^2$, and ideality factors of around 1.9. The measured diode current-voltage characteristics are compared to numerical simulations of thermionic field emission with sub-bandgap states in the semiconductor, which we attribute to spatial variations in metal stoichiometry of amorphous Zn-Sn-O. To the best of our knowledge, this is the first demonstration of vertical Schottky diodes using solution-processed amorphous metal oxide semiconductor. Furthermore, the in situ chemical modification method developed here can be adapted to tune interface properties in many other oxide devices.
PEN: Power and Energy
Numerical Computation of Parameter Space Disturbance Recovery Boundary by Exploiting Topology of Stability Boundary

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Determining parametric influences on the stability of systems that are described by nonlinear differential equations is of interest in numerous application areas including transient stability of power systems. Behavior of such systems can be decomposed into a disturbance phase followed by a post-disturbance phase. The initial condition of the post-disturbance phase is variable and depends on parameters through an implicit map. It is useful to characterize sets of parameter values for which the post-disturbance initial condition lies on the stability boundary of a stable equilibrium point, corresponding to the boundary between recovery and undesirable behavior. Classical results concerning the partition of the stability boundary into certain attractive sets are extended to incorporate parameter variation. Under reasonable assumptions, there will exist a special equilibrium point on the stability boundary associated with any particular disturbance. It is shown that locally varying parameter in order to maximize the time in a neighborhood of the special equilibrium point will drive the post-disturbance initial condition onto the stability boundary. These theoretical results motivate novel algorithms for numerically computing the border that separates parameters that lead to recovery from parameters that lead to undesirable behavior, and for finding the point on the border that is closest to a given point parameter space. The algorithms are applied to a modified version of the IEEE 37-bus test feeder.
Renewable Voltage Regulation, Transformer Parameters, and a Tapping Tradeoff

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Load-tap-changing (LTC) transformers provide voltage regulation in subtransmission and distribution networks, but these expensive devices can only tap so many times before they fail. Fluctuations due to renewable energy can cause excessive tapping, accelerating aging. We address the question of how voltage regulation at renewable sources influences tapping frequency. In particular, we show that loose regulation results in excessive downstream (distribution) transformer tapping, while tight regulation causes upstream (subtransmission) tapping. We use yearlong simulations of a simple test network to generate tap trajectories and trade-off curves, illuminating the trade-off between subtransmission and distribution transformer wear. Many parameters influence these curves, including renewable node voltage setpoints, transformer voltage setpoints, and transformer timing parameters. We illustrate the effects of varying these parameters, further exploring the transformer tradeoff.
**Reduced Order Multi-Physics Model for the Dynamics of Permanent Magnet Synchronous Machines**

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In electric/ hybrid electric vehicle (EV/HEV) powertrains, electric machines are strategic components of the vehicle powertrains. Studying dynamics of the electric machines is critical for powertrain-level design, simulation, and optimization. Magnetic force excitations inside the machine structures cause undesired noise and vibrations with broadband frequency spectrum. The magnetic forces acting on the stator are detected as a main source for vibrations inside the machine. Hence, it is essential to study its dynamics, efficiently and accurately to improve noise, vibration, and harshness (NVH) of the vehicle. In this study we develop a computational model using the finite element analysis (FEA) to investigate dynamics of the stator for permanent magnet synchronous machines (PMSMs) by considering the strongly coupling between magnetic flux density problem and stator elastic deformation. This model enables studying vibrations problem of the stator by considering its strongly coupling with the magnetic field problem. The model is computationally efficient since the FEA is only used for weekly coupled magnetic force calculations.
Hidden Cost and Requirement of Direct Air Capture Integration into the Existing Power Infrastructure

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The current carbon emission pathway calls for carbon removal technologies that can undo a significant portion of our past emissions to meet the climate target. One such technology includes direct air capture (DAC), which chemically scrub carbon dioxide from the ambient air. Most literature on DAC tended to a single plant level feasibility and cost analysis.

This research quantified the hidden cost and requirement to operate DAC plants on a large-scale when they were integrated into the existing power infrastructure. This was performed by integrating DAC into the developed model which computes least-cost technological carbon mitigation pathway over 2050. First, emissions penalty stemming from the dirty grid mix is estimated to increase the overall cost of DAC by 43%, higher than 30% as anticipated in the existing literature. This was due to the feedback effect not easily observed in the plant-level analysis. Secondly, large-scale deployment of DAC resulted in a significant amount of additional power infrastructure, all of which need to come from renewable energy. The financial needs to install this additional clean energy can even outweigh the overall cost of DAC plants.

These results bring up important lessons on the climate strategies with DAC. DAC is to be used to mitigate carbon emissions from recalcitrant sources, such as vehicles, shipping, and aviation. This challenges the argument found in some of the existing literature that identifies DAC as a competitor to conventional carbon capture and storage technology for fossil fuel power plants.
An AC-QP Optimal Power Flow Algorithm Considering Wind Forecast Uncertainty

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While renewable generation sources provide many economic and environmental benefits for the operation of power systems, their inherent stochastic nature introduces challenges from the perspective of reliability. Existing optimal power flow (OPF) methods must therefore be extended to consider forecast errors to mitigate in an economic manner the uncertainty that renewable generation introduces. This work presents an AC-QP OPF solution algorithm that has been modified to include wind generation uncertainty. We solve the resulting stochastic optimization problem using a scenario based algorithm that is based on randomized methods that provide probabilistic guarantees of the solution. The proposed method produces an AC-feasible solution while satisfying reasonable reliability criteria. Test cases are included for the IEEE 14-bus network that has been augmented with 2 wind generators. The scalability, optimality and reliability achieved by the proposed method are then assessed.
Improving Grid Resiliency in Real-Time with Model-Predictive Control

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Growing numbers of distributed energy resources including renewable generation, energy storage, and FACTS devices offer opportunities to improve the control of power systems. Unfortunately, choosing the best actions during an emergency is complex and system operators may not have time to analyze such a wide range of choices. Model-predictive control (MPC) has been shown to handle this challenge well by identifying optimal decisions in real-time while accounting for future system behavior.

This research combines two previously separated control objectives into a single MPC formulation. MPC has successfully resolved both transmission congestion and long-term voltage instability as isolated phenomena in the past. In reality, these issues are often related and may even present conflicting control priorities. This work combines both objectives in a single MPC formulation while using a unique model of transformer tap-changing dynamics to regulate voltages.

Results demonstrate MPC’s ability to resolve transmission congestion and unstable voltages simultaneously. In situations with conflicting control objectives, MPC optimally balances the effects of both phenomena to minimize overall system degradation. This process fits naturally into present energy management systems and can operate autonomously or act as a guide for human operators by identifying beneficial control actions across a wide range of devices.
The Influence of Noise and Parameter Heterogeneity on TCL Aggregate Models

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This work studies the fidelity of aggregate models used to simulate and control a large population of thermostatically controlled loads (TCLs) and analyzes the influence of noise and parameter heterogeneity on TCL aggregate dynamics. At first, a homogeneous TCL population is considered which exhibits sustaining power oscillations following temperature synchronizing events. The commonly used discrete bin-based aggregate models can capture such behavior with a significantly large number of bins. However, decreasing the numbers of bins causes the model performance to worsen considerably. Hence, the different sources of error have been investigated. The tradeoff between accuracy and computational burden have also been analyzed. TCL populations are, however, heterogeneous in practice. Moreover, their dynamics can be affected by various sources of uncertainty. While heterogeneity and noise can add damping to the system and cause power oscillations to decay faster, the quantification of the decay rate is a challenging task. System identification based techniques can be used, but are computationally intensive and the results are parameter specific. Hence, two alternative techniques, based on ‘temperature unwrapping’ and ‘phase de-synchronization’, have been proposed. While a TCL’s temperature moves within a fixed dead-band, the first method uses an unwrapped normalized temperature based representation to express the TCL dynamics, and the second uses phase differences. Using these representations, analytical tools have been developed to estimate the influence of noise and heterogeneity on damping of oscillations. Finally, the implications of our analysis in predicting the damping, and in designing efficient demand response strategies have also been discussed.
Carbon Mitigation Potential of Grid-Scale Energy Storage Systems for Peak Load Shifting

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We presented a method to evaluate the environmental benefits of energy storage for providing load shifting service to the grid. In the peak load shaving application, energy storage displace gas turbines while charging with efficient combined-cycle generating units. We used dynamic program to obtain the optimal operating strategy for battery that maximize the net emissions reduction from electricity generation. The dispatch model also examine the incremental cost of carbon dioxide abatement for range of storage sizes and capacities. We evaluated this by computing the avoided-cost of peaker plants operation and amortizing the cost of batteries over its lifetime. Our proposed method use simplistic approach to estimate the value of environmental characteristics of energy storage on the grid and assessed the sensitivity of results for storage technology and grid characteristics. The model was implemented for the ERCOT (Electric Reliability Council of Texas) grid load data and estimated the potential of 41.7 – 58.0 Tons CO₂/yr/MWh of storage capacity at the marginal cost of $568 - $918/Ton CO₂.
Simulated Cyclic Capacitive Loading of Thin-film Batteries

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Cyclic loading of power sources is common in microelectromechanical systems (MEMS), e.g. piezoelectric and electrostatic actuation. Simulation of these types of systems can allow for improved design and control. This work incorporates physical phenomena of cyclic capacitive loading into a full battery discharge model. This requires handling of dynamics at the two very different time scales of the switching and overall battery dynamics. Here we present an approach that adequately captures the experimentally observed dynamics at the fast time scale, and projects the states of the system over many cycles to reduce the numerical expense of understanding dynamics at the much longer time scale of the full battery discharge. We are able to show a significant reduction in numerical cost with our projection scheme. In addition to the model development and validation we analyze the error that occurs due to the projections used.
Mechanical Modeling of Agglomerate in Lithium-Ion Battery Electrodes

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Mechanical degradation is a significant mechanism that shortens the lifetime of lithium-ion batteries. During the operations of lithium-ion batteries, lithium ions are intercalated to or extracted from the electrode active particles, leading to stress generation inside the particles. The stress may result in cracks and even particle fracture, and further cause battery degradation.

Mathematical modeling is an important approach to investigate the stress inside the particle. Previous models assumed a single solid particle without internal structure. However, some active materials, e.g. LiNiₓCoᵧAl₂O₄, are in the form of agglomerate structure. In such materials, many nanometer-scale primary particles agglomerate to form a micrometer-scale secondary. The secondary particle is porous rather than solid, and electrolyte is soaked into the agglomerate.

The objective of this work is to develop an electrochemical and mechanical coupled model for a secondary particle with agglomerate structure. The electrochemical model accounts for the electrolyte and electrochemical reactions inside the secondary particle. In the mechanical model, the secondary particle is assumed as a continuum with effective properties, and the intercalation-induced stress is calculated through an analogy to thermal stress. Several important factors affecting the stress generation behaviors are discussed: 1) A strong dependence of open circuit potential on the concentration results in small stress; 2) Larger magnitude of over-potential at the particle surface leads to greater stress; 3) Large primary particle size is helpful to reduce the stress. 4) Stress in a porous secondary particle is much smaller than that in a solid particle of the same size.
Using Demand Response to Improve Electric Power System Stability Margins

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High penetration of renewables causes power system operating closer to their stability margins. Demand response has already been used to reduce system costs and improve power system reliability. This paper presents a new DR strategy that reallocates load to different buses while keeping the total load constant, to improve power system stability margins. This strategy only need actions from flexible loads, and does not require any change in generations. Its goal is to find the most stable load distribution with maximum smallest singular value of Jacobian matrix. A corresponding optimization model is formulated to describe such spatial DR problem. Also, an algorithm using eigenvalue sensitivity method is developed to solve the problem. Two test cases are used to numerically illustrate the correctness and effectiveness of the algorithm.
CSS: Climate and Space Sciences
Modeling the Impacts of Competition and Meteorological Conditions on Root Water Uptake in a Northern Temperate Forest Stand

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It is estimated that nearly two-thirds of terrestrial water cycles back to the atmosphere through plant vascular systems via the process of transpiration. The capacity for plants to meet atmospheric demands for water depends on the ability of their root systems to access soil water reserves. Detailed studies of single plant systems have shown the ability of root systems to adjust zones of uptake due to the redistribution of local water potential gradients, thereby delaying the onset of stress under drying conditions. An ongoing question of interest is how lateral interactions and competition among neighboring plants impact individual and community resilience to water stress. While computational complexity has previously hindered the implementation of microscopic root system structure and function in larger scale hydrological models, newer hybrid approaches allow for the resolution of these properties at the plot scale. Using a modified version of the PFLOTRAN model, which represents the 3-D physics of variably saturated soil, we model root water uptake in a one-hectare temperate forest plot for three separate lateral interaction scenarios (mild, medium, and heavy interaction). Variations in root hydraulic architecture and degree of interaction produce variable local response to water limitation and provide preliminary insights on individual and community response to changing meteorological conditions. These results further illustrate how improved representation of root zones processes in land surface models will help better quantify the margins of heat and drought resilience for forest ecosystems under changing climate.
Energetic particle bursts in association with dipolarization events within Mercury’s magnetotail have been a source of curiosity and controversy since Mariner 10. Mariner 10 observed particle events analogous to injection and dipolarization events at Earth, but instrumental effects prevented an unambiguous determination of species, flux, and energy spectrum. At Earth, such energetic particle events closely correlate with sudden increases in the northward component of the near-tail magnetic field, termed dipolarization events, typically near substorm onset. Results from the Energetic Particle Spectrometer aboard MESSENGER have shown that energetic particle bursts at Mercury are composed entirely of electrons with energies from ~30 – 300 keV. Here we use the Gamma-Ray Spectrometer (GRS) high time resolution (10 ms) energetic electron (>50 keV) measurements and the Magnetometer data to discover the relationship between energetic electron bursts and dipolarizations of the magnetic field in Mercury’s magnetotail. From March 2013 to April 2015, we identified 1655 electron burst events within the magnetotail, of which 229 were closely associated with dipolarization. The dipolarizations were detected on the basis of their rapid (~1 s) increase in the northward tail field (ΔBz ~ 35 nT), which persist for ~10 s. The GRS energetic electron bursts are typically coincident with the leading edge of the dipolarization event and last for ~8 s. Surprisingly, these events display a strong dawn-dusk asymmetry with more events on the dawn side of the magnetotail.
Simulating 3D Spacecraft Constellations for Low Frequency Radio Imaging

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Constellations of small spacecraft could be used to realize a low-frequency phased array for either heliophysics or astrophysics observations. However, there are issues that arise with an orbiting array that do not occur on the ground, thus rendering much of the existing radio astronomy software inadequate for data analysis and simulation. In this work we address these issues and consider the performance of two constellation concepts. The first is a 32-spacecraft constellation for astrophysical observations, and the second is a 5-element concept for pointing to the location of radio emission from coronal mass ejections (CMEs).

For the first, we fill the software gap by extending the APSYNSIM software to simulate the aperture synthesis for a radio interferometer in orbit. This involves using the dynamic baselines from the relative motion of the individual spacecraft as well as the capability to add galactic noise. The ability to simulate phase errors corresponding to positional uncertainty of the antennas was also added. Error plots that show how well the dirty image matches the input image as a function of integration time were made. For the second concept we performed radio interferometric simulations of the Sun Radio Interferometer Space Experiment (SunRISE) using the Common Astronomy Software Applications (CASA) package. The results of our analysis show that SunRISE can localize the radio emission originating from the head or flanks of the CMEs in spite of the phase errors introduced by uncertainties in orbit and clock estimation.
Analysis of Ion Phase Space Distributions Detected by the Ion Mass Analyzer aboard Mars Express

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We present observations of planetary ion phase space distributions from the Ion Mass Analyzer (IMA) onboard the Mars Express (MEX) satellite. The magnetometer data from Mars Global Surveyor is used to obtain a rough estimate of the interplanetary magnetic field (IMF) orientation. The orientation of this field organizes certain characteristic features of the velocity space distributions of ions escaping Mars’ atmosphere. This study focuses on the high (keV) energy ions, as well as the relative importance of a high-altitude magnetosheath source of escaping planetary ions. Comparisons to virtual detections using a test particle simulation will also provide insight into ion origins and trajectories.
Heliospheric Suprathermal Electrons during Filament-Associated ICMEs

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We are undertaking a study of solar wind plasma and suprathermal electron pitch angle distributions (PADs) during interplanetary coronal mass ejections (ICMEs) to trace the plasma back to its solar origins, addressing the magnetic topology and initial structure of the ICME. We present initial results for case-studies of filament-associated ICMEs observed by ACE/SWEPAM and ACE/SWICS. Counterstreaming suprathermal electrons are widely regarded to be a signature of closed heliospheric magnetic field lines associated with coronal mass ejections (CMEs). Thorough investigation indicates that counterstreaming electrons are not observed continuously or consistently in ICMEs. While very narrow suprathermal electron strahl are commonly observed in ICMEs. We present initial findings on the occurrence of counterstreaming suprathermal electrons and narrow electron strahl during a case study of filament-associated ICME events.
TCB: Tissue, Cellular, and Biomolecular Engineering
Exploiting Rheological Characteristics of Biofilms for Novel Treatment and Remediation Methods

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Medical device infections are one of the leading causes of bloodstream infections in the United States. These device related infections are predominately caused by bacteria forming sessile communities, known as biofilms, which are often antibacterial resistant. The objective of this research is to approach the treatment of bacterial biofilms from a complex fluid perspective. By applying engineering principles and external stimuli we believe that it is possible to manipulate the rheological characteristics of the bacterial communities and prevent or remediate biofilm growth. Using a model catheter system, biofilms grown under physiological conditions show signs of cell death when exposed to flowing media at temperatures above 50°C. Using confocal microscopy, it has been determined that there are variations in cell viability relative to the thickness of the biofilm suggesting that heat transfer in the plane perpendicular to the biofilm surface is significant. Furthermore, we have investigated the effects of flow and shear stress on biofilm development and shown a positive correlation between increased shear and biofilm detachment. It is hypothesized that the effects of heat and flow shear can be coupled with antibiotics, possibly leading to increased antibiotic susceptibility. These are promising steps in the development of an in situ treatment/remediation method for biofilm growth in medical devices.
Bacterial Adhesive Dynamic Simulation of FimA Mutant with Low Uncoiling Force

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Uropathogenic \textit{Escherichia coli} type 1 fimbria allows bacterial adhesion to human epithelial cells, a critical step to urinary tract infections. Type 1 fimbria is structurally composed of FimH, the adhesion domain, tethered by a spring like helical structure formed by polymerization of thousands of FimA subunits. While FimH is responsible for the adhesive property of \textit{E. coli} through the formation of catch bonds, of which bond lifetime increases under higher tensile force, the function of the FimA tether has not been fully understood. Previous simulations of cell adhesion under shear demonstrated that yielding elasticity of the FimA tether is critical for bacteria to remain adhered under high shear. Here, we modified the FimA mechanics of an established cell adhesion simulation to further investigate the role of FimA on bacterial adhesion. We also compared our simulations to experiments, which were tested on wild type \textit{E. coli}, as well as a mutant with mutations in the FimA protein. Longer travel distance at high shear observed in the mutant compared to the wild type in experiments can be explained by the higher uncoiling rate of mutant FimA. However, quantitative difference between the simulations and experiments on mutant suggest that other factors may also contribute to the difference in behavior of the mutant and wild type. Successful development of a validated model of the mutant adhesive dynamic under flow would provide insights in inhibiting bacterial adhesion to prevent urinary tract infections as well as other catch bond adhesive systems with yielding tethers.
Staphylococcus Epidermidis Alters a Fibrin Clot – Insights into Septic Thromboembolism

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Bacterial infection causes a three-fold increase in the risk of venous thromboembolism, a leading cause of death and disability. Here we show that the common pathogen and biofilm former Staphylococcus epidermidis influences an in vitro model of a blood clot by retarding its formation, increasing its elasticity, and generating a heterogeneous structure. The model clot is a fibrin network produced by thrombin catalyzed polymerization of fibrinogen. When S. epidermidis is introduced, the resultant, steady-state material, termed an infected clot, has a bulk elasticity about 3.7 times larger than a clot of pure fibrin. By confocal microscopy, we observe that the infected clot has a heterogeneous structure characterized by two different network mesh sizes, rather than a single one as observed in a pure fibrin clot. Using multiple-particle tracking microrheology, we correlate the higher bulk elasticity to this heterogeneous microstructure via direct measurement of the fiber dynamics. Finally, by combining time-lapse microscopy and photography, we observe that the fibrin network of an infectious clot continues to increase its heterogeneity with a void structure that progresses over time from microscopic to macroscopic scales. Our results provide insight into the correlation between bacterial infection and thromboembolism: The higher elasticity of the infected clot may be associated with embolism, a condition that has previously been linked to high fibrin rigidity. Moreover, the continuous increase in heterogeneity of infected fibrin clots suggests that S. epidermidis has the capacity to remodel and eventually rupture a fibrin clot.
Development of Novel Stable Cell System with Fluorescently Tagged Hypoxia Inducible Factor 1α and 2α

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All solid tumors become hypoxic as they progress, and this hypoxia is the major driving force in the advanced progression of tumors. Hypoxic response is transcriptionally regulated by hypoxia-inducible factors (HIFs), which are heterodimeric transcription factors that comprises a constitutive subunit, aryl hydrocarbon nuclear translocator (Arnt), and a hypoxia-inducible alpha-subunit. Under normoxic conditions, HIF’s are degraded through Von Hippel-Lindau protein. There are three different isoforms of HIF: HIF-1α, HIF-2α and HIF-3α. HIFs are master regulators, with over 300 direct gene targets having been identified. HIF-1α and HIF-2α are of particular interest due to their role in several cancers. Currently, the temporal dynamics of HIF-1α and HIF-2α are not clear since there are no effective methods to determine their real-time expression. The primary goal of this project is engineer cell lines with O6-alkylguanine-DNA-alkyltransferase based enzymatic tags on HIFs that will then be used to quantify and localize HIF-1α and HIF-2α expression in real time simultaneously. We have designed guideRNA (sgRNA) for our CRISPR Cas9 system, and created stable cell lines to confirm the cut sites. Additionally, we have characterized parent NIH/3T3 cell for HIF expression under hypoxia and the hypoxia mimic, FG-4592 compound. Our engineered cell lines will also allow for the characterization HIF-1α and HIF-2α activity under various stressors. This will be the first integrated characterization of HIF-1α and HIF-2α dynamics, and will be critical for HIF-based therapies.
The function of chemical cues, adhesion signals, and transcription factors have been studied intensively to understand how cells in the embryo differentiate into specific lineage. However, not much attention has been put studying mechanical stresses to which cells are exposed to in understanding the role of forces (i.e. tensile, compression) in guiding human embryonic stem cell (hESC) differentiation. In this work, we investigate the role of external forces in hESCs by utilizing from Acoustic Tweezing Cytometry (ATC), an ultrasound-based subcellular mechanical stimulation technique. Approximately 1,000,000 undifferentiated single hESCs (H1 and H9) were seeded on matrigel coated 60mm dishes and approximately 500,000 cells localized in the area where ATC is applied. The next day, microbubbles functionalized with RGD were linked via integrin to dissociated single hESCs. Ultrasound pulse (1 MHz center frequency, 10 Hz pulse repetition frequency, and 50% duty cycle) with ramping amplitudes (0.025, 0.04, 0.06 to 0.08 MPa) was applied to the cells at a 45 degrees angle beneath the petri dish for 30 mins at each amplitude. Surprisingly, stress induced shuttling Oct3/4 and Nanog from nucleus to cytoplasm in time dependent manner, while Sox2 was not affected. The stress-induced shuttling occurred as early as 2 hours after the onset of ATC application. Nucleo-cytoplasmic Nanog and Oct4 may direct cell prograning and determine the cell lineage in early embryo development. These findings might help us to better understand the effect of mechanical forces during development and help us correct defects and to treat diseases.
Self-assembled Iron Sulfide Supraparticles as Artificial Viruses

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Gene therapy has been widely used for treatment of inherited or acquired genetic diseases. Efficient delivery of therapeutic agents has become a significant barrier in clinical applications due to the toxicity and instability of the vectors and complex intracellular environment. Among non-viral vectors, inorganic nanoparticles have become a popular strategy for nucleic acid delivery due to their similarities with proteins. We synthesized L-cysteine stabilized iron-based inorganic nanoparticles which self-assemble into supraparticles. Transmission electron microscopy (TEM), TEM tomography and dynamic light scattering (DLS) were used to characterize the supraparticles size, shape, and charge. To understand how these supraparticles interact with DNA, we incubated them with pEBB-cherry plasmid overnight and we tested these complexes in circular dichroism, UV-Vis spectroscopy and electrophoretic mobility shift assay. Our results indicate that supraparticles contain continuous compartments, are positively charged (32 mV) and 74 ± 21 nm in diameter. DLS results suggest supraparticles are wrapped with DNA like histon proteins are wrapped with DNA during chromosome formation. Due to the charge of the supraparticles and DNA, it is assumed that electrostatic interactions are responsible for the formation of these complexes. Since iron sulfide is a natural material, it presumably has low cytotoxicity and high biocompatibility. Supraparticles can condense DNA, protect it against degradation, penetrate through cellular membranes and facilitate endolysosomal escape in gene therapy. Therefore, development of these particles can be used as an effective delivery tool for gene therapy.
The Influence of Fiber Stiffness on Directed Cell Migration in Aligned Fibrillar Microenvironments

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While cell migration has traditionally been studied on rigid flat surfaces coated with extracellular matrix proteins, it is now widely accepted that in many physiologic settings the physical structure of the surrounding matrix is a key factor influencing migration (e.g. the migration of cancer cells through the fibrous stroma required for intravasation and eventual metastasis). Towards a better understanding of how ECM structure and mechanics impact cell migration, we designed a synthetic fibrous biomaterial with tunable mechanics and user-defined architecture. Our material system affords independent control over several key attributes of fibrous ECMs including fiber stiffness, alignment, density, and diameter, a capability unachievable in previously established models such as type I collagen gels. Using time-lapse microscopy, we examined how matrix stiffness alters cell migration speed in matrices of aligned fibers, mimicking the organization of the stroma surrounding several types of solid tumors. Interestingly, our results demonstrate a biphasic relationship between stiffness and migration speed. At higher stiffnesses, cells were unable to deform the matrix. Conversely, at lower stiffnesses, a portion of cell traction forces were absorbed by deformation of the matrix. Optimal migration speed appeared to be achieved at a medium stiffness where slight matrix deformation helped propel the cell forward. Further improving our understanding of how matrix mechanics affects cell migration may aid in the design of materials that improve cellular engraftment in implantable materials, guide cells to a specific tissue for regenerative purposes, or confine what would otherwise be metastatic cells to the primary tumor.
Abstracts – Richard and Eleanor Towner Prize for Outstanding Ph.D. Research
Data-Driven Optimization for Early Detection of Prostate Cancer

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Prostate cancer (PCa) is the most common cancer among men in the United States. Recent advances in the development of new technologies for the early detection of cancer have the potential to improve patient survival by catching cancer at an early stage when health outcomes are most favorable for patients. However, there is little research investigating the long-term health and economic implications of these new technologies. For example, magnetic resonance imaging (MRI) and new biomarker tests have been proposed as potential minimally invasive ways to achieve early detection of PCa, but whether and when to use them is unclear due to the high cost and imperfect nature of these tests.

We present a stochastic modeling framework for PCa onset and progression that incorporates partial observability of a patient’s health status. We used statistical learning algorithms and clinical datasets combined with expert clinical knowledge of our collaborators to formulate and validate the models. New technologies, such as MRI and biomarker tests, are incorporated into the models using a probabilistic simulation of test outcomes to represent the information these tests provide about the true health status of the patient. We used our model to design testing strategies that tradeoff the harms and benefits of using these new technologies. Our results show that these strategies can lead to significantly improved health outcomes and they are cost-effective relative to established norms for societal willingness-to-pay.

The methodological approaches we present could be applied to many other chronic diseases, including bladder, breast, and colorectal cancer.
High-Efficiency Microfluidics for Single Cell Phenotypic and Genotypic Analysis of Rare Cancer Cells

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Recent research suggests that cancer stem-like cells (CSCs) are the key subpopulation for tumor relapse and metastasis. Due to the cancer plasticity in surface antigen and enzymatic activity markers, functional tumorsphere assays are promising alternatives for CSC identification. To reliably quantify rare CSCs (1-5%), thousands of single-cell suspension cultures are needed. While microfluidics is a powerful tool in handling single cells, previous works provide limited throughput and lack automatic data analysis capability required for high-throughput studies. In this work, we present the scaling and automation of high-throughput single-cell-derived tumor sphere assay chips, facilitating the tracking of up to ~10,000 cells on a chip with ~76.5% capture rate. The presented cell capture scheme guarantees sampling a representative population from the bulk cells. To analyze thousands of single-cells with a variety of fluorescent intensities, a highly adaptable analysis program was developed for cell/sphere counting and size measurement. Using Pluronic\(^{\circledR}\) F108 (Poly(ethylene glycol)-block-poly(propylene glycol)-block-poly(ethylene glycol)) coating on Polydimethylsiloxane (PDMS), a suspension culture environment was created to test a controversial hypothesis: whether larger or smaller cells are more stem-like defined by the capability to form single-cell-derived spheres. Different cell lines showed different correlations between sphere formation rate and initial cell size, suggesting heterogeneity in pathway regulation among breast cancer cell lines. More interestingly, by monitoring hundreds of spheres, we identified heterogeneity in sphere growth dynamics, indicating the cellular heterogeneity even within CSCs. These preliminary results highlight the power of unprecedented high-throughput and automation in CSC studies.
Uncovering Security Failures with Internet-Wide Measurement

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Historically, the vast majority of the devices connected to the public Internet have remained out of sight to the research community. However, as the diversity of devices and the role they play in critical infrastructure has increased, understanding the dynamics of and securing these devices has become of paramount importance. We introduce ZMap—a network scanner capable of surveying the entire IPv4 address space in under an hour—more than 1300 times faster than existing tools and Censys—a framework that maintains an up-to-date snapshot of the hosts and services running across on the public Internet. We show that the global perspective provided by these tools enables the research community to uncover new classes of vulnerabilities, understand how network protocols have evolved beyond their original specifications, and measure the real-world challenges to protocol deployment on the Internet.
Bridging Scales Using High-Order Adaptive Mesh Refinement for Idealized Simulations in a Global Atmospheric Model

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Extreme atmospheric events such as tropical cyclones or atmospheric rivers are inherently complex multi-scale phenomena. Such extremes are a challenge to simulate in conventional atmosphere models, which typically use rather coarse uniform-grid resolutions. Adaptive Mesh Refinement (AMR) techniques seek to mitigate these challenges by dynamically placing high-resolution grid patches over user-defined features of interest. This provides sufficient local resolution over e.g. a developing cyclone while limiting the total computational burden of requiring such high-resolution globally. Studying such techniques in idealized simulations enables the assessment of the AMR approach in a controlled environment and can assist in identifying the effective refinement choices for more complex, realistic simulations. We present a non-hydrostatic, finite-volume dynamical core, which implements refinement in both space and time on a cubed-sphere grid. Several test cases are discussed, including an idealized tropical cyclone simulation, for both the 2D shallow water equations and the full 3D model. These simulations test the effectiveness of both static and dynamic grid refinements as well as the sensitivity of the model results to various adaptation criteria. Finally, we assess AMR as a possible technique to study scale discrepancies in atmospheric models.
Supersonic combustion ramjets are a class of air-breathing engines that could one day revolutionize hypersonic transport and single-stage-to-orbit vehicles. Here, the ingested air is fluid mechanically compressed through a complex system of shocks. However, the sensitivity of this flow to external perturbations can be detrimental to the compression ratio, affecting ignition and decreasing thrust. Ensuring efficient fuel/oxidizer burning at supersonic speed is also challenging given the supersonic fluid speed inside the engine. Since propulsive thrust is linked to the ability to compress incoming air, loss of either one will lead to engine failure. Both the shock train's complex response to external perturbations and the mechanics of supersonic combustion are therefore key design considerations.

In this collaborative study with NASA, massively parallel computations called direct numerical simulations (DNS) were used to understand the mechanism of shock train formation and combustion in such scramjet engines. For instance, many of the calculations used 5000-10000 processors simultaneously for 24-72 hour period, enabling first-time access to flow regimes and conditions. It was found that there exists a resonance feature, whereby external flow perturbations of certain frequencies are amplified but others are filtered out by the high-speed viscous fluid and shock structure. Further, molecular processes that are subject to fast chemical transformation do not have the time to relax to so-called thermal equilibrium, which affects the ignition process in the engine. These studies have provided new insights into scramjet design, including new injector design concepts and shape-changing inlets.
Designing Durable Icephobic Surfaces

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Ice accretion remains a costly, hazardous hindrance worldwide. Icephobic materials reduce the adhesion between ice and a surface. However, only a handful of the icephobic systems reported to-date reduce the ice adhesion sufficiently for the facile removal of ice under its own weight or by mild winds. The majority of these amply-icephobic surfaces have relied on sacrificial lubricants, which may be depleted over time, drastically raising the ice adhesion. In contrast, here we show that surfaces utilizing interfacial slippage to lower their adhesion to ice may remain icephobic indefinitely (including after severe mechanical abrasion, acid/base exposure, 100 icing/de-icing cycles, thermal cycling, accelerated corrosion, and exposure to Michigan wintery conditions over several months). By tailoring the crosslink density of different elastomeric coatings, irrespective of material chemistry, we are able to design a library of extremely durable icephobic systems. Moreover, we propose a new, universally applicable and theoretically consistent model that accurately predicts the adhesion of ice to surfaces exhibiting interfacial slippage. This model allows one to rationally engender icephobicity in essentially any polymeric system. As such, we present several new, extremely icephobic systems, fabricated from a wide range of materials including common engineering plastics and sustainable natural oils. These environmentally friendly, icephobic systems may significantly reduce ice accumulation on airplane wings, wind turbine blades, car windshields or boat hulls.
Advanced Ultrasound-Based Mechanical Property Characterization and Stimulation of Engineered Tissue Constructs

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Polymer- and protein-based hydrogels are widely used as injectable matrices for regenerative tissue engineering. Mechanical properties of these materials are essential in regulating cell functions. However, conventional mechanical testing methods usually involve sample destruction, and most ultrasound electrography techniques provide only semi-quantitative results. We have implemented a dual-mode ultrasound elastography (DUE) system to measure the viscoelastic properties of biomaterials nondestructively and noninvasively. Additionally, we are developing an ultrasound-based therapy to promote tissue development via acoustic straining in engineered tissues. The DUE system consists of a focused ultrasound transducer for inducing compression and a higher frequency imaging transducer for tracking deformation. Both the bulk properties and the cellular scale strain distribution within construct can be obtained. Quantitative physical parameters were extracted by fitting creep and recovery curves to established mechanical models. The spatiotemporal distribution of viscoelastic properties of hydroxyapatite-doped agarose, fibrin, collagen hydrogels as well as in cell-seeded collagen constructs have been revealed using DUE. We also have demonstrated DUE’s capability of resolving small-dimension samples and delineating phase differences within hydrogel constructs. Combinations of acoustic pressure level, pulse repetition frequency and pulse duration that induce over 0.5% strain were applied to human mesenchymal stem cell-seeded constructs at selected dosages, and enhancement in osteogenic differentiation and mineral deposition have been observed. DUE is a valuable tool in characterizing microscale mechanical properties and matrix remodeling noninvasively. Furthermore, the acoustic straining effect presented by DUE may lead to development of an ultrasound-based therapy to facilitate bone regeneration in conjunction with biomaterial-based stem cell delivery.
Sub-Millimeterwave Radar Systems for Short Range Applications

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In recent years, the increasing demand on high resolution imaging radars has pushed the research activities to the sub-millimeterwave frequency range. Important applications that can benefit from such systems include short-range autonomous navigation radars used in vehicles and aircrafts, as well as high resolution radars for standoff imaging of persons and hidden objects, including illicit drugs and explosives. These systems have the potential to approach the resolution of optical imaging while operating under adverse conditions of weather.

This research investigates the unique advantages as well as the performance limitations of radar systems operating at 240 GHz working in typical outdoor environments. The research has three main objectives which are: 1) developing novel scattering models that can accurately describe the propagation and scattering of electromagnetic wave in realistic communication channels, 2) material characterization of different synthetic and artificial targets found in typical radar environments, and 3) developing novel microfabrication techniques that rely on piezoelectric micro-actuators to fabricate an electronic beam steering radar system in a reliable and very compact fashion.
A New Theory of Exploration in Reinforcement Learning with Rich Observations

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Recently, Reinforcement Learning (RL) has achieved impressive successes in video game playing and mastering the game of Go (AlphaGo). In general, RL agents learn from data to act in unknown environments, which requires a learning module (to learn from collected data) and an exploration module (to collect data from all different situations). While the use of function approximation techniques, such as deep neural networks, has improved the learning module substantially and helped RL deal with complex sensory inputs (or rich observations, such as raw camera images), advances in improving the exploration module have been rather limited, and even state-of-the-art RL algorithms can be ineffective when non-trivial exploration is required. On the other hand, exploration has been studied for a long time in RL theory, but most methods only apply to simple problems where the environment has a small number of discrete states.

In this work, we provide the first data-efficient algorithm that provably explores in problems with rich observations. Our algorithm requires the problem to satisfy a particular rank condition. We show that a broad range of RL problems, including some most sophisticated environments tackled by practitioners nowadays, satisfy this condition, hence can be effectively solved by our algorithm.
Materials and Device Optimization of Transition Metal Oxides-based Memristors

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Memristors are electronic devices with inherent memory effects and have attracted enormous interest recently for applications in non-volatile memory and neuromorphic computing. Resistive switching (RS) effects in memristors originate from internal, microscopic ionic migration and associated electrochemical processes, which modulate the electrical and other physical properties of materials. To optimize the device performance for practical applications with large-size arrays, it is necessary to control the internal ionic transport and redox reaction processes at the atomic scale. Here we show that the RS characteristics in Ta$_2$O$_5$-based memristors can be systematically tuned by inserting a graphene film with engineered nanopores. In this structure, the graphene film effectively blocks ionic transport and redox reactions, thereby the oxygen vacancies required during the RS process are only allowed to transport through the engineered nanosized openings in the graphene layer, leading to effective modulation of the device performance by controlling the nanopore size. We also theoretically study the electronic and optical properties of Ta$_2$O$_5$ polymorphs and oxygen vacancies using first-principles calculations based on density functional theory to provide insights on the physical mechanism of the RS behavior for material and device optimization. Our calculated results (e.g., band gap, thermodynamic and optical transition levels) are in excellent agreement with experimental results, elucidating the fundamental atomistic properties of oxygen vacancies. Based on the theoretical calculations, we propose microscopic processes involving charge transition between charged and neutral vacancies during the RS, which can provide an additional degree of control on the RS characteristics of memristors.
The Phonovoltaic Cell and Tuned Graphene

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The phonovoltaic cell harvests optical phonons like a photovoltaic harvests photons. That is, in a phonovoltaic cell, a non-equilibrium population of optical phonons more energetic than the band gap generates electron-hole pairs through the electron-phonon coupling. Then, a \(p-n\) junction separates them to generate power. If this occurs faster than the optical phonon population thermalizes and becomes heat through the phonon-phonon coupling, then the phonovoltaic cell can convert the precursor of heat, the optical phonon, into energy much more efficiently than the thermoelectric generator converts heat. However, few crystals combine the required material properties, i.e., few have (i) an optical phonon energy greater than the band gap and much greater than the thermal energy and (ii) an electron-phonon coupling stronger than the phonon-phonon coupling. Indeed, most materials exhibit an optical phonon energy an order of magnitude smaller than their band gap. Tuned graphene (h-C) is one of the few exceptions. An analytical tight-binding model predicts that opening a band gap in graphene through the manipulation of the sub-lattice symmetry enables a substantial phonovoltaic figure of merit, and \textit{ab initio} (DFT-LDA) calculations validate this prediction. Indeed, a h-C:BN phonovoltaic can double the thermoelectric efficiency, even at 300 K. Moreover, the tight-binding model predicts that h-C:BN is not unique in this regard: Other tuned graphene structures, like a bilayer of graphene under an electric field, should reach a similar efficiency.
Determining Hurricane Structure and Intensity from CYGNSS Observations

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The Cyclone Global Navigation Satellite System (CYGNSS) constellation of eight small satellites, each with a 4-channel GPS bi-static radar receiver, is designed to measure ocean surface wind speed over the full dynamic range of wind speeds experienced in a hurricane. CYGNSS is unique for two main reasons: 1. Unlike the existing network of Earth observing satellites, CYGNSS will provide estimates of surface wind speed in all precipitating conditions—a universal failure in other satellite observations. 2. CYGNSS uses a constellation of small satellites, so many can be flown to improve sampling.

In preparation for the first observations of hurricanes made by CYGNSS in 2017, several CYGNSS-based hurricane science data products are being developed to support the needs of the research and forecasting communities. The maximum sustained wind speed (VMAX), radius of maximum wind (RMW), and 34-, 50-, and 64-kt wind radii parameters are commonly used to characterize the potentially destructive wind field of a hurricane. This work develops unique algorithms to estimate these hurricane parameters from CYGNSS observations. CYGNSS-based VMAX, RMW, and wind radii estimation algorithms have been developed which take advantage of the unique properties of CYGNSS observations, as well as overcome potential challenges of CYGNSS observations. Performance of these science data products is validated using a prelaunch mission simulator. The in-flight products will be available in time for the 2017 Atlantic hurricane season.
The Stratospheric Changes Inferred from 10 Years of AIRS and AMSU-A Radiances

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We analyze global-mean radiances observed by AIRS (Atmospheric Infrared Sounder) and AMSU-A (Advanced Microwave Sounding Unit) from 2003 to 2012. We focus on channels sensitive to emission and absorption in the stratosphere. Optimal fingerprinting is used to obtain estimates of changes of stratospheric temperature in five vertical layers due to external forcing in the presence of natural variability. The results show a cooling rate of 0.75±0.10K decade⁻¹ (2-σ uncertainty herein) in the upper stratosphere above 6hPa due to external forcing. The cooling rate due to external forcing in two middle stratospheric layers (6-14hPa and 14-30hPa) is ~0.5±0.24K decade⁻¹. The cooling rates in the lower stratosphere (30-60hPa) and in the lowest part of the stratosphere (60-100hPa) are small and statistically insignificant. The joint use of passive infrared and microwave radiance permits disambiguation of trends of carbon dioxide and stratospheric temperature, reduces uncertainty and increases vertical resolution of detected stratospheric temperature trends. This study, for the first time, applies optimal fingerprinting to observed high spectral resolution IR radiances to detect climate change signals. Furthermore, it demonstrates the merit of well-calibrated spectral infrared and microwave radiance in the monitoring of global climate, as well as the synergies in infrared and microwave global satellite observations for detecting climate change signals.
A Molecular Thermodynamic Model of Complex Coacervation in Oppositely Charged Polyelectrolytes with Explicit Account of Charge Association/Dissociation

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Into the classical Voorn-Overbeek (VO) free energy model for polyelectrolyte complexation and phase behavior, we incorporate counterion condensation, cross-chain ion pairing, and charge regulation by treating each as a reversible chemical reaction using laws of mass action. The importance of each reaction is controlled by a corresponding standard free energy parameter that needs to be determined separately via experimentation or molecular simulations. Our model also includes free energy terms accounting for Born (or ion solvation) energy, van der Waals energies as well as the translational entropy and electrostatic energies present in the VO model. In monophasic systems, the proposed model can qualitatively explain the observed shifts in acidity and basicity observed in potentiometric titration of weak polyions in the presence of salt and oppositely charged polyions in accordance with Le Châtelier's principle. We demonstrate how a competition between counterion condensation and ion pairing can explain the complex coacervation of strongly charged polyions. Binodal diagrams predicted in our model are most sensitive to ion pairing strength both for weak and strong polyions. Our model predicts that when a freshly mixed system undergoes coacervation, the extent of ion pairing increases in the dense phase that forms, at the expense of reduced counterion condensation. We compare binodal diagrams predicted by our model against experimental data, and find a plausible parameter set that leads to agreement between them. Our model yields a picture of coacervation driven primarily by ion pairing rather than by long-ranged electrostatic free energy as envisioned by the original VO model.
Molecular Engineering of Polymers to Realize High Thermal Conductivity in Amorphous Systems

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Low thermal conductivity (κ ~0.1–0.5 Wm⁻¹K⁻¹) of polymers has impeded their use in applications that require efficient heat dissipation. Commonly used techniques like compositing and chain-extended fibers suffer with numerous disadvantages such as unwanted physical properties, high cost, loss of processability etc. For practical applications, high κ polymers that are more compatible with conventional manufacturing processes (e.g., injection molding) are desired, yet no strategy to achieve all-polymeric material with κ > 0.6 Wm⁻¹K⁻¹ has been reported. Here, we demonstrate two design strategies to engineer the polymer chains’ morphology and interactions to realize high κ in all-polymeric amorphous systems.

In the first approach, we employed hydrogen bonds between a short rigid polymer chain (Poly(N-acryloyl piperidine), PAP) and a long flexible one (Polyacrylic acid, PAA) to hold the latter in extended chain conformation. In addition to improving intra-chain thermal transport through the extended PAA chains, H-bonds also strengthened inter-chain heat transfer resulting in significant enhancement in κ with value as high as 1.5 Wm⁻¹K⁻¹ achieved in nanoscale thin films. The second approach involved using columbic repulsion field along the backbone of a polyelectrolyte (PAA) to achieve isotropically expanded chains. Polymer chain confirmation was systematically varied from tightly coiled up unionized chains (at low pH) to a swollen ionized one (at high pH) through controlled ionization of the acidic side groups. Thermal conductivity in a typical spun-cast amorphous film increased linearly with the degree of ionization of PAA, reaching up to ~1.2 Wm⁻¹K⁻¹ in film with >90% ionized PAA chains.
Bioengineered *in vitro* Model for Peri-implantation Human Embryogenesis

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Implantation is a critical developmental milestone for early human embryogenesis and successful pregnancy. During implantation, the pluripotent epiblast gives rise to the squamous amnion and the columnar embryonic disc, which together enclose the amniotic cavity to form an asymmetric cystic structure called the amniotic sac. While amniogenesis marks the first differentiation of the epiblast, the amniotic sac sculpts the morphology of peri-implantation human embryo and patterns the embryonic disc for gastrulation. Despite its fundamental and clinical significance, the development of the amnion and the amniotic sac in humans is poorly understood due to inefficient *in vivo* studies and the lack of *in vitro* methods. Here, we report the first *in vitro* model for peri-implantation human embryogenesis, by culturing human pluripotent stem cells (hPSCs) in a bioengineered niche that mimics the implantation microenvironment. Specifically, we find that hPSCs can undergo spontaneous, self-organized development *in vitro* that resembles the differentiation of amnion and the morphogenesis of human amniotic sac *in vivo*. Our findings show that implantation-like physical niche cues are both sufficient and necessary for the amniogenesis by hPSCs in an otherwise self-renewal-permissive biochemical context. We molecularly profile the hPSC-derived early amniotic cells and show the bipolar amnion-epiblast patterning in the amniotic sac embryoid generated *in vitro*. We further unveil an autonomous BMP-SMAD signaling underlying peri-implantation human embryogenesis. Together, our findings provide the first *in vitro* system for modeling early human embryonic development during implantation and early gastrulation, generating new insights that will advance both fundamental human embryology and clinical reproductive medicine.
Structured Perfect Bayesian Equilibrium in Infinite Horizon Dynamic Games with Asymmetric Information

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In dynamic games with asymmetric information structure, the widely used concept of equilibrium is perfect Bayesian equilibrium (PBE). This is expressed as a strategy and belief pair that simultaneously satisfy sequential rationality and belief consistency. Unlike symmetric information dynamic games, where subgame perfect equilibrium (SPE) is the natural equilibrium concept, to date there does not exist a universal algorithm that decouples the interdependence of strategies and beliefs over time in calculating PBE. In this paper we find a subset of PBE for an infinite horizon discounted reward asymmetric information dynamic game. We refer to it as Structured PBE or SPBE; in SPBE, any agents' strategy depends on the public history only through a common public belief and on private history only through the respective agents' latest private information (his private type). The public belief acts as a summary of all the relevant past information and it's dimension does not increase with time. The motivation for this comes the common information approach proposed in Nayyar et al. (2013) for solving decentralized team (non-strategic) resource allocation problems with asymmetric information. We calculate SPBE by solving a single-shot fixed-point equation and a corresponding forward recursive algorithm. We demonstrate our methodology by means of a public goods example.
Global Optimization: Branching-Point Selection for Trilinear Monomials in Spatial Branch and Bound

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Spatial branch and bound (sBB) is the workhorse algorithmic framework to solve global mathematical optimization problems. Formulating a problem using this paradigm allows both the non-linearities of a system and any discrete design choices to be modeled effectively. This means that the techniques are used in a wide variety of applications, from chemical engineering problems to the design of energy systems. Due in part to their generality these problems are very difficult, and consequently the best way to implement many algorithmic details is not wholly understood. In this work we provide some analytic results guiding the implementation of sBB for a simple but frequently occurring function ‘building block’.

In particular, we use volume as a geometric measure to compare the impact of different branching variable and branching point choices in the context of sBB. We do this for functions involving trilinear monomials (or any three quantities multiplied together), an incidence that occurs frequently in global-optimization models. We demonstrate that the problem of obtaining the optimal branching point can be solved by finding the minimum of a (parameterized) convex function; we also provide tight bounds on where this minimum falls. In addition, we stipulate guidance regarding which branching variable to select under various appropriate conditions. As opposed to showing that our techniques work for a particular library of test problems, we establish analytically that our results hold for all problems of the given form. In this way, we demonstrate that analytic results are indeed obtainable for algorithm implementation decisions.
Identifying Crystals Using Machine Learning

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Colloidal and nanoscale particles are objects with sizes in between those of molecules and macroscopic matter. They are interesting building blocks to use in new materials because they combine the best of both of these worlds: they are small enough to obey statistical mechanics, but still large enough for individual particles to be easily observed and analyzed. While atoms and molecules are limited to the periodic table of elements and have rigidly-defined interactions, colloids and nanoparticles are much more customizable in design and can be “made to order” to have target properties and defined interactions. Computer simulations have proven immensely helpful in designing new systems on the colloidal- and nanoscale, but studies are often limited in breadth by human analytical capacity and by the difficulty of designing automated tools to detect structure within simulated systems. Here we employ common machine learning methods to identify the crystal structures formed in self-assembly simulations, reducing the human work required to analyze data sets by two orders of magnitude and enabling more comprehensive studies.
Dynamic Market Mechanisms for Wind Energy

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Electricity generation from wind is intermittent and uncertain. A wind generator does not have complete control over her generation in advance and dynamically learns about her generation capacity and wind condition over time. However, the current two-settlement market architecture, which consists of a forward market followed by a real-time market, is mainly designed for conventional generators that have (almost) perfect knowledge and control over their generation in advance. As a result, in addition to technical challenges, the integration of wind energy into electricity markets gives rise to market design challenges. In our work, we study the problem of market design for wind energy. We propose a dynamic market architecture that addresses the intermittent and dynamic nature of wind generation. We determine a set of dynamic market mechanisms for wind energy procurement that provide a coupling between real-time and forward markets over time. We show that the dynamic mechanisms outperform the common practices for the integration of wind generation, namely inclusion of wind generation in real-time and forward markets. Therefore, we demonstrate the advantage of adopting dynamic market mechanisms over static mechanisms for the integration of wind energy in the emerging smart grids. We show that the proposed dynamic market mechanisms provide a richer space of market allocations than forward and real-time markets, allow for flexible generation of wind energy, incorporate all the information that arrives over time into the market, and provide forward commitment of wind producers that is necessary for system operation and reliability.
An LCM-based Simplified Coupling Scheme to Facilitate Distributed Simulation in the Building Energy Analysis Domain

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A distributed simulation framework helps in understanding the integrated effects of systems by connecting and exchanging information across real systems, simulation models and humans. In the building energy analysis domain, several coupling based tools have been created in the past and Building Control Virtual Test Bed, MLE+, and Functional Mock-up Interface are the most commonly used frameworks by researchers for developing coupled systems. However, these tools are inherently complex which makes it difficult for the facility managers and other decision makers to understand and adopt. Also these tools are tightly coupled, which means the framework itself lacks the flexibility to incorporate tools and simulation programs of our choice. Hence the main of this study is to address this gap by creating a simple and generalized coupled framework using the capabilities of Lightweight Communications and Marshalling (LCM), a tool mainly used by the robotics community.

As a case study demonstrating this new framework, the thermal comfort of occupants in an office building is simulated using an Agent Based Model and is coupled with an energy simulation tool to analyze the real-time energy effects. In the ABM, occupants also adapt their behavior according to the building ambient conditions as well as external interventions. Measuring all these variables in a real building for a long period is cumbersome and thus coupling and simulation tools offer a good way of analyzing this. Initial results show opportunities for achieving significant energy savings while maintaining sufficient thermal comfort to the building occupants.
A Viscoelastic Biomechanical Model for Predicting Maternal Levator Ani Muscle Tears During Vaginal Delivery

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Approximately 15\% of first time mothers suffer pelvic floor muscle tears during vaginal birth. These tears can lead to pelvic organ prolapse and incontinence for which 11\% of US women later undergo surgery. So we are developing a method that should allow physicians to identify women at risk so they can be delivered by alternative means, including C-section, to prevent these tears.

We developed a geometric model of the fit between the fetal head diameter and the mother's birth canal diameter as determined by four morphological parameters (Tracy et al. 2016). We have since refined the model by adding viscoelastic relaxation of the soft tissues forming the birth canal by deriving a constitutive model validated using in vivo human data. The results suggest the mothers with smallest 15\% of birth canals are at risk with an average fetal head size.

The refined model has permitted demonstration of (1) why a vacuum delivery results in lower tear rates than forceps (and suggests how forceps could be modified to reduce injury risk); and (2) the effect of episiotomy incision depth on levator tear risk and length of delivery, two variables of considerable interest to obstetricians. The final step is to compare tear risk with actual outcomes observed using ultrasound in a large clinical trial that has been completed. If validated, the model will be ready for a prospective trial in the labor and delivery room.
Using the Method of Manufactured Solutions for the Verification of a Neutron Transport Code

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The Method of Manufactured Solutions (MMS) is the most rigorous method for verifying scientific computing codes. It has great flexibility and has seen wide applications in many engineering fields. However, limited application has been seen in the field of neutron transport, particularly eigenvalue problems. This is partially due to the high dimensionality of the Boltzmann transport equation governing neutron transport but primarily due to the introduction, propagation and coupling of errors caused by various approximations in the spatial, angular, and energy variables. In this work, the applicability of MMS to numerical methods for neutron transport is investigated and demonstrated for both fixed source and eigenvalue problems. A suite of test problems is devised to serve this purpose. The proposed idea of isolating and removing errors due to certain approximations from the overall error proves effective. Two methods are developed for eigenvalue problems, including the manufactured source method and the manufactured cross section method. The manufactured source method leads to an inhomogeneous eigenvalue problem that admits multiple solutions. Consequently, systematic approaches are taken to ensure convergence to the correct eigenvalue and eigenfunction. The numerical results demonstrate that both the criticality eigenvalue and the corresponding scalar flux show the expected order of accuracy for the $S_N$ method. This MMS methodology has been extended to the method of characteristics (MoC), which is critical to building the credibility and reliability of MPACT, a state of the art MoC-based neutron transport code under joint development by the University of Michigan and Oak Ridge National Laboratory.
Paramagnetically Enhanced Optical Activity of Chiral Nanoparticles

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Chirality is a property unifying both electromagnetic waves and matter that typically manifests in light-matter interactions as the difference in absorption left- and right circularly polarized light, known as circular dichroism (CD). Although the studies of chiral effects associated with the magnetic component of light have long history and date back to M. Faraday, our sense is that the nexus of magnetism and chirality represents an underexplored area of science. Despite importance for fields of multiferroics, skyrmions, spintronics, and homochirality of Earth’s life, magnetooptical effects are generally much weaker than their electrooptical analogs. Although the use of this effects in memory, optoelectronics, information processing devices, and catalysis has much technological appeal, the requirements of temperatures around \( T=5-7 \) K and magnetic fields of \( B = 1.2-7.5T \) complicates their implementation. Difficulties of molecular design of traditional chiral materials capable of combining chiral and magnetic centers or long-distance coupling of magnetic spins also hinders exploring of the effects.

Emergence of the new field of inorganic chiral nanoparticles (NPs) provides new opportunities for materials design of magnetooptics. Magnetic NPs can enhance both local magnetization of the chiral “centers” and their interaction with photons without externally applied magnetic fields. Here we demonstrated highly enhanced optical activity of NPs by synthesizing them using transition metal components. The chiral paramagnetic NPs exhibited \( \sim 10x \) stronger optical activity compared to conventionally synthesized NPs. The tunable strong optical activity of NPs should contribute to chiral catalysis, chromic filters and display devices.
Intrinsic Engineering Properties of Soils through Image Analysis

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The intrinsic properties of soil including particle gradation, sphericity, and roundness control their macroscopic engineering properties such as packing density, limit index porosities, strength, compressibility, hydraulic conductivity, erodibility and others. However, due to difficulties in reliably and expediently determining them, intrinsic properties have not received their deserved attention and usage in practice. This research has facilitated rapid and precise quantification of intrinsic properties using optical-image techniques. Extensive laboratory tests were performed on sands of various gradations, angularities, sphericities and geologic origins to develop relationships between their intrinsic properties and fundamental soil properties. The models have proven to be highly accurate. They can readily be used by engineers and scientists for estimation of soil behavior in construction, geology, soil science and geoenvironmental engineering. More importantly, the models have led to fundamental understanding of soil behavior based on first principles and thus are essential to advances in soil micromechanics.
Abstracts – Afternoon Session
ATE: Automotive and Transportation Engineering
Study of Effects of Thermal Insulation Techniques on a Catalytic Converter for Reducing Cold Start Emissions

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Cold start emissions constitute around 60% to 80% of all the hydrocarbon & CO emissions in present day vehicles. The time taken to achieve the catalyst light-off temperature in a three-way catalytic converter significantly affects the emissions and fuel efficiency. The current work aims at development of a method to retain heat in catalytic converter, thus avoiding the need for light-off and reducing cold start emissions effectively. The study uses an after treatment simulation model coupled with vehicle driveline, which was developed at W.E. Lay auto lab, to study the effect of various insulation techniques on a catalytic converter using real world drive cycle data. The catalyst blocks in the model under study are thermally connected to a chamber filled with phase change material which absorbs heat and are insulated by a layer of vacuum. Although the existing model retains heat for long periods and usually reduces cold start emissions, it fails to reduce the fully cold start emissions due to the thermal mass delaying the catalyst light-off temperature time during a fully cold start. The current work is aimed at avoiding cold start emission performance degradation, and to effectively insulate the thermal masses to increase the catalyst cool down temperature. Various techniques under study involve trapping maximum heat from exhaust gases downstream of catalyst bricks, composite insulation with different materials and geometry optimization of the phase change material around the catalyst bricks to increase the heat absorption rate and storage capacity for very long cool down periods.
Dimethyl Ether – Glycerol Blend: Soot-Free Combustion Fuel with Ultralow Greenhouse Gas Impact

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Due to impending regulations that feature the sharp reduction in pollutants and greenhouse gas (GHG) emission, both governmental and industrial organizations are now in desperate need to secure innovative solution to satisfy the standards. Move from petroleum-based liquid fuel to renewable, clean-burning liquid fuel can be both the feasible and innovative solution. Dimethyl ether (DME) has been considered as a promising diesel oil alternative in compression-ignition engines because of its similar ignition quality to diesel, soot-free engine exhaust emission, and extremely low GHG impact. However, application of neat DME to conventional fuel supply system results in operational problems such as pump leakage and premature injector wear due to its extremely low viscosity and lubricity. This research aims to improve the viscosity and lubricity of DME by blending it with “glycerol”, a highly viscous liquid resulting from biodiesel synthesis process, while securing the main attraction points of DME as diesel alternative. Immiscibility problem between DME and glycerol is resolved by adding glycol co-solvents. Viscosity improvement is achieved up to the level of No.2 diesel oil depending on the type of co-solvent and blending ratio. Engine test is planned to be conducted with DME-Glycerol blend in the near future to ensure extremely alleviated, if any, pump leakage and injector wear problems. Comprehensive engine combustion/emission analysis by using this blend will also follow as the next stage of this research.
Advanced Ignition Systems for Heavy-Duty Natural-Gas Engines

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Natural gas (NG) is a promising alternative fuel for heavy-duty truck engines due to its superior compressibility and clean combustion products. However, igniting NG is challenging, especially when it is lean and diluted by exhaust-gas recirculation, due to the high autoignition temperature and reduced flame-speed. In an experimental program to identify improved ignition systems and implement them into an NG-operated heavy-duty engine, we have extensively surveyed ignition systems in use and under development, and we have identified corona ignition and turbulent-jet ignition (TJI) as the technologies with the highest potential for this application. In conventional igniters, a single ~1-mm spark is generated and heats up the combustible mixture to the autoignition temperature to create a flame kernel that must grow across the chamber. By contrast, corona ignition utilizes multiple ~5-25 mm non-equilibrium plasma streamers to ignite a larger volume, distributing the input energy into the preferred electronic energy levels (rotational and vibrational, rather than translational) within the combustible mixture. TJI uses a pre-chamber in which a rich air/fuel mixture is ignited. High-energy, turbulent flames jet out of nozzles from the pre-chamber into the main chamber and ignite the air/fuel mixture contained therein. Ultra-lean mixtures can be ignited in this way. We are building a dual-axis, infrared borescope/camera setup to study the ignition and resultant flame-kernel growth produced by these ignition systems in a modified production heavy-duty engine. We will characterize the performance of each system using high-speed infrared imaging in order to guide implementation in truck fleets.
Set-Membership Condition Monitoring Framework for Dual Fuel Engines

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Condition monitoring and condition-based maintenance can reduce maintenance costs and improve operation safety of vehicles across the full spectrum of transportation domain, including automotive, rail, air and marine applications. In this paper, a set-membership condition monitoring framework is proposed to detect aging and health degradation for dual fuel engines based on simultaneous input and parameter estimation techniques. Dual fuel engines operate in two modes, a diesel mode or gas mode, and can burn either diesel fuel or natural gas fuel. To improve health parameter identifiability, we exploit transient data from mode transitions between the diesel mode and gas mode. Simulation results based on a nonlinear mean-value model of the engine are reported, demonstrating that the proposed set-membership estimation algorithms can provide tight overbound of the health parameters.
CPH: Chemical Physics
Effect of Densification Conditions on the Electrochemical and Interfacial Stability of 75Li$_2$S-25P$_2$S$_5$ Solid Electrolyte against metallic Lithium

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Solid-state electrolytes have garnered significant attention for their potential to enable solid-state batteries for electric vehicles with metallic Li as an anode. However, the stability between solid-state electrolytes and metallic Li is not well understood. In this work, the effect of densification conditions on the electrochemical and interfacial stability of 75Li$_2$S-25P$_2$S$_5$ (LPS) against metallic lithium was investigated. LPS was densified by compacting at room temperature, and hot pressed between 130-300 °C. The relative density (80% for all samples) was not affected by the hot pressing temperature, which was likely due to insufficient heat to promote densification. The meta-stable crystalline phase (thio-LiSICON III analog) precipitated from the mother glass when hot pressing between 170 - 250 °C and the stable Li$_3$PS$_4$ phase formed when hot pressing at 300 °C. The electrochemical stability was characterized as a function of current density between 0.001 - 1.0 mA·cm$^{-2}$. Two phenomena were observed; first, as the current density increased, deviation from Ohmic behavior was observed, manifested in an increase in polarization voltage. Second, as the current density was further increased, a drop in cell potential was observed followed by a voltage instability; likely consistent with short-circuiting caused by Li metal propagation. The highest maximum tolerable current density resulted when hot pressing at 170 °C, reaching 1.0 mA·cm$^{-2}$. In general, hot pressing LPS glass-ceramic increased electrochemical stability. It is believed that further atomic/microstructure optimization can improve the maximum tolerable current density of LPS.
Light Diffraction Response of Colloidal with Structural Color by Electric Field Assisted Assembly

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This study seeks to build upon existing knowledge of low-voltage direct current (DC) electric field assisted self-assembly to investigate and quantify the light scattering responses of isotropic and anisotropic colloidal particles assemblies. These colloidal crystals can potentially display biomimetic structural color. The light scattering responses – which are optical diffraction patterns – can be related to the structure of the colloidal crystal. In this research, a small-angle light scattering (SALS) experimental setup was designed, built, and tested. The results demonstrated that this new design setup improves the sensitivity of the measured scattering responses and provides a one-to-one mapping between CCD pixel array and the scattering angles with polystyrene colloidal suspensions used as a standardized test. The colloidal crystals are created rapidly (10 min) with spheres that vary in size from as large as 1.4 \( \mu \text{m} \) to as small as 0.3 \( \mu \text{m} \). The light scattering patterns of the DC electric field-assisted spherical colloidal assemblies are presented. Potential methods to improve the quality of light diffraction response are discussed.
The Unraveling of a Polymer Chain in an Entangled Network under Strong Extensional Flow

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The dynamics of entangled polymeric fluids has long been a fascinating topic for scientists and researchers. To achieve a high throughput with low consumption of energy and materials, industry is in need to know and predict the flow behavior of polymeric fluids. Polymer melts of high molecular weight chains form an entangled network through which the physical spatial constraints limit the mobility of polymer molecules. These entanglements play an important role in flow characteristics of molten polymers like stress and dimension evolution. By assuming that in strong extensional flow a polymer molecule is quickly driven into folded or kinked state in which drag and entropic forces dominate over Brownian force, we derive kink dynamics equations that describe the unraveling of the molecule under extension. Although unable to provide the early stage evolution of the chain, the kink dynamics can successfully predict the terminal polymer contribution to stress at final stages of deformation. Our results match pretty well with more detailed but time-consuming simulation techniques like slilinks simulations or modified Brownian dynamics.
Putting Together the Building Blocks of Non-Equilibrium Self-Assembly

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In equilibrium materials, self-assembly is observed as a consequence of entropy. Particle anisotropy, i.e. shape, influences the maximal entropy configuration and thus the final self-assembled structure. In a simple example, spheres in a box will exhibit cubic close packing, while cubes will exhibit simple cubic packing. However, many real-world systems, such as those in biology, are not in equilibrium, raising the intriguing question: what role does particle anisotropy have on the self-assembly behavior of non-equilibrium materials? To answer this question, we use an “active” system, in which particles are driven out of equilibrium by an applied force. In such active systems, isotropic particles have been shown to self-assemble into “living crystals” that dynamically dissolve and reform at steady state. Recent work has additionally shown that particle anisotropy can change the density and applied force at which the onset of living crystals is observed. However, the impact of particle anisotropy on the non-equilibrium self-assembled structure has not yet been explored. Here, we show that non-equilibrium driving forces combined with shape entropy result in shape-dependent self-assembled structures that correlate with those seen in equilibrium systems. Further understanding of this process could allow for access to self-assembled structures not reachable in equilibrium systems.
Highly Selective Catalysts for Bio-oil Upgrading

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The desire to decrease global CO₂ emissions and to continue using liquid transportation fuels has motivated research to produce liquid fuels from biomass. Fast pyrolysis is an attractive method for converting biomass to oil, however, the resulting bio-oil is corrosive, has poor heating value, and is thermally unstable. Upgrading via selective hydrogenation can improve the properties of the bio-oil by increasing its thermostability and energy density. Considering the molecular character of pyrolysis bio-oil, crotonaldehyde was chosen as the model compound for this work as it is a simple aldehyde and can be used to probe a variety of reaction pathways.

Molybdenum carbide (Mo₂C) based catalysts are highly active for reactions of importance in upgrading bio-oils. In addition, Mo₂C based catalysts can be multifunctional (acidic, basic and/or metallic sites) depending on the synthesis and treatment conditions, and are stable under the conditions of fast pyrolysis. Potassium promotion of Mo₂C has been shown to cause dramatic shifts in the selectivity of some hydrogenation reactions, including CO hydrogenation to ethylene at similar extents of conversion. We synthesized a series of Mo₂C catalysts with increasing amounts of potassium loading, and characterized the changes in their acid and base site densities and selectivities for crotonaldehyde hydrogenation. Increasing potassium loading increased the base site density and decreased the acid site density, while also significantly shifting product selectivity. We have statistically linked the changes in selectivity to the increase in the base site density.
Polymer Blends with an Order of Magnitude Higher Thermal Conductivity

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The main bottleneck for heat transfer in bulk polymers is believed to be weak inter-chain bonds. These bonds are typically weak Coulombic or van der Waals interactions. Strengthening these inter-chain bonds have shown to increase thermal conductivity of polymers in recent experiments, however, some other experiments do not show any enhancement or even a reduction in thermal conductivity upon using stronger inter-chain bonds.

In this work we use molecular dynamics simulations to study heat transfer in polymers with various inter-chain bonds to resolve these discrepancies in experimental results. We examine bulk polymer mixtures to find the effect of hydrogen bonding formation (a bonding stronger than vdW) on heat transfer. In addition to hydrogen bonding we investigate many other polymer characteristics on heat transfer including the stiffness of the chains. We find that inter-chain bonding is effective if it can change the morphology of the system.
Heterogeneous Catalysts for the Aldehyde Water Shift Reaction

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The aldehyde-water shift (AWS) reaction is a clean, atom economical method for the preparation of hydrogen and carboxylic acids from aldehydes using H\(_2\)O as the terminal oxidant (see equation 1).

\[
\text{CH}_3\text{CHO} + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{COOH} + \text{H}_2 \quad (1)
\]

The development of AWS catalysts has been focused primarily on homogeneous catalysts [1]. To our knowledge, this reaction has not been reported for a heterogeneous catalyst system. The research described in this paper explores the use of heterogeneous catalysts including Mo\(_2\)C, Mo\(_2\)N, CeO\(_2\), and Al\(_2\)O\(_3\) supported metal (Au, Pt, Cu) catalysts for the AWS reaction, drawing inspiration from materials active for the analogous water-gas shift (WGS) reaction [2].

The support-type was found to have a significant impact on the activities and selectivities. Among all the catalysts tested, the Mo\(_2\)C supported materials possessed the highest activities; they were typically an order of magnitude higher than other materials. The Pt/CeO\(_2\) catalyst had the highest rate among the CeO\(_2\) supported materials. While no H\(_2\) was detected for the Al\(_2\)O\(_3\) support, the Cu/Al\(_2\)O\(_3\) and Pt/Al\(_2\)O\(_3\) catalysts produced small amounts. The Mo\(_2\)C and Mo\(_2\)N catalyst were 60% selective toward acetic acid (AWS reaction); this selectivity increased with the addition of Au, Cu, or Pt to the Mo\(_2\)C support. The Al\(_2\)O\(_3\) based materials primarily produced crotonaldehyde via aldol condensation. The research described in the paper will provide further insights regarding heterogeneous catalysts for mild oxidations with H\(_2\)O.

References:
EBS: Engineering in Biological Systems
Biomaterial Scaffolds for the Detection, Treatment and Study of Cancer Metastasis

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In most types of cancer, the formation of distant metastasis is the point at which the disease becomes lethal. At present, there is no clinical method to detect metastatic dissemination and colonization of distal sites until radiologically evident, at which point the function of the organ has often already been compromised. The Shea lab has developed a biomaterial implant that recruits metastatic cancer cells in xenogeneic human and syngeneic mouse models of breast cancer. Scaffold implantation has facilitated detection of metastasis prior to colonization of organs and has been shown to reduce metastatic disease burden, ultimately resulting in enhanced survival with surgical intervention. We performed a resection experiment at day 6 and day 10-post tumor inoculation to investigate if the observed tumor burden reduction could translate into a survival benefit. With resection at day 6 we were unable to discern a difference in animal survival. Subsets of both the mock and scaffold groups survived indefinitely without succumbing to metastasis (~40% survival). For day 10 resection 40% survival was observed for mice that received a scaffold but no mice receiving a mock surgery survived indefinitely. This indicates that the scaffold increases the time over which a therapeutic intervention, such as surgical resection, can be performed and provide a survival benefit. Biomaterial scaffolds capable of recruiting metastatic tumor cells in vivo represent a transformative approach that can not only to serve as a platform for early detection and intervention, but also serves as a defined site in vivo to study metastasis.
Age and Stress-Induced Venous System Changes in Murine Models

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Venous diseases represent a significant problem worldwide, with venous thromboembolism (VTE) affecting an estimated 900,000 people in the US each year.¹ Animal models provide a critical tool for investigating disease treatment and prophylaxis due to limitations in the human pathogenesis timescale and the inability to take a biopsy of a human thrombus. Quantifying age-related changes in the venous system is crucial, as VTE incidence increases dramatically over the age of 60 in both men and women², and impaired thrombus resolution has been observed in aged murine models of venous thrombosis.³ The purpose of this work was to quantify how the murine venous system changes with age, providing a foundation for understanding the aged cardiovascular system as well as age-dependent differences in male and female models of VTE.
Deformable Particles for Vascular-Targeted Drug Delivery: Softer is Not Always Better

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Vascular-targeted drug carriers (VTCs) are designed to preferentially localize to the site of disease, thereby decreasing systemic side effects while simultaneously increasing therapeutic delivery to the disease site. This is achieved by harnessing disease protein expression patterns; as the expression of certain surface proteins increase in disease states, corresponding targeting ligands with a high affinity for those proteins can be attached to the VTCs. The ability of VTCs to localize and bind to a targeted, diseased endothelium determines their overall clinical efficacy. Size and shape are known physical parameters that prescribe VTC vascular wall localization and adhesion. Here, we present the first investigation into the role of particle deformability in adhesion of VTCs to the vascular wall under realistic physiological blood flow conditions. At low shear, deformable particles show favorable adhesion, while at high shear, rigid particles show superior adhesion. Mechanistically, particle collisions with leukocytes drive these trends. For both VTC sizes examined, more deformable particles adhere better than rigid counterparts to inflamed endothelium in vivo in mouse mesentery vessels with low shear blood flow. Overall, this work demonstrates the importance of VTC modulus as a design parameter for enhanced VTC interaction with vascular walls, and thus, contributes important knowledge for development of successful clinical theranostics with applications for many diseases.
Application of Elevated Pressures in Culturing Hydrogen-Oxidizing Bacteria

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The use of atmospheric pressure as a parameter to manipulate the growth and production of cell cultures has recently begun to be thoroughly investigated. The variability of effects on different cell types and species indicates that there is much more to learn about the use of elevated pressures (up to 10 bar) within bioreactors and how to best utilize this asset. When elevated pressures are applied to aerobic bacterial cultures, increases in metabolic activity are witnessed as the result of increased dissolved oxygen concentrations. Additionally, excess carbon and energy supplies are created within the cell which result in phenomena of biotechnological interest. In this study we are examining the effects of elevated atmospheric pressures on hydrogen-oxidizing bacteria, with particular focus on the bacterium, Cupriavidus necator.
A Molecular Dynamic Study to the Chiral Graphene Quantum Dots

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Similar to metals and semiconductors in nanotechnology, graphene-based materials enrich physical and chemical phenomena associated with optical properties of chiral nanostructures and facilitate their applications in biology. Here, we used molecular dynamic (MD) simulation to study the biocompatibility of chiral graphene quantum dots (GQDs) to the cellular membrane. We determined the equilibrium geometries of chiral GQDs. We revealed the dynamics of a GQD entering the cellular membrane, and found a barrier at the center of membrane preventing GQDs entering cells. In addition, in vitro evaluation of GQDs with liver cells demonstrated their low cytotoxicity and differentiation of cytotoxicity between GQD stereoisomers. Our simulations showed that membrane was selective to the chiral groups on the GQDs. This result implied that cellular membranes were likely to play the central role in the chiral differentiation.
Exposing the Injection Machinery Dynamics of T-even Bacteriophages through Multi-Scale Modeling

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T-even bacteriophages (T2, T4, T6) are one of the most common and complex tailed viruses, from family \textit{Myoviridae}, which infect the \textit{E.coli} bacterium using an intriguing nanoscale injection machine including an elastic contractile tail sheath which powers the injection process. The sheath is composed of helical strands of protein that attaches to a large multi-protein capsid by neck at one end and connects to a baseplate at the other end. During the injection, the sheath simultaneously rotates about and translate along the tail assembly axis and creates a suddenly collapse from an energetic, extended conformation prior to infection to a relaxed, contracted conformation. This coupled translation and rotation of injection machinery creates a combination of thrust force and torque that pierces the host membrane. Finally, the genomic DNA is transferred from capsid into the host cell.

Despite extensive progress in resolving the structure of T-even phages, the dynamics of the genome-delivery machine remains largely unknown, including the process time scale and energetics. In this study, a multi-scale dynamic model is developed to approximate the three-dimensional nonlinear dynamics of the injection machinery. In proposed model, the sheath strands are represented by interacting helical rods that are coupled to the capsid represented by a massive cylinder. Simulation process is exemplified by phage T4 injection machinery. Dynamic simulations reveal the time scale, the pathway of sheath contraction, and the energetics driving the injection process. The resulting model and methodology may inform the future design of nanotechnology injection devices.
Neuronal Network Robustness: Where to Look for Synaptic Deficiencies in the Brain

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Synaptic deficiencies are known to be a hallmark of neurodegenerative diseases but the diagnosis of impaired synapses on the cellular level is not an easy task. Nonetheless, the changes in the dynamics of neuronal networks with damaged synapses can be detected using smaller resolution. This work investigates how the structure of neuronal networks influences their dynamics when they suffer from synaptic loss. We construct different neuronal network structures by specifying their degree distribution. Networks with bimodal degree distribution resemble small world networks and consist of rich clubs as well. We define two dynamical metrics to compare activity of networks with different structures: persistent activity as the self-sustained activity of the network upon removal of the initial stimulus and quality of activity as the percentage of neurons which participate in the persistent activity. Our results show synaptic loss affects the persistent activity of networks with bimodal degree distributions less than random networks. The robustness of neuronal networks enhances when the distance between the modes of the degree distribution increases since the highly connected cores of networks with distinct modes keep the whole network active. However, our results show a tradeoff between the quality of activity and the persistent activity of networks. We propose different selection methods to impair synapses in the network, which may correspond to different pathological conditions. Regardless of the network structures, the results demonstrate that synaptic loss has more severe effects on the activity of the network if the impairments are correlated with the activity of the neurons.
Breast Cancer Cells Acquire Chemoresistant, Metastatic and Invasive Phenotypes when Exposed to Pulsatile Fluid Shear Stress in a Novel 3D Bioreactor Platform

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Cancer cells experience a range of shear stresses in the tumor microenvironment and in vitro 3D models fail to include dynamic physiological effects. To address this, we developed a 3D bioreactor that applies pulsatile shear stress, for 24 or 72 hours, to MCF7 breast cancer cells suspended in agarose-collagen hydrogels. Finite element modeling was used to determine that hydrogels and cells within experienced a homogeneous shear profile within the bioreactor. The effect of shear was characterized with immunohistochemistry for Phalloidin (cell shape), Ki67 (proliferation) and, Cox-2 (mechanotransduction). Gene expression changes under shear were monitored using qPCR arrays. The effects of the mechanotransduction were inhibited using Celecoxib, and resistance to chemotherapy under shear was investigated with the drug, paclitaxel.

Cells exposed to shear had significantly higher aspect ratios (1.3±0.01 to 1.4±0.02) compared to unstimulated control cells (1.1±0.09), indicating a motile phenotype with shear stress. Gene expression analysis of sheared cells demonstrated >2-fold changes in several genes modulating invasiveness, tumorigenicity, and chemoresistance (SERPINE1, PTGS2, TP53, BLC2, ABCG2). Celecoxib inhibited the effect of shear and subsequent mechanotransduction on cells, demonstrated by a lack in change of cell shape factors under shear conditions compared to unstimulated control cells. Lastly, shear exposed MCF7 cells were more resistant to paclitaxel (~80% viable), compared to unstimulated static cells (55% viable), indicating a chemoresistant phenotype. Our data indicate that these shear forces promote cancer cell metastasis, invasion, and chemoresistance in MCF7 breast cancer cells. This work is supported by the DOD OCRP Early Career Investigator Award W81XWH-13-1-0134 (GM).
Mitigating RF Peak Amplitude and Power Limitations for Simultaneous Multislice Excitation MRI

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Simultaneous multislice (SMS) excitation for magnetic resonance imaging (MRI) has recently gained recognition as an effective means of accelerating imaging, especially after the incorporation of parallel imaging techniques using multiple receive coils. By acquiring multiple slices at once, MR imaging applications that have particularly demanding time resolution demands such as functional MRI (fMRI), diffusion imaging, and cardiac imaging have made significant advances and wider integration into clinical practice. Even still, SMS RF pulses have flip angle and multiband factor (number of simultaneous slices) limitations for each given application that are usually dictated by either the RF pulse peak amplitude limit or power deposition, which both roughly scale linearly with multiband factor [1]. Many methods have been proposed to address the RF limitations of SMS excitation, but usually only RF power or peak amplitude are addressed individually with the provided solution. In this abstract, we propose the design of SMS RF pulses with direct constraints on integrated RF power and peak amplitude. We solve the RF pulse design iteratively for a single transmit RF pulse following the small tip angle approximation [2] using a least-squares optimization. The advantage of this dual-constraint design method is that it is universal and adaptable for RF design parameters such as flip angle (up to 90°) and multiband factor. We demonstrate this pulse design with an example of an SMS pulse for a fMRI resting state scan that is a part of a standard practice protocol for the Human Connectome Project [3].

References:
Immune cell trafficking to biomaterial implants that model the cancer pre-metastatic niche

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The progression of cancer to metastasis usually results in patient death. It has been shown that specific immune cell populations can promote metastasis to other organs, most notably in the formation of a pro-tumor microenvironment termed the pre-metastatic niche. The Shea lab has developed an implantable polymer scaffold that serves as an artificial pre-metastatic niche. The scaffold has been shown to recruit specific immune cells as well as metastatic tumor cells in both syngeneic and xenogeneic mouse cancer models, thus recapitulating a localized metastatic site. Immune cell trafficking dynamics to the artificial pre-metastatic niche have been probed in mice by using adoptive transfer of fluorescently labeled immune cells. In the presence of a primary tumor, CD11b+ Gr1-hi Ly6C- cells increase dramatically in the scaffold, suggesting they are important in the formation of the pre-metastatic niche. Further understanding the trafficking of immune cells and tumor cells systemically and locally at the niche can lead to the identification of key targetable interactions that are necessary for metastasis to occur.
FAT: Fluid Dynamics, Acoustics, and Thermal Science
Imaging of Temperature Variations in the Near-wall Region of an Internal Combustion Engine

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Predicting heat transfer processes within internal combustion (IC) engines is important for engine development and design due to their impact on performance, efficiency and emissions. This requires an understanding of the behavior of thermal boundary layers that develop near the combustion chamber walls. However, boundary layer flows in IC engines are transient in nature, and are not fundamentally understood. Recently developed laser-based imaging techniques have shown the capability of providing instantaneous flow visualization in combustion systems, and are now used extensively to substantially resolve the flow inside IC engines. This work aims to characterize the thermal boundary layer in an optical IC engine using the technique of laser-induced fluorescence (LIF). It presents two-dimensional relative temperature fields of the near-wall region collected at low-speed rate from a motored engine test at 500 rpm. These planar LIF images were taken early and late in the compression stroke at 250° and 350° crank angle, respectively, in two different tests, and then calibrated to the polytropic temperature calculated from the in-cylinder pressure trace. Results show increasing thermal stratification towards the end of compression as temperature modulation increases and spatial scales of temperature variations decrease. Transition to high-speed high-resolution planar LIF thermometry is being prepared to investigate the evolution of thermal inhomogeneity near the walls. Future work includes performing simultaneous heat transfer measurements in addition to exploring different imaging techniques to obtain measurements of absolute temperature.
A Study to Investigate Pyrolysis of Wood Particles of Various Shapes and Sizes

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Pyrolysis of wood particles with various shapes and sizes was studied. Two classes of shapes known as Prolate and Oblate ellipsoids of revolution were chosen to be representative of particle geometry for computation. Model simulation showed satisfactory agreement with literature and experimental data. Mass loss and center temperatures were presented and compared with different cases. Particle aspect ratio, equivalent radius, surface/volume ratio were chosen to represent particle geometric information. A power correlation function between conversion time and surface/volume ratio was found and verified by experiment. Particle aspect ratio was found to affect pyrolysis conversion time by changing heat transfer rate. Yields of char and tar are affected by volume/surface ratio while the gas product is not significantly affected. The effect of shape on pyrolysis yield is ignorable when particle size is small but becomes significant when particle size becomes large.
Remote acoustic sensing of mechanical changes in a plate in an unknown reverberant environment

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An experimental method for remote acoustic sensing of changes in radiating structures in an unknown reverberant environment is presented. Acoustic radiation from a mechanical structure due to oscillatory forcing may be described by a frequency response function (FRF) dependent on the structure’s material, geometry, and boundary conditions. Mechanical changes may alter the structure’s FRF in detectible and potentially predictable ways. However, collecting suitable FRF measurements may be difficult in reverberant environments over the necessary extended measurement times due to the importance of reflected and scattered sound. Here, experimental results are presented for the remote acoustic detection of mechanical changes to a vibrating 0.3-m-square by 3-mm-thick aluminum plate in a reverberant environment. The plate has nominally clamped edges and is subject to swept-frequency base excitation. Sound from the plate with and without a mechanical change is recorded remotely with a 15 microphone linear array. These recordings are then processed using Synthetic Time Reversal to reconstruct a single radiated sound signal that is corrected for the environment’s unknown reverberation, and this corrected signal is examined to detect mechanical changes to the test plate. Results from the proposed technique are compared with equivalent results from conventional approaches. [Sponsored by NAVSEA through the NEEC]
Nanofabricated thermal probes for studying thermal transport in one-dimensional systems

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With the advent of nanotechnology, researchers have encountered a number of thermal phenomena that cannot be explained by classical heat transfer theory. Two outstanding challenges in the field of nanoscale thermal transport are to achieve high thermal conductive materials for mitigating electronic device heating and to realize low thermal conductivity for thermoelectric materials. Addressing these challenges require a deep understanding of nanoscale thermal transport. Many researchers have investigated to reveal thermal transport phenomena in 2- and 3-dimensional (D) materials. However, probing thermal transport in 1-D materials remains elusive due to experimental challenges. For example, no experimental research has been performed to investigate the possibility of thermal conductance quantization at room temperature. This is in stark contrast to the extensive explorations of electrical conductance quantization. To elucidate 1-D thermal transport phenomena, it is necessary to develop novel scanning probes that can resolve heat currents with very high sensitivity and resolution. This poster illustrates the design and fabrication of a novel thermal probe and its thermal performance. Specifically, the noise floor and sensitivity of this probe are found to be 100 pW/√Hz and 400 μV/K. In addition, the stiffness of the probe cantilever is 100N/m by incorporating a T-shaped beam. This novel thermal probe is expected to reveal many interesting nanoscale thermal transport phenomena through 1-D systems, such as single organic molecular or atomic junctions.
Singular value decomposition for rapid simulation of a hypersonic vehicle

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A reduced order model method based on singular value decomposition and correlation is developed to capture the nonlinear flight behavior of a hypersonic vehicle. A set of state space training samples are collected using the complex-step method and used to identify a set of ordered bases which describe the variation of the state matrices. Surrogate functions are used to relate these bases to the states and may be used to estimate state matrices beyond the training set. The dynamics of a hypersonic vehicle may then be rapidly simulated while preserving most behaviors of the full nonlinear system. The speed, efficiency, and accuracy of this method are compared against the University of Michigan High-Speed Vehicle code and classically linearized state space representations of the same hypersonic vehicle.
Separation control of flow over a backward-facing ramp

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Wall bounded turbulent flows [Frisch, 1995] occur in wide range of engineering [Hinze, 1959], [Richardson, 1922], [Wimmer-Schweingruber, 2003]. In such flows, the onset of instability inside the boundary layer generally results in flow separation and subsequent deviation of flow behavior. Such separated flows are generally known to have adverse effect on flow that is characterized by increased drag for example, on airfoil of wing of wind turbine blades and wings of aircraft, thereby reducing its aerodynamic efficiency. Moreover, the highly nonlinear behavior of flow makes the complete understanding of flow physics rather more difficult. Experimental investigations on large scale are expensive and need time and sophisticated setups. Due to large losses of energy associated with boundary layer separation in many applications it is important to be able to control the boundary layer separation. The fundamental idea behind separation control is to energize the boundary layer by entraining momentum from the free stream to the near wall region by increasing turbulent mixing. The solid obstacles placed inside the boundary layer are referred to as vortex generators (VGs) [Lin et al., 1989]. The motivation of the present study is to use a high-fidelity wall resolved Large Eddy Simulation (LES) approach to control flow separation of a spatially evolving turbulent boundary layer. The geometry of choice in this study is a 25° backward-facing ramp, which is observed in many applications like an expansion nozzle, the rear end of an automobile. A wall resolved LES will help us capture the detailed time-dependent flow features which will in turn help us to control separation.
Enhanced radiative heat transfer in the far-field

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For over a hundred years, Planck’s law has been the de facto framework for understanding thermal radiation. Starting from Planck’s fundamental equation describing the spectral emissive power from an ideal blackbody, one can derive the maximum radiative heat transfer (RHT) between bodies. However, this derivation of the RHT relies on two main assumptions: 1) The distance between bodies, and 2) the size of the bodies are much larger than the thermal wavelengths of the exchanged radiation. A natural question then arises: how can we understand RHT between bodies when Planck’s second assumption is violated, i.e. when the bodies themselves are very small? To date, there has been a complete lack of theoretical and experimental studies examining this size effect. Here, I present the results of an experimental study, enabled by picowatt-resolution resistance thermometry-based calorimetry, that quantitatively probes the radiative heat transfer between adjacent micron-sized structures separated by a 20 μm vacuum gap. Orders of magnitude enhancements in the RHT over the predictions of Planck’s law were measured at room temperature when a critical dimension of the structures was reduced to ~100 nm. These experimental results are supported by computational modelling based on the framework of fluctuational electrodynamics, which relates this super-Planckian RHT to an enhanced absorption cross-section of the structures. These new experimental and computational observations have important ramifications for energy conversion and thermal management technologies.
IOF: Industrial, Operations, and Financial Engineering
Multi-job Production Systems

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Multi-job production (MJP) is a class of flexible manufacturing systems intended to produce different products (job-types) according to a given product-mix and build-schedule. In MJP systems, all job-types are processed by the same sequence of manufacturing operations, but with different processing times at some or all machines. To characterize MJP, we introduce the work-based (rather than the traditional part-based) model of production systems, which is “insensitive” to whether a single- or multi-job manufacturing takes place. Using this model, we develop a method for performance analysis of MJP serial lines with the emphasis on their throughput and bottlenecks as functions of the product-mix. We show, in particular, that for the so-called conflicting job-types, there exists a range of product-mixes, where the throughput of MJP is larger than that of any individual job-type involved. To characterize the global behavior of MJP systems, we introduce the notion of Product-Mix Performance Portrait, which represents the system throughput and bottlenecks for all feasible product-mixes. Finally, we apply the results obtained to a section of the underbody assembly system at an automotive assembly plant, calculate its performance portrait, and evaluate the efficacy of potential continuous improvement projects.
Incorporating Downstream Disruptions in Robust Planning and Recovery

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When disruptions occur in the network, airlines have to make recovery decisions to recover and minimize future cancellations, delays, passenger missed connections etc... These decisions are often made solely based on the current state of the system. We develop a simulation tool to evaluate different recovery strategies that takes into account correlation and propagation of delays to mitigate future disruptions.
The inspection of deteriorating water distribution pipes is an important process for utilities. It helps them gain a better understanding on the state of the system and aids decision making regarding replacement and rehabilitation operations. Due to physical and regulatory constraints, utilities can only inspect a small fraction (~2% typically) of the system annually. There exists a need for an optimization process that enumerates candidate paths that both capture pipes that are at high risk of failure and accounts for the physical limitations of inspection tools. Such limitations include, reducing the number of feature changes along the path (material, diameter etc.) to avoid numerous recalibrations, as well as avoiding any branching or looping structures. This paper examines the use of various optimization algorithms (Genetic Algorithm, Simulated Annealing, Greedy Search) in identifying inspection paths that will maximize the highest risk pipes being included while reducing the number of pipe feature changes along the path. A scoring system was developed to compare various candidates and the optimization algorithms were applied to an example grid network as well as a virtual water distribution system. Both case studies demonstrated that genetic algorithms were most effective in identifying inspection paths satisfying the goals of capturing high-risk pipes.
Optimal Return-to-Play from Concussion

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In the United States up to 3.8 million sports-related concussions are estimated to occur each year. A key component of the concussion management protocol is the return-to-play (RTP) decision. Premature RTP can lead to increased risks for secondary injury, post-concussion syndrome, and second impact syndrome. Late RTP can lead to financial or opportunity losses for the athlete. We consider the RTP decision and model the sequential decision-making problem as a finite-horizon MDP. We present structural properties for each model and present preliminary computational results, highlighting the differences between a potential physician’s and athlete’s optimal policy.
Effect of Secondary Task Modality and Road Curvature on the Safety of Horizontal Curve Driving

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Driving on horizontal curves requires more research attention since it causes more accidents than on straight roads. Several studies have found that horizontal road curvature and secondary task’s sensory modality are two of the major factors which affect driving performance and safety on horizontal curves. However, the studies have been limited: less diverse types of modality and road curvature. This article reports a driving simulation study that was conducted to investigate the impact of both secondary task’s modality and road curvature on the safety of driving on horizontal curves. Eye movements, lane keeping performance, and subjective workload were measured from 24 participants. The results showed that drivers performing a visual-manual type of secondary task fixated on the road less frequently and shorter compared to other modalities. Also, when driving on the sharper curve, drivers looked at the road more frequently and longer. Meanwhile, driving on sharper curves caused more unstable lane keeping performance (i.e., more standard deviation of lane position and standard deviation of steering wheel angle). Participants reported higher visual demand when preforming visual-verbal type of task compared to auditory-manual type of task. In general, no significant interaction between modality and road curvature was found. The practical implications for driving safety on horizontal curves were discussed.
Scheduling Medical Requests with Conflicting Personal Requests

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In scheduling medical residents, the objective is often to maximize resident satisfaction across the space of feasible schedules, relative to the many hard constraints that ensure appropriate patient coverage, adequate training opportunities, etc. A common metric of resident satisfaction is the number of time-off requests that are granted. Simply maximizing this total, however, may lead to undesirable schedules since some requests have higher priority than others. For example, it might be better to grant one resident’s request for a family member’s wedding in place of two residents’ requests to attend a football game. Another approach is to assign a weight to each request and maximize the weighted sum of granted requests, but determining weights that accurately represent residents’ and schedulers’ preferences can be quite challenging. We propose to instead identify the exhaustive collection of maximally-feasible and minimally-infeasible sets of requests which can then be used by schedulers to select their preferred solution. Specifically, we have developed two algorithms, which we call Sequential Request Selection Via Cuts (Sequential RSVC) and Simultaneous Request Selection Via Cuts (Simultaneous RSVC), to identify these sets by solving two sequences of optimization problems. We present these algorithms along with computational results based on a real-world problem of scheduling residents at the University of Michigan C.S. Mott Pediatric Emergency Department. Although we focus on the problem of resident scheduling, our approach is applicable to a broad class of scheduling problems with soft constraints.
Improving Patient Flow in an Outpatient Cancer Center

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Patient visits in an outpatient cancer center are often a long, multi-step process. Patients may go through a combination of getting blood work done in the lab, visiting their physician in the clinic, and having the pharmacy prepare their drugs all before receiving their treatment. This process often results in complicated system flow, increased potential for delays, and longer wait times for the patients. Collaborating with nurses and physicians in the clinical environment, we use data collection and analysis, simulation, and optimization techniques to develop ways to improve the patient experience and reduce delays in this complex series of activities.
Title Improving Make-ahead Chemotherapy Drug Policies in the Outpatient Infusion Center Pharmacy

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In collaboration with the University of Michigan Comprehensive Cancer Center (UMCCC), we have developed an optimization-based approach to improve make-ahead policies for chemotherapy drugs in order to help reduce overall patient waiting time.

A typical patient visit consists of getting blood work done, seeing their physician, having the pharmacy prepare their chemotherapy drug, and receiving their infusion. At every step during their visit (blood draw, clinic, pharmacy, infusion), variability can lead to patient delays and overworked staff. One major opportunity to reduce patient delays is optimizing drug preparation at the pharmacy. Drugs can be prepared ahead of time to reduce patient delays, but the majority are not mixed in advance for fear that these costly drugs may be wasted. If the drug cost is low enough, and/or the probability of treatment being deferred is small enough, then the expected cost of wasting the drug may be outweighed by the combined benefits of decreasing nurse overtime and reducing patient wait times. The current deterministic optimization model prioritizes how many and which drugs to pre-mix. Given a finite amount of time for pre-mix, we considered how best to use that time by maximizing the difference between expected saved wait time and expected waste cost- a variation of the classic knapsack problem formulation. We then present a GUI the pharmacist can use to utilize our optimization model. This approach will help reduce patient waiting times at the UMCCC and other Cancer Centers.
An Integrated Facility Location and Network Restoration Model Under Repair Time Uncertainty

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We propose a two-stage stochastic programming model for an integrated facility location and network restoration problem in a disaster-prone region where facility location decisions should be made in the pre-disaster stage. We capture uncertainty in the network availability by incorporating the repair times required to restore the damaged arcs. In contrast to other models that ignore repair times, our model locates some facilities in remote, low-demand areas that are unreachable for a certain number of periods following a disaster.
Simulation-Based Framework for Colonoscopy Scheduling

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Scheduling colonoscopy procedures in an endoscopy clinic involves the coordination of several activities related to the intake, procedure, and recovery processes. Due primarily to pre-procedure bowel preparation and patient absenteeism, the system operates with a great degree of uncertainty. Additionally, multiple criteria must be balanced when considering how to schedule colonoscopy procedures (e.g., patient wait time vs. provider overtime vs. procedure quality). Uncertainty combined with the need to trade off many criteria makes colonoscopy scheduling a complex task. We developed a simulation-based framework for designing and evaluating sequencing and scheduling schemes, recognizing both absenteeism and the significant variability in procedure duration.
Twofold Error Propagation Modeling and Analysis for Roll-to-Roll Manufacturing Systems

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Roll-to-Roll (R2R) manufacturing systems with high-volume and high-speed production capability require reliable system performance and precise quality control. Due to the growth of new technological development of R2R processes in various applications, increasing challenges are faced by manufacturers in product quality control and improvement that induced by complex interactions among sequential operations and product quality variations. These challenges have led to the need to develop methodologies for R2R system modeling, diagnosis, quality control and process design optimization. This paper aims to understand the quality variation propagation in R2R processes. A multistage modeling technique is developed to model the twofold error propagation – product-centric error propagation and process-centric error propagation, and its relationship with product quality evolution. The modeling employs both physics-based analysis (torque equilibrium and Hooke’s law for tension propagation) and regression models (censored regression and logistic regression) using multi-sensor signals. The estimation results from the model can serve as a virtual sensing and virtual metrology tool to increase the system visibility and be applied for process monitoring and quality control.
Evaluating and Improving Access to Specialty Care in Endocrinology

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Recurrent patient visits add tremendous complexity to modeling capacity utilization for healthcare professionals. To assist an endocrinology clinic at the University of Michigan, we present a temporal database that takes prospective patient appointment and provider ability data and enables capacity analysis through a compilation of daily snapshots. Using this database, we investigate the clinic's issues regarding access and adherence to the program's highly structured timeline.
Contextual Markov Decision Processes for Robust Dynamic Programming

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Markov decision process (MDP) models are commonly used for optimization of sequential decision-making in uncertain environments. However, the model parameters in MDPs are often subject to variation and the optimal policy may not be robust to these variations. We propose a new Contextual MDP (CMDP) framework for finding policies that are robust to uncertainty in the model parameters. We do so by encoding possible realizations of the uncertainty into the contexts of the CMDP. We will discuss exact and approximate algorithms for finding policies that are robust to this uncertainty. We will analyze the runtime and performance bounds of our algorithms and compare these algorithms to the nominal and robust (maximin) solutions. We will illustrate these findings with a case study of patients with type 2 diabetes using a CMDP that accounts for ambiguity in risk models proposed in the literature. Our results show how our CMDP framework can produce robust policies for optimal control of cholesterol and blood pressure for prevention of myocardial infarction and stroke.
Multicriteria Optimization for Brachytherapy Treatment Planning

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High Dose Rate Brachytherapy (HDR-BT) has become a popular mode of radiation therapy for its ability to deliver high dose localized to the tumor, resulting in lower risk of side effects. The goal is to allow the physician to explore trade-offs via an intuitive GUI with respect to multiple dose-volume criteria (also known as value-at-risk) among high quality plans. The underlying problem is non-convex and therefore is not practically solvable. The desire to generate plans quickly, i.e., within the 30 minutes while the patient is under anesthesia, motivates solving convex approximations (based on conditional value-at-risk) instead. Our method is retrospectively tested on various cancer sites.
A Systematic Analysis of Procedures, Cleanability & Manufacturer Cleaning Instructions of Surgical Instrument Processing

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CHEPS Surgical Instruments team has been working with the University of Michigan Health System to address effectiveness & productivity challenges in surgical instruments reprocessing. To ensure the quality of instrument reprocessing, the team has analyzed the current procedures and manufacturer Instructions for Use (IFUs) guidelines. To properly allocate limited resources, the team has focused on developing the instrument ‘Cleanability Index’ (CI) tool with time & difficulty data for individual instruments & sets. With the results from both analysis & CI tool, the team recommended the hospital to establish a standardized reprocessing procedure guideline and adjust staffing & equipment accordingly.
IVM: Integrated Circuits, VLSI and Microsystems
Low-Noise MEMS Gyroscope System for Navigation

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The goal of this project is to develop a MEMS gyroscope system with high precision and high rotational sensitivity. Applications for this system include GPS-free navigation, active vehicle safety systems, robotics, and autonomous vehicles. Our gyroscope, named the birdbath resonator gyroscope (µ-BRG), is made with fused silica using a micro-blowtorching process and has n=2 wineglass modes at approximately 10kHz. The quality factor of the µ-BRG in 1mTorr vacuum is approximately 480,000, which results in a reduced Brownian noise floor, and the potential for use as a navigation sensor. However, in order to achieve navigation-grade performance we must develop low-noise interface electronics for sensing sub-micron rim displacements of the vibrating µ-BRG. A control system is also needed to improve stability and robustness to fabrication mismatch, structural asymmetry, and changes in environmental factors such as temperature and pressure. Our readout and control system is implemented using a combination of custom integrated circuits, FPGA, and software. The system achieves a scale factor on the order of 10-20 mV/deg/s, an angle random walk (ARW) of 0.55 deg/hr/rt(Hz), and a bias instability of 0.1 deg/hr.
Phase Change Optical Shutter

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Optical shutters and modulators are needed in variety of reconfigurable optical components such as wave front shaping, couplers, fiber optics, spectroscopy, atomic clocks, etc. [1]. This reconfigurability could either come from the change in the structure as in mechanical modulators or the optical indices as is the case in electro-optical modulators. Mechanical modulators offer high modulation index but are slow, bulky, non-reliable, and consume high power. Electro-optical modulators have a smaller index but are fast and more reliable [2]. State of the art of electro-optical modulators use index changing materials such as liquid crystals [3], Germanium (Antimony) Telluride [4], Vanadium Dioxide [5], etc. with two significantly different refractive index values at two different phases to achieve amplitude modulation. We report on a high-contrast optical modulator with amplitude modulation index of 27 dB and forward loss of < 3 dB at 1.5 μm. The high contrast is achieved by utilizing slit and surface plasmon resonances (SPP) in an array of gold lines filled with a phase change material (Germanium Telluride-GeTe). Stacking multiple layers of gold arrays with 450 nm period enabled development of the high-index modulator in chip scale dimensions. Coupling the SPP of multiple layers results in such a high contrast when GeTe goes through crystallographic phase transition. Both phases of GeTe are stable at room temperature, unlike Vanadium Dioxide, resulting in zero static power. The phase change phenomenon in GeTe can be achieved optically or through Joule heating and is proven to be reliable, fast, and repeatable.

References:
Low-power Readout for Resonant IR Sensors

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IR sensors are crucial elements in vision systems, especially IR cameras. The IR sensors would enable sensing human objects both in day and night as well as in unclear environments. In this work, we have built the fundamental theoretical modeling, and fabricated Aluminum Nitride (AlN) based micromechanical resonators as un-cooled thermal IR detector arrays, integrated with CMOS readout circuitry, in collaboration with InvenSense Company. Our purpose in this project is to develop IR sensors with lower power consumption and reduced size. The challenge with AlN-based resonant IR detector specifically and with monolithically integrated readout circuit in general is low-power consumption, achieving a promising IR detection sensitivity, controlling the ambient temperature and fast conversion of input frequency to output voltage. Such challenges are mitigated in the work through developing new readout electronics and designing uncooled resonators. AlN-based IR sensors (resonators), with high quality factor, $Q$, and high temperature coefficient of frequency, TCF, were designed and fabricated, instead of the conventional bolometer based IR sensors. Each sensor pixel is covered with an IR absorber layer (SiN in this case) and its temperature changes due to the IR absorption. Then resonance frequency of each sensor pixel (resonator) shifts due to IR absorption and the temperature change caused by that. The absorbed IR intensity on each sensor pixel can be determined by extracting the shift in the resonance frequency ($\Delta f_{\text{res}}$). In this project the ring-down based readout method is used to extract the frequency shift because of its low power consumption and high speed.
130 Second Ring-Down Time and 3.98 Million Quality Factor in 10 kHz Fused Silica Micro Birdbath Shell Resonator

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We achieved a 130.0 second ring-down time constant for the 9.736 kHz \( n = 2 \) wine glass mode of a birdbath shell microresonator, corresponding to a quality factor of 3.98 million. The resonator is a fused silica shell with an outer radius of 2.5 mm, anchor radius of 0.5 mm, height of \( \sim 2.1 \) mm, and thickness ranging from \( \sim 15–70 \) µm. This is the longest reported ring-down time and quality factor to date for any micro resonator at this frequency. We also measured an extremely low 138 mHz frequency split between wine glass modes at 10.389 kHz with a low damping mismatch of \( 7.1 \times 10^{-5} \) Hz. This unprecedented result is a considerable achievement for microresonators and will pave the way to the development of next generation navigation-grade MEMS gyroscopes with \( 10 \times 10^{-3} \)°/hr bias stability.
Micro-Additive Manufacturing using Electrohydrodynamic Jet Printing

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Electrohydrodynamic jet (e-jet, EHD) printing is a candidate technology for maskless, additive manufacturing at the microscale. E-jet printing achieves orders of magnitude improved printed spatial resolution compared to inkjet printing, and e-jet printing has a wider range of acceptable inks. In this work, atomic force microscope scans and micrographs of e-jet-printed high viscosity inks, sub-2 µm polymer features, and electrodes are presented. We demonstrate submicron precision in droplet-to-droplet positioning with in situ monitoring. Rapid, sub-optical measurement of printed patterns provides a unique method for characterizing e-jet printing performance with specific interest in the applications of liquid resist patterning for nanoimprint lithography and the direct printing of thermally-sinterable conductive lines for sensor and actuator fabrication. Directions for the development of e-jet printing for manufacturing are discussed.
An X-Band Reconfigurable Bandpass Filter Using Phase Change RF Switches

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We report on a reconfigurable bandpass filter for X-band applications. The filter is composed of coupled $\lambda/2$ microstrip line resonators. Center frequency tuning of each resonator is achieved using an RF switch based on a phase change chalcogenide compound, germanium telluride, which switches in and out a loading capacitor. A combination of electric and magnetic coupling between the resonators realizes a near constant absolute-bandwidth as the filter is tuned. The center frequency of the filter is switched between 7.45 and 8.07 GHz, with a 3-dB bandwidth of ~500 MHz, insertion loss of less than 3.2 dB, and return loss of better than 18 dB. The measured third-order intermodulation intercept point (IIP3) and 1-dB power compression point (P1dB) are better than 30 dBm at frequency offset of 1 kHz and 25 dBm, respectively. Measured and simulated results are in good agreement. To our best knowledge, this is the first time implementation of a tunable filter using germanium telluride based phase change switches.
MDM: Multidisciplinary Design, Manufacturing, and Mechatronics
Optimization of Highly Flexible Aircraft Wings Using Next Generation Composite Materials

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The demand for more efficient transport aircraft by airlines has pushed aircraft manufacturers to design a higher aspect ratio wing in order to reduce induced drag. However, increasing the aspect ratio of the wing incurs a weight penalty, and also leads to aeroelastic issues due to the higher flexibility. To address this issue, many have started to investigate how to utilize the next generation of materials to enable higher aspect ratio wings that do not incur a prohibitive structural weight penalty.

One material technology of current interest are tow-steered composites. Tow steering is a new composite manufacturing technique whereby a machine is used to manufacture composites with fiber angles that vary continuously throughout the structure. Since the stiffness of a composite laminate is highly dependent on the orientation of these fiber angles, this gives the designer much more control over the stiffness properties of the structures. There are currently machines that manufacture tow-steered composite structures, but manufacturers have not yet taken full advantage of this capability due to a lack of numerical tools to design these new composites.

My research looks at designing a tow-steered composite wing through numerical optimization. This process will optimize both the composite layup as well as the local structural thicknesses. In this work a high-fidelity aerostructural analysis is used, accounting for the wing’s flexibility through the coupling of the aerodynamic and structural disciplines. In addition to the structural sizing and composite fiber tow angles the wing shape is also optimized simultaneously.
Novel aircraft configurations and technologies can be used to reduce the contribution of the aircraft industry towards global warming by reducing the rate of fuel burn for commercial transport aircraft. To quantify the effectiveness with which these configurations and technologies reduce fuel burn, we leverage high-fidelity computational tools. In this work, we use these tools to measure the effectiveness of morphing wing technology. To capture the level of fidelity necessary to produce a meaningful comparison of an aircraft with and without a morphing trailing edge, we use RANS-based aerodynamics with an SA turbulence model, coupled with a high fidelity structural model. By comparing the results of optimizations of the structural members in the wingbox and the shape of the wing’s outer mold line on both an aircraft with and without a morphing trailing edge, we can measure the fuel burn reductions produced by the morphing technology. The baseline configuration for the optimizations is the undeformed Common Research Model. For a seven point stencil centered around the nominal cruise condition, we measured a fuel burn reduction of more than 5% for the aircraft with the morphing trailing edge. A reduction of the structural weight enabled by active maneuver load alleviation contributed significantly to this reduction. We performed a similar comparison for a configuration with an aspect ratio of 13.5, and found active morphing to be more effective for high aspect ratio aircraft.
Friction stir spot welding (FSSW) process has been successfully applied for joining aluminum alloy 6061-T6 to TRIP 780/800 steel. Cross sections of weld specimens show the formation of the hook with a swirling structure. Higher magnified SEM view with EDS analysis reveals the swirling structure to be composed of alternating thin layers of steel and Al-Fe intermetallic compounds (IMCs). Effects of tool plunge speed and dwell time on the weld strength were studied through the design of experiments and analysis of variance. It is shown that dwell time is a more dominant parameter in affecting the weld strength than plunge speed. During the lap shear tests, cross nugget failure is the only failure mode. Cracks are initiated in the swirling structure at the tensile side of the weld nugget and cleavage feature can be observed on the fractured surface.
Development of a Robust and Streamlined Multifidelity Optimization Methodology

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Multifidelity design optimization combines information from different levels of fidelity to obtain an optimal solution to a design problem. There is currently a large activation energy to properly harness multiple information sources intelligently. Our current research focuses on developing tools to efficiently combine data from these information sources. This research is divided into two main thrusts: the development of an open-source low-fidelity aerostructural optimization package and the creation of an automated geometry engine to join different levels of fidelity.

OpenAeroStruct is an open-source low-fidelity aerostructural optimization program built upon NASA's OpenMDAO framework. Aerodynamic effects are modeled using a vortex lattice method and structural components are modeled using six-degree-of-freedom spatial beam elements. OpenAeroStruct uses a Newton-Krylov solver with coupled adjoint derivatives to converge the system. Aerostructural optimization can be run in seconds on a desktop computer.

To marry high- and low-fidelity simulations, we need a geometry engine that can transfer information across different levels of fidelity. To achieve this, a central geometry representation is stored and then translated to different representations as needed for each simulation type. We have developed an automated process that finds geometric features, such as bodies or intersections, and creates structured meshes so that we can run high-fidelity simulations. Because this is done for each optimization iteration, we can explore design spaces that include drastic geometry changes.
Bond Formation and Parameter Effects in Al/Cu Ultrasonic Welding

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Aluminum (Al) and copper (Cu) are common materials used as cathode and anode respectively in automotive lithium-ion battery cells. Due to the high electrical and thermal conductivity, and significant different melting points, joining of these two materials is very challenging using conventional fusion. One of the solutions to these difficulties is ultrasonic welding (USW), a solid state welding process. This study aims to investigate the bond formation process and major bonding mechanisms in USW of Al and Cu. Microstructural analysis indicates that severe plastic deformation plays a major role in the bond formation with current setups. Meanwhile, elemental dispersive spectroscopy (EDS) analysis shows that diffusion occurs as assistance to strengthen the bond. The effects of major process parameters including clamping pressure, vibration amplitude, and weld energy was also studied through design of experiment (DOE). The bonding strength was measured by U-tensile test, and correlated to different bond formation period via optical microscope imaging. Process window was also defined based on bonding strength and failure structures.
Biaxial Testing Procedure for Additive Manufacturing of Silicone Elastomer

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This study presents biaxial testing methods for materials made through 3D-printing of moisture cured silicone elastomers. The biaxial tensile test was performed using four linear actuators. The biaxial specimen maintained in the center location during the testing. The strain is computed using the digital image correlation (DIC) methodology. The elasticity and fracture strength were measured through utilization of the cruciform specimens. Normal and shear strains in x and y direction and were examined to study the biaxial deformation and breaking strength. The displacements and strains of biaxial specimen were computed using the DIC. The forces were measured by two dynamometers during the stretch of specimen. The biaxial test was performed through equal displacement for x and y direction (equibiaxial tension was applied to the specimen). The hyperelastic model are then acquired by incorporating the stress and strain relationship. The hyperelastic model are then validated to check its accordance to the experiment result.
MSE: Materials Science and Engineering
Short Crack Growth and Very High Cycle Fatigue Behavior of Magnesium Alloy WE43

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Despite their potential, magnesium alloys are currently underdeveloped with critical mechanisms in magnesium not yet fully understood. In this study, the short crack growth and very high cycle fatigue behaviors of the hot-rolled rare-earth magnesium alloy WE43 were investigated using displacement-controlled ultrasonic fatigue (USF) instrumentation and a novel combination of USF and scanning electron microscopy, termed UFSEM. The role of heat treatment and microstructure on fatigue life and crack propagation behavior in the T5, underaged and T6 conditions were investigated. The effect of grain boundary misorientation on short crack propagation was studied in the large-grained underaged and T6 conditions using basal-oriented notches, and was observed to play a significant role in crack growth retardation at grain boundaries. UFSEM was used to characterize micro-scale fatigue damage mechanisms.
Smooth, all-solid, omniphobic surfaces

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Surfaces which are resistant to wetting by a broad variety of liquids are relevant to numerous industrial applications. Omniphobic surfaces are capable of self-cleaning, resisting chemical attack and corrosion, and may play a key role in fields ranging from enhancement of phase-change heat transfer, prevention of contamination of medical devices by biological agents, and manipulation of sub-microliter volumes of liquids. Typical non-wetting surfaces rely on one of three approaches – incorporation of re-entrant nanoscale texture to entrap air beneath the liquid, incorporation of an immiscible non-volatile liquid impregnated into the texture, or surface modification with a reactive low surface energy molecule. These approaches each have potential drawbacks which limit their long-term stability, scalability to industrial applications, or generalizability to a wide range of substrate materials. In this study we have developed a facile deposition method for a highly fluorinated coating on a wide range of substrate materials, rendering them repellent to a wide range of liquids. Liquids including water, hexadecane, toluene, ethanol, and silicone oil exhibit low contact angle hysteresis (<10°) on these surfaces and can easily slide off without leaving a trail.
Understanding Spatial Packing through Variable Shape

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The onset of spatial packing is well defined, but non-trivial to solve. In statistical physics, particles are said to pack when they arrange under infinite pressure, and the ideal packing shape for a particle has been found for a variety of methods detailed in previous literature. But the ideality of a packing shape in a structure is not an instantaneous phenomenon; there must exist an onset to this “packing behavior” in shapes at a lower, finite pressure. This onset provides useful insight into particle stability in assembling these structures, as well as the notion that “packing behavior” may not directly coincide with the densest packing shape, challenging the supposition of these packing shapes as ideal candidates for assembly. In order to understand the evolution of particle shape through this change in behavior, we use the recently developed Alchemical Monte Carlo (AMC) move to explore a statistical ensemble with variable shape, known as shape-space. We define the onset of packing behavior as a numerical convergence of shape diversity and alchemical potential in shape space in several crystal systems.
Templated Synthesis of Shape-Controlled Polymer Nanofibers via Polymerization in Anisotropic Media

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The two essential components for a chemical reaction are reagents and reaction media. Chemical reagents can determine the chemical structures of the final reaction product. Reaction media, on the other hand, controls the reaction kinetics and defines the morphology (e.g. size, shape and surface texture) of the final products. In this study, we utilize one typical anisotropic medium, liquid crystals (LCs), as reaction media to create arrays of functional polymer nanofibers though a vapor-based polymerization process. When substituted [2,2]paracyclophanes were polymerized in liquid crystals (LCs) via chemical vapor deposition, the molecular alignment inside LCs guided the propagation of polymer chains and facilitated the formation of arrays of high-aspect ratio nanofiber. In addition, by tuning the properties of the LCs or polymerization parameters, we can control the size, shape and surface chemistry of the nanofibers, as well as introduce chirality to the nanofibers. We further demonstrated our finding can be utilized as a method to create nanofiber arrays on complex geometries and for capturing biomolecules. We believe that our work opens a new platform for designing functional polymer nanostructures to target a wide range of technological applications, including bio-sensing, affinity filtration, and catalyst supports.
Atomic Self-Assembly of 3D Nanocomposites

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Atomic self-assembly by way of phase separation allows for fabricating nanoscale features currently unachievable in currently-employed fabrication techniques. Here we report on the morphology development in co-deposited binary and ternary metallic thin films at elevated temperatures with feature sizes as small as 5-10 nanometers. Combining the deposition and annealing steps allows for control over the direction of constituent domain separation via the deposition rate and substrate temperature. Holding deposition rate constant and increasing the substrate temperature, we observe a transition from lateral phase concentration modulations to vertical concentration modulations. Holding substrate temperature constant and increasing the deposition rate, we observe the opposite transition; from vertical concentration modulations to horizontal concentration modulations. After some critical deposition rate and temperature, the system randomly phase separates into a tortuous, bicontinuous structure. We show that the morphology evolves during deposition in a way consistent with a surface inter-diffusion controlled process.
pH-mediated Hybridization of Complementary Dynamic Covalent Oligomers

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Dynamic covalent chemistry has been introduced as a method of assembling molecular architectures that are both durable and precise when compared to classic molecular self-assembly mechanisms. We incorporate boronic acid and catechol moieties into peptoid-based oligomers that were designed to undergo a dynamic covalent reaction and assemble into molecular ladders. Here we describe the synthesis of the precursor oligomers and the resulting assembled structures from reactions between homopolymers of boronic acids and catechols as well as the hybridization of single complementary oligomer chains that were comprised of both dynamic covalent functional groups. The generated structures were characterized using matrix-assisted laser desorption/ionization mass spectrometry confirming successful molecular ladder fabrication. The described work is helping to lay the foundation for a method that will enable a route to the facile fabrication of complex and robust proteomimetic nanostructures.
Nanoscale Spectroscopy of Electronic States in Nitride Nanostructures & 2D Materials

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We explore the nanoscale structure of two-dimensional materials and its influence on the band structure using a combination of scanning tunneling microscopy/spectroscopy (STM/STS), scanning thermoelectric microscopy (SThEM) and atom probe tomography (APT). Using SThEM and APT, we explore the ionization of Si dopants within and outside of InAs QDs. Using STM and STS, we determine the relative influences of strain fields associated with threading dislocations vs. those associated with buried QDs on the formation of InGaN/GaN QDs and their corresponding energy band offsets. With high-precision, variable separation STS we explore the surface of the set of topological insulators $(\text{Bi}_{1-x}\text{Sb}_x)\text{Te}_3$ as a function of composition and directly access the topological surface states. The study of these materials are useful for optoelectronic\textsuperscript{1,3} and thermoelectric applications\textsuperscript{1,3}.

References:
Kinetics Study of Carbon Nanotube Alignment via Real-time Polarized Raman Spectroscopy

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Carbon nanotubes (CNTs) have remarkable mechanical properties that the addition of CNTs into polymer matrix significantly improves polymer’s mechanical properties. Thus it is potentially cost-effective to reinforce polymers/polymer-composites with CNTs. Because of CNTs’ unique highly anisotropic structure, further enhancement can be achieved by manipulating the CNT alignment in the CNT/polymer composite.

We have developed a polarized Raman spectroscopy to characterize CNT alignment in real time. Electric field, magnetic field and shear force are common methods to induce CNT alignment in polymer. Magnetic fields (especially high fields) have the advantage of not touching the materials (while in an electric field setup, electrodes have to be immersed in the composite solution) and are free from Joule heating (caused by the current in electric fields) that can disturb the polymerization of the composite as well as CNT alignment. We have integrated a low magnetic field (max 1 Tesla) to the polarized Raman spectroscopy and are collaborating with the National High Magnetic Field Lab (MagLab).

The shear force alignment has a high potential for large-scale production. Besides, alignment kinetics purely depends on CNT’s diameter and length, not affected by the electromagnetic susceptibility. A shearing stage (from Linkam Scientific, UK) has just been integrated to the Raman spectroscopy, inside which CNTs are aligned by the torsional flow generated from two parallel disks. Preliminary results indicate CNTs align faster under higher shear rates. CNT bundling or aggregation occurs for high shear rates.
Dynamics of Star-Shaped Polystyrene Molecules: From Arm Retraction to Cooperativity

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The frequency $\omega$ dependent storage $G'(\omega)$ and loss $G''(\omega)$ moduli of star-shaped polystyrene (SPS) molecules of a range of functionalities $f$ and molecular weights per arm $M_a$ were measured under small amplitude oscillatory shear conditions. Star-shaped macromolecules are composed of an inner region, core, where the chain segments are stretched and the “packing” density is higher than that of the outer region, corona. The frequency dependencies of $G'(\omega)$ and $G''(\omega)$ for low functionality molecules ($f < 8$) with long arms $M_a$ are well described by the model of Milner and McLeish, indicating that the translational dynamics are facilitated by an arm retraction mechanism. With increasing values of $f$ and decreasing $M_a$ the model fails—the arm retraction process is no longer valid—due largely to the increasing size of the core in relation to the overall size of the molecule. The molecules exhibit evidence of spatial structural order due to entropic, intermolecular interactions, and the translational dynamics of these molecules occur via a cooperative process, akin to that of soft colloids, for sufficiently large values of $f$ and small $M_a$. The overall dynamics may be summarized in a diagram delineating different mechanisms that facilitate flow as a function of $f$ and $M_a$. 
Impact of Alloy Fluctuations on Recombination Rates and Efficiency of InGaN Quantum Wells

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Indium gallium nitride (InGaN) and its applications in light-emitting diodes play an integral role in efficient solid-state lighting, as recognized by the 2014 Nobel Prize in Physics. Despite its many successes, InGaN still suffers from issues that reduce the overall efficiency of devices. Optical experiments and structural characterization indicate that InGaN exhibits significant atomic-scale composition fluctuations. In this work, we study the effect of local composition fluctuations on the radiative recombination rate, Auger recombination rate, and efficiency of InGaN/GaN quantum wells (QWs). We use a commercial software package (nextnano) to simulate band edges, wave functions, and wave function overlaps of quantum wells with fluctuating alloy distributions based on atom probe tomography data. Our results are compared to calculations of quantum wells with uniform alloy distributions and to published work.
Hidden Anisotropy in Gold Nanorods

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Understanding symmetry of nanoscale object is fundamental to study physics, chemistry, and biology of functional nanostructures. Assigning correct symmetry to dispersed nanocolloids is, however, problematic due to structural complexity and dynamics of nanomaterials. Gold nanorods (Au NRs) have been considered as centrosymmetric structure based on their electron microscopic images that usually visualize only the metal cores but not the organic shells around them. Here, we demonstrate that Au NRs have distinct anisotropy of surface charge density by various microscopic techniques including off-axis electron holography and Kelvin force microscopy. We found that this anisotropy of the electrostatic potential in Au NR is associated with unequal number of cetyltrimethylammonium (CTA) moieties capping two ends of NRs and obtained nearly perfect symmetry of plasmon resonance map after removing of excess CTA on one of the ends. Moreover, the retardation-corrected second harmonic generation studies of Au NR composite films indicated that asymmetry of NRs is observed both for individual particles and in large ensembles. These findings explain previously puzzling discrepancies in non-linear optical effects in metallic nanostructures and will aid in interpretation of chemical, optical, biological, and other properties of nanostructures.
Sugar Coating the Answer to Virus Binding: Glycocalyx-mimetic Interfaces

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The glycocalyx is a membranous structure composed of glycoproteins and carbohydrate residues. This sugary forest that sheaths our cells is responsible for protecting us from pathogen invasions and forms a crucial component of our cells immune machinery. The first step of viral infection is binding to the glycocalyx. Virus-glycocalyx interactions are poorly understood and a detailed study of these interactions is hindered by the tendency of the native glycocalyx to collapse during in vitro studies. Hence we have developed a simplified synthetic model system for the glycocalyx to identify and understand physicochemical parameters that shape its interactions of viral pathogens. We have developed a library of carbohydrate-based monomers, including mannose, glucose and galactose, which recapitulate the chemical complexity of the glycocalyx. Though our carbohydrate-functionalized surfaces are inert to non-specific protein adsorption, they exhibited strong binding to lectins. In addition to specific affinity based interactions, we have also engineered electrostatically mediated interactions into our surface to enable capture of negatively charged species such as viruses and bacteria. In this work, we assess glycocalyx-mimetic abilities of our biomimetic surfaces by studying interactions with viruses and proteins and by evaluating the tunability of these interactions. By combining non-fouling properties of the polymer brush, non-specific (electrostatic) and specific carbohydrate-lectin interactions, a multifunctional glycocalyx mimic was developed. Our tunable surface can be employed to develop design rules for ant-viral coatings and to visualize the onset of infectious diseases.
The ductility of metallic glasses (MGs) correlates with the intensity of high-frequency mechanical relaxations (beta relaxations). In order to understand the microscopic origin of ductility, we compared the flow defects in a La-based MG with strong beta relaxation with those in a Al-based MG without pronounced beta relaxation. Quasi-static anelastic relaxation measurements using a combination of bending and nanoindenter cantilever techniques were conducted on amorphous Al$_{86.8}$Ni$_{3.7}$Y$_{9.5}$ and La$_{55}$Ni$_{20}$Al$_{25}$. Direct spectrum analysis yielded relaxation-time spectra with distinct peaks. These peaks correspond to a quantized hierarchy of shear transformation zones (STZs), which are clusters of atoms that undergo dissipative shear. STZ properties, such as time constant, volume and volume fraction of potential STZs were compared between these two MGs. While the increment in STZ volume corresponding to two adjacent spectrum peaks for Al-based MG is very close to the atomic volume of Al (major component in the MG), La-based alloy shows small-atom increment, which may be related to the observation that the activation energy for beta relaxation and diffusion of the smallest atom are similar. The volume fraction of potential STZs for the Al-based MG increases monotonically and steeply, but that for the La-based MG does not. One possibility for this behavior is that potential STZ of La-based alloy is a cluster of small atoms since the probability of high-n small atom clusters decreases with n.

References:
Assembly of Colloidal Microspheres and Measurement of Their Structural Color

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This project uses direct current (DC) electric field to assist self-assembly of spherical particles into colloidal crystals. We measure the iridescent structural color as well as the defect density of these colloidal crystal arrays. The structural color here arises due to light diffracted from the periodically spaced microspheres. Structural color has potential applications because the color arises from dielectric properties that are not prone to chemical degradation, such as photobleaching.

For the self-assembly, we constructed a capacitor-like electric field device and produce close-packed colloidal crystals in the solvent dimethyl sulfoxide (DMSO) with 0.1mM tetrabutyl ammonium chloride (TBAC). The colloidal spheres are polystyrene with diameter varying in the range of 0.3 - 1 μm. We assess the quality of the crystals by analyzing confocal microscopy images of the colloidal crystals so as to compute their defect density after assembly. Structural color are observed for the ordered assemblies of colloids with diameters from 0.3 to 0.7 μm. Spectrophotometry is used to measure optical properties and these are compared to predictions from Bragg scattering. This work supports the design and control of the spectral response of structural color materials.
Post-synthetic Modification of Covalent Organic Frameworks for Gas Separation Membranes

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Improving the efficiency of membrane-based gas separations remains a formidable challenge owing to the compromise between attaining high selectivity and high permeability; thus, further research is required to fully realize the potential of these materials to displace conventional gas separation approaches. Although there have been a range of studies on metal-organic framework (MOF)-based membranes, there is currently a dearth of studies on membranes based on porous organic materials such as covalent-organic frameworks (COFs) despite their several advantages.

In this project, COF particles were synthesized via imine condensation reactions from tetrahedral monomers. The resultant porous organic particles were characterized using nitrogen adsorption/desorption isotherms, scanning electron microscopy, and X-ray diffraction to determine surface area, porosity, and particle size. The crystalline COF particles were then surface functionalized and copolymerized with methacrylate monomers to obtain thin films, and the gas separation properties of the attained films were characterized.
Selective Wettability Membranes for Enhanced Liquid Separation and Fouling Prevention

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Access to clean water is one of the greatest challenges worldwide, and effective purification methods should be cheap, low energy, and capable of processing many forms of contaminated water. Billions of barrels of oily wastewater are produced each year, and traditional separation methods are slow, expensive, or ineffective with stabilized emulsions, especially with oil droplets below 10 \( \mu \text{m} \) in diameter. Membrane technologies can meet these shortcomings and be modified based on the oil droplet size and chemical interactions with the surface, but the decline in flux, due to fouling, is the greatest limitation of membranes. To address this difficulty, we study the modification of several common membrane materials and pore sizes, to prevent fouling due to the adsorption of oils and surfactants and to extend the membrane life. Our membrane’s selective wettability for water over oil also decreases fouling that may occur during process startup, maintenance, and stop-and-go operation. These selective wettability membranes are capable of separating surfactant-stabilized, nano-sized oil-in-water emulsions, even after heavy oil exposure, in both batch and continuous flow operations. The application of our methodology to ceramic cross-flow membranes shows that >60\% of the initial flux can be maintained after 500 hours of operation – a three-fold improvement over the unmodified membrane. We expect that our methodology will provide a robust, flexible, and scalable means of purifying oily water in a variety of industries.
Nature has developed highly specific and efficient catalysts that can synthesize complex organic compounds, such as the synthesis of sugars in photosynthesis. Due to the efficiency of these reactions, great effort has been put towards developing artificial reaction schemes that can replicate the complexity found in nature. Inorganic nanoparticles are a plausible choice for the development of a biomimetic system due to similarities with proteins found in nature. The advancement of NPs allows for tunable size, shape, charge, and surface functionality, allowing them to self-assemble into terminal superstructures similar to biological components. These superstructures, also known as supraparticles (SPs), can achieve the same catalytic functionality as natural enzymatic systems, and show improved functionality over their NP constituents due to collective and synergistic interactions.

The development of SP assemblies does not only provide a cost-effective and more stable alternative to enzymes but they can improve current inorganic NP catalysts. The tight structural integration of NPs in SPs present the capacity to enhance the stability of catalysts, and mitigate the aggregation of individual constituents by offering separation while remaining immobilized. SPs are capable of combining the individual properties of constituents to produce enhanced catalysts through synergistic interactions.

This work focuses on the formation of hybrid (organic – inorganic) SPs and FeS$_x$-based inorganic SPs to highlight the collective effect of SPs as catalysts.
Viscoelastic Materials for Impact Protection

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It is well-known that an unprotected human skull subjected to an impact load is at risk of sustaining a traumatic brain injury, so athletes playing football, lacrosse, baseball, and a number of other sports are encouraged, and often required, to wear helmets. Many commercial sports helmets limit the force applied to the wearer’s skull, but depending on the duration of the impact, the impulse transmitted to the head during the impact event may dominate the brain’s mechanical response, and so should also be considered in helmet design. In order to achieve a reduction in transmitted impulse, it is necessary to dissipate energy. Because viscoelastic materials can be cycled without significant losses in energy damping capability, they are well-suited for use in reusable helmets. In order to take full advantage of viscoelastic materials’ damping abilities, the design of the helmet must ensure that the timing of the impact event and the time dependence of the helmet material’s viscoelastic properties are compatible. Taking these separate time-scales into account, a mathematical model of an impact event with simplified geometry is presented and used to obtain guidelines for viscoelastic material selection for different types of impact.
Wettability Engendered Templated Self-Assembly (WETS) for Fabricating Polymer Particles for Drug Delivery

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Polymer nanoparticles have demonstrated significant potential in treating cancer though both in vitro and in vivo studies. However, a large obstacle that polymer nanoparticles face in transitioning to clinical applications is upscaling production. Current laboratory-scale methods for producing nanoparticles usually have small yields and involve steps, such as sonication, that are difficult to reproduce on an industrial scale. In addition, more complicated nanoparticle architectures with additional functionalities (e.g. drug, fluorescent dye, or magnetic nanoparticles), coatings, or phases are often more difficult to fabricate reproducibly. To address these issues, our lab has been developing a novel, scalable method, termed Wettability Engendered Templated Self-Assembly (WETS), to produce monodisperse, polymer micro- and nano-particles with various shapes, sizes, and compositions. WETS utilizes surface chemistry to create patterned templates consisting of omniphilic domains (wettable by all liquids) with well controlled sizes on top of an omniphobic (repel all liquids) substrate. This template is then dip-coated into a polymer solution (may contain any desired functionality), which when withdrawn causes the polymer to self-assemble within the omniphilic domains, and to completely recede from the omniphobic background, leaving behind polymer particles in the exact shape of the omniphillic domains. Multiphasic particles can be fabricated in a layer by layer fashion using successive dip-coats as each new polymer layer is deposited on top of the previous polymer layer. Using WETS, particles of different sizes, shapes, and with different phases and functionalities have been produced showing that WETS has the potential to serve as an industrial-scale polymeric particle fabrication methodology.
The Influence of Aluminum Content on Recrystallization and Grain Growth in Alpha Titanium Alloys

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Recrystallization and grain growth are important microstructural phenomena in commercial titanium alloys. In this study, we concentrate on recrystallization and grain growth of the dominant $\alpha$-phase. The static recrystallization behavior of model binary $\alpha$-Ti alloys were studied by performing room temperature compression tests followed by recrystallization heat treatments. Electron backscatter diffraction (EBSD) is used to quantify the extent of recrystallization after various heat treatment times by calculating the grain orientation spread (GOS) of each grain. GOS is a measure of the degree of misorientation throughout a grain which will be high in a deformed grain and low in a recrystallized grain. Using this method, the kinetics of recrystallization is captured for various alloys. The effects of processing conditions and solute concentration on the recrystallization kinetics are then modeled using the JMAK model. Increasing aluminum content was observed to lead to significantly slower recrystallization kinetics. The effect of solute concentration on the grain growth kinetics is also investigated by annealing fully recrystallized samples of multiple alloys. The grains are imaged using polarized optical microscopy and measured using the line intercept method. The addition of aluminum to titanium was observed to also significantly slow down the grain growth kinetics. The results from these experimental studies have been used to parameterize a phase-field model of recrystallization and grain growth in single phase titanium.
Li⁺ Conducting PEO-Based Solid Electrolytes Containing Active or Passive Ceramic Nanoparticles

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Solid nanocomposite electrolytes incorporating ceramic nanoparticle fillers into polymeric matrices have attracted much attention as an alternative to replacing liquid electrolytes for high energy density Li batteries. In this study, three types of fillers, liquid-feed flame spray pyrolysis synthesized amorphous Li₁.₃Al₀.₃Ti₁.₇(PO₄)₃ (LATP), TiO₂, and fumed silica nanoparticles are dispersed in poly(ethylene) oxide (PEO) polymer matrices. These materials, of which the first is considered an active, and the other two passive fillers, are chosen for comparative purposes. Nanocomposite electrolytes are prepared with up to 20 wt. % particles loading. PEO-LiClO₄ with 10 wt. % LATP nanoparticles exhibits an ionic conductivity of 1.70×10⁻⁴ S cm⁻¹ at 20°C, the highest among the surveyed systems. Even though the degree of crystallinity and glass transition temperatures of LATP-filled nanocomposites are higher than those of the other systems, they exhibit one to two orders of magnitude enhancement in the ionic conductivity. We attribute this remarkable performance to cation transport within the interphase region surrounding the particles, which achieves percolation at low nano-particle loading. The development of this interphase structure is influenced by the active nature of the LATP filler, and we estimate that the inherent conductivity of the interphase is about three to four times higher than the maximum measured value.
Shape Evolution of In-rich InGaN Disc-in-Nanowire Heterostructures

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InGaN nanowires have been intensively investigated for the use of optoelectronic devices, especially LEDs and lasers. One challenge in the growth of infrared InGaN disc-in-nanowire lasers is to incorporate a large amount of In. It has been shown that as the amount of In increases, branching and faceting occurs. This work focuses on examining the shape evolution and compositional distribution of InN/InGaN nanowire heterostructures. The n-i-p structure of nanowires were designed with active region of 3nm InN layers separated by 12 nm In₀.₄Ga₀.₆N barriers. Scanning electron microscopy shows that increasing In composition changes the growth mode and the crystal shape of the nanowires heterostructures. The active regions take on a polyhedral shape and appear at the top, suggesting that the p-GaN does not grow on the c-plane of the nanowire. Indeed, scanning transmission electron micrographs reveal that the InN regions are enveloped by quasi-conformal GaN shell. Energy-dispersive X-ray spectroscopy (EDS) shows that the polyhedral shapes are enriched in Ga on their upper half, and enriched in In on their bottom half and encased in a Ga-rich shell. Line profiles suggest that there is In segregation into the barrier layers. Occasionally, cracks develop near the center of the polyhedral, indicating the relief of significant amounts of lattice mismatch strain. Despite the complex morphology of the nanowires, strong luminescence was frequently observed. Low temperature photoluminescence measurement shows a primary peak at 1.6 μm and a secondary peak at 1.3 μm.
Processing Flame Made Nanoparticles to Free Standing Li$^+$ Conducting Thin Film Membranes

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Ceramic Li$^+$ conductors are the key component in the realization of all-solid-state batteries that outperform conventional Li-ion batteries as well as offer inherent safety. Identifying materials with ionic conductivities similar to the liquid counterpart has been the main focus in the research community for the past several decades. LiTi$_2$(PO$_4$)$_3$ (LTP) and Li$_7$La$_3$Zr$_2$O$_{12}$ (LLZO) doped with selected aliovalent ions have been down-selected as promising candidates, which show optimal electrochemical and microstructural properties when processed to high density monoliths. Given ceramics must be sintered to high temperatures to achieve ideal microstructures, often >1000°C where Li$_2$O volatilizes, it has been difficult to replicate the bulk properties in thin film forms at thicknesses <50μm, the required form factor for actual application. Hence, successful examples of processing Li$^+$ conducting membranes are scarce. Furthermore, the production must involve low-cost, easily-scaled processes readily translatable to mass-production. We show that casting-sintering of flame made nanopowders result in flexible Li$^+$ conducting membranes of LTO and LLZO at thicknesses <30μm with ionic conductivities >1mS cm$^{-1}$, equal to liquid electrolytes. Both processes are commonly practiced in industry for mass-producing nanopowders and ceramics in flat geometry. These Li$^+$ conducting oxide membranes greatly increase the selection of complementary cell components and simplify battery configurations broadening opportunities for cell designs. In a broader perspective, we show that high surface free energies of nanoparticles drive densification such that microstructures normally obtained by sintering at higher temperatures or longer times, or even with pressure, can be achieved at a much lower energy input via simple conventional sintering.
SCE: System and Communication Engineering
Consider a communication system in which there are multiple measuring devices each observing a source. Suppose the sources are statistically correlated. Each device is equipped with a transmitter. The transmitters encode the data obtained by the measuring devices, and communicate necessary information to a central receiver. The receiver wishes to reconstruct the sources losslessly. In this setup, the transmitters cannot communicate with each other. The goal is to design a coding strategy to for transmission of the sources reliably and efficiently. The case when there are only two transmitters is well studied in the literature. The Cover-El Gamal-Salehi's (CES) scheme is introduced for this setup, and achievable rates is derived. In this work, we study the three-user version of this problem, and investigate sufficient conditions for transmission of correlated sources. An extension of the CES scheme is introduced. We observe that certain algebraic structures in the sources can be exploited to improve upon unstructured random codes. Based on this observation, we use a combination of CES with linear codes to propose a new coding strategy. Our results indicate that this coding strategy outperforms the CES scheme.
Enforcement of Security and Privacy Properties: An Interface-based Approach using Event Insertions

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We study the enforcement of opacity, an information-flow security property, using insertion functions that insert fictitious events at the output of the system under the framework of discrete event systems. The intruder is characterized as a passive external observer whose malicious goal is to infer system secrets from observed traces of system events. We consider the problems of enforcing opacity under the assumption that the intruder either knows or does not know the structure of the insertion function; we term this requirement as public-private enforceability. In this poster, we address both the weak and strong requirement of enforceability, i.e. private enforceability and public-private enforceability. The private case assumes that the intruder does not know the form of the insertion function, while the public-private case requires that opacity be preserved even if the intruder knows or discovers the structure of the insertion function. We focus on the latter one and formulate the concepts of public-private enforceability, which leads to the notion of public-private enforcing (PP-enforcing) insertion functions. We then identify a necessary and sufficient condition for an insertion function to be PP-enforcing. We further show that if opacity is privately enforceable by the insertion mechanism, then it is also public-private enforceable. Using these results, we present a new algorithm to synthesize PP-enforcing insertion functions by a greedy-maximal strategy. This algorithm is the first of its kind to guarantee opacity when insertion functions are made public or discovered by the intruder.
Designing Cyber Insurance Policies: Mitigating Moral Hazard Through Security Pre-Screening

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Cyber-insurance has been studied in the literature as both a method for risk-transfer, as well as a potential incentive mechanism for improving the state of cyber-security. However, in the absence of regulated insurance markets or compulsory insurance, the introduction of insurance deteriorates network security. This is because by transferring part of their risk to the insurer, the insured agents can decrease their levels of effort. In this report, we consider the design of insurance contracts by an (unregulated) profit-maximizing insurer, and allow for voluntary participation. We propose the use of pre-screening signals by the insurer to limit agents' effort reduction after they enter a contract. We consider the use of this signal to offer premium discounts to the higher effort agents. We show that such premium discrimination not only helps the insurer attain higher profits, but we also show that it leads the agents to improve their efforts compared to the no pre-screening scenario. In other words, the availability of pre-screening signals benefits both the insurer, as well as the state of network security.
Impact of Community Structure on Cascades

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The threshold model is widely used to study the propagation of opinions and technologies in social networks. In this model individuals adopt the new behavior based on how many neighbors have already chosen it. We study cascades under the threshold model on sparse random graphs with community structure to see whether the existence of communities affects the number of individuals who finally adopt the new behavior. Specifically, we consider the permanent adoption model where nodes that have adopted the new behavior cannot change their state. When seeding a small number of agents with the new behavior, the community structure has little effect on the final proportion of people that adopt it, i.e., the contagion threshold is the same as if there were just one community. On the other hand, seeding a fraction of population with the new behavior has a significant impact on the cascade with the optimal seeding strategy depending on how strongly the communities are connected. In particular, when the communities are strongly connected, seeding in one community outperforms the symmetric seeding strategy that seeds equally in all communities.
Scalable Control of Cyber-Physical Systems

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Cyber-Physical Systems are emerging engineering systems including smart energy systems, communication systems, cyber-physical security, smart health and transportation systems, etc. These systems are large, dynamic, and with imperfect information for the decision maker. Controlling these systems is a future challenge. We present two scalable approximation approach for controlling these systems. The first approach maps the information state to a finite state space. The second approach divides the system into subsystems controlled by local controllers. To do so, the influence graph is defined using system dynamics. This graph is clustered into sub-graphs controlled by local controllers. The communication between the local controllers is designed to share important information for control of their sub-systems.
Finite Block-Length Codes Trump Random Coding over Infinite Length Blocks

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In this work we investigate the structures of optimal coding schemes for communication over networks. It is well-known that in order to exploit the redundancy of the source in point-to-point data compression, it is necessary to compress large chunks of the source simultaneously. More precisely, optimality is only possible as the length of the coding blocks approaches infinity. However, we show that as the code-length increases, the outputs of distributed quantizers become less correlated. So, random coding over large block-lengths is detrimental to the ability of encoders in a network to coordinate their outputs. Hence, it is sometimes advantageous, that in the interest of cooperation, smaller block-length codes be used instead. Furthermore, we show that in large classes of multi-terminal problems, the optimal encoding function at each terminal decomposes into finite block-length encoding functions. We conclude that the coding strategies available in the literature do not approach optimality in these classes of problems. This is contrary to our usual understanding in Shannon theory that optimality is achieved by increasing block-length. We characterize a group of coding schemes called Single-Letter Random Coding (SLRC) schemes. These SLRC schemes include the random coding schemes used in the two terminal problems in network information theory. We show that no SLRC scheme can generate an encoding function which operates ‘close’ to optimality in these multi-terminal communication settings.
Descending Price Algorithm for Determining Market Clearing Prices in Matching Markets

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Matching Markets, first studied by Gale and Shapley, are critical and have many real-world applications such as Google selling web slots to advertisers, organ donor exchange, and marriage. Since the revenue equivalence theorem does not hold in matching markets, different pricing mechanisms may yield higher expected profits for sellers when anticipating buyers’ strategic behavior. Hence, algorithm design in search of the maximum market clearing price is a problem deserving of study. In our work, a two-sided matching market is considered and a valuation matrix is used to represent buyers’ different private value toward goods. To determine market clearing prices, a skew-aided descending price algorithm based auction mechanism is proposed in this work. With an intelligent choice of set of good for price reduction, called reverse constricted sets, we prove that the algorithm converges in a finite number of rounds for any non-negative real valuations. Then specializing to the rank-one valuation matrix in sponsored search markets, we provide an alternate characterization of the set of all market clearing prices, and use this to prove that the proposed algorithm yields the maximum market clearing price. Some open problem such as maximum return in general valuation matrix, an efficient algorithm in search of the most skewed set, and the analysis of strategic concerns are deferred for future work.
Approximately Envy-Free Spectrum Allocation with Complementarities

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With spectrum auctions as our prime motivation, in this work we analyze combinatorial auctions where agents' valuations exhibit complementarities. Assuming that the agents only value bundles of size at most $k$ and also assuming that we can assess prices, we present a mechanism that is efficient, approximately envy-free, asymptotically strategy-proof and that has polynomial-time complexity. Modifying an iterative rounding procedure from assignment problems, we use the primal and dual optimal solutions to the linear programming relaxation of the auction problem to construct a lottery for the allocations and to assess the prices to bundles. The allocations in the lottery over-allocate goods by at most $k-1$ units, and the dual prices are shown to be (approximately) envy-free irrespective of the allocation chosen. We conclude with a detailed numerical investigation of a specific spectrum allocation problem.
Path Partitioning Algorithms for Personalized PageRank

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PageRank, introduced by Google founders Larry Page and Sergey Brin, provides a means of identifying important nodes in a network. Originally intended for Internet search, it has since been applied to domains as diverse as road networks, biology, and even ranking sports teams. Similarly, Personalized PageRank (PPR) is a measure of the importance of nodes from the perspective of a single node (or distribution of nodes). PPR has been used in many applications, such as recommending who a particular user should follow on Twitter.

A closely related problem is PPR search, in which one wishes to compute the PPR of a set of target nodes $T$ from the perspective of a source node $s$. For example, $s$ may represent a user searching a name on a social network, $T$ may represent the set of users on Twitter with that name, and, by sorting nodes in $T$ by PPR, one can identify which users are most relevant to $s$.

In this work, we explore extensions to the Bidirectional-PPR algorithm of P. Lofgren, S. Banerjee, and A. Goel, currently the state-of-the-art solution for PPR search. We present an interpretation of Bidirectional-PPR that leads us to define a larger class of similar algorithms we call Path Partitioning Algorithms. We explore two algorithms in this class, which we believe to be useful in PPR search. Theoretical bounds and numerical results suggest that our algorithms offer improvement over the state-of-the-art.
SIC: Signal and Image Processing, Computer Vision
Predicting the Asymptotic Performance of Rank-1 PCA with Heteroscedastic Data

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Principal Component Analysis (PCA) is a method for estimating a subspace given noisy samples. It is useful in a variety of problems ranging from dimensionality reduction to anomaly detection and the visualization of high dimensional data. PCA performs well in the presence of moderate noise and even with missing data, but is also sensitive to outliers. PCA is also known to have a phase transition when noise is independent and identically distributed; recovery of the subspace sharply declines at a threshold noise variance. Effective use of PCA requires a rigorous understanding of these behaviors. This work provides a step towards an analysis of PCA for samples with heteroscedastic noise, that is, samples that have non-uniform noise variances and so are no longer identically distributed. In particular, we provide a simple asymptotic prediction of the recovery of a one-dimensional subspace from noisy heteroscedastic samples. The prediction enables: a) easy and efficient calculation of the asymptotic performance, and b) qualitative reasoning to understand how PCA is impacted by heteroscedasticity (such as outliers).
Limited Angle Breast Ultrasound Tomography with *A Priori* Information and Artifact Removal

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Recently, it has been shown that by delineating suspected, relatively homogeneous structures in B-mode images from dual-sided ultrasound, one can enhance limited angle tomography to produce speed of sound images in the same view as X-ray mammographic tomography (DBT). This could allow better breast cancer detection and discrimination, as well as improved registration of the ultrasound and X-ray images because of the similarity of SOS and X-ray contrast in the breast. However, this speed of sound reconstruction method relies strongly on the B-mode or other reflection mode segmentation. If that information is limited or incorrect, artifacts will appear in the reconstructed images. Therefore, the iterative speed of sound reconstruction algorithm has been modified in the manner of simultaneously utilizing the image segmentations and removing most artifacts. The first step of incorporating *a priori* information is solved by any nonlinear-nonconvex optimization method while artifact removal is accomplished by employing the fast split Bregman method to perform total-variation (TV) regularization for image denoising. The proposed method was demonstrated in simplified simulations of our dual-sided ultrasound scanner. To speed these computations two opposed 20-element ultrasound linear arrays with 0.5 MHz center frequency were simulated for imaging two cylinders in a uniform background. The proposed speed of sound reconstruction method worked well with both bent-ray and full-wave inversion methods. This is the first demonstration of successful full-wave, limited angle, medical ultrasound tomography. The presented results lend credibility to possible translation of this method to clinical breast imaging application.
Female Pelvic Synthetic CT Generation Based on Joint Shape and Intensity Analysis

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Purpose: This study develops a method to estimate electron density information (Synthetic Computed Tomography) from Magnetic Resonance Imaging (MRI) scans and evaluates its utility in supporting radiotherapy treatment planning for female pelvic patients.

Methods: A single imaging sequence (T1_VIBE_Dixon) was acquired for 10 patients. This sequence yields 3 useful image volumes of differing contrast (“in-phase” T1-weighted, fat and water). A pelvic bone shape model was trained from 30 CT pelvic bone images and used to generate a rough bone mask for each patient. A modified fuzzy c-means tissue classification was performed on the multi spectral MR data, with a regularization term that utilizes the prior knowledge provided by the bone shape model and addresses the intensity overlap between different tissue types on MRI. A weighted sum of classification probabilities of tissue types with attenuation values of corresponding tissues yielded Synthetic Computed Tomography (MRCT) volumes. Treatment planning using both actual CT and MRCT was performed and compared.

Results: MRCT image volumes presented contrast similar with CT image volumes. Calculated doses were comparable for plans generated using actual CT and MRCT. Maximal dose difference on plan target volumes and various organs at risk (including pelvis, bowel and sacrum) is smaller than 1Gy across patients. This difference is negligible as compared to the prescribed doses for patients (range from 45 to 58.25 Gy).

Conclusion: MRCT based on a single imaging sequence in the female pelvis is feasible, with acceptably small variations in attenuation estimates and calculated doses to target and critical organs.
Sparse Equisigned PCA

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Principal Component Analysis (PCA) is a dimensionality reduction technique for multivariate data. However, when the dimensionality of the data is of similar order to the number of samples, PCA breaks down: the eigenvectors of the sample covariance matrix are inconsistent estimates of the population eigenvectors. Nevertheless, when the eigenvectors are sparse, there are consistent estimators. Unfortunately, many such estimators are multi-stage procedures or are complicated iterative methods. Placing a second structural assumption on the data leads to a simplification: if the data are either non-negative or non-positive, a one-stage algorithm yields consistent estimates of the population eigenvectors. We examine the consistency, performance, and theoretical limits of eigenvector estimation under these conditions.
Algorithms for Estimating a Rank One Matrix in Noise With Triple Kronecker Product Structured Principal Singular Vector

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We consider the problem of estimating a rank one signal buried in noise, which has, without loss of generality, a triple Kronecker product structured principal left singular vector. We assume that the Kronecker components are unknown, but their dimensions are known. This is also equivalent to the estimation of an appropriately reshaped rank one tensor signal buried in noise. This model arises in a wide variety of signal processing applications such as Space Time Adaptive Processing and vector-sensor array processing.

We propose eight new algorithms for the estimation of this signal matrix, based on a rearrangement operator introduced by Van Loan and Pitsianis, which use Singular Value Decomposition (SVD) and the rearrangement operator in different ways. We find that the algorithm which first computes the singular vector estimate using the SVD, and then fits the Kronecker product structure to it outperforms the algorithm which first estimates the Kronecker components by exploiting the Kronecker product structure. Using insights from random matrix theory, we approximate the estimation performance of all algorithms. Our analysis also uncovers that each algorithm has a different, sharp phase transition boundary between reliable estimation performance and algorithm breakdown. These breakdown points depend upon the dimensions of the Kronecker components and sample size in a way that can be made explicit. Such a characterization determines the right algorithm to select depending upon the dimensions of the Kronecker components or tensor modes in any given application.
Digital Breast Tomosynthesis Reconstruction with Detector Blur and Correlated Noise Model

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Digital breast tomosynthesis (DBT) has been developed to reduce the problem of overlapping tissue in conventional 2-D mammography. We propose a new reconstruction method for DBT. The new method incorporates detector blur into the forward model. The detector blur introduces correlation in the measurement noise. With the approximation that the reconstructed image consists of high-frequency structures and a low-frequency background, we formulate the reconstruction as a quadratic optimization problem with data-fit term that accounts for the non-diagonal noise covariance matrix. Considering the fairly uniform thickness of the compressed breast in DBT, we made a further approximation that the standard deviations of the quantum noise and the readout noise are constant for a given projection angle, which dramatically simplified the inversion of the noise covariance matrix. We also applied an edge-preserving regularization to control the noise level. The optimization problem was solved with a slightly modified separable quadratic surrogate (SQS) algorithm. This new reconstruction method is referred to as SQS with detector blur and correlated noise (SQS-DBCN). The SQS-DBCN method was applied to DBT reconstruction of breast phantoms and human subjects. The contrast-to-noise ratio (CNR) and full width at half maximum (FWHM) of microcalcifications (MC) and the visual quality of mass margins were analyzed and compared to those by the commonly used simultaneous algebraic reconstruction technique (SART). The results demonstrated the potential of the new method in improving the image quality of reconstructed DBT images. This work is our preliminary step towards a model-based iterative reconstruction (MBIR) for DBT.