Abstract Booklet

12th Annual Engineering Graduate Symposium

Friday, November 10th, 2017

College of Engineering, University of Michigan, Ann Arbor
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Morning Poster Session:
10:30 am - 1:00 pm
CDR: Controls, Dynamics, and Robotics
Supratransmission in a metastable modular metastructure for tunable nonreciprocal wave transmission

Z. Wu\textsuperscript{1}, Y. Zheng\textsuperscript{1,2}, K.W. Wang\textsuperscript{1}

\textsuperscript{1} Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI
\textsuperscript{2} State Key Laboratory for Strength and Vibration of Mechanical Structures, Xi’an Jiaotong University, Xi’an, China

In this research, we theoretically and numerically investigate the nonlinear energy transmission phenomenon in a metastable modular metastructure. Numerical studies on a 1D metastable chain provide clear evidence that when driving frequency is within the stopband of the periodic structure, there exists a threshold for the driving amplitude, above which sudden increase in the energy transmission can be observed. This onset of transmission is due to nonlinear instability and is known as supratransmission. We show that due to spatial asymmetry of strategically configured constituents, such transmission thresholds are considerably different when structure is excited from different ends and this discrepancy creates a region of nonreciprocal energy transmission. We demonstrate that when the loss of stability is due to saddle-node bifurcation, the transmission threshold can be predicted analytically using a simplified nonlinear-linear system model, and analyzed via combining harmonic balancing and transfer matrix methods. These investigations elucidate the rich and complex dynamics achievable by nonlinearity and metastabilities, and provide tunable bandgaps and nonreciprocal wave transmissions.
Fuel Cell Thermal Management: Modeling, Specifications and Correct-by-Construction Control Synthesis

Liren Yang\textsuperscript{1}, Amey Karnik\textsuperscript{2}, Benjamin Pence\textsuperscript{2}, Md Tawhid Bin Waez\textsuperscript{2}, Necmiye Ozay\textsuperscript{1}

\textsuperscript{1}Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI
\textsuperscript{2}Ford Research & Advanced Engineering, Dearborn, Michigan

Thermal management is crucial for safe and efficient operation of fuel cells. The goal of this work is to algorithmically synthesize a provably-correct controller for a fuel cell thermal management system. For this purpose, we start with developing a control-oriented model for the fuel cell thermal management system and list the associated requirements. Then, we identify some structural properties of the system dynamics that can be leveraged for making the abstraction-based synthesis algorithm computationally efficient. Finally, we synthesize a controller for this system and demonstrate the closed-loop system behavior via simulations.
Calibrated Mixed Reality for Scalable Multi-Robot Experiments

Victoria Edwards\textsuperscript{1}, Edwin Olson\textsuperscript{2}

\textsuperscript{1}Robotics Institute, University of Michigan, Ann Arbor, MI
\textsuperscript{2}Department of Computer Science and Engineering, University of Michigan, Ann Arbor, MI

Researchers who test multi-robot teams are often faced with two options: test on real robots, where the number of robots is low but the fidelity is high, or test in simulation, where the fidelity is low but the number of robots can be high. This becomes a problem for robots with sophisticated sensing and planning systems which rise in cost as robots require more realistic environments. We propose a mixed-reality testing framework in which a number of real robots interact with virtual counterparts. This framework allows us to have a large team of robots that interact with the environment with high fidelity. However we have introduced a new problem: the simulated robots must behave like their real teammates. So we focus on calibrating parameters for virtual robots so that the results of a mixed-reality experiment are meaningful. In particular, we take advantage of the fact that virtual robots can be used to elicit behaviors from physical robots in order to empirically measure their kino-dynamic characteristics.
Stealthy Deception Attacks for Cyber-Physical Systems

Romulo Meira Goes, Stephane Lafortune

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

We study the security of Cyber-Physical Systems (CPS) in the context of the supervisory control layer. Specifically, we propose a general model of a CPS attacker in the framework of Discrete Event Systems (DES) and investigate the problem of synthesizing an attack strategy for a given controlled system. Our model captures a class of deception attacks, where the attacker has the ability to modify a subset of sensor readings and mislead the supervisor, with the goal of inducing the system into an undesirable state. We introduce a new type of a bipartite transition structure, called Insertion-Deletion Attack structure (IDA), to capture the game-like interaction between the supervisor and the environment (which includes the system and attacker). This structure is a discrete transition system that embeds information about all possible attacker’s stealthy actions, and all states (some possibly unsafe) that become reachable as a result of those actions. We present a procedure for the construction of the IDA and discuss its properties. Based on the IDA, we discuss the characterization of successful stealthy attacks, i.e., attacks that avoid detection from the supervisor and cause damage to the system.
Enforcement of security and privacy properties: An interface-based approach using event insertion and erasure

Yiding Ji, Stéphane Lafortune

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

We study the enforcement of opacity, an information-flow security property, using edit functions that insert fictitious events or erase the observed 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 problem of enforcing opacity under the assumption that the intruder either knows or does not know the implementation of the edit 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 edit function, while the public-private case requires that opacity be preserved even if the intruder knows or discovers the structure of the edit 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) edit functions. We further define constraints for edit functions and develop a novel tripartite transition system which embeds all feasible privately safe edit functions. Based on this structure, we discuss synthesizing (PP-enforcing) edit functions under both deterministic and nondeterministic settings. In both cases, we present synthesis algorithms and analyze their performance. This work is the first of its kind to explore opacity enforcement from both deterministic and nondeterministic perspectives when edit functions are made public.
Semantic Mapping: Revisiting Put That There in Real Domestic Environment

Zhen Zeng$^1$, Yunwen Zhou$^2$, Odest Chadwicke Jenkins$^3$

$^1$Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI
$^2$Robotics Institute, University of Michigan, Ann Arbor, MI
$^3$Department of Computer Science and Engineering, University of Michigan, Ann Arbor, MI

Service robots are becoming increasingly capable of assisting people with their daily activities. They require, however, an interface that allows the user to easily communicate the goal of a task, such as organizing a living room by putting different things at proper positions. In this work, we present a semantic mapping method where a robot can map domestic environment with localized objects, such as furniture and groceries. Then user can directly command the robot to organize the domestic environment by moving objects in the semantic map on a browser. We propose a discriminatively informed generative semantic mapping method to detect and estimate object poses in observed RGB-D stream, and its effectiveness is demonstrated on a real robot performing put that there tasks.
Generating provably-correct 2D push recovery controllers by patching 1D controllers

Zexiang Liu, Necmiye Ozay

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

In this work, we study how control synthesis can be applied to the push recovery on a 2D plane, i.e. an uneven ground with holes or areas forbidden to step onto. We consider an abstraction-based synthesis approach. To avoid state space explosion in abstractions, we ask whether the robot can do push recovery on 2D plane using only 1D controllers. We develop an algorithm that extracts a finite set of 1D controllers that can handle a certain 1D map with holes, that when used together, can guarantee recovery on the 2D topology. Moreover, an incremental algorithm is developed, to synthesize 1D controllers from an ideal 1D controller that operates on a map without holes, by taking advantage of the action inclusion relation in the fixed point operations for synthesis. This local patching significantly improves the computation time. Our numerical simulations with a linear inverted pendulum model of the robot demonstrates the efficacy of the proposed approach.
Stochastic Feedback Combustion Control at High Dilution Limit

Bryan Maldonado\textsuperscript{1}, James Freudenberg\textsuperscript{2}, Anna Stefanopoulou\textsuperscript{1}

\textsuperscript{1}Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI
\textsuperscript{2}Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI

Cycle-to-cycle variability in the combustion process of spark ignition engines imposes limits when operating at highly diluted conditions. When exhaust gas recirculation (EGR) is used to achieve higher fuel efficiency, the combustion variability (CV) increases due to the reduction in flame propagation speed. A slower combustion process will locate peak pressure later in the power stroke, reducing brake torque. Hence, spark advance (SA) needs to move accordingly to locate combustion phasing at the optimal value. As EGR levels increase, the CV reaches a limit where drivability is compromised and partial burn and misfire cycles sporadically occur. A tight control is required to operate close to such limit with minimum variability to maximize EGR benefits. A linear quadratic Gaussian (LQG) controller has been designed to drive the system towards a high efficiency condition with high EGR without deteriorating CV. The controller manipulates SA and EGR-valve opening to target a desired operating condition. The closed-loop system however does not need to be designed only for transient response but also for steady state operation maintaining low CV. The directionality of the open-loop system at the target condition is shown to be problematic. Rejection of disturbances along the directions with low plant gain requires large control signals that could drive the system towards misfiring conditions. Moreover, such control commands could be perceived by the driver as torque fluctuations, jeopardizing drivability. This limitations at the high dilution limit are discussed and simulated results are provided.
Legged Robot State-Estimation Through Combined Forward Kinematic and Preintegrated Contact Factors

Ross Hartley¹, Josh Mangelson¹, Lu Gan¹, Maani Ghaffari², Jeffery M. Walls³, Ryan M. Eustice², Jessy W. Grizzle¹

¹Robotics Institute, University of Michigan, Ann Arbor, MI
²Department of Naval Architecture and Marine Engineering, University of Michigan, Ann Arbor, MI
³Toyota Research Institute, Ann Arbor, MI

State-of-the-art robotic perception systems have achieved sufficiently good performance using Inertial Measurement Units (IMUs), cameras, and nonlinear optimization techniques, that they are now being deployed as technologies. However, many of these methods rely significantly on vision and fail when visual tracking is lost because of lighting or scarcity of features. In addition, such systems are formulated such that the system is independent of the operating platform. This work presents state-estimation technique for legged robots that takes into account the robot's kinematic model as well as its contact with the environment. This is achieved by introducing forward kinematic factors and preintegrated contact factors into a factor graph framework that can incrementally solved in real-time. The forward kinematics factor relates the robot's base pose to a contact frame through noisy encoder measurements. The preintegrated contact factor provides odometry measurements of this contact frame, while accounting for possible foot slippage. Taken together, the two factors constrain the graph optimization problem allowing the robot's trajectory to be estimated. The work evaluates the method using simulated and real sensory IMU and kinematic data from experiments with a Cassie-series robot designed by Agility Robotics. These experiments show that using the proposed method in addition to IMU significantly decreases drift and improves localization accuracy, suggesting that its use can enable successful recovery from loss of visual tracking.
A Nonparametric Approach to Scene Estimation with Inter-object Relations towards Goal-directed Manipulation

Karthik Desingh\textsuperscript{1}, Zhen Zeng\textsuperscript{2}, Odest Chadwicke Jenkins\textsuperscript{1}

\textsuperscript{1}Department of Computer Science and Engineering, University of Michigan, Ann Arbor, MI
\textsuperscript{2}Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI

Personal robotics is a rapidly growing field of research where assistive robots are being developed to help people with disability. These robots must sense, perceive and understand indoor environments to be able to assist people. A typical indoor environment is composed of many objects including graspable objects such as food products, and kitchen utensils. The robot must grasp and manipulate these graspable objects to perform meaningful tasks such as putting food into a fridge or setting a table for dinner. In order to grasp and manipulate an object, the robot must perceive both the label and pose of the object instance. In reality, the robot will have to perceive several objects in arbitrary poses at a time. Perceiving object poses in a cluttered scene composed by multiple objects with various inter-object relations is a challenging problem. The inter-object relations create partial observations of objects making harder to perceive their poses. In this work, we propose a nonparametric scene estimation framework to estimate the scene as a collection of object poses. We make use of information such as a) the object interactions in the form of a scene graph, b) object labels from an object detector and c) the observed RGBD sensor data, to generatively estimate poses of all objects in a scene. The problem is formulated as a pairwise Markov random field (MRF), a probabilistic graphical model where each hidden node is a continuous pose variable and the edges denote the inter-object relations between the poses.
Equalized performance is an intuitive property for estimators to ensure that the estimation error does not increase. Therefore, it is shown to be useful in output feedback correct-by-construction control. Previously, designing to achieve this property meant performing an optimization in which a triangle-inequality derived expression played a role in the constraints. In this work we extend this result by defining a less conservative, improved solution to the optimization problem and presenting a novel guarantee for the error at times further in the future than previously considered by leveraging ideas from the dual problem of affine finite horizon optimal control design. In the case of time horizons greater than one, the condition can be thought of as ensuring a “recovery” to some desired performance level after a lapse due to some unknown but bounded disturbance. We compare this new approach to the original triangular inequality based approach on simulations.
Synchronous and Asynchronous Multi-Agent Coordination With cLTL+ Constraints

Yunus Emre Sahin, Necmiye Ozay
Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI

Planning trajectories for multiple agents in a way to guarantee that their collective behavior satisfies a certain high-level specification is crucial in many application domains. Motivated by this problem, we introduce a new logic called counting linear temporal logic plus (cLTL+). This logic enables specifying multi-agent tasks over possibly infinite horizons in a compact manner. We then propose an optimization based method that generates trajectories for individual agents that, when implemented together, guarantee the satisfaction of a given cLTL+ formula. We further discuss how these results can be extended to generate trajectories that can be asynchronously implemented by the agents while preserving the satisfaction of the desired cLTL+ specification. In particular, we show that when the asynchrony between agent trajectories is bounded, it is possible to generate trajectories robust against such asynchrony with an appropriate modification of the optimization problem.
CEE: Civil and Environmental Engineering
Construction is known as one of the most stressful occupations due to its involvement with physically and psychologically demanding tasks performed in a hazardous work environment. Because workers’ stress is a critical factor that adversely affects workers’ productivity, safety, and well-being, an understanding of workers’ stress should take precedence for the management of excessive stress. Various instruments for subjective measurement towards one’s perceived stress have been used, but they rely on imprecise memory and reconstruction of feelings in the past, which limits their use in the field. Recent advancements in wearable Electroencephalography (EEG) devices possess a potential for continued measurement of human stress without interfering with workers’ ongoing work. However, its capability of measuring field workers’ stress under real occupational stressors remains questionable due to significant noises and absurd signals. To address these issues, we propose a comprehensive and efficient stress measurement framework by; 1) acquiring high-quality EEG signals via advanced signal processing to remove prevalent artifacts at a job site; 2) automatically recognizing construction workers’ stress in the field based on workers’ brain activities by supervised learning algorithms (e.g., SVM: Support Vector Machine); and 3) recognizing real-time stress by applying a novel Online Multi-Task Learning (OMTL) algorithms. Results yielded a high of 80.13 % accuracy using SVM. In case of real-time stress recognition, our framework achieves 77.61% in recognizing workers’ stress with OMTL. These results are very promising given that stress recognition with an exquisite and wired EEG device in the clinical domain has at most the similar level of accuracy. This EEG based stress detection approach is expected to better understand workplace stressors and to improve workers’ productivity, safety, and well-being by early detection and mitigation of the factors that cause stress.
Ordinary Camera-Mounted Drone Based Human Centric Scene Understanding for Construction Hazard

Daeho Kim, SangHyun Lee
Department of Civil and Environmental Engineering, University of Michigan, Ann Arbor, MI

Most construction tasks involve physically demanding labors and significant interactions with heavy machinery, which imposes severe safety risks (e.g., struck-by hazard and ergonomic risk). While on-site manual observation has been commonly used in practice, it is time-consuming, costly, and error-prone. To address these limitations, we utilize an ordinary camera-mounted drone and develop computer vision methods augmented with deep learning techniques to automate this observation process. Toward this end, we focus on human-centric scene understanding that automatically detect an entity’s spatial and kinematic attributes (i.e., location and pose) at this stage, which is the most basic but a fundamental task for human-level scene understanding. Specifically, the following technologies have been applied: (i) an ordinary camera-mounted drone for capturing dynamic construction sites comprehensively and continuously; (ii) deep convolutional neural network frameworks for robust and prompt object detection and pose estimation; and (iii) single view-based rectification to restore original geometry of a scene, thereby estimating accurate spatial and kinematic information. The proposed method outputs the spatial coordinates of objects (e.g., workers and equipment) as well as their joint locations, which in turn enables automated safety hazard recognition such as proximity detection and ergonomic risk analysis. Demonstration on a real scene video shows the promising performances of the proposed method. Its accuracy in proximity detection was more than 95% (i.e., average distance error < 0.9 meters). In case of ergonomic risk, the developed method can estimate the ergonomic risks close to and even better than experts’ estimation (i.e., average of total 16 ergonomic professionals) on a near real-time basis.
System-Level Reliability-Based Design Optimization for Uncertain and Dynamic Wind-Induced Large-Scale Building Systems

Arthriya Suksuwan, Seymour M.J. Spence
Department of Civil and Environmental Engineering, University of Michigan, Ann Arbor, MI

This research aims to develop a methodology for solving wind-induced reliability-based design optimization problems posed on uncertain and dynamic building systems characterized by a large number of design variables and system-level constraints. One of the main challenges in the field of reliability-based design optimization is due to the tremendous growth in computational demand as the number of design variables increases. This difficulty has posed a limitation on solving practical design optimization problems involving large-scale infrastructure systems. In this contribution, an efficient simulation-based methodology is developed to tackle large-scale design optimization problems constrained by system-level performance targets. In particular, a novel decoupling strategy is developed based on defining and solving a sequence of an approximate system-level subproblem. Each subproblem is formulated using information derived exclusively from a single simulation carried out at a current design point. This property allows the reliability-based design optimization problems to be solved efficiently in a limited number of cycles notwithstanding the dimension of design variable vectors. To illustrate the applicability and efficiency of the proposed method, a case study is presented in which a wind-excited high-rise building system is optimized to satisfy the system-level reliability constraint.
Development of a Wireless Sensor Network Architecture for Dense and Rapid Deployment in Smart Cities

Katherine A. Flanigan, Jerome P. Lynch
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Unlike traditional urban environments, smart cities rely on automation and connectivity as central features of both physical (i.e. infrastructure) and social systems. As practical applications of smart city technologies such as autonomous vehicles, structural health monitoring, and automated water systems emerge, there is a growing need for an adaptable sensing platform that allows for the rapid deployment of dense sensor networks in cities for data collection. To address this need, a novel, ultra-low power wireless sensor architecture called Urbano was developed to serve as a versatile foundation of future automation and monitoring solutions in smart cities. Urbano consists of a low-power embedded microcontroller, flexible sensing interface, and uses a wireless cellular modem so that deployed systems do not require tethered or extensive wireless communication infrastructure which are not feasible in urban environments. The integration of a cellular modem into Urbano’s network architecture allows for connection to the internet, high precision time synchronization, and very high data rates. In addition, the embedded microcontroller is used for extensive on-chip data processing as part of a larger edge-computing structure associated with smart cities. An array of GPS enabled mobile air quality sensing nodes are deployed on food trucks in the city of Grand Rapids to serve as a validation of the proposed system. This network, which can easily be deployed on other modes of transportation such as city busses and school busses, also allows the city’s transportation officials to observe the behavior and locations of food truck vendors.
Performance of Foam Filled Tubular Steel Braces under Seismic Loading

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Extensive structural damage and subsequent economic losses resulting from seismic hazards are providing impetus for a paradigm shift toward resilience based design. With the prevalence of steel structures in seismic zones, there is a glaring need for supplemental damping systems that reduce the vulnerability of braced frames to premature fracture and provide a more stable structural response under seismic loading. To address these limitations, a novel system that employs lightweight, pourable and expandable polyurethane foam within the voids of round hollow structural section (HSS) braces is tested. Specifically, experimental results from six steel tubular braces with different diameter-to-thickness ratios tested under quasi-static cyclic loading are presented. The test data suggests that foam filled braces are effective in delaying the initiation of local buckling and thus prolonging the fracture life of braces when compared to their unfilled counterparts. To augment the experimental testing, a significant numerical parametric study will be undertaken to assess the influence of diameter-thickness and slenderness ratios on filled brace performance.
Developing Rapid, Accurate, and Field-Adaptable Sediment Testing by SedImaging

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Remediation efforts for America’s water systems is a time-consuming and expensive process. These efforts often involve testing and classification of the sediments of river bottoms and adjacent floodplains. Traditional sediment classification efforts require sending field samples to an off-site lab. The costs incurred from this can be prohibitive if large numbers of samples are to be tested. Additionally, it can take several days to weeks for the classifications to be performed. These high costs and extensive timelines have led to the need for development of alternative testing methods for classification that are rapid, accurate, and low-cost. A research program has been initiated at the University of Michigan to undertake this task. The overarching goal is to remove Polychlorinated biphenyl (PCB), (a likely carcinogenic hydrocarbon that has been banned within the United States since 1979) from a river system in Western Michigan. Sediment testing for classification is required in order to identify areas where PCB concentrations are expected. The research will employ a previously-developed SedImaging device to rapidly classify sediment samples from a portion of the river. The SedImaging device relies on image processing to classify, within a matter of minutes, a sample of soil sedimeted through a column of water. The soil classifications generated from the SedImaging device were compared to results obtained by traditional testing techniques, and the results showed excellent correlation. A low-cost, field-adaptable SedImaging device that will be used for full-scale field sediment testing along the river system is presently under development.
Adaptive perception, planning, and execution for robotized construction joint filling

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In order for a construction robot to perform work on a construction workpiece, the robot must determine the workpiece’s relative position, orientation, and shape, and then use that information to form a kinematic work plan. Due to large uncertainties in the robot’s own pose and differences between the workpiece’s actual and designed geometry, the robot must travel to the workpiece and perceive it in place to obtain sufficiently precise estimates of the relative pose and shape. The robot must then adapt its kinematic work plan to accommodate the circumstances it encounters. This research explores techniques for estimating the relative pose and shape of a workpiece in situ, converting the generated workpiece model into an adapted kinematic work plan, and executing the adapted plan. Although many elements of this research can be generalized and applied to other construction tasks, we focus on joint filling, namely caulking, as our example application for the development and evaluation of our methods. A robot’s performance capabilities are evaluated using a real industrial robotic arm to determine how well it can perceive, plan, and execute adaptive caulking on joint specimens of unexpected pose and shape. A 2D laser profiler is used for workpiece sensing, and a robotic caulking tool is presented for caulk dispensing. Using our methods, the robot was found capable of planning its joint filling process with a mean absolute positioning error of 0.5 mm and standard deviation of 0.2 mm.
How Accessible Are Our Cities? A Cross-sectional Analysis of Access to Green Space

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Adapting our cities requires us to resolve the contentious issue of social justice in access to core urban services. Green spaces provide a wide range of health and community benefits, and their access has been subject to much analysis. However, the generalizability of many existing conclusions is limited by both scope and resolution of analysis. Here, we evaluate access to green space in multiple US cities to: a) Investigate whether systemic inequity exists across US cities; and b) Assess the sensitivity of these conclusions to measures of amenity quality. This large-scale, fine-resolution analysis incorporates uncertainty and enables us to draw enhanced insights to answer these questions, essential to designing livable cities.
EBS: Engineering in Biological Systems
Biomaterial scaffolds recruit an aggressive population of metastatic tumor cells in vivo

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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 organ function 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. While survival has been shown to be a function primarily of immunomodulation caused by the scaffold, the behavior of scaffold-recruited tumor cells has been unknown. Human tumor cells were isolated from scaffolds, primary tumor, and bone metastasis using Miltenyi MACS kit. Cell lines were generated from each location and investigated for functional differences via scratch, migration, invasion, mammosphere, cancer stem cell markers, RNA-seq and qRT-PCR in vitro. Additionally, cell lines were inoculated into mice and investigated for metastatic ability. Cells derived from the scaffold were found to be more aggressive in vitro and more metastatic in vivo indicating the scaffold may capture a key population of tumor cells. 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.
A computational study of growth-driven folding patterns on shells, with application to the developing brain

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We consider the development of folds, or sulci (troughs) and gyri (crests), of the brain. This phenomenon, common to many gyrencephalic species including humans, has attracted recent attention from soft matter physicists. It occurs due to inhomogeneous and predominantly tangential growth of the cortex, causing circumferential compression and leading to a bifurcation of the solution path into a folded configuration. The problem can be framed as one of buckling in the linearized elasticity regime. However, the brain is a very soft solid subject to large strains due to inhomogeneous growth. As a consequence, the morphomechanics of the developing brain demonstrates an extensive post-bifurcation regime. Nonlinear elasticity studies of growth-driven brain folding have established the conditions necessary for the onset of folding and for its progression to configurations broadly resembling gyrencephalic brains. The reference, unfolded, configurations in these treatments have a high degree of symmetry--often spherical. Depending on the boundary conditions, the folded configurations have patterns of symmetry or anti-symmetry. However, these configurations do not approximate the actual morphology of, e.g., human brains, which display unsymmetric folding. More importantly, from a neurodevelopmental standpoint, many of the unsymmetric sulci and gyri are notably robust in their locations. Here, we initiate studies on the physical conditions and parameters responsible for the development of primary sulci and gyri. In this preliminary communication we work with idealized geometries, boundary conditions and parameters to perform computations aimed at understanding the formation of the first fold to form: the Central Sulcus.
Heat as a novel treatment of *Staphylococcus epidermidis* biofilms in an *in vitro* catheter model

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Bacterial biofilms are a leading cause of hospital-acquired infections. The development of biofilms on medical devices, such as hemodialysis catheters, can be understood as a consequence of adsorption, growth, and detachment; each effect is governed by self-assembly, fluid mechanics, and transport phenomena which are governed by fundamental chemical engineering principles. Here we show how the fundamental chemical engineering principles of fluid dynamics and heat transfer can be applied to prevent and/or remove bacterial biofilms in an *in vitro*, flow cell model of a dialysis catheter. Using *Staphylococcus epidermidis*, the most common bacterial species isolated from infected medical devices, we grow biofilms under physiologically relevant flow conditions and expose them to thermal degradation using a pre-warmed fluid that is injected into the model catheter. We establish that exposing biofilms to elevated temperatures changes the biofilm morphology and cell viability. Further, we discuss the mechanism by which this degradation occurs in light of the two parameters temperature elevation and exposure duration. Finally, we probe the resilient, adaptive nature of bacterial cells to investigate if they develop thermal resistance when exposed to the heat treatment. Understanding the response of these bacterial cells under thermal stress is a promising step toward the development of an *in situ* treatment/remediation method for biofilm growth in medical devices.
Multiparametric MRI Defines Temporal and Spatial Heterogeneities in Thrombosis: Towards Precision Medicine in Deep Vein Thrombosis

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Venous thromboembolism (VTE), consisting of deep vein thrombosis (DVT) and its sequelae pulmonary embolism, is an elusive illness affecting an estimated 900,000 people in the United States each year. Despite the dynamism of venous thrombosis research in the last decades, the standard treatment of anticoagulants has remained unchanged since the 1950s and carries significant bleeding risk. Alternative treatments such as catheter directed thrombolysis are only successful in early stages of thrombus progression. We aimed to develop MRI techniques to determine thrombus composition in two murine inferior vena cava models, representing the two possible clinical scenarios of a fully occlusive or partially occlusive thrombus. Multiparametric sequences were optimized for visualizing heterogeneities within the thrombus via T1- and T2-weighted fast spin echo, and T2*-weighted gradient echo sequences. Mice were imaged at days 2, 6, 14, and 21 following thrombus induction. Thrombus composition varied spatially and temporally in all subjects. Low T2* signal, indicating structured material such as a fibrin mesh, was most prevalent at day 2 in both models. Regions with high T2 signal were more prevalent at all time points studied in the stasis model compared to the blood flow model, indicating an increased inflammatory response in fully occlusive thrombi. This work demonstrates for the first time that non-contrast multispectral MRI can provide information on thrombus composition. This methodology could eventually be used clinically to predict patient-specific susceptibility to DVT lysis therapies, which would reduce risk of death and improve quality of life.
A Polymeric Nanoparticle Platform for the Prevention of Relapsing-Remitting Experimental Autoimmune Encephalomyelitis

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Polymeric nanoparticles have been utilized to induce antigen specific clinical tolerance in multiple immune models by several groups and are currently undergoing clinical development. Methods of antigen delivery by nanoparticles general utilize either surface coupling or encapsulation methods which are often limited by poor polydispersity, uncontrollable Ag loading and release, and possible immunogenicity. We introduce a nanoparticle platform formulated by conjugation of antigenic peptides to poly(lactide-co-glycolide) and subsequent emulsion synthesis to form antigen-polymer conjugate nanoparticles (acNPs). Importantly, acNPs exhibit modular loading of single or multiple antigens, low burst release, and minimally exposed surface antigen. In vitro assays were conducted to decouple the role of NP size, concentration, and Ag loading on regulatory T cell (T_{reg}) induction. CD4+CD25+Foxp3+ T_{reg} induction depended on acNP size, but CD25 expression of CD4+ T cells did not. When applied prophylactically in relapsing-remitting experimental autoimmune encephalomyelitis (RR-EAE), a murine model of multiple sclerosis, acNPs limited disease progression induced by a single peptide or multiple peptides. This platform provides a simple, modular, and well-defined method to synthesize particles with highly-controlled physicochemical properties and will be valuable as a tool to answer complex mechanistic questions related to nanoparticle-induced tolerance.
Effects of three-dimensional MT topology on kinesin-mediated nanotransport

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In order to transport cargoes inside cells, kinesin motors must navigate through complex cytoskeleton structures including three-dimensional microtubule topologies. Revealing kinesin transient dynamics in the complicated track system can give important information about the mechanisms that govern the powerful intracellular transport. We have recently developed a stochastic quantitative model to study the effects of microtubule topologies on single/multiple kinesins walking motion and cargo diffusion. Our model predicts different dynamics kinesin use to overcome mechanical barriers of nearby or intersecting microtubules and adjust transportation direction. The further development of the model can provide a deeper understanding of the cytoskeleton mediated intracellular trafficking machinery.
Morphological-Feature-Based Cancer Cell Migration Prediction Using Artificial Neural Network (ANN)

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Metastatic disease causes death of most patients with breast cancer and other solid malignancies. The ability of a cancer cell to migrate critical determines metastatic potential. Identification of cancer cells with high potential to migrate typically relies on markers for epithelial-to-mesenchymal transition (EMT), a process that increases cell migration and metastasis. Marker-based approaches are limited by inconsistencies among patients and types of cancer and existence of partial EMT states. As an alternative strategy, we sought to identify morphological features of cancer cells directly correlated with cell migration. Using a single-cell microfluidic migration chip and high-content fluorescent imaging, we extracted morphological features and recorded migratory direction and speed of 1,358 SUM159 breast cancer cells. By applying Random Decision Forest (RDF) and Artificial Neural Network (ANN) methods, we achieved over 99% prediction accuracy for movement direction and 82% for moving speed. We also pinpointed features determining cell migration, including not only known features related to cell polarization but also novel ones that can drive future mechanistic studies. We further validated key features by comparing wild-type cancer cells with doxorubicin-treated and selected highly migratory cell populations. Predicting cell movement by computer vision establishes a ground-breaking new approach to analyze cell migration and metastatic potential.
Gene expression profiling of tumor cell subpopulations derived from implantable biomaterial scaffolds in mice with metastatic breast cancer

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Metastasis is a complex process in which circulating tumor cells migrate from the primary tumor to other tissues through the bloodstream or lymphatic system colonizing distant sites in the body. The primary tumor secretes various diffusible factors and chemokines to attract immune cells such as macrophages and lymphocytes conditioning the target site of metastasis and forming a pre-metastatic niche. This pre-metastatic niche has been found to contribute towards tumor cell colonization, and a strategy for effectively identifying the factors promoting metastatic cell homing can help in limiting the process of tumor cell metastasis. Based on the concept of the premetastatic niche, a biomaterial scaffold that recruits metastatic breast cancer cells through local immune response in vivo was implanted in mice. RNA was isolated from the scaffold captured tumor cell line and qRT-PCR analysis was conducted to establish a novel gene expression signature as an important determinant of in vitro functional behavior. The scaffold recruited tumor cell line showed elevated expression levels of CD151, PTEN and P53 while the primary tumor cell line showed elevated expression levels of ADAMTS18, BRCA2, CD163, IL8, IL23A and SPEN.
Serially passaging ovarian cancer spheroids in vitro in 3D hanging drop array as a model for emergence of chemoresistance and enrichment of cancer stem cell population

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Despite a usual good initial response to chemotherapy, over 85% of patients treated for ovarian cancer relapse due to chemoresistance and metastasis (Ip, C. K.M. et al, Scientific Reports 6, 2016). The development of chemoresistant tumors with malignant ascites, leads to increasing difficulty in treatment and spread of disease that can cause the formation of intraperitoneal tumors. Still, there are few studies to examine the emergence of chemoresistance. In this study, we describe a novel chemoresistance model that further elucidates role of cancer stem cells in metastases and chemoresistance.

Ovarian cancer spheroids were serially passaged on a 3D hanging drop array from each of the following: the OVCAR3 cell line, patient-derived ascites cells (Pt224), and a patient tumor sample (Pt412OV). The spheroids from passage 0 (P0) to passage 6 (P6) were evaluated for proliferation, and response to treatment with cisplatin and an ALDH inhibitor, Compound 673A, as well as levels of expression of cancer stem cell markers ALDH1A and CD133. Serially passaged spheroids had increased cellular proliferation when comparing P0 to P6. Resistance to cisplatin treatment increased with serial passage, along with increased sensitivity to Compound 673A. Furthermore, both ALDH1A and CD133 positivity increased significantly from P0 to P6. Lastly, tumorigenicity increased with serial passage. The data indicates that serial passaging of ovarian cancer spheroids in vitro enhanced proliferation and chemoresistance, enriched the population of cancer stem cells, and led to faster tumor initiation. This data indicates the usefulness of this model for examining the emergence of chemoresistance.
FAT: Fluid Dynamics, Acoustics, and Thermal Science
Laser-Optical Investigation of Highly Radiative, High Temperature Homogeneous Combustion

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Homogeneous Combustion (HC) and its various variants, have emerged as attractive techniques to abate NO\textsubscript{x} emissions (produced via the “thermal” route or Zel’dovich mechanism) and enhance efficiency of various combustion systems. It has been conclusively shown (in existing literature) that for homogeneous combustion, Damköhler number (Da) (ratio of reaction rate and advective transport rate) must be very close to unity. As Da increases, inhomogeneity increases, constraining the combustion to thin regions of intense reaction (flames), which in turn, aggravate NO\textsubscript{x} emissions. In applications such as engines or gas turbines, since the useful output is work, low temperature reactions are an excellent way to combat NO\textsubscript{x} emissions. However, for high temperature applications (industrial heating/furnaces), especially with enriched oxidizer streams ($x_{O_2} > 0.21$), if heat is not transferred fast enough from the reaction zone, reaction rates are accelerated (Da increases) and promote flaming tendencies. This work explores usage of fuel blends containing small proportions of sooting fuels (ethylene) with the conjecture that radiative heat transfer would be enhanced by presence of soot particles in the reaction zone as their emissivity is higher in comparison to the combusting gases. The relationship between quantity of soot (in terms of volume fraction, determined by laser extinction) in different control volumes and heat radiation from these is also investigated. It is shown that the addition of ethylene increases the heat radiation from the reaction zone for similar temperature distributions. There exists an optimal blend ratio though, exceeding which causes a flame-dominated global reaction for the current geometrical configuration.
Kelvin-Helmholtz evolution in subsonic cold streams feeding galaxies

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The most prolific star formers in cosmological history lie in a regime where dense filament structures carried substantial mass into the galaxy to sustain star formation without producing a shock. However, hydrodynamic instabilities present on the filament surface limit the ability of such structures to deliver dense matter deeply enough to sustain star formation. Simulations lack the finite resolution necessary to allow fair treatment of the instabilities present at the stream boundary. Using the Omega EP laser, we simulate this mode of galaxy formation with a cold, dense, filament structure within a hotter, subsonic flow and observe the interface evolution. Machined surface perturbations stimulate the development of the Kelvin-Helmholtz (KH) instability due to the resultant shear between the two media. A spherical crystal imaging system produces high-resolution radiographs of the KH structures along the filament surface. The results from the first experiments of this kind, using a rod with single-mode, long-wavelength modulations, will be discussed.
Output Error Control for Unsteady Flow Simulations

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We present a numerical error control strategy for unsteady flow problems based on unsteady r-adaptation, i.e. mesh motion. The method uses discrete unsteady sensitivities to compute an error estimate in a scalar output of interest. This estimate yields an error indicator that identifies regions in space and time where refinement is required to reduce the output error. Rather than employing standard refinement techniques that increase computational degrees of freedom, we adapt the mesh by moving its nodes. This allows elements to grow or shrink without increasing the degrees of freedom. The mesh motion is performed using analytical contraction/expansion functions and node-interpolated motion driven by a spring analogy. We demonstrate the ability of such motion to reduce output error in Euler equations with some preliminary results. In one sample result, we demonstrate our r-adaptation functionality with an airfoil encountering a vortex. We perform two solutions for this case, one for a static mesh and one for an r-adapted mesh. The lift integral output error on the static mesh is estimated to be $-1.6 \times 10^{-3}$. On the other hand, the lift integral output error on the r-adapted mesh is estimated to be $-2.54 \times 10^{-5}$. This case exhibits a significant output error reduction from the static mesh to the r-adapted mesh. Our research on r-adaptation helps the solver to produce more accurate solutions.
Numerical Analysis of Local and Global Hydroelastic Response to Wetdeck Slamming Events on Multihull Vessels

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Catamarans operating in a large sea state encounter slamming events on the wetdeck that lead to structural failure. Wetdeck slamming is a non-linear process which involves complex free-surface topology, high-velocity water jets, and breaking waves interacting with the bow and deck-hull geometry. The slamming process generates large pressures and loads that are time dependent and concentrated in space. The structure responds in a coupled manner to the complex fluid loading. Common approaches to design for the limiting slamming loads include analytical models or segmented model tests. Analytical slamming models assume a linear free-surface, prescribed velocities, and simplified geometries. These simplified assumptions make it difficult to apply to realistic cases. Experimental model tests capture slamming loads by using segmented models attached to a backspline. It is difficult to scale results to full-scale and to recreate model scale conditions that lead to the limiting load cases.

It is proposed to use a high-fidelity fluid-structure interaction solver to study a simplified impact problem and slamming on a catamaran. The canonical problem is a flat plate impacting a curved water surface. The curvature of the water surface will be varied in both directions to examine the influence of non-planar hull-wave impact. The influence of non-planar impacts is a critical missing link in the applications of analytical impact theories. Catamaran slamming simulations will be studied while modeling both local and global hydroelastic effects. The full field data provided by the numerical solver will be used for careful evaluation of existing impact models.
Radiative Heat Transfer in a Particle Laden Flow: Numerical Methods

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Radiative transfer through a discrete particle cloud presents a series of difficult problems which can only be answered with high fidelity modeling. Our work investigates the heat transfer through a cloud of small (12 micron) particles in a square, turbulent test chamber. Two infrared sources are considered: a incoherent conical source and a coherent Gaussian source. Monte Carlo ray tracing techniques have proved to be the only feasible means to perform these calculations. Furthermore, one must parameterize a series of geometric and physical parameters. Properly calibrated, one can construct models which predict transmission well within experimental error (a project currently being carried out at Stanford University). Moreover, we have shown that our models are most sensitive to geometric parameters.
High-Capacity Thermal Energy Storage Materials: Identification by Computational Screening and Machine Learning Analysis

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Thermal energy storage (TES) can be used in a variety of applications and temperature ranges to either regulate a system’s temperature or store generated heat. Hydration/dehydration reactions are promising methods for the storage of thermal energy due to their simplicity, cost effectiveness, and potential for reversible operation at moderate temperatures. The goal of this work is to identify thermal energy storage materials that can outperform known compounds. High-throughput Density Functional Theory calculations were performed on metal halide hydrates and metal hydroxides from the Inorganic Crystal Structure Database. In total, 265 hydration reactions were characterized with respect to their gravimetric and volumetric energy densities, and their operating temperature range. Promising reactions were identified for applications that fall into three temperature ranges: low (< 100°C), medium (100°C - 300°C), and high (> 300°C). Energy density trends amongst the salt hydrates and metal hydroxides are discussed. Additionally, machine learning techniques such as Principal Component Analysis and Decision Tree learning were used to explore correlations between fundamental material properties and thermal storage. Our study suggests new materials for TES, and identifies pathways for additional performance optimization.
High-Speed Imaging Studies of Gasoline Fuel Sprays at Fuel Injection Pressures from 300 to 1500 bar

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High-pressure gasoline fuel injection is of considerable interest due to the improvements in fuel atomization and mixing that occur with higher injection pressure to improve combustion efficiency and lower emissions. The objective of this study was to quantify the effects of high fuel injection pressure on transient gasoline fuel spray development for a wide range of injection pressure including pressures over 1000 bar. The spray development was investigated in a constant volume combustion chamber using high-speed imaging. Reference grade gasoline was injected at fuel pressures of 300, 600, 900, 1200, and 1500 bar into the chamber which was pressurized with nitrogen at 1, 5, 10, and 20 bar at room temperature (298 K). The bulk spray data were used to quantify spray penetration distance rate, and spray cone angle. The near-nozzle data were used to evaluate the early spray development. All imaging data were evaluated for potential effects of cavitation. The bulk characteristics of the high pressure gasoline sprays were consistent with results from lower fuel injection pressures, e.g. where sprays with higher cone angles were produced with increasing chamber pressure at constant fuel injection pressure. The sprays approached a similar penetration rate after the spray break-up time. The experimental results for a majority of the conditions were under-predicted by most of the empirical models derived from previous diesel and gasoline studies. The near-nozzle experiments produced interesting phenomena at the very early times of the sprays (times much earlier than the spray break-up time) for some experimental conditions.
Mass-Varying Aerothermoelastic Hypersonic Vehicle Modeling and Simulation

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This work represents the continued development and expansion of the University of Michigan’s High-Speed Vehicle (UM-HSV) simulation framework, developed at the Active Aeroelasticity and Structures Research Laboratory. Hypersonic vehicles are characterized by their high energy flight environment, where high thermal loads and high dynamic pressures induce powerful interactions between the thermodynamics, structural dynamics, and unsteady aerodynamics. Multi-physics and multi-fidelity reduced order modeling techniques have been developed to balance analytical models that are computationally fast and couple well but make several simplifying assumptions to represent a real system, and advanced numerical simulations that produce high fidelity individual physics models but cannot couple well among the disciplines and, moreover, make rapid simulation computationally infeasible.

Hypersonic vehicle trajectories can be divided into three regimes: the boost phase, cruise phase, and terminal phase. In the boost phase, typically a booster vehicle burning solid propellant is used to accelerate the hypersonic vehicle along an ascent trajectory to a target velocity and altitude. This flight regime complicates the time simulation as the inertial and structural characteristics must be constantly updated as the fuel depletes. The drastic change in velocity and altitude also presents more dynamic aeroheating conditions and further optimization techniques must be used in order to maintain accuracy and maximize computational speed. This poster is meant to showcase the development and reduced order modeling techniques for a boosted hypersonic vehicle used in the UM-HSV framework.
Flow Control Using Passive Vortex Generators

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In wall-bounded turbulent flows [Frisch, 1995] [Richardson, 1922], the onset of instability inside the boundary layer results in flow separation and subsequent deviation of flow behavior. Such separated flows are generally associated with adverse effects such as increased drag on airfoil of wing thereby reducing its aerodynamic efficiency. Moreover, the highly nonlinear behavior of flow makes the complete understanding of flow physics rather more difficult. Experimental investigations are expensive and need time and sophisticated setups. Due to losses of energy associated with boundary layer separation it is important to be able to control the separation. The idea behind separation control is to energize the boundary layer by adding momentum through some mechanism to the near wall region by using solid bluff bodies placed inside the boundary layer that 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 identify the mechanisms that help in modulating flow behavior to mitigate separation. Here we use single cube as a passive VG to modulate turbulent flow over 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. The flow behavior depends on the size and shape of the VG and accordingly the mechanisms that enable flow control may differ.
Big data analysis for damage characterization of aerospace structures based on nonlinear guided wave simulation tool UM/LISA

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The purpose of the research is to develop efficient damage detection algorithms for effective characterization of various damage features inside aerospace structures, based on a large data library of damage scenarios generated by the nonlinear guided wave simulation tool UM/LISA. UM/LISA is a very efficient and versatile tool that is developed in A2SRL laboratory at the U-M's CoE for guided wave simulations in structures, considering features such as non-reflective boundary, piezoelectric coupled multi-physics field, strain-based damping model, nonlinear contact dynamics, and the capability for multiple GPU platform. The numeric simulation not only helps us understand guided wave interactions with structural damages, it also plays a vital role in the damage characterization algorithms, through building a large database of simulation cases with virtually all possible damage scenarios, and then correlating test signal with the database to obtain the information about the damage. Matching pursuit algorithm for extracting time and frequency centers from the signals is adopted to localize and estimate possible damage on typical aerospace structures, and big data analysis is performed on the damage library to determine most obvious signal features. The overall damage characterization framework for typical aerospace structures will be given, and the damage detection algorithm computes a special distribution of matching merit metric to illustrate regions of high likelihood of having damage while also providing the corresponding damage size estimation. The work will also look into some practical examples in an effort to demonstrate the effectiveness of the algorithms for complex engineering structures.
Multi-artery heat-pipe spreader: monolayer-wick receding meniscus transitions and optimal performance

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For high heat flux and low thermal resistance, the multiple-artery heat-pipe spreader uses distributed high-permeability arteries (posts) for liquid supply and high-capillary pressure monolayer wick for liquid spreading and evaporation. Experiments indicate the receding meniscus transitions in monolayer play a role in sudden drop in thermal resistance prior to dryout. Using monolayer SEM images and the minimum surface energy principles, the meniscus dynamics up to dryout is analyzed, and the meniscus location, capillary pressure, effective thermal conductivity, and permeability are also predicted for heterogeneous, periodic sintered copper-particle (including bimodal particle size) unit cells. The liquid thickness is nonuniform within the heterogeneous unit cell, and with increase in the wick superheat local dryout occurs (meniscus snaps) in the loose-packed region influencing the wet-wick properties and the occurrence of the minimum thermal resistance. The monolayer wick continues to function under local dryout (away from post) until a receding dry front is formed followed by complete dryout. These predictions are in good agreement with experiments. The optimal wick thermal-hydraulic performance, i.e. dimensionless ratio of heat flux to thermal resistance (wick figure of merit $Z_m$) is sought through analysis. The uniform, sintered, close-packed 30–50 µm particles give the highest $Z_m$ over a range of superheat in the wet regime, and 30 µm particles give a record low resistance near 2.5 µK/(W/m²). For further study, a canopy wick can be implemented to the post-monolayer structure to remove the vapor and to increase the heat transfer efficiency using flow boiling phenomena.
IVM: Integrated Circuits, VLSI, and Microsystems
Many technologies rely on GPS for navigation, but a reliable signal is not always available. Inertial sensors can supplement GPS, which has been demonstrated with large-scale sensors in satellites and airplanes. Shrinking the size and cost of these sensors will have widespread benefits for a range of defense and consumer applications, including munitions, autonomous vehicles, and drones; however, at the micro-scale mechanical and electronic noise can dominate the signal. This research focuses on developing a resonator for a micro-gyroscope that aims to quiet the noise and provide a reliable means of navigation by reducing energy dissipation and maximizing symmetry.

This poster addresses the challenges of creating 3D micro-shell resonators out of fused silica, and explains how we accomplished it with a unique blowtorch molding technique. It examines common fabrication defects, considering their contributions to energy dissipation, and discusses the steps we have taken to mitigate them. Applying the knowledge gained from our experiments has led us to create resonators with very low energy dissipation, leading to micro-shells with the longest ring-down times and some of the highest quality factors in the world. We believe our resonators will lead to high-performance micro-gyroscopes that could enable widespread affordable inertial navigation.
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. We report the latest experimental results from a fused-silica Birdbath Resonator Gyroscope (BRG) with a quality factor of 450k and a resonant frequency of 9058 Hz. The BRG and its readout/control system achieve an angle random walk (ARW) better than 0.0087 deg/√hr and a bias stability of 0.0391 deg/hr. This result was obtained using a force-rebalanced control architecture without temperature control or additional compensation. The device performance is improved by driving the resonator at displacements near 10% of the nominal electrostatic gap. The low gyroscope noise is attributed to a relatively large measured scale factor of 100 mV/deg/s. Our readout/control system is implemented using a combination of custom integrated circuits, FPGA, and software.
RF-Echo: Decimeter Accurate, Long Range Localization System Using Low Power ASIC Tag for Public Safety Applications

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Long-range low-power localization is a key technology that enables a host of new applications of wireless sensor nodes. We present RF-Echo, a new low-power RF localization solution that achieves decimeter accuracy in long range indoor non-line-of-sight (NLOS) scenarios. RF-Echo introduces a custom-designed active RF reflector ASIC (application specific integrated circuit) fabricated in a 180nm CMOS process which echoes a frequency-shifted orthogonal frequency division multiplexing (OFDM) signal originally generated from an anchor. The proposed technique is based on time-of-light (ToF) estimation in the frequency domain that effectively eliminates inter-carrier and inter-symbol interference in multipath-rich indoor NLOS channels. RF-Echo uses a relatively narrow bandwidth of ≤80 MHz which does not require an expensive high sampling rate analog-to-digital converter (ADC). Unlike ultra-wideband (UWB) systems, the active reflection scheme is designed to operate at a relatively low carrier frequency that can penetrate building walls and other blocking objects for challenging NLOS scenarios. Since the bandwidth at lower frequencies (2.4 GHz and sub-1 GHz) is severely limited, we propose novel signal processing algorithms as well as machine learning techniques to significantly enhance the localization resolution given the bandwidth constraint of the proposed system. The newly fabricated tag IC consumes 62.8 mW active power. The software defined radio (SDR) based anchor prototype is rapidly deployable without the need for accurate synchronization among anchors and tags. Field trials conducted in a university building confirm up to 85 m operation with decimeter accuracy for robust 2D localization.
Researchers have continued to explore approaches to develop miniaturized sensors and actuators with improved performance, enhanced functionality, smaller size and lower cost. Innovations are made possible with significant advances in design/analysis techniques, ICs, micro/nano fabrication and packaging technology. Biological systems in nature provide us with inspiration for engineering and one common structure is the “hair”. Large array of hair is promising candidate for a MEMS multi-transducer platform that may offer improved sensitivity and selectivity, redundancy, robustness, and increased dynamic range. In this research, we developed the microfabrication technology to build a unique 3D biomimetic hair structure for multi-transducer platform. Direct integration with CMOS will enable signal processing of dense arrays of MEMS transducers within a small chip area. Based on this structure, we built and tested capacitive and threshold MEMS accelerometer arrays. The novel process circumvents the stringent requirements on DRIE of thick (1mm) silicon. The device can achieve sub-μg resolution (< 1μg/√Hz) and high sensitivity (1pF/g/mm²), having an area smaller than any previous precision accelerometers with similar performance. This technology is suited for forming MEMS transducer arrays including: 1) high performance inertial measurement units that require large dynamic range, high resolution, as well as robustness and fault tolerance; and 2) large arrays of miniaturized detectors and actuators with high temporal and spatial resolution, analogous to high-density CMOS imagers.
A Charge-Mode In-Memory Computing Deep Neural Network

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In this work, we propose an all layers all weights on-chip deep learning accelerator based on pulse width modulation. Key challenges of a comprehensive deep learning system include layer to layer connections, energy and latency constraints from data movement, implementation of non-linear functions such as sigmoid and ReLU. Our proposed system modulates input images into pulse width and computes dot-product as charge integration of SRAM’s read buffer currents over pulse widths. With this in-memory computing approach, energy and delay for weight retrieval can be removed. Dot-product outputs are stored as analog voltages, and converted into pulse width again by comparison to non-linear signals. Outputs modulated in pulse width enable layer to layer connection simple and fast, as standard digital buffers can easily drive pulse signals without information loss. Maxpooling, which is a common computation in modern convolutional neural network can easily be implemented with OR gate. Intermediate values during inferences all remain in analog domain either as voltages or pulse widths, removing analog to digital conversion overhead and allowing an energy efficient high-throughput accelerator. A test chip with 17 convolutional layers, an average pooling layer, and a fully connected layer is being fabricated in CMOS 28nm technology. The chip area is 11.5mm² and consumes 300mW to 700mW power in simulation.

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Air-vehicle systems (AVS) show a promising capability to conduct both indoor and outdoor missions in a confined environment by reducing the size to micro-air-vehicles (MAVs) and nano-air-vehicles (NAVs). To extend the operation time, it is essential to reduce the payload and power dissipation of sensors and controllers especially for navigation of next-generation NAVs. Traditionally, AVS used separate image sensors and digital processors/controllers, however these additional components result in high payload and additional power consumption, especially for communicating among components. Recently, integration of image sensing arrays and processing units together on chip has shown promising results in low-power optic flow generation. Several object recognition chips have been reported for navigating MAVs. However, these systems still need additional sensors to provide crucial information for navigation, such as obstacle avoidance and self-status, which can be acquired from optic flow sensors.

We report a single-chip vision-based navigation chip, which is the first attempt to provide both object recognition and bio-inspired 2D optic flows (OF) to suppress the payload and the power dissipation. Among many feature-extraction methods, we implemented the histogram-of-oriented-gradients (HOG) because of its robustness against illumination variation and complicated background. However, the HOG feature and support vector machine require a complicated calculation, huge memory and high-resolution images. In this work, we implement the gradient orientation with 2b spatial difference images and cell-based classification to save both payload and power. The system achieved 75% memory size reduction and 272.49 pJ/pixel for object recognition and 2D optic flow generation.
Time Synchronization in a Network of Bluetooth Low Energy Beacons

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Time synchronization is a vital feature in many wireless sensor networks with applications ranging from structural health monitoring systems to body area sensors used for rehabilitation and sport medicine. While different wireless protocols have been utilized in sensor networks, Bluetooth Low Energy (BLE) has drawn a lot of attention in the past years due to its low-power architecture and availability in many consumer electronics. Moreover, the added non-connectable beacon mode has increased its functionality for Internet of Things (IoT) and sensor fusion. However, in this mode as devices are not paired with each other no synchronization service is available. In this work, we present a synchronization protocol based on BLE beacons that can be used in conjunction with BLE software stacks provided with a commercial Bluetooth System-on-Chip (SoC). Offset and frequency-drift estimation techniques are discussed, and the effects of number of synchronization packets and their intervals on the overall synchronization accuracy are investigated. Experimental results show that without any resynchronization in ten minutes, average synchronization errors of less than 350 ns per minute (single hop) can be achieved.
**In Situ Acoustomagnetic Interrogation of a Glaucoma Valve with Integrated Wireless Microactuator**

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This work describes the design, fabrication and *in situ* evaluation of a system developed for interrogation of an actuator-integrated glaucoma valve. An implanted glaucoma valve facilitates drainage of aqueous humor from the eye to help lower intraocular pressure in patients with glaucoma. Over time, adhesion of endothelial cells can lead to fibrosis around the valve which, in turn, increases the resistance to aqueous humor outflow. Here, a customized magnetoelastic actuator is integrated on the valve to limit the fibrosis and encapsulation of the valve that can otherwise lead to implant failure. An interrogation system is needed to facilitate in vivo studies and confirm the vibration of the actuators after implantation. The system described here excites the actuator magnetically and verifies the actuation by sensing the acoustic signals generated by the vibrating actuator. This work focuses on increasing the wireless range, reducing signal feedthrough, and establishing the clinical utility of the system. Physical domain decoupling, i.e., sensing the acoustic signal from the magnetically excited actuator, reduces the signal feedthrough. A series of signal processing techniques are implemented to improve the signal to noise ratio and thus wireless range. *In vitro* experiments performed with the system demonstrate a signal-to-noise ratio of \(\approx 140\). *In situ* experiments, performed with the actuator-integrated valves implanted in porcine eyes, achieve a signal to noise ratio of 3-6. Successful *in situ* experiments verify the functionality of the actuator even after implantation. These are the first recorded acoustic signatures through tissue from an implanted magnetoelastic device.
IOF-1: Industrial, Operations, and Financial Engineering Session 1
The role of behavior in undermining the effectiveness of adaptive measures in reducing long-term vulnerability to natural hazards

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How to defend the world’s cities from natural hazards is the subject of intense debate. Allegedly some adaptive measures increase vulnerability to unforeseen events. Here, we quantitatively examine how vulnerability changes using different adaptive strategies. As an example, we developed a cellular automaton model of land use change to measure a town’s vulnerability to repeated tsunamis. We compare alternative sea wall heights with increasing community awareness of the hazard to determine how a coastal community’s risk of building stock damage evolves over time when subjected to repeated tsunami events. We find that while hard adaptive measures protect against expected events, they increase development’s vulnerability to future, larger events, as occurred leading up to the 2011 Great East Japan Tsunami. Actions to avert development from risk zones appear more effective. These results quantitatively challenge existing practice for hazard adaptation and demonstrate maladaptation due to hard-adaptive measures.
The replacement of deteriorating distribution pipes is an important process for water utilities. It reduces water main breaks which in turn lowers water loss, capital spending on emergency repairs, and improves customer satisfaction. To assist the development of an effective renewal plan, statistical models have been used to provide forecasts of the future likelihood of breaks to guide inspection and replacement planning. This process is difficult for utilities with older systems due to the lack of readily available pipe network data. This study examines whether accurate and useful predictive models can be built in the complete absence of pipe-feature data, using road segments as a spatial proxy of the system combined with publicly available demographic and environmental data. Using a 51-month historical break record from a Mid-Atlantic utility, multiple classification algorithms were attempted which includes: linear models, tree-based models, ensemble methods, and boosting algorithms. This study shows that while predictive accuracy suffers with the lack of pipe-level detail, it is still possible to create a model suitable for informing inspection planning.
Eye tracking: a promising method for measuring trust in automation in real time

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Trust miscalibration, a mismatch between a person’s trust in automation and the system’s actual reliability, is a major concern for human-automation interaction. Trust miscalibration can lead to misuse or disuse of automated systems. To be able to study and address this issue, a valid and reliable measure of trust is needed. To date, most research on trust calibration has relied on subjective ratings. However, providing such ratings can be disruptive of task performance and yields only snapshots of momentary trust. Understanding the process of trust calibration requires a real-time trust measure instead. The present study investigated whether eye tracking can be used for this purpose. Participants were asked to monitor video feeds from six simulated unmanned aerial vehicles (UAVs) to detect possible targets with the assistance of onboard automation. They were informed, in advance, of the overall reliability of the target detection systems (TDS; 50% and 95%, respectively). It was expected that high reliability would result in higher trust and less monitoring of the respective UAV. Various eye tracking metrics reflected different trust levels, closely mirroring subjective ratings. Participants’ total visit duration, average visit duration, total fixation duration and average fixation duration were significantly longer for low reliability TDSs (50% reliable), compared to high reliability TDSs (95% reliable). Total fixation counts were also significantly higher for low reliability automation, and they were particularly sensitive to real-time changes in automation performance. In summary, these findings confirm that eye tracking is a very promising tool for supporting future research into trust calibration.
Visual and auditory feedback to improve touchscreen usability in a turbulent environment

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Touchscreens are being introduced to various mobile environments that are, at times, affected by vibrations and turbulence, such as modern car cockpits or flight decks of commercial and military aircraft. To date, very few studies have investigated the nature and severity of potential difficulties with touchscreen usage in those conditions and domains. To help fill this gap, the current study examined the performance effects of turbulence on a (simulated) modern flight deck on two tasks, flight plan entry and electronic checklist use. In two experimental conditions, visual or auditory feedback on touchscreen entries was presented to support error detection, fast completion times and multitasking. Nineteen pilots performed the two tasks in both calm and turbulent conditions, during manual flight or on autopilot. Results show that unaided performance (no feedback on touchscreen entries) suffered significantly in turbulence, in terms of the number of errors and completion time for both tasks. The availability of visual or auditory feedback did not significantly reduce errors, improve error detection or decrease response time. An increase with response time was even observed when visual feedback was provided for the flight plan entry tasks. However, feedback improved overall performance as pilots were better able to timeshare the manual flying and the touchscreen tasks. Subjectively, pilots preferred auditory feedback for text entry during manual flight and in turbulence. The findings from this study can inform the design and certification of touchscreens for a wide range of mobile environments.
Smart Production Systems: Theory and Application

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Smart Production Systems (SPS) are production systems capable of self-diagnosing and designing optimal continuous improvement projects, leading to the desired productivity improvement. SPS may operate in two regimes – semi-autonomous and autonomous. In the semi-autonomous regime, SPS computes the optimal continuous improvement project, while the Operations Manager authorizes its implementation (manager-in-the-loop). In the autonomous regime, the SPS-designed continuous improvement project is submitted for implementation without an external approval.

To be “smart”, a production system must be equipped with an Advising Tool (AT) consisting of Information Unit (IU), Analytics Unit (AU), and Optimization Unit (OU). The IU utilizes sensing/computing/communication devices (e.g., Industry 4.0 technology) to monitor machine parameters and performance metrics. The AU utilizes the theory of Production Systems to analyze system’s health and investigate various “what if” scenarios of potential improvement. The OU utilizes the methods of Artificial Intelligence to select the optimal advice for achieving the desired productivity improvement (if possible).

In this research, we construct the foundations of SPS advising tool and implement it on simulated and real production plants.
Comparing Two Goods-to-Person Order Picking Systems for Online Retailing

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Using simulation modeling and an on-line retail setting, we compare the performance of two types of goods-to-person order picking (OP) systems, namely, the Kiva system and the Miniload-AS/RS with a conveyor loop (to connect the pick stations). The two systems are compared on the basis of quantitative factors such as expected throughput (line items picked per hour), expected picker and material handling equipment utilizations, and order completion times. We also compare the two systems in terms of qualitative factors that are relevant for OP systems.
Micromechanics-based Modeling of additively manufactured metallic parts

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Nowadays, 3D printing of metallic materials plays an important role in manufacturing technology due to its unique capability of printing strong and complicated components with high precision. Recently, the approach to obtain some specific mechanical properties in 2D printed metallic parts is a challenging and expensive iterative process. Using computational models to predict the mechanical behaviors of SLM metallic alloys based on their microscopic features can be leveraged to reduce the iteration cost for obtaining the desired mechanical properties. An accurate computational model will also be a superior tool to explore practical modifications in the processing parameters to improve the functional performance of 3D printed metals. In this study, a novel technique is developed to investigate the correlation between microstructural features, including melt pools and grain structures, and the macroscopic mechanical properties of additively manufactured metallic parts. Crystal plasticity is utilized, and calibrated to represent the material properties of materials. The capability of the model in considering the role of texture, process defects, and mechanical loading direction on the mechanical behavior of SLM parts are evaluated. The good agreement between the obtained results and the reported experimental data confirms the accuracy of the developed micromechanics model.
Design and Trajectory Optimization of a Morphing Wing Aircraft

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Wing morphing is not a new concept. The Wright Brothers utilized morphing wings to control their famous Wright Flyer in 1903. Some modern work has focused on variable camber wings and aero structural optimization of morphing wing aircrafts. Fundamentally wing morphing gives the wing designer more freedom by allowing the shape to change throughout the flight. However, the ability to alter the shape begs the question: what shape should it be?

To correctly answer this question, we must design the wing, morphing inputs, and mission trajectory simultaneously. In this work, we perform gradient-based aerostructural optimization for a morphing wide-body commercial airliner wing while controlling its nominal shape, morphing shape across its mission, and its mission altitude profile. Optimizing all of these factors together produces an optimal design that is not achievable by designing each portion individually. Additionally, we explore the cost savings when optimizing the wing shape, mission, and aircraft allocation across a realistic set of airline routes as a subproblem. This is done with a non-morphing wing as a step towards including morphing design variables in the full allocation-mission-design problem.
MTR: Medicine and Translational Research
Functional assessment via linearization of 2-compartment model of gadoxetic-acid uptake in dynamic contrast enhanced magnetic resonance imaging

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Dynamic gadoxetic-acid enhanced magnetic resonance imaging (MRI) allows investigation of liver function through observation of the perfusion and uptake of contrast agent in the parenchyma. Assessment of contrast uptake rate ($k_1$) through the standard dual-input two-compartment model can be linearized to a simpler more robust model. To evaluate estimated $k_1$ values using this linearized analysis, high temporal resolution gadoxetic-acid enhanced MRI scans were obtained in 11 patients, and $k_1$ maps were created using both the models. Comparison of liver $k_1$ values estimated from the two methods produced an average correlation coefficient of 0.87 across the 8 livers that could be used. Temporally sparse clinical MRI data with gadoxetic acid uptake were also used to create $k_1$ maps of 28 exams using the linearized model. Of 20 scans, the created $k_1$ maps were compared to overall liver function as measured by indocyanine green (ICG) retention, and yielded a correlation coefficient of 0.72. In the 28 $k_1$ maps created via the linearized model the mean liver $k_1$ value was 3.66 $\pm$ 1.61 mL/100mL/min, consistent with prior studies. The results indicate that the linearized model provides a simple and robust method for assessing the rate of contrast uptake that can be applied to both high-temporal resolution dynamic contrast enhanced MRI and typical clinical multi-phase MRI data and that correlates well with both the results of two-compartment analysis and independent whole liver function measures.
Transport analysis of antibody-drug conjugate bystander effects and payload tumoral distribution: designing effective clinical therapies

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Antibody-drug conjugates (ADC) have emerged as sophisticated therapeutics for molecular targeting of cancer, with four FDA-approved ADCs, but there is limited understanding of how heterogeneous, perivascular distribution of ADCs in tumors relates to overall efficacy. Development of effective payloads is also challenging, owing to their complexity and limited availability of design criteria. No experimental techniques exist to directly measure tumoral payload distribution; therefore we developed a predictive computational model using partial differential equations to study payload distribution as a function of controllable design parameters: antibody dose, payload dose (drug-antibody ratio, DAR), and payload physicochemical properties that determine bystander potential. Optimization involves adjusting these parameters based on target tissue (receptor expression, internalization rate, etc.) to reach the maximum number of cells with a toxic payload dose. Our simulations highlight that: (1) heterogeneous distribution of ADCs impacts efficacy, and increasing antibody dose improves penetration and efficacy. (2) Increased penetration of payloads with bystander effects can partially compensate for poor antibody penetration, but direct cell targeting from increased ADC penetration still results in better efficacy over bystander killing. (3) Bystander effects are important for killing antigen negative cells in heterogeneous clinical tumors, and can be maximized by optimizing payload physicochemical properties. When the dimensionless Damköhler number (describing payload cellular uptake versus extracellular diffusion) is ~ 3, bystander payloads accumulate to their maximum levels throughout the tumor. This corresponds to an 'ideal' payload LogD (measure of lipophilicity) between 3 and 4. This work presents strategies for optimizing payload physicochemical properties to match potency with tumor distribution for improving ADC efficacy.
Two-step emulsion solvent evaporation technique for fabricating biodegradable rod-shaped drug carriers

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Recently, there has been growing interest towards utilization of non-spherical carriers in targeted delivery applications. These particles benefit from lower immune clearance and increased adhesion to the vascular wall. The current methods developed for rod fabrication have expensive and complicated set up with low production rates. Emulsion solvent evaporation (ESE) technique has been recently utilized for rod fabrication using a very simple and scalable set up. In this method, rods are fabricated by stretching the emulsion droplets with shear. However, this technique has been unable to fabricate rods within the size range applicable to in vivo and clinical applications without imposing the risk of embolism.

In this work, we have modified the ESE technique to a two-step fabrication method where the droplet formation and emulsification steps are separated to fabricate smaller sized rods. The size of the particles is fixed in the first emulsification step. After completion of the droplet formation, we stretch the initially formed droplets by a step change in the viscosity of our system. With this system and optimization of the fabrication conditions, the size of the poly(lactic co-glycolic acid), PLGA, rods fabricated with the ESE technique were scaled down to major axis sizes of 3.5 µm and minor axis sizes of 700 nm while maintaining the rod fabrication yield at 70% or higher. Our work has introduced a simple method for fabricating non-spherical carriers in a range of sizes for targeted delivery applications, with rod volumes equivalent to or greater than a 1.1 µm spherical particle.
Role of Red Blood Cell Deformability on Cellular and Particle Dynamics in Blood Flow

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The symptoms of many blood diseases are often attributed to irregularities in blood cells, particularly red blood cells (RBCs). Contingent on the disease and its severity, RBCs can be afflicted with increased membrane rigidity, amongst other changes. Others have extensively modeled complex blood flow to postulate how RBC rigidity may disrupt normal hemodynamics. However, little experimental work has been conducted towards understanding the effect of RBC rigidity on cellular and vascular-targeted carriers (VTCs) dynamics in physiologic blood flow. Currently, there lacks clear understanding of how rigid RBCs affect the segregation behavior, known as margination, and the resulting change in localization of other types of blood cells while in flow. We utilize an in vitro blood flow model to examine how different RBC rigidities and volume fractions of rigid RBCs impact cell margination and the downstream effect on white blood cell (WBC) adhesion in flow. Healthy RBC membranes are rigidified and reconstituted into whole blood to be either perfused over activated endothelial cells under physiologically relevant shear conditions or utilized with confocal microscopy to investigate the effect of rigid RBCs on blood cell distribution. Rigid RBCs are shown to reduce WBC adhesion by up to 80%, contingent on the RBC rigidity and amount of treated RBCs present in blood flow. VTC adhesion is similarly reduced in the presence of rigid RBCs. Overall, the obtained results suggest an impact of RBC rigidity on cellular dynamics and WBC adhesion, which may contribute to the pathological understanding of diseases characterized with significant RBC rigidity.
Towards a physiologically-relevant in vitro model for oral drug product delivery in the human gastrointestinal tract

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Hydrodynamics induced by gastrointestinal system (GIS) motility is a key parameter in in vivo drug dissolution, but compendial dissolution methods fail to model the critical in vivo parameters that govern drug product dissolution. A dissolution system is designed to simulate in vivo hydrodynamics conditions. The dissolution vessels and stirrer is designed in a way that can replicate the in vivo range of shear rates. In addition, a wide variety of physico-chemical properties of drug and the gastrointestinal system which influences drug dissolution rate such as gastrointestinal fluid's composition, pH, buffer capacity, viscosity, gastric emptying rate, and hydrodynamics was implemented in the GIS simulator. Moreover, a mathematical model with all the aforementioned variables is developed to predict mass transport phenomena in the in vitro dissolution apparatus. This model also highlights the impact of the system's hydrodynamics and the pH of the media in the dissolution of ibuprofen as a BCS II drug. This modernized GIS will provide powerful predictions for tablet formulation design as well as for physically meaningful and rationally designed in vitro experiments.
Development of Restricted Diffusion Model for Differentiation of Tumor from Normal Tissue in Glioblastoma

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Restricted water diffusion in solid tumors has been suggested by preclinical studies. However, conventional apparent diffusion coefficient (ADC) derived from diffusion weighted images (DWIs) by a mono-exponential fitting often shows poor differentiation of tumor from edema in glioblastoma (GBM). This research aims to develop a restricted diffusion model and to characterize GBM, edema and normal tissue.

Equations of the restricted diffusion model that accounts for cell size distribution, intra- and extra-cellular water diffusion, and bi-polar diffusion gradient modulation were derived. The model was fitted to DWIs acquired with 11 b-values (0 - 2500 s/mm\textsuperscript{2}) from 30 patients with GMB to yield four parameters: cell radius ($R$), intracellular and extracellular diffusion coefficients (respective $D_{\text{in}}$ and $D_{\text{ex}}$), and intracellular fractional volume $V_{\text{in}}$ using Simplex algorithm in Matlab. The parameters in hyper-cellular tumor volume (HCV) defined previously were compared to those in frontal white matter (WM), genu, deep gray matter (dGM), cortex and edema by Student’s t test. The parameters were also compared to ADC.

Three parameters ($R$, $V_{\text{in}}$ and $D_{\text{ex}}$) were significantly greater in HCV than other tissue types ($p<0.01$), in which $R$ and $V_{\text{in}}$ were able to completely separate HCV from other tissue types. Edema had significant smaller $V_{\text{in}}$ and $R$ than HCV ($p<0.01$). ADC did not show any significant differences between tissue types.

The restricted diffusion model can differentiate hyper-cellular GBM from other tissues, particularly edema, better than conventional ADC. Future studies will investigate the T2 effects on diffusion imaging and models.
OPS: Optics, Photonics, and Solid-State Devices
Increased Blocking Voltage in Solution Processed ZTO HVTFTs through Drain Offset

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Solution processing is an attractive thin film deposition technique because solution processing does not require vacuum equipment enabling inexpensive and large-area applications. Solution processed zinc tin oxide (ZTO) is an attractive amorphous oxide semiconductor (AOS) because ZTO has a higher mobility compared to amorphous silicon (a-Si) and a wide bandgap of ~3 eV. With a wide bandgap, similar to that of SiC and GaN, ZTO may enable a new generation of thin film power devices, i.e. high voltage thin film transistors (HVTFTs) and rectifiers. In this work, we have shown that HVTFTs can be fabricated using solution-processed amorphous ZTO. The blocking voltage is increased from 45 V for a device with no offset to over 100 V with a 3 µm drain offset. The devices have ohmic source and drain contacts, using sputtered molybdenum as the contact metal, and show excellent linear and saturation behavior with > 200 μA on current. Improving the electric field distribution through drain offset increases the breakdown voltage, as shown through Silvaco Atlas simulations, but also increases the on-resistance of the device. The offset region is not under gate control; therefore, the conductance cannot be modulated and the low conductance in the offset region dominates the on resistance of the ZTO HVTFTs.
Reliable, all-phosphorescent stacked white organic light emitting devices with a high color rendering index

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High efficiency solid state lighting devices have the potential to significantly reduce lighting energy usage while also offering good color rendering and longer lifetimes than conventional lighting sources. While organic light emitting diodes are promising candidates for this application, their operational lifetime is limited by the blue phosphorescent chromophore. We demonstrate stacked white phosphorescent light emitting devices (SWOLEDs) with lifetimes (as determined from the time it takes to lose 30\% of the initial luminance of 1000 cd/m\textsuperscript{2}) of up to 80,000 hours. The correlated color temperature of the devices ranges between 2780-3300 K with color rendering index as high as 89. The three emitter devices (red, green, and blue) contain up to five stacked elements, and employ red emitting blocking layers, stable charge generation layers, graded doping, and hot excited state management to achieve long lifetime. The materials and layer structures used and design principles for SWOLEDs are discussed.
A High Speed, High Sensitivity, and Universal Graphene Vapor Sensor for Both Polar and Non-polar Molecules

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The burgeoning of wearable health technology has made direct current (DC) driven nanoelectronic chemical detection one of the most attractive candidates due to its simple circuitry. To date, nearly all existing DC sensing methodologies are based on charge transfer between the sensor and the adsorbed vapor molecules. However, the high binding energy at the charge-trapped sites significantly limit those sensors’ response to tens to hundreds of seconds and also makes it inherently difficult for non-polar molecule detection, of which donor and acceptor effect is quite poor. Here we report a radically different sensing mechanism by exploiting the incomplete screening effect due to the semi-metallic nature of graphene. Molecular absorption induces capacitance change on the graphene transistor, which can be amplified intrinsically by the graphene transistor’s transconductance and measured conveniently as DC current change. Rapid (down to sub second) and sensitive (down to ppb) detection of a broad range of vapor analytes, including 17 polar and non-polar molecules, are achieved on a centimeter-area graphene field effect transistor covered with a micro fabricated flow channel. Specifically, we demonstrated, for the first time, alkane detection based on pristine CVD graphene. Our results not only pave the way to a universal gas sensor technology which offers high speed and high sensitivity to nearly all types of analytes, but also provide an ideal test bed for probing physisorption kinetics between hydrocarbon and π system.
Leaky Mode Coupling in Asymmetric Subwavelength Gratings

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Asymmetric subwavelength dielectric gratings can couple to symmetry-protected leaky modes, enabling normal incidence filtering. Finite element simulations calculate the transmittance profile and dispersion relation of a two-step high contrast grating. Further, linewidth broadening due to leaky mode coupling and angular dependence are established.
Spin-coated zinc tin oxide film made via metal-organic decomposition route

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Here, we investigate the effect of relative humidity and pre-annealing temperature on multi-layer, solution-processed amorphous zinc tin oxide films. The different pre-annealing temperature showed to significantly change the chemical composition of zinc tin oxide films. Films pre-annealed at higher temperatures exhibit tin-rich, hydroxide-poor compositions, which lead to thin-film transistor performance enhancement, with an increase in field-effect mobility from 0.75 cm²V⁻¹s⁻¹ to 5.91 cm²V⁻¹s⁻¹ and a decrease in subthreshold voltage swing from 1.37V/decade to 0.44V/decade.

By using high-temperature anneals of spin-coated inks based on acetate-precursors, we can induce metal-organic decomposition and complete dehydroxylation (MOD), which helps to form high-quality amorphous oxide semiconductor films under a variety of ambient humidity conditions. Intentional, controlled variation of relative humidity (RH) during film deposition from 10% RH to 83% RH results in little change in electron mobility (3.76 to 5.62 cm²V⁻¹s⁻¹) or subthreshold swing (0.23 to 0.39 V/decade). This wide process window distinguishes the MOD route from sol-gel processes, which are known to be humidity-sensitive. Such uniform film properties over a wide humidity range indicates the utility of the MOD approach for producing high-quality solution-processed semiconductors for large-area and printed electronics.
Fundamentals and Applications of Organic-Inorganic Hybrid Semiconductors

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In this work we present the fundamental physics and potential applications for a new class of heterogeneous semiconductors known as organic-inorganic hybrid semiconductors. Since many interesting charge transport and energy transfer phenomenon in semiconductors are determined by their interfacial properties, we will study the behavior of charges and excitons at hybrid organic-inorganic semiconductor heterojunctions (OI-HJs). We will describe a new excitonic state that exists at the OI-HJs, known as the hybrid charge transfer exciton (HCTE), and demonstrate our ability to manipulate its properties by tuning the dimensionality of the semiconductor material systems. The experimental data will be shown to match first-principles quantum mechanical description of the HCTE. We will also present experimental data for OI-HJ based diode and show that the data match with the predictions of our theory. We will conclude with discussing potential applications for the HCTE and future pathways for development of the nascent field of organic-inorganic hybrid semiconductors.
Pulsed laser deposition of In$_2$O$_3$-SnO$_2$: from films to nano-wires

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As micrometer sized device structures approach their limits in performance, nano-structures, such as nano-wires (NW) are being considered for high efficiency energy conversion and storage devices.$^{[1]}$ Metal oxides have been identified as promising materials for lithium ion batteries$^{[2]}$ and UV lasers.$^{[2]}$ Furthermore, metal-oxide NWs have been embedded in field-effect transistors, lasers, solar cells, and various chemical sensors.$^{[4]}$ Typically, metal-oxide NW are prepared by vapor deposition$^{[3]}$ or thermal evaporation.$^{[5]}$ Pulsed-laser deposition (PLD)$^{[6][7][8]}$ has emerged as a promising approach for the fabrication of tin-doped indium oxide (ITO), with film or NW growth determined by the choice of a reactive (O$_2$) or inert (N$_2$) atmosphere.$^{[6]}$ To date, cubic NW with $\leq$10 % Sn incorporated into In$_2$O$_3$ have been reported. However, a mechanistic understanding of the influence of growth parameters and substrates on the morphology, composition, and crystal structure of the deposited film is needed. Additionally, PLD of various In$_2$O$_3$-SnO$_2$ mixtures has yet to be considered. We report on PLD of various In$_2$O$_3$-SnO$_2$ mixtures, onto c-plane sapphire and Inconel substrates. Using an inert atmosphere, we have identified parameters to obtain smooth films; pyramid-shaped nano-scale clusters; sparse, tapered nano-rods; and high density, vertically oriented NWs, with and without catalyst spheres. We will present high-resolution transmission electron microscopy (HRTEM) images and selective-area electron diffraction (SAED) patterns illustrating the structure and composition of the films, nanowires, and catalyst. The photoluminescence emission from NWs and films, the electronic transport properties of individual NWs will also be discussed.
Self-referenced single-shot THz detection

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We demonstrate a self-referencing method to reduce noise in a single-shot terahertz detection scheme. By splitting a single terahertz pulse and using a reflective echelon, both the signal and reference terahertz time-domain waveforms were measured using one laser pulse. Simultaneous acquisition of these waveforms significantly reduces noise originating from shot-to-shot fluctuations. We show that correlation function based referencing, which is not limited to polarization dependent measurements, can achieve a noise floor that is comparable to state-of-the-art polarization-gated balanced detection. Lastly, we extract the DC conductivity of a 30 nm free-standing gold film using a single THz pulse. The measured value of $\sigma_0 = 1.3\pm0.4 \times 10^7$ S m$^{-1}$ is in good agreement with the value measured by four-point probe, indicating the viability of this method for measuring dynamical changes and small signals.
Photo-assisted Capacitance-Voltage Characterization of Interface States in SiO$_2$/β-Ga$_2$O$_3$ (010) MOS Capacitors

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Beta-Gallium Oxide (β-Ga$_2$O$_3$) is a wide bandgap semiconductor with great potential for power devices due to its high expected Baliga's figure of merit. When choosing a dielectric for Ga$_2$O$_3$ metal-oxide-semiconductor (MOS) devices, the conduction band offset (ΔE$_c$) between the dielectric and semiconductor needs to be considered. A large ΔE$_c$ is ideal to minimize thermal leakages in MOS devices, but the large (~4.6eV) bandgap of β-Ga$_2$O$_3$ limits the options. Silicon dioxide (SiO$_2$) has shown to be a promising dielectric for β-Ga$_2$O$_3$ with a ΔE$_c$ of 3.1eV. A low interface trap density (D$_{it}$) is also ideal for minimizing the threshold voltage variations in MOSFETs. Traditional D$_{it}$ extraction techniques cannot measure traps deep within the bandgap of β-Ga$_2$O$_3$ due to their extremely long electron emission time constants. The photo-assisted capacitance-voltage (CV) method uses deep-UV illumination during a depletion bias to ensure all traps will be measured. SiO$_2$/β-Ga$_2$O$_3$ (010) MOSCAPs were fabricated and the photo-assisted CV method was performed to estimate a total interface trap and border trap density. The method was performed with illumination of various wavelengths including 265nm to 660nm. The AC conductance method was also performed for a comparison of the two techniques. This work was supported by the University of Michigan M-Cubed program and a National Science Foundation Graduate Research Fellowship.
Charge transport in highly doped (010) β-Ga$_2$O$_3$ single crystals made by edge-defined film-fed growth

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Recently, a new wide bandgap material called gallium oxide, Ga$_2$O$_3$, has been discovered as a potential material for the next generation of power devices. The main advantages of Ga$_2$O$_3$ over currently used materials for power electronics such as silicon carbide (SiC) and gallium nitride (GaN), are its ultra-wide bandgap of 4.5 – 4.9 eV and the ease of high-quality mass production using melt-growth techniques. There are five crystal polymorphs of gallium oxide: α, β, γ, δ and ε. Of the five, β-Ga$_2$O$_3$ is the most stable one and β-phase substrates are commercially available. Temperature-dependent charge transport of unintentionally-doped (UID) β-Ga$_2$O$_3$ with (201) and (100) surface orientations and of highly-doped (201) β-Ga$_2$O$_3$ has been previously reported. However, the (010) orientation is the most promising because the [010] direction has the highest thermal conductivity, allowing heat extraction through the top and bottom of the substrate. Moreover, the best high-power devices made so far were fabricated using (010) β-Ga$_2$O$_3$. In this work, we report on temperature-dependent Hall measurements of highly-doped (010) β-Ga$_2$O$_3$ from 1.7K to 500K using a van der Pauw structure. Low-temperature measurements were performed using the PPMS DynaCool Hall system, and high-temperature measurements were taken using the HL5500PC Hall system. We observe a maximum mobility that is the highest reported value so far for the heavily doped β-Ga$_2$O$_3$. Additionally, we show that variable range hopping through an impurity band dominates electron transport at low temperatures.
Metal-organic phosphors can achieve theoretical internal quantum efficiencies four times higher than their fluorescent counterparts in electroluminescence devices by harvesting triplet excitons through intersystem crossing, but they suffer from stability issues as a result of the weak metal–ligand bonds, as well as the increasing cost of transition metals like iridium or platinum, which discourages commercialization of OLEDs for solid-state lighting. Hence, there is interest in developing all-organic phosphorescent OLEDs. The elimination of the heavy metals brings with it new challenges, such as facilitating spin–orbit coupling interactions in an organic crystal to enhance the intersystem crossing rates and suppressing vibrations in order to prevent non–radiative decay, before efficient room-temperature phosphorescence can be achieved. In all-organic systems, the enhanced spin-orbit coupling necessary for phosphorescence is thought to be due to the halogen bonding that is present in the crystalline form. To elucidate the underlying mechanism, the electronic and optical properties of purely organic phosphor candidates are investigated using density functional theory (DFT) and time-dependent density functional theory (TDDFT). These calculations are compared with the absorption, fluorescence, and phosphorescence experimental spectra in crystalline and dissolved forms to clarify the role of halogen bonding in promoting phosphorescence. Our results can be used to guide future metal-free organic phosphors.
Highly Sensitive Photodetectors Based on Hybrid Organic-Inorganic Interface

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In summary, we report highly sensitive photodetectors based on MoS₂ and j-aggregate molecules. Due to the significant enhancement of absorption by j-aggregates, the photo responsivity of the MoS₂ photodetector was enhanced all over the visible spectrum with the maximum enhancement occurring at 590 nm, which corresponded to the overlap of the emission and absorption spectra of j-aggregate and MoS₂, respectively. Such a device efficiently utilizes the high absorption property of organic molecules as well as the high charge mobility in inorganic materials, thus offering the best of both the worlds. By understanding the energy transfer mechanism between organics and inorganics, we will be able to design energy efficient optical and photonic devices.
Coherence Transfer in CdSe Colloidal Quantum Dots Revealed by 2D Optical Spectroscopy

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Colloidal quantum dots (CQD), which are nanocrystals of ~100-10,000 atoms synthesized in solution, have been the continued focus of intense study due to their wide range of applications such as biological tagging, photovoltaics, and tunable light absorbers/emitters. Strong coupling occurs between excitons and LO phonon modes, resulting in ladders of vibronic ground and excited states separated by the phonon energy. Due to strong inhomogeneous broadening however, study of the carrier-phonon dynamics is difficult.

A technique that can circumvent the inhomogeneous broadening of CQD is 2D spectroscopy, in which a four-wave mixing (FWM) signal is recorded as a function of 2 time delays between the 3 generating laser pulses and Fourier transforming. Choosing the second-third inter-pulse time and the emission time after the last pulse as the scanned delays gives a so-called “0-quantum” 2D spectrum, in which intraband Raman coherences are correlated with their emission energies. We use this technique to study CdSe CQD with ground/excited state resonances of ~605nm, and the evolution of resultant 0-quantum spectra with increasing time delay τ shows the appearance of a sideband corresponding to a Raman coherences. The dynamics of this sideband and the zero frequency peak suggest the contribution of interband coherence transfer, and agrees with simulation. Coherence transfer has thus far been observed primarily in molecular systems, and its surprising observation will aid in both the fundamental understanding of CQD and in the design of optoelectronic devices that incorporate them.
Studying Semiconductor/Liquid Junctions with Ultramicroelectrodes

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Theoretical and experimental studies of semiconductor-liquid interfaces using individual ultramicroelectrodes (UMEs) will be presented. Two hypotheses will be discussed. First, semiconductor/liquid contacts with areas ≤ 10 μm\textsuperscript{2} will afford more reproducible and more accurate measurements of heterogeneous electron transfer rates than are currently available in the literature. These platforms will allow more detailed tests of microscopic theories of charge transfer, while also providing more precise measurements of band edge positions and diode quality factors. Additional processing and surface passivation techniques were employed during fabrication in order to reduce the interface defect density. Atomic force microscopy and electrochemical measurements (Mott-Schottky plots, pH dependent study) indicate a clean semiconductor/liquid interface that behaves according to the bimolecular rate law. Possible further improvements to the surface quality through the use of non-aqueous systems and smaller contacts will be presented.

Second, the low and controllable density of states in a liquid solution will impart distinct differences in the current-voltage responses of small semiconductor/electrolyte heterojunctions as compared to similarly sized semiconductor/metal Schottky contacts. These data will aid in the understanding and development of photovoltaic systems for energy conversion/storage. The prospect for semiconductor/liquid (and organic/inorganic semiconductor) nano-Schottky contacts will also be introduced.
Artificial Plasmon: a design-friendly alternative for micro-biosensing and high speed millimeter-scale communication

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'Artificial' or 'Spoof' Surface Plasmon Polariton is a relatively new class of subwavelength mode which offers flexibility in designing the operating frequency at TeraHertz and below by shaping the geometry of the metamaterial. The energy of the mode can be squeezed into a space manifold smaller than its free space wavelength, and it can propagate chip scale distances without significant decay. These properties can be leveraged to design spoof plasmon based compact microbio-sensors with ultrasensitivity. On top of that, we showed that a handful number of unit cells are sufficient to support spoof plasmon mode, and designed a very compact resonant-tunneling SSPP structure with large Q-factor and Purcell Factor. The sharp resonant mode shows great sensitivity to the external perturbation, which paves the way for refractive index based biosensor design. In parallel to this bio-interaction based application, we capitalized the property of subwavelength confinement to design closely spaced SSPP metamaterial based channels on-chip to enable high-speed communication with large bandwidth density. A comprehensive analytical modeling of spoof plasmon mode in planar SSPP structure has been developed by us, which is utilized to determine the theoretical limit of bandwidth density and signal propagation length of SSPP based data-bus, which turns out to be 20 Gbps/µm bandwidth density at a propagation length of 15 mm. The CMOS compatibility of the structure in conjunction with its ability of cross-talk suppression can make it a strong candidate for future interconnect technology replacing the conventional electrical interconnects.
Nearly Polarization Independent Longwave Infrared Transmission Filters via Two-Dimensional Subwavelength Dielectric Gratings

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We demonstrate a longwave infrared narrowband transmission filter using a subwavelength dielectric grating in simulation and demonstrate fabrication. These gratings operate at nearly-normal incidence and are nearly independent of the polarization of incident light due to their two-dimensional symmetry. Background rejection is achieved from 8 μm to 10.5 μm with a transmission peak falling in this range; appropriate grating geometry selection determines the location of the transmission peak in this range.
Microscopic theory for local semiconductor excitations and nanostructures

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The continuing miniaturization of electronic and optoelectronic devices can make quantum effects become more important, potentially leading to non-classical behavior. At the same time, there is a growing interest in using the exceptional properties of excitons (like its large absorbance) in so called opto-excitonic devices. In both cases, a better understanding of the formation, interaction, and transport of carriers and excitons in nanostructures is necessary for developing and advancing future generations of such devices.

We present a microscopic theory following the ideas of Ref. [1] to use a Wigner-function based approach, and derive local semiconductor Bloch equations by applying second quantization and cluster expansion [2]. Even though this is a fully quantum mechanical model, the equations of motion interestingly recover the classical motion of an interacting electron and hole distribution in form of the Liouville equation. However, the momentum and electrostatic potential are renormalized by many-body effects.

To validate our theoretical description, we study an experiment [3] where a quantum well is excited by an ultrashort, diffraction limited laser pulse resonant to the $1s$ exciton. A second time delayed probe pulse, which can also be scanned across the optically excited region, is used to measure the nonlinear response. As a result, one can study the excitation dynamics with spatial and temporal resolution.

In the poster we discuss the theoretical framework and present a comparison between experimental and numerical results.
Quantum Spectroscopy with Extreme Nonlinearities

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Quantum spectroscopy [1] is based on the idea that distinct photon correlations can directly excite highly correlated excitation clusters in interacting many-body systems. In principle, this would lead to ultimate control of quantum devices. Moreover, one can use the quantum fluctuations of light to gleam information from nonlinear optical systems, which otherwise would be difficult to obtain. Specifically, when studying nonlinear optical effects, the difficulty lies in isolating the particular pathway of interactions between constitutive quasiparticles that results in the desired effect. The cluster-expansion approach [2] identifies a strictly sequential build up of clusters from singlets to doublets to triplets and so on. Inconveniently, laser-spectroscopy initiates the sequential cluster dynamics from the lowest rung, singlets, hindering the ability to either observe or control high order clusters.

Unfortunately, quantum-light sources with the desired properties are not readily available at this time. However, a recent work [3] introduced a robust scheme to project ordinary laser-spectroscopy measurements to quantum-optical responses with the Cluster-Expansion Transformation (CET) [4]. Using this approach, quantum spectroscopy has already led to exciting progress, such as the discovery of the dropleton [5]. Despite the fact that the CET relies on an integration over all excitation powers, I will show, relying on fundamental properties of quantum responses, how CET can be applied even when the classical response scales extremely nonlinearly, possibly diverging at high field strengths. As a proof of concept, CET is used to determine how quantum light modifies experimentally measured nonlinear light scattering of gold nanorods [6].
Modeling of Thermoelectric Transport in Polycrystalline Organic Semiconductors

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The last five years have seen a growing interest in organic semiconductors for thermoelectric (TE) applications owing to their low cost, material abundance, tunable properties, mechanical flexibility, non-toxicity, and ease of processing and manufacturing relative to conventional inorganic materials. The Seebeck coefficient \(S\), is a fundamental parameter which governs the performance of TE devices and provides insights into the entropy transported by charge carriers. In inorganic semiconductors, \(S\) is primarily dependent on the details of band structure and the scattering events. In organic semiconductors (OSCs), however, the electron-phonon coupling is prominent and strengthens with temperature which modifies the band structure drastically and leads to carrier localization. In addition, the grain boundaries in polycrystalline thin films of OSCs, pose an energy barrier and filter out the low energy charge carriers which may lead to an enhancement in the Seebeck coefficient at certain doping concentrations. In this work, we model the dependence of thermoelectric properties of polycrystalline organic semiconductors, on temperature and carrier concentration. We have characterized, for the first time, the combined effect of material properties such as electron-phonon coupling parameter, grain size and density of trap states on the thermoelectric trends observed in these materials. The predictions of the model are corroborated towards experimental data gathered by several authors on polycrystalline pentacene and rubrene.
AlN/h-BN Nanowire Heterostructures for Deep Ultraviolet Photonics

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Al-rich AlGaN and AlN are ideal choices for achieving solid-state deep ultraviolet (DUV) light sources. To date, however, the realization of high efficiency DUV optoelectronic devices has been limited by the presence of dislocations and the inefficient p-type conduction in conventional planar AlGaN structures. In this work, AlN/h-BN nanowire heterostructures were grown on silicon substrate by plasma-assisted molecular beam epitaxy under nitrogen rich conditions. Following the growth of AlN nanowires, a h-BN thin layer was subsequently deposited using an in situ electron beam source. The AlN/h-BN nanowire heterostructures exhibit stronger photoluminescence emission at 210 nm compared to the AlN nanowires without the h-BN capping layer, attributed to the reduced surface recombination. We have further demonstrated, for the first time, a functional AlN/h-BN nanowire light emitting diode that operates at 210 nm. The underlying AlN segment is doped n-type using Si. By exploiting the acceptor-like boron vacancy formation, we have discovered that h-BN can function as a highly conductive, DUV-transparent p-type electrode. As a consequence, the AlN/h-BN device shows excellent current-voltage characteristics, with a turn-on voltage < 6 V. Moreover, the electroluminescence intensity of such an AlN/h-BN nanowire LED device is more than one order of magnitude stronger than AlN p-i-n LEDs without a BN layer, which is attributed to the enhanced hole injection and reduced electron overflow.
Structural Color Filters: Fundamentals and Opportunities for Real-world Applications

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Structural color filters, which generate distinctive colors employing optical resonant properties in the nanostructures, have attracted much attention in recent years. They offer various advantages over the existing color filters that rely on the organic dyes or pigments to absorb a spectral portion in the visible wavelength range for the color generation, thus opening the door to many potential applications, including color displays, image sensor technologies, and anti-counterfeit tagging.

In this presentation, wide-angle, polarization-independent structural reflective colors from both directions are investigated employing materials of high refractive index. The proposed structures offer significant advantages over existing colorant-based filters in terms of high efficiency, slim dimension, long-term stability, being free from photobleaching, but most importantly for their unique metallic and iridescent appearance. Considering that only the one-step deposition method is required in the fabrication process, this new strategy holds great promise for mass production with well-controlled manufacturing cost and has been successfully applied as the vehicle exterior paints for Lexus LC 500h model that is being rolled out in 2018. In addition, angle-insensitive reflective filters that can simultaneously transmit the broadband complementary light to the reflected color have also been demonstrated. They are used for highly-efficient colored solar cells by simply integrating them with commercial crystalline silicon solar panels beneath. At the current stage, these passive filters have been adapted into active solar cells, thereby further boosting the efficiency performance. This facile method presents great feasibility for future building-integrated photovoltaics and electric cars to harvest the wasted solar energy.
Low Temperature Carrier Transport Measurements on Low Doped HgCdTe

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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 $n = 2.0 \times 10^{15}$ cm$^{-3}$ and $\mu = 23,500$ cm$^2$/Vs. Our data indicates two distinct values, including a lower doped layer with $n = 7.54 \times 10^{13}$ cm$^{-3}$ and $\mu = 196,000$ cm$^2$/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.
Photovoltaic Infrared Energy Harvesting for Bio-Implantable Devices

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The progress in wireless biomedical implantable devices and low power microelectronics at the mm-scale supports a variety of applications for monitoring physiological signals and identification and tracking. Nevertheless, these widespread applications are limited by current energy harvesting technologies from ambient sources. Several energy harvesting approaches including kinetic, radio frequency and radiative sources have been used for implantable devices. However, miniaturization to mm-scale and reliability of these sources have been inadequate. In this work, we show that photovoltaic cells on the mm-scale can provide highly efficient subcutaneous energy harvesting under extremely low-flux illumination from ambient sunlight or intentional illumination through the near-infrared transparency window of tissue between the 700nm and 1100nm wavelength range. Photovoltaic cells optimized for the near-infrared were based on two established material systems, silicon and GaAs. In particular, optimized passivation layers were studied to minimize perimeter/sidewall recombination losses and optical reflection, where LPCVD Si$_3$N$_4$ was used for Silicon and (NH$_4$)$_2$S surface treatment with subsequent PECVD Si$_3$N$_4$ was used for GaAs. The power conversion efficiency values were 17.82% for silicon and 31.63% for GaAs under 1.06μW/mm$^2$ LED illumination at 850nm wavelength. Beyond the energy harvesting from the single PV cell, a series/parallel PV network to power directly to the implantable system or to charge a battery without the requirement for DC-DC voltage up-conversion is studied.
SMR: Structural Material Research
Interaction of Glide Dislocations with Extended Precipitates in Mg-Nd alloys

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The unit processes of precipitate-dislocation interaction in dilute Mg-Nd alloys are elucidated through in situ indentation experiments in TEM. Results suggest that pinned dislocations can glide along the broad facets of extended β1 precipitates, a common strengthening phase in Mg-rare earth (RE) alloys. A dislocation-theory based analysis suggests that the shape, spacing and orientation (with respect to the glide plane) of β1 precipitates may favor glide of pinned dislocations along interfaces as opposed to the classical mechanism of bowing and looping around the precipitate.
Molecular Dynamics Study of the Polycondensation of Water at a Polyimide/Cu(100) Interface

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Accurate modeling of structural developments during polyimide cure at a polymer/metal interfaces can provide critical information with regard to the incorporation of water formed via polycondensation and how its presence influences the structure and mechanical properties and interfacial interactions. A previous study of bulk polyimide demonstrated that a newly-developed dynamic polymerization technique combining molecular dynamics and Monte Carlo methods can generate a more realistic bulk structure in the absence of an interface. In this work the algorithm is used to explore polyimide cure in the vicinity of a Cu(100) interface. The relevant interfacial effects, including spatial confinement, molecular dissociation, adsorption, and charge transfer are explored. Results are compared with literature data for monomer/substrate and polymer/substrate interfacial interactions. Network structure and hydration behavior are tracked throughout the course of the polymerization reaction. This system is used to investigate the effects of water concentration and the proximity the interface on hydration behavior of this material.
Integrated Imaging of Self-Organized Modified Eutectics

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During eutectic solidification, a liquid transforms into two or more self-organized solid phases at the same time. A common method of improving the mechanical properties of eutectics is through the deliberate addition of trace amounts of metal impurities which influence microstructure formation during solidification. Such modification usually alters the morphology of the eutectics from a coarse, plate-like network into a finer, more fibrous one. Several models have been proposed since the 1960s and onwards to explain the mechanisms leading to refinement and twinning in the impurity-modified alloys, most of which lack experimental verification. We have examined the solidification pathways of an Al-51.6wt\%Ge eutectic with and without trace metal impurities (0.1wt\%Na). By monitoring the solidification process \textit{in situ} via synchrotron-based, 4D (3D space- and time-resolved) X-ray tomography (4D-XRT), we found that the Ge lamellae in the modified alloy develop curved solid-solid interfaces as growth proceeds, anomalous for a faceted phase. We attribute this curvature to the greater intralamellar misorientation of the Ge phase in the modified eutectic, as determined from electron backscatter diffraction (EBSD) analysis of the fully-solidified specimen. The local distribution of Na was investigated at nanometer resolution by aberration-corrected scanning transmission electron microscopy (STEM) and X-ray energy-dispersive spectroscopy (EDS), coupled with atomic resolution electron energy loss spectroscopy (EELS) mapping. Further analysis of our integrated dynamic and \textit{ex situ} characterizations aims at relating the segregation of Na in the alloy to the crystallographic features, thereby extending Hellawell's impurity-induced twinning model of irregular eutectic solidification.
The Effect of Ti on the High Temperature Oxidation of Ni-based Alloys

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Though nickel-based alloys have been developed to have superior strength, toughness, and creep resistance in a variety of high-temperature conditions, their lifetimes are often limited by their vulnerability to oxidation. For this reason, elements such as chromium and aluminum are added to promote the formation of a slow-growing, passive oxide scale which protects the underlying alloy from further attack by oxidation. To have a useful lifetime, a protective scale should have slow oxidation kinetics at high temperature, and should be adherent to the underlying alloy under a variety of conditions. It is well-established that the addition of small amounts of dopants such as yttrium result in a significant improvement in the scale lifetime due to reduced oxide growth kinetics and enhanced scale adherence. Though progress has been made in understanding the mechanisms of these dopant effects, there are still many open questions about this phenomenon, including the differing effects of different dopants and the effect of varied dopant amount. Titanium, an alloying element often present in Ni-based superalloys, has an unclear effect on oxidation behavior in the literature. The objective of this work is to clarify several mechanisms of aluminum oxide formation and growth on Ni-based alloys by examining the effect of titanium additions using advanced microscopy techniques such as atom probe tomography and transmission electron microscopy.
Local Control of Dislocations in Colloidal Materials

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Dislocations are linear defects which form in crystalline matter with predominantly isotropic bonding. This category of materials famously includes atomic metals, but surprisingly also includes colloidal crystals. Our research shows that simulated colloidal solids (held together only by external pressure, without attractive inter-particle bonds) are well-behaved linear elastic media. Dislocations in these colloidal systems also have strain fields closely mirroring classical dislocation strain field solutions.

It is well understood how the migration of dislocations due to externally applied stress permits plastic flow for metallic systems. In colloidal solids, new opportunities exist because of the large scale of the ‘meta-atom’ particles comprising the crystal. At this scale, forces can be applied locally to individual dislocations, creating intentional microstructures with tailored properties, or causing bulk sample shape change through dislocation re-arrangement.

This research involves creating Monte-Carlo optimization schemes to create interstitial particles which interact strongly with colloidal dislocations. By changing the interstitial particles’ anisotropic pair potentials, the strength of interaction between them and nearby dislocations can be tuned. Through HOOMD-blue molecular dynamics simulations of systems approximating hard sphere crystals, we show that it is possible to drive colloidal dislocations into glide using local forces exerted by rod-shaped interstitial particles.

Developing these techniques for locally re-arranging dislocations brings us closer to the point where arbitrary microstructure could be created as desired. Total microstructural control would represent a large step forward for the concept of ‘designer materials’.
A substantial amount of research effort has been made aiming to fabricate anisotropically aligned well-defined conjugated polymer (CP) films to realize the unique anisotropic optoelectronic properties of CPs in the solid-state. However, directed CP alignment is a challenging task and most previous studies have been conducted for developing film fabrication techniques rather than material design. Our research has been focused on establishing molecular design principle of CPs to elucidate structure-property correlation for directed self-assembly and alignment capability of CPs. In this study, we designed and synthesized a series of liquid crystalline conjugated polymers and systematically analyzed their liquid crystalline behavior and alignment capability. Their optoelectronic properties were also investigated for plastic electronics. The findings from this project provide insight into molecular design features to achieve intrinsic self-assembly and directed alignment of CPs for high performance organic electronics.
Use of Wavelet Analysis for an Objective Evaluation of the Formation of Pills in Nonwoven Fabrics

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We have developed an objective and quantitative measure for abrasion of nonwoven fabrics that involves minimal human interpretation. We apply two-dimensional, discrete-wavelet transforms to images of nonwoven fabrics and have determined an optimal approach to eliminate the background from characteristic information about the pills. We describe the degree of damage in terms of a gray-value ratio that is extracted from the details of the wavelet characterization, and show that this parameter correlates well with an independent qualitative assessment of damage.
Isolation of Aramid Nanofibers for Strong Polymeric Composites

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Aramid fibers are famous for their high specific strength and energy absorption properties, and have been intensively used for soft body armor and ballistic protection. However, the use of aramid fiber reinforced composites is barely observed in structural applications. Aramid fibers have smooth and inert surfaces that are unable to form robust adhesion to polymeric matrices due to their high crystallinity. Here, a novel method to effectively integrate aramid fibers into composites is developed through utilization of aramid nanofibers. Aramid nanofibers are prepared from macroscale aramid fibers (such as Kevlar\textsuperscript{®}) and isolated through a simple and scalable dissolution method. Prepared aramid nanofibers are dispersible in many polymers due to their improved surface reactivity, meanwhile preserve the conjugated structure and likely the strength of their macroscale counterparts. Simultaneously improved elastic modulus, strength and fracture toughness are observed in aramid nanofiber reinforced epoxy nanocomposites. When integrated in continuous fiber reinforced composites, aramid nanofibers can also enhance interfacial properties by forming hydrogen bonds and π-π coordination to bridge matrix and macroscale fibers. Such multiscale reinforcement by aramid nanofibers and continuous fibers results in strong polymeric composites with robust mechanical properties that are necessary and long desired for structural applications.
Simulation of Micro-Scale Shear Bands Using Peridynamics with an Adaptive Dynamic Relaxation Method

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A peridynamic (PD) implementation of crystal plasticity with an adaptive dynamic relaxation method is presented in this report. PD is a new non-local approach for naturally modeling phenomena such as distributed contact and crack problems that are too complex for finite element methods (FEM). PD and molecular dynamics (MD) have similar computational structures, as both compute the force on a particle by summing the forces from surrounding particles. However, the difference arises from the origin of the force; in MD, the forces come from an interatomic potential whereas, in PD, the forces come from a continuum constitutive model. This study has proposed a new PD model with an adaptive dynamic relaxation method. Emphasis is placed on the efficiency and accuracy of the new explicit method working with the crystal plasticity constitutive model. The computation efficiency of the explicit PD model is demonstrated to be superior to an implicit PD model by more than 20%. Simulations on micro-scale shear bands are conducted with this new model. These shear bands or strong strain localizations are the main reasons of formations of fractures and cracks. The stress field distribution, texture formation, and homogenized stress-strain response predicted by the new explicit PD model are compared with FEM. Sharper localization bands are observed in PD results. The origin and evolution of these shear bands studied by PD simulations during deformation of polycrystals will be compared to experiments in the future.
Matrix Cracking and Fiber Breaks in SiC/SiC CMCs Using In Situ Tomography Techniques

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In-situ mechanical testing of a SiC/SiC composite was performed in Beamline 8.3.2 of the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory. Composite samples were loaded at room temperature and imaged at incremental loads through fracture. Both uniaxial and cross-ply laminates were tested. The tomography images were used to quantify damage accumulation such as fiber breaks and matrix cracks in the composites. Measurements of matrix cracking and fiber breaks were compared to predictions from existing models.
Richard and Eleanor Towner Prize for Outstanding Ph.D. Research Poster Session:
1:00 pm - 3:00 pm
Compute Caches

Shaizeen Aga, Supreet Jeloka, Arun Subramaniyan, Satish Narayanasamy, David Blaauw, Reetuparna Das

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Our world today increasingly relies on processing massive amounts of data to solve important problems facing us. However, current architectures tackle this data deluge inefficiently as they are compute centric. Conventional processor's narrow vector units fail to exploit the high degree of data-parallelism present in data centric applications. Also, they expend a disproportionately large fraction of time and energy in moving data over cache hierarchy and in instruction processing, as compared to the actual computation.

This poster presents Compute Caches, a novel technique which tackles these inefficiencies and addresses the needs of data centric applications. We do that by empowering processor caches, which today occupy large on-chip area but are only used to store and retrieve data, to instead also perform in-place computations. This unlocks massive amounts of data parallelism as individual elements inside caches can compute concurrently. Further, this also significantly reduces the overheads in moving data between different levels in the cache hierarchy.

Compute Cache architecture harnesses SRAM circuit technology of bit-line computing which helps re-purpose existing cache elements as active very large vector computational units. We also present solutions to satisfy new constraints imposed by Compute Caches such as operand locality. Compute Caches increase performance by 1.9x and reduce energy by 2.4x for a suite of data-centric applications, including text and database query processing, cryptographic kernels, and in-memory checkpointing. Applications with a larger fraction of Compute Cache operations could benefit even more, as our micro-benchmarks indicate (54x throughput, 9x dynamic energy savings).
Dual-Polarized Fully-Populated Common-Aperture Cavity-Backed Slot Antenna for Empowering Broadband Full-Duplex Communication

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In this work, a broadband dual-polarized 2×2 common-aperture Cavity-Backed Slot Antenna array (CBSA) for enabling full-duplex wireless communication is proposed. The antenna consists of a thin rectangular cavity appropriately loaded with metallic septa to excite multiple resonances of similar desired field distribution to achieve consistent radiation characteristics over a wide bandwidth. Four radiating cross slots are cut out on one of the broad walls of the cavity all of which are fed by a single cross slot on the opposite broad wall of the cavity. The cavity is excited by an end-launch waveguide to coaxial transition to generate one of the orthogonal polarizations. The other polarization is excited by a fork-shaped air-dielectric millistrip line (metallic strip of a few millimeters width suspended over the ground plane) symmetrically crossing over the other slot of the feeding cross slot. Keeping its size smaller than 1.28 λL×1.28 λL×0.27 λL (where λL is the free space wavelength at the lowest frequency), the antenna provides a minimum of 10 dB gain for both polarization and exhibits more than 25 dB polarization isolation within the main beam over the entire band. The designed antenna is fabricated by 3D-printing using Direct Metal Laser Sintering (DMLS) technology out of Aluminum. Due to the out-of-phase coupling from the arms of the fork-shaped millistrip lines to the waveguide feed, this dual-type feed configuration provides very high isolation between orthogonal channels over 45% fractional bandwidth. In that capacity, the proposed antenna paves the way towards broadband full-duplex wireless communication.
Designing Self-Healing Superhydrophobic Surfaces with Exceptional Mechanical Durability

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Water beads up and effortlessly rolls off a superhydrophobic surface (SHS) due to its combination of low surface energy and texture. This capability of SHSs has earned increasing interest in the past decade, particularly for its applications in drag reduction, stain repellency, self-cleaning, fog harvesting, or heat transfer (to name a few). The durability of an SHS is critical in all of these applications. Although a handful of purportedly durable SHSs have been reported, there are still no criteria available for systematically designing a durable SHS. In the first part of this work, we discuss two new design parameters that can be used to develop mechanically durable SHSs. These parameters aid in the rational selection of material components, and allow one to predict the capillary resistance to wetting of any SHS from a simple topographical analysis. However, even the most durable SHSs can eventually become damaged, and ideally should be able to recover. In the second part, we utilize our design parameters to guide the fabrication physically and chemically self-healing SHSs via spray deposition of blends of polymers and hydrophobic small molecules. The developed surfaces can recover their superhydrophobicity even after being abraded, scratched, burned, plasma-cleaned, flattened, sonicated, and chemically attacked.
The Role of Socio-Cognitive Mechanism in Construction Workers’ Safety Behaviors

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Construction is one of the most dangerous industries in the U.S. Previous studies have noted that vast majority construction accidents are associated with workers’ unsafe behaviors. This study investigates how workers' cognitive processes and their interaction with the environment (e.g., coworkers, managers, site risk) affect their safety behaviors. An interdisciplinary research framework that integrates empirical studies, computer simulations of organizational behaviors, and analyses of physiological sensing data has been developed. The mechanism of social influence has been investigated using behavioral economic experiments and surveys. An agent-based model is developed to incorporate social influence into the cognitive process of workers’ safety behaviors. The model then is used to conduct experiments to examine the effectiveness of various safety management strategies to reduce the incident rates in different site risk conditions. Also, the potential in using physiological sensory data (e.g., heart rate, electrodermal activity, and skin temperature) collected from wearable devices to understand the cognitive processes is investigated using filed experiments. The results indicate that stricter managers’ safety feedback have positive but limited impacts on reducing workers’ unsafe behaviors. Also, it is found that stimulation of workers’ project identification has potential to create synergies for reducing workers’ unsafe behaviors. Finally, the results demonstrate that wearable devices can be used to explore workers’ risk perception from diverse construction tasks in a non-intrusive and affordable way. This study will provide insights into how we can elicit constructive interactions between construction workers and environment to improve their safety behaviors.
Real-Time 3D Compton Imaging

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Compton imaging uses multi-interaction Compton scattering events to reconstruct radiation distribution images around gamma-ray detectors. With the information of the detector position and orientation, it is possible to locate the back-projected Compton cones and estimate the source distribution in a 3D space. However, since the mesh size of a typical 3D imaging space and the number of collected events are both very large, the speed of reconstruction is limited and the memory usage is not practical for iterative algorithms. To accelerate the 3D reconstruction, an incremental iterative algorithm was applied, which provides real-time reconstruction speed while preserving reasonable statistics, and environmental information was fused to exclude voxels in the air and build a sparse 3D imaging space. A recent detector system was built using two 3×3 arrays of 2×2×1.5 cm³ CdZnTe crystals with pixelated 11×11 array anodes and a planer cathode. A simultaneous localization and mapping (SLAM) system with two cameras was mounted on the radiation detector to provide environmental information. We also collaborated with Carnegie Mellon University by mounting a single-crystal detector on a robot, to achieve real-time 3D Compton imaging and autonomous source searching.
Probing Thermal Transport and Energy Conversion at the Nanoscale

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The study of thermal energy transport and conversion at the nanoscale is of fundamental interest, and holds great promise for the development of a variety of technologies including heat management in nanoelectronics, thermoelectrics and thermophotovoltaics. Although vastly more attention has been directed to the investigation of optical and electronic properties at the nanoscale, thermal properties on length scales ranging from the atomic scale to few nanometers have been barely explored due to experimental challenges. Here we describe a series of our experimental efforts to understand thermal transport and energy conversion at the nanoscale. Specifically, by employing custom-fabricated picowatt-heat-resolution calorimetric scanning probes, we observed quantized thermal transport at room temperature in metallic wires that are only single-atom wide and verified the validity the Wiedemann-Franz law down to the single atom limit. Moreover, we measured radiative heat transfer in angstrom and nanometer scale gaps and observed heat fluxes that are several orders of magnitude larger than that predicted by Planck’s Black body limit. Furthermore, we studied thermoelectric energy conversion of organic molecule junctions and observed molecular-scale refrigeration phenomena due to Peltier effects. These findings set the stage for rational design of thermally-efficient nanoscale devices and are expected to enable future development of environmentally-friendly energy saving solutions.
Preprogrammed long-term pulsatile Parathyroid Hormone delivery to strengthen bone and promote bone regeneration

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Parathyroid Hormone (PTH) is the only FDA approved anabolic agent for osteoporosis treatment and its efficacy and minor side effects in increasing bone mineral density, promoting bone formation, has been well established. Current PTH treatment requires pulsatile administration by daily injection, which is not a convenient or a favorable choice of patients and physicians. PTH also exhibited temporal-dependence that long-term administration is necessary to cover the effective therapeutic window. Thus, there is a clear clinical need for an implantable and biodegradable device capable of long-term pulsatile delivery of PTH. Here, we designed two types of devices, which deliver PTH in distinct manners, pulsatile and continuous, using surface erosion biodegradable polyanhydrides. The pulsatile device delivered 21 pulses of PTH (one pulse/day) and the continuous device delivered PTH in a linear continuous manner for 3 weeks. We demonstrated the systemic pulsatile PTH release was able to increase bone via enhanced bone remodeling, whereas the continuous PTH release resulted in bone resorption via elevated osteoclast resorption activity. We also repurposed the anabolic action of pulsatile PTH releases in a local bone defect regeneration model. We found that the local PTH continuous release inhibited the bone repair, whereas local PTH pulsatile release significantly promoted the bone formation. The local PTH pulsatile release also showed better regeneration effects compared to the standard PTH injection treatment. In addition, the devices are biodegradable and absorbable in vivo. Therefore, these biodegradable PTH delivery devices hold promise for treating conditions of bone loss without the burden of daily injections and repeat explantation surgeries.
Optimally Weighted PCA for High-Dimensional Heteroscedastic Data

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Principal Component Analysis (PCA) is a classical method for reducing the dimensionality of data by projecting them onto a low-dimensional subspace that captures most of their variation, and it has numerous applications ranging from environmental sensing to anomaly detection and visualization to name just a few. However, conventional PCA treats all data uniformly and does not exploit any knowledge we may have of the relative quality of each sample. If the noise variance of each sample is known, a more natural approach is to give less noisy samples more weight, i.e., to use a weighted PCA. Common choices for weights include binary weights (i.e., throwing away noisier samples) and inverse noise variance (i.e., maximum likelihood weighting). This work analyzes the statistical performance of weighted PCA for high-dimensional data drawn from a low-dimensional subspace and degraded by heteroscedastic noise (i.e., noise that has non-uniform variance across samples). The analysis shows that the common choices produce sub-optimal asymptotic estimation of the underlying low-dimensional subspace. In particular, we provide a simple expression for asymptotic recovery as a function of data properties (e.g., noise variances, samples-to-dimension ratio, etc.) and the weights that can be optimized to find the best weights given the data properties. Furthermore, the expression can be used to calculate the performance lost by using sub-optimal weights: sometimes it is practically optimal to throw away noisier samples and other times doing so significantly degrades performance.
Securing Modern Appified Platform through Systematic Program Analysis and Design

Yunhan (Jack) Jia
Department of Computer Science and Engineering, University of Michigan, Ann Arbor, MI

Appified platform where software application (app) development is open to third-party developers has drastically changed the way software is produced and consumed and how users interact with smart devices over the last couple of years. In appified ecosystems such as Android, and even the emerging smart home platforms, there is an app for almost everything, and the market entrance barrier is low, attracting many (sometimes unprofessional or despiteful) developers. It not only enriches user’s experience, but also raises security and safety risks by allowing untrusted 3rd-party code, which can potentially be vulnerable or malicious, to control user's device.

Our work try to address this challenged posed on the application security by looking into the design flaws and malice in the apps from the program analysis point of view. Specifically, we demonstrate that systematic program analysis of apps lead to: (1) an understanding of design and implementation flaws across different platforms that can be leveraged in miscellaneous attacks; (2) the development of security mechanisms that limit the potential for these attacks. Concretely, we contribute security and safety oriented app analysis support for three modern appified platform -- smartphone, smart home, and autonomous vehicle. Our analysis reveals the lack of context-based access control as a main enabler for attacks, and we propose a set of program analysis based techniques (OPAnalyzer, ContexIoT, and AVGuard) to provide advanced vetting support and better access control on these platforms, therefore reducing the potential for attacks.
Computational Multi-Physics Analysis and Modeling for Improved High-Speed Vehicle Performance

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This research considers the nonlinear and unsteady loads environment of an agile high-speed aerospace vehicle with an unconventional jet-based control system and structural degrees of freedom to account for the flexibility of the slender vehicle. At supersonic flow conditions the jet flow interacts with the external flow and induces a complex pressure distribution on the vehicle surface. This interaction has been documented in the literature for jets mounted on rigid structures and considering steady-state flow. However, the unsteady fluid-structure interaction must be considered for a slender vehicle due to increased flexibility. This coupled multi-physics interaction problem is analyzed with high-fidelity computational simulations to understand the various interactions and aid in engineering model development. Time-accurate dynamic results have been created that provide insight into the various degrees of coupling among interactions. A reduced order model is being developed based on the high-fidelity results that captures the main physics within this complex process and enables rapid, robust, and accurate simulation of the fully coupled system. The results and innovations in modeling methodologies and fundamental phenomenological understanding coming from this research aid in the development of future high-speed aerospace vehicles with increased operating capability and performance.
Directing Biointerfacial Events Using Polymer Brushes

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The overarching goal of this dissertation is to control interactions between the complex environment within living organisms and synthetic materials using biomimetic polymer brushes. Polymer brushes of tunable composition, architecture and biological functionality can be created by growing biomimetic polymer chains from substrate-bound initiator sites through controlled radical polymerization (CRP). In this work, CRP has been employed extensively to create robust and modular polymer brush interfaces that can fulfill design criteria for numerous biomedical applications. By using theoretical and statistical models to guide coating design and synthesis, four challenges in the design of biomedical coatings were addressed. First, a property-prediction tool was developed to identify polymer brush attributes that would maximize the rate of human embryonic stem cell proliferation, which poses a critical engineering challenge in regenerative medicine. Secondly, glycoalyx-inspired carbohydrate brushes were designed and interfacial attributes that promote viral binding were identified, allowing us to learn from nature and formulate design rules for virus-resistant coatings. Third, a substrate-independent and facile strategy was developed to synthesize micropatterned polymer brushes, paving the way for geometric control over protein adhesion in applications ranging from high throughput arrays, biosensors and cellular patterning. Finally, carbohydrate-functionalized brushes were used to selectively capture pro-regenerative macrophages, which in turn could promote healing in diabetic wounds. By applying insights from polymer chemistry, surface science, and thermodynamics, we acquired an intimate understanding of biointerfacial phenomena. This understanding enabled us to establish a platform based on multifunctional polymer brushes, ultimately addressing diverse problems at the interface of polymers and biology.
Understanding and controlling resistive switching in oxide-based memristors for memory and neuromorphic computing

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Rapid advances in artificial intelligence, mobile devices, and sensors require efficient, real-time storage and analysis of large amounts of data. However, current hardware systems are not optimized for these data-intensive tasks. Neuromorphic computing systems, taking inspiration from human brain, can potentially offer enormous computing capability through massive parallelism at extremely low power consumption for “big data” tasks. Resistive switching memristors have attracted broad interests as promising building blocks for high-density memory and neuromorphic computing. However, atomic-level thermodynamic and kinetic descriptions of resistive switching in oxide-based memristors have not been comprehensively developed yet, which are essential for continued device design and optimization. Specifically, there are contradictions in the general description on the microscopic mechanism of memristors. For example, resistive switching is known to occur via the migration of oxygen vacancy, leading to the formation/rupture of conductive filaments. Since the ion migration is facilitated by an electric field, oxygen vacancies in resistive switching are generally considered positively charged. However, strong repulsive forces expected due to Coulomb interactions are contradicted by the experimentally observed stable filaments with high vacancy concentrations. In this work, we performed predictive atomistic calculations in combination with electrical measurements under visible-light illumination to understand interactions between oxygen vacancies in tantalum pentoxide memristors. We proposed a series of charge-transition processes during resistive switching that enable the drift and aggregation of vacancies. The developed model was validated by our experimental measurements. Our results provide comprehensive understanding of the microscopic resistive switching mechanism and guide the design of memristors for improved performance.
Multiscale Investigation of Shape Memory Alloy Fatigue

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This work investigates the durability of a remarkable class of metals called shape memory alloys (SMAs) that can recover unusually large deformations and absorb large amounts of mechanical energy. Current and promising SMA applications include scenarios for which failure must be avoided, but predicting SMA failure exceeds the present understanding of structural fatigue. To address this knowledge gap, this work developed new experimental approaches with unprecedented precision to examine the relationships between cracking (fatigue/fracture) and the solid-to-solid phase transformations that underlie the unique properties of SMAs. New insights on the interacting roles of microstructure and phase transformation were quantified for the first time, including why certain grain sizes and crystallographic textures impart better fatigue crack growth resistance. Furthermore, a method was developed for reducing error in a popular measurement technique (digital image correlation, or DIC) by 60%, and definitive guidelines were established for optimizing sample preparation for DIC. These insights will enhance the performance of existing and future SMA applications in a broad range of critical areas, from biomedical devices to aerospace structures. Furthermore, this work enhances techniques for investigating other materials for which fatigue is important, such as composites and lightweight metals. Also, it adds new scientific knowledge about solid-to-solid phase transformations in the presence of cracking that is important for the advancement of many other active materials beyond SMAs, including magnetocaloric and Heusler alloys.
Prostate cancer staging involves the determination of the spread of cancer (metastasis) via bone scan (BS) and/or CT scan. Standard clinical guidelines indicate the need for BS and CT scan only in patients with certain unfavorable characteristics; however, there is no consensus about the optimal use of BS and CT scan for men with newly-diagnosed cancer. To develop state-wide, evidence-based imaging criteria, we collaborated with the Michigan Urological Surgery Improvement Collaborative (MUSIC), a quality-improvement collaborative comprising 90% of the urologists in the state. The goal of this project was to determine which patients should receive imaging and which patients can safely avoid imaging. Because not all men with newly-diagnosed cancer received an imaging, we used an established method to correct for verification bias to evaluate the accuracy of published imaging guidelines. In addition to the published guidelines, we implemented advanced classification modeling techniques to develop accurate classification rules identifying which patients should receive imaging on the basis of individual risk factors. We proposed a new algorithm for a classification model considering the extraction of data of patients with nonverified disease and the high cost of misclassifying a metastatic patient in its learning framework. We employed a bi-criteria based approach to determine the Pareto optimal guidelines with respect to expected number of positive outcomes missed and expected number of negative studies. MUSIC implemented these guidelines, which were predicted to reduce unnecessary imaging by more than 40% and limit the percentage of patients with missed metastatic disease to be less than 1%.
Numerical hydroelastic algorithm for the analysis of the interaction between structures and dense fluids with high forward speed

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In this poster we will present the application of a tightly-coupled fluid-structure interaction (FSI) methodology to simulate the hydroelastic effects during slamming events of high-speed vessels. While a majority of the studies of water entry problems have been focused on pure vertical motion, in this study we specifically introduce large forward speed and study its effect on the structural loading.

The tightly-coupled approach takes into account the time-dependent wetness of the structure, and accurately obtains the fluid loading and structure deformation through time. The fluid solution is determined using computational fluid dynamics (CFD) with the volume of fluid (VoF) approach to track the complex non-linear free surface. The structural domain is simulated using a dynamic solver within the commercial software Abaqus with a modal decomposition approach.

The numerical method is used to study the experiment of water entry of a rectangular flat plate at high horizontal speed (Iafrati et al., 2015). The experiments were designed and conducted for the aerospace problem of ditching, but they are very suitable for high-speed planning craft slamming.

A $\gamma_{\varphi} = 0.6853$ was estimated by the fine grid and a $\gamma_{\varphi} = 0.6884$ was measured for the experimental data, where $\gamma_{\varphi}$ is defined as $p/\rho U^2$. Excellent agreement on the total normal force acting on plate, dimensionless plate pressure distribution, jet root propagation velocity and strains were achieved between the medium, fine and experimental data. Results and detailed comparison between the numerical simulation and experimental data will be presented during the poster session.
In recent years, magnesium and its alloys have been studied extensively for their use in structural applications due to their low density and excellent strength to weight ratio. These materials offer good fatigue strength but they display a strong in-plane tension-compression asymmetry during deformation processing and therefore, mechanical twinning plays an important role in deformation of these materials. The twinning and detwinning behavior of wrought pure Mg was investigated using in-situ high energy x-ray diffraction (HEXRD) under displacement controlled, fully-reversed low cycle fatigue conditions. This is the first time these results have been reported in literature for pure magnesium. Macroscopic uniaxial strain was monitored independently using an extensometer during each test. In this study, three strain amplitudes were investigated: 0.45%, 0.85%, and 1.2% at a cycle frequency of 0.25 Hz. The initial texture was such that the c-axis in most grains was perpendicular to the loading direction, which is an orientation where extension twinning is favored under compressive loading. Tension-compression loop asymmetry was observed during cyclic loading which can be related to twinning and detwinning during the compressive portion of the cycles. The twinning and detwinning were characterized by monitoring the evolution of texture throughout a cycle. In-situ HEXRD results show that twinning occurs during compression and most twins are removed under reversed loading. However, it was also found that the number of grains that remain twinned upon reversal from compression to tension gradually increases with increasing number of cycles applied.
Discriminating Materials Using a Multi-particle Approach in an Active Interrogation Environment

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Spectroscopic transmission radiography using MeV--class radiation is a powerful method for identifying and quantifying the elemental composition of dense objects. Of special interest is the identification of special nuclear material (SNM), which relies on characteristic signatures such as energy-dependent transmission or the presence of delayed radiation. Fast neutron and gamma-ray probes have proved their usefulness in this application space in the past, but neither type of probing radiation by itself is universally applicable, nor are they sufficient to confirm or exclude the presence of SNM. We demonstrated a method that integrates both neutron and gamma transmission spectroscopic signatures to deduce specific material properties based on the $^{11}\text{B}(d,ng)^{12}\text{C}$ reaction using an organic scintillator. Further, the presence of fissionable material was detected using a capture-based neutron detector, which measured the time-dependent buildup and decay of delayed neutron emission from $^{238}\text{U}$. Future work will continue to advance material identification using the $^{11}\text{B}(d,ng)^{12}\text{C}$ reaction by using neutron time-of-flight techniques to measure the transmission over a broad range of neutron energies and merged with additional spectroscopic photon transmission by principle component analysis to provide a more accurate measurement of the effective atomic number. Finally, uranium isotopes will be identified by exploiting the differences in their respective characteristic long-lived delayed neutron groups. This work will use a single multi-particle multi-energy source and single type detector for the first time to perform neutron and photon radiography simultaneously and distinguish between uranium isotopes based on the long-lived delayed neutron decay and buildup.
Deep Design: Product Aesthetics for Heterogeneous Markets

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Aesthetic appeal is a primary driver of customer consideration over product designs such as automobiles. Product designers must accordingly convey design attributes (e.g., ‘Sportiness’) that the customer will prefer, a challenging proposition given subjective perceptions of customers belonging to heterogeneous market segments. We introduce a scalable deep learning approach that aims to predict how customers across market segments perceive aesthetic designs, as well as visually interpret “why” the customer perceives as such. An experiment is conducted to test this approach, using a Siamese neural network architecture containing a pair of conditional generative adversarial networks, trained using large-scale product design and crowdsourced customer data. Our results show that we are able to predict how aesthetic design attributes are perceived by customers in heterogeneous market segments, as well visually interpret these aesthetic perceptions. This provides evidence that the proposed deep learning approach may provide an additional means of understanding customer aesthetic perceptions complementary to existing methods used in product design.
Flexible Supply Chain Network Design under Correlated Uncertainty

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Traditional Supply Chain Network Design (SCND) models assume demand values at different markets and for different products are independent and the demand distributions are given. These assumptions are not accurate when correlation among the demand of different products exists. In this research, we propose a decision model for designing flexible supply chain networks (SCNs) operating under correlated uncertainties through capacity planning. We extend the current models by coordinating several SCNs of common commodities of different products. To study the correlation across uncertain parameters in the model, we employ distributionally robust optimization with given marginal probabilities for demand, exchange rate, and freight cost uncertainties. Initial results indicate that our model often deploys more capacity than the traditional stochastic models for a profit-maximization problem where positive correlations can lead to profit loss.
Today, aircraft design and performance analysis depend greatly on our ability to run high-resolution flow simulations. Such simulations allow engineers to see the intricate details of the flow and explore a larger design space. Faster turnaround time and lower cost per design iteration, as compared to wind tunnel tests, have also made computational simulations the backbone of the early stage of the aircraft design process. This research project focuses on improving the efficiency of the current computational simulation workflow by introducing automation to the most time-consuming and user-intensive task. Currently, mesh adaptation and generation rely heavily on user’s experience, creating robustness issues and causing difficulties in producing high-quality meshes. This is particularly problematic when dealing with unsteady, turbulent flows around complex geometry, and even more so when increasing flow resolutions. One possible solution is to develop an algorithm that systematically places all nodes within the mesh at their optimal locations. Here, we explore various optimization problem formulations to guide the node placement. A unique feature of our algorithm is the ability to warp mesh elements to better approximate flow features. With only marginal increase in computational cost and no additional software complexities, warping mesh elements can reduce error by at least a factor of two and allow us to run higher-resolution simulations using relatively coarse meshes. The importance of fully-automated mesh adaptation and generation that produce high-quality meshes becomes more significant as we run higher-resolution simulations and aim to take advantage of exascale computing resources, as specified in NASA’s Computational Fluid Dynamics vision for 2030.
Out-of-Band Acoustic Fields: Theory and Applications

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As is well-known, a harmonic oscillator driven with a sinusoidal input force responds with motion that matches the same frequency, though with possible variations in amplitude and phase. Similarly, in linear acoustics, a broadband acoustic source creates acoustic fields which contain the same frequency content. As a result, nearly all signal processing of acoustic fields is performed at the “in-band” frequencies, or the range of frequencies included in the signal’s bandwidth. In this research, a nonlinear product of frequency-domain acoustic fields forms the “autoproduct”, which, within some limitations, can very closely mimic a genuine acoustic field at frequencies significantly above or below the original signal’s bandwidth, or in other words, an “out-of-band” acoustic field. Theoretically, it has been found that autoproducts mimic genuine out-of-band acoustic fields when the in-band field is well-described by acoustic rays. Further analysis also considered the effects of diffraction, and the relationship between autoproducts and the field of bilinear time-frequency analysis. In terms of applications, being able to shift to a very different frequency band allows for a significant level of signal processing customization. Remote sensing, particularly source localization, has been found to be rich with opportunities for out-of-band signal processing, especially for much lower frequencies. Numerous simulations and experiments have found source localization performance using out-of-band techniques in regimes that conventional in-band techniques available in literature would completely fail. Through this research, the theoretical limitations of the autoproduct have been explored and identified, and many out-of-band remote sensing applications were found to out-perform conventional techniques.
The impact of airborne pollen on precipitation via the aerosol indirect effect

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Aerosols influence the climate system indirectly by affecting the formation of clouds and precipitation. While pollen grains are too large to influence cloud formation, pollen can rupture into subpollen particles (SPP) under wet and humid conditions. SPP are submicron particles that comprise the pollen grain and that have been shown, potentially, to be efficient as cloud condensation nuclei (CCN). Thus, SPP may influence climate via the aerosol indirect effect, changing cloud albedo, lifetime and cloud-associated moisture processes like rain. In this study, we investigate if SPP are able to have a regional impact on precipitation via the aerosol indirect effect. We introduce a mechanism to simulate the rupture of pollen grains to SPP based on lab-determined parameters into a regional climate model, RegCM4, which simulates the transport of pollen and SPP on regional scales, as well as contribution of SPP to CCN and the aerosol indirect effect. We study the sensitivity of precipitation to the addition of SPP to constant background CCN concentrations. We simulate a single spring pollen season (March – June) over the continental United States using 10-member ensemble simulations. The monthly average change in the CCN number among four subregions in the United States is small (e.g., < 1%), while localized precipitation patterns change by over 30%. These model results suggest that the spatial pattern of precipitation can be affected by pollen and the generation of SPP. Key model uncertainties are the background concentrations of CCN as well as the number of SPP generated by the rupture mechanism.
A number of recent high-profile outbreaks, including severe acute respiratory syndrome (SARS), Middle East respiratory syndrome (MERS), Ebola, Zika, and influenza are caused by human enveloped viruses. These viruses are composed of an outer lipid membrane (i.e., envelope), proteins, and a genome. Genome-based tests on patient samples suggest that certain enveloped viruses can be shed in human excreta and enter water environments. At this point, research on the environmental survivability of highly pathogenic enveloped viruses is limited due to qualified researchers and high-level biosafety facilities. Previous research shows that virus persistence in the environment varies widely amongst viruses, even when they are closely related. Therefore, a mechanistic understanding of how molecular properties of enveloped viruses impact their persistence in the environment would help specialists predict the behavior of highly pathogenic and emerging viruses. In this study, we examined the mechanistic fate of enveloped virus Phi6 with two common disinfectants, namely, free chlorine and UVC. Virus infectivity was tracked along with reactions in the viral genome, proteins, and lipids with the increases of exposure to disinfectants. Specifically, we applied virus infectivity assays, real-time reverse transcription polymerase chain reactions (RT-qPCR), and high-resolution mass spectrometry to identify the locations within the virus particle that are most susceptible to disinfectants. This work provides a framework for understanding inactivation mechanisms of other enveloped viruses via a bottom-up approach. The outcomes of the study can be applied in future pandemic and epidemic viral diseases to design effective disinfection strategies that protect human health.
Afternoon Poster Session:
1:45 pm - 4:15 pm
ACS-SPS: Atmospheric, Climate Sciences, Space and Planetary Sciences
Satellite-derived SIF Observations Show Coherent Responses to Interannual Climate Variations

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Gross primary production (GPP) is the single largest carbon flux in the Earth system, but its sensitivity to changes in climate is subject to significant uncertainty. Satellite measurements of solar-induced chlorophyll fluorescence (SIF) offer insight into spatial and temporal patterns in GPP at a global scale and, combined with other satellite-derived datasets, provide unprecedented opportunity to explore interactions between GPP and climate variability. To explore potential drivers of GPP in the Northern Hemisphere (NH), we compare monthly-averaged SIF data from the Global Ozone Monitoring Experiment 2 (GOME-2) with observed anomalies in temperature (T; CRU-TS), liquid water equivalent (LWE) from the Gravity Recovery and Climate Experiment (GRACE), and photosynthetically active radiation (PAR; CERES SYN1deg). Using observations from 2007 through 2015 for several NH regions, we calculate month-specific sensitivities of SIF to variability in T, LWE, and PAR. These sensitivities provide insight into the seasonal progression of how productivity is affected by climate variability and can be used to effectively model the observed SIF signal. In general, we find that high temperatures are beneficial to productivity in the spring, but detrimental in the summer. The influences of PAR and LWE are more heterogeneous between regions; for example, higher LWE in North American temperate forest leads to decreased springtime productivity, while exhibiting a contrasting effect in water-limited regions. These data shed light on the drivers of interannual variability in GPP, and may provide improved constraints on projections of long-term carbon cycle responses to climate change.
Multi-fluid MHD simulations of Europa’s interaction with Jupiter’s magnetosphere

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Several distinct physical processes generate the interaction between Europa, the smallest of Jupiter’s Galilean moons, and Jupiter’s magnetosphere. The 10˚ tilt of Jupiter’s dipole causes time varying magnetic fields at Europa’s orbit which interact with Europa’s subsurface ocean to induce magnetic perturbations around the moon. Jovian plasma interacts with Europa’s icy surface to sputter off neutral particles, forming a tenuous exosphere which is then ionized by impact and photo-ionization to form an ionosphere. As jovian plasma flows towards the moon, mass-loading and interaction with the ionosphere slow the flow, producing magnetic perturbations that propagate along the field lines to form an Alfvén wing current system, which connects Europa to its bright footprint in Jupiter’s ionosphere. The Galileo mission has shown that the plasma interaction generates significant magnetic perturbations that obscure signatures of the induced field from the subsurface ocean. Modeling the plasma-related perturbations is critical to interpreting the magnetic signatures of Europa’s induction field, and therefore to magnetic sounding of its interior, a central goal of the Europa Clipper mission. Here we model the Europa-Jupiter interaction with multi-fluid magnetohydrodynamic simulations to understand how these physical processes affect the plasma and magnetic environment at Europa. Compared to previous simulations, this multi-fluid model allows us to more accurately determine the precipitation flux of jovian plasma to Europa’s surface, which has significant implications for space weathering at the moon. Our simulations incorporate the effects of separate ion-electron bulk motion throughout the interaction, and reveal noticeable asymmetries and small-scale features in the Alfvén wings.
Empirical modeling of ICMEs using ACE/SWICS ionic distributions

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Coronal Mass Ejections (CMEs) are some of the largest, most energetic events in the solar system releasing an immense amount of plasma and magnetic field into the Heliosphere. The Earth-bound plasma plays a large role in space weather, driving geomagnetic storms that can damage space and ground based instrumentation. As a CME is released, the plasma experiences heating, expansion and acceleration; however, the physical mechanism supplying the heating as it lifts out of the corona still remains uncertain. Previous work has shown the ionic composition of solar ejecta undergoes a gradual transition to a state where ionization and recombination processes become ineffective rendering the ionic composition static along its trajectory. This property makes them a good diagnostic of thermal conditions in the corona, where the CME plasma likely receives most of its heating. We model this so-called ‘freeze-in’ process in Earth-directed CMEs using an ionization code to empirically determine the electron temperature, density and bulk velocity along its trajectory. ‘Frozen-in’ ions from an ensemble of independently modeled plasmas within the CME are added together to fit the full range of observational ionic abundances collected by ACE/SWICS during an ICME event. The models derived using this method will be used to estimate the CME energy budget to determine a heating rate used to compare with a variety of heating mechanisms that can sustain the required heating with a compatible timescale.
3D Hall MHD-EPIC Simulations of Ganymede’s Magnetosphere

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Fully kinetic modeling of a complete 3D magnetosphere is still computationally expensive and not feasible on current computers. While magnetohydrodynamic (MHD) models have been successfully applied to a wide range of plasma simulation, they cannot capture some important kinetic effects. We have recently developed a new modeling tool to embed the implicit particle-in-cell (PIC) model iPIC3D into the Block-Adaptive-Tree-Solarwind-Roe-Upwind-Scheme (BATS-R-US) magnetohydrodynamic model. This results in a kinetic model of the regions where kinetic effects are important. In addition to the MHD-EPIC modeling of the magnetosphere, the improved model presented here is now able to represent the moon as a resistive body. We use a stretched spherical grid with adaptive mesh refinement (AMR) to capture the resistive body and its boundary. A semi-implicit scheme is employed for solving the magnetic induction equation to allow time steps that are not limited by the resistivity. We have applied the model to Ganymede, the only moon in the solar system known to possess a strong intrinsic magnetic field, and included finite resistivity beneath the moon’s surface to model the electrical properties of the interior in a self-consistent manner. The kinetic effects of electrons and ions on the dayside magnetopause and tail current sheet are captured with iPIC3D. Magnetic reconnections under different upstream background conditions of several Galileo flybys are simulated to study the global reconnection rate and the magnetospheric dynamics.
AEP: Applied Electromagnetics and Plasma Science
A Position-Independent Highly-Efficient Wireless Power Transfer Based on Coupled Nonlinear Resonant Circuits

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Near-field resonant-based wireless power transfer (WPT) systems are highly sensitive to the relative position of the power transmitter (TX) and receiver (RX). A new approach to address the power transfer efficiency's (PTE) strong dependence on the TX/RX transfer distance and alignment is presented in this work. This approach is simple, yet efficient, and requires no active feedback/control circuits or varying the frequency of operation. In particular, a nonlinear resonant circuit is employed as a part of the WPT system to automatically compensate for the PTE degradation as the coupling factor (k) varies. The self-adaptive nonlinear resonant based WPT is realized using simple passive nonlinear devices and experimentally verified using an inductively coupled WPT prototype capable of transferring 60 W at 2.25 MHz. A PTE of 90% with +/-4% is achieved over a distance variation of up to 20 cm, lateral misalignment offset of up to ±50% of the coil diameter, and angular misalignment up to ±70°. The new design approach enhances the performance of WPT systems by significantly extending their efficient charging zone.
GPS Constellation Power Monitor System for High Accuracy CYGNSS L1B Calibration/Validation: Design, Implementation and Calibration

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The Cyclone Global Navigation Satellite System (CYGNSS) uses the Global Positioning System (GPS) constellation (32 satellites) as the active source in a bi-static radar configuration, with CYGNSS acting as the passive radar receiver. A knowledge of Equivalent Isotropically Radiated Power (EIRP), based on transmit power and antenna pattern of GPS satellites, is of great importance in the accurate calibration of L1B data (bistatic radar cross section, BRCS) of the CYGNSS mission. However, the current knowledge of the EIRP of GPS satellites is limited. There exists an uncertainty of transmit power, and only 20 laboratory-measured antenna patterns have been published. Due to the azimuthal asymmetry of the patterns, the yaw attitude of GPS satellites may affect the EIRP. Therefore, a ground-based GPS constellation power monitor (GCPM) system has been built to accurately and precisely measure GPS signals in watts and, from that, estimate the transmit powers and antenna patterns of all GPS satellites. Measurement data without absolute calibration demonstrates that the GPS yaw attitude does affect the received power. A low noise amplifier (LNA) and calibration subsystem implemented on a PID controlled thermal plate is calibrated with a liquid nitrogen source, showing stable and reasonable results. For GPS PRN 29, GCPM received power agrees with DLR/GSOC's measurement using a 30 m dish antenna at Weilheim ground station. With the absolute calibration of GPS signals, the retrieved GPS parameters will serve as inputs to the CYGNSS L1B calibration algorithm to improve the data accuracy.
Zero-dimensional modeling of the Hall thruster breathing mode

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The breathing mode is a common instability observed in Hall thrusters that is often reproduced with multi-dimensional simulations but hard to accurately capture with a zero-dimensional (0D) model of the device. A temperature-dependent linear perturbation model proposed in the literature is examined by assessing the sensitivity of its predicted growth rate to several key parameters. Deficiencies in the implementation of the model are identified and the issues with determining 0D input parameters is addressed. To improve the model, a simplified Ohm’s law is included to allow perturbations in electric field strength. The stability predicted by the model is investigated over a range of electron velocities and anomalous collision frequencies corresponding to a nominal discharge current. Reformulation of the model utilizing physics in an ionization front-centered frame of reference is considered. It is found through numerical experiments that temperature dependence alone leads to an unconditionally stable system, even accounting for the fact that the input parameters for the model have strong spatial dependence. Adding Ohm’s law does not allow for any unstable behavior unless an anomalous collision frequency with a non-Bohm- like functional dependence is assumed. Analysis of the ionization front model indicates that it is unconditionally unstable, and thus that an instability akin to the breathing mode can be recovered with a 0D model.
Sampling Requirements for Wideband Autocorrelation Radiometric (WiBAR) Remote Sensing of Dry Snowpack and Lake Icepack

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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 passive microwave remote sensing technique, known as wideband autocorrelation radiometry (WiBAR), offers a direct method to remotely measure the microwave propagation time difference of multi-path microwave emission from low-loss layered surfaces such as dry snowpack and freshwater lake icepack. The microwave propagation time difference through the pack yields a measure of its vertical extent; thus, this technique is a direct measurement of depth. It is also a low-power sensing method since there is no transmitter.

We present a simple geophysical forward model for the multipath interference phenomenon and derive the system requirements needed to design a WiBAR instrument. An X-band instrument fabricated from components-off-the-shelf (COTS) measured the thickness of freshwater lake ice at the University of Michigan Biological Station. Ice thickness retrieval is demonstrated from nadir to 59°. The WiBAR was able to directly measure the lake icepack thickness of about 36 cm with an accuracy of 2 cm over this range of incidence angles.
High order harmonic generation with femtosecond mid-infrared laser

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There has been growing interest in high order harmonic generation (HHG) from laser-solid interactions as a compact source of coherent x-rays. The ponderomotive potential in laser-plasma interactions increases with longer laser wavelength, so there may be significant differences in the physics of harmonic generation and other phenomena when experiments are conducted with mid-infrared lasers. Previous experiments, however, have been done almost exclusively with near-infrared lasers. In this work, we report the results of experiments performed with millijoule, 40 fs, 2 µm laser pulses generated by an optical parametric amplifier (OPA) which are focused onto solid targets such as silicon and glass. The HHG efficiency, polarization dependence, and x-ray emission are studied and compared to measurements with near-infrared lasers.
Intrinsically Switchable and Miniaturized Ferroelectric Bulk Acoustic Wave Filters

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Frequency-agile communication systems are receiving considerable attention due to the growth of the multi-standard RF front ends required for emerging smart devices. Reconfigurable bulk acoustic wave (BAW) filters and resonators are essential building blocks for such systems. Intrinsically switchable thin film bulk acoustic resonator (FBAR) filters based on the ferroelectric barium strontium titanate (BST) are designed and fabricated by the authors. In this work, a low insertion loss (IL) 1.5 stage \(\pi\)-network ladder type intrinsically switchable bulk acoustic wave (BAW) filter based on ferroelectric barium strontium titanate (Ba0.5Sr0.5TiO3) thin film bulk acoustic resonators (FBARs) is presented. The filter is designed and fabricated utilizing switchable BST FBARs with \(Q_m=300\) and \(K_T^2=6\%\). When a DC bias is applied to the FBARs, the switchable filter turns on and provides an insertion loss of 2.25 dB with 3-dB bandwidth of 58 MHz at 2.08 GHz center frequency. The switchable BST filter presented in this work provides the lowest IL as compared to the previously reported BST filters. The size of the active area for this miniaturized filter unit cell is 80 µm × 110 µm, which is significantly smaller than conventional piezoelectric based BAW filters.
Metamaterial Bessel Beam Radiator

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A coaxially fed device that generates Bessel beams over a broad bandwidth is presented. The concept of quasi-conformal transformation optics is employed to engineer an inhomogeneous, isotropic dielectric region that bends the waves emitted by an electrically small monopole into a paraxial Bessel beam. The axicon angle remains relatively constant over a large frequency range. As a result, non-diffracting, highly localized pulses (X waves) can be emitted under a pulse excitation. The design methodology and the metamaterial implementation of the launcher are discussed. The device is currently being fabricated.
Low-Frequency Plasma Oscillations in the Plume of a Low Temperature Magnetic Nozzle

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Many radio frequency electric propulsion devices incorporate magnetic nozzles, or axially diverging magnetic fields, to facilitate conversion of thermal to directed, bulk motion. However, without a mechanism of detachment from field lines, the flowing ionized exhaust of the nozzle will follow magnetic field lines downstream of the nozzle and potentially circle back to the front of the thruster, preventing any net thrust. While detachment has been observed in magnetic nozzles before, the mechanism responsible is not clear. Many theories have been proposed for detachment in nozzles, including collisional diffusion, electron demagnetization, and instability driven transport. Development of plasma instabilities is often driven by a difference in electron and ion velocities and yields an effective collision frequency that provides an FxB drift across field lines. These instabilities are expected to be found in the azimuthal direction to correspond with the greatest electron drift motion driven by potential and pressure gradients. While potential signals of turbulence correlating with detachment have been observed, a full study of the presence of turbulence and the relation to detachment has not been conducted.

We also set up a FastCam downstream of the thruster to observe high frequency azimuthal oscillations in density, using light intensity as a proxy for density. Data from the Magnetic Detachment Experiment at the University of Michigan are analyzed and compared to turbulent fluid theory.
Scalable Phased Array Architectures with a Reduced Number of Tunable Phase Shifters

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The goal of this research is to reduce the complexity, size, and cost of phased arrays, facilitating their widespread commercialization. The phased array in this work can be incorporated into automotive radars for advanced driver assistance systems (ADAS) and in mobile terminals for 5G communications.

An electronically controlled phased array consists of an ensemble of antennas capable of beamforming and steering by adjusting the relative phase and amplitude of the signals received or transmitted by each antenna element. The spatial selectivity offered by phased arrays allows for reducing the required transmit power in telecommunication systems, reducing multipath fading and co-channel interference, and an increased channel capacity and data rate without requiring extra bandwidth. Phased arrays can also enhance cross-range resolution and signal-to-noise ratio in radar systems. Considering their unique capabilities, phased arrays are very attractive for commercial applications. The main obstacles hindering widespread use of phased arrays in commercial applications are their complexity, size, and cost.

In phased arrays, phase shifters are the key components responsible for adjusting the signal phase across the array elements. Phase shifters and their control circuitry play a significant role in determining the complexity, size, and cost of phased arrays.

This work presents a new technique for designing scalable phased arrays. This technique significantly reduces the number of phase shifters in a phased array by integrating the phase shifting function into a new RF feed network through vector summation. The described technique can be utilized for designing receive as well as transmit phased arrays.
Dispersion relation measurements of plasma modes in the near-field plume of a 9-kW magnetically shielded thruster

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Hall thrusters are a form of crossed-field plasma device commonly employed for in-space electric propulsion. A strong magnetic field confines the lighter species of the plasma, electrons, which ionize the propellant, while an applied electric field accelerates the ions downstream. Ideally, the electrons would be confined by the magnetic field, serving as an efficient ionization source. However, it has been found experimentally that electrons can cross field lines in these devices at rates orders of magnitude higher than can be explained by classical effects. To date, no self-consistent model has been developed for this anomalous electron transport. Recent experiments and particle-in-cell simulations imply anomalous transport may be induced by the growth of ion-acoustic instabilities associated with high frequency (MHz) fluctuations of plasma density and electric field in the azimuthal direction. However, questions concerning the role of the acoustic-like modes for cross-field transport remain. It is not evident whether or not the amplitude of these oscillations is sufficiently large to explain the effective mobility measured in the plume.

This work directly measures the dispersion relation in the near field of a 9-kW magnetically shielded Hall thruster using ion-saturation probes. In each direction, axial, radial and azimuthal, two ion-saturation probes are closely spaced to measure fluctuations in ion density. Using the histogram technique of Beall gives the distribution of wavenumbers in frequency space yielding an experimental dispersion relation. Quasilinear theory for turbulent-induced transport is then applied to estimate the effective mobility in the plume due to these oscillations.
Scattering of Lossy Dielectric Surfaces in Full Wave Simulation of Maxwell’s Equations with Dense Grid and Neighborhood Impedance Boundary Conditions

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In this work, we propose a new method to calculate the scattering of surfaces with a high dielectric constant, e.g., ocean surfaces. With a high dielectric constant, a dense grid as up to 64 points per wavelength is necessary to get correct results by using Method of Moments. Rigorous solution of solving Maxwell Equation will result in a high CPU and memory consumption with such a dense grid. What is more, the impedance matrix is usually ill conditioned which needs plenty of iterative steps to get converged. The proposed new method exploits the band nature of the impedance matrix formulated by the extinction theorem in the lower medium. Different from the usual Impedance Boundary Condition (IBC) which assumes a simple relation between local electric and magnetic fields, our new method have related the electric and magnetic fields using a distance within a designated threshold. We have studied the scattering problem of ocean surface under wind speed 5 m/s to 20 m/s. Results show that our new method is both accurate and fast and yet saves a lot of CPU and memory.
Scaling Laws of Rotating Magnetic Field Field-Reversed Configuration Thrusters

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The electrodeless Lorentz force field-reverse configuration thruster (FRC) is an electric propulsion concept that utilizes plasmoids confined in a field-reversed configuration for pulsed propulsion. FRCs are an attractive option for in-space propulsion due to their high specific impulse and ability to use a multitude of propellants. While the principles of forming plasmoids in a field-reverse configuration for confinement have been well established in the fusion community, key aspects of their use as thrusters remains poorly understood, including propellant utilization efficiency and thruster performance.

Research on FRCs has steadily grown over the past decade. Prototypes of FRC thrusters exist and have been tested with a variety of propellants. In addition, numerical analyses have been performed to investigate the scaling of FRCs with already formed plasmoids. However, there are still open questions about how the thrust and mass utilization efficiencies depend on the thruster operating conditions. Current scaling laws that capture the formation and ejection of the plasmoid do not provide a relation to the coil currents and how the presence of a plasmoid influences them.

This study details fundamental scaling laws for FRC thrusters utilizing a rotating magnetic field for azimuthal current generation. A magnetohydrodynamics hierarchy coupled with a basic circuit analysis is used to establish relationships for parameters that effect ideal thruster performance. Operating parameters of these devices such as current, voltage, and thruster geometry are related to performance parameters including impulse and efficiency.
ATE: Automotive and Transportation Engineering
Steering Torque Disturbance Modeling for Control of Electric Power Steering System

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Electric power assist steering (EPAS) has gradually become one of the most vital components of majority of commercial vehicles. The ever increasing need to satisfy the expectations on driver comfort have placed a huge emphasis on exhausting all engineering methods to improve the assist action of EPAS for both routine and atypical conditions. In the automotive industry, the steering assist torque required for driving on flat roads have been successfully modeled and tuned over time to provide a sufficiently decent driving experience. However, the torque required to eliminate steering disturbances arising due to road profiles with banks or crowns and potholes or truck ruts have mostly been modeled by either performing iterative learning or by designing disturbance observers. This research attempts to model these disturbances, in the form of disturbance torque acting on the steering hand wheel, by using the dynamic models of the tire and the vehicle. A four degree of freedom model for the vehicle and a transient slip model for the tire contact patch have been developed, simulated, and validated using the data from an actual vehicle driving over different road profiles. The resulting hand wheel torques help to isolate the steering disturbances arising due to such road profiles and would be used to create new or modify the current EPAS control algorithms for more effective disturbance rejection that is believed to provide better assist to the driver at the steering wheel.
Intelligent Cruise Control of Diesel Powered Vehicles Addressing the Fuel Consumption Versus Emissions Trade-off

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Intelligent cruise control with traffic preview introduces a potential to adjust the vehicle velocity and improve fuel consumption and emissions. This work presents trade-offs observed during velocity trajectory optimizations when the objective function varies from fuel-based targets to emissions-based. The scenarios studied consider velocity optimization while following a hypothetical leader executing the federal test procedure (FTP) velocity profile with distance constraint, instead of the classical legislated velocity constraint, to enable the flexibility in optimizing the velocity trajectory. The vehicle model including longitudinal dynamics, fuel consumption and tailpipe NOx emissions is developed for a medium-duty truck with a diesel engine and verified over the FTP. Then, dynamic programming is applied on a reduced-order model to solve the constraint trajectory optimization problem and calculate an optimal vehicle velocity profile over the temperature stabilized phase (Bag 2) of the FTP. Results show 59% less tailpipe NOx emissions with an emission-optimized drive cycle but with 17% more fuel consumption compared to a non-optimized baseline. Whereas, a fuel-optimized cycle improves the fuel efficiency by 18% but with doubled tailpipe NOx emissions. Moreover, it is shown that for a diesel powertrain, including the aftertreatment system efficiency associated with the thermal dynamics is crucial to optimize the tailpipe NOx emissions and cannot be ignored for problem simplification.
Impact of Bulk Modulus and Speed of Sound of Jet Fuels on Unintended Fuel Injection Timing Shift

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Bulk modulus and speed of sound of fuel are important physical properties to understand the difference in fuel injection behavior when different types of fuels are applied to internal combustion engine. Especially, in mechanically-driven fuel supply system, difference in bulk modulus and speed of sound can cause unintended shift in start of injection (SOI) because mechanically-driven fuel supply system, unlike electronically-controlled injection system, cannot directly mandate its SOI. Meanwhile, United States Army is gearing toward to apply jet fuels in their ground vehicles for the good of flexibility of the fuel usage, thus initiating the need to investigate the effect of difference in physical properties of jet fuels from diesel fuel on engine operation. Thus, authors measured the bulk modulus and speed of sound of 6 types of jet fuels and investigated the correlation between them and fuel injection timing shift in a single-cylinder diesel generator. Bulk modulus measurement results showed that jet fuels have about 10%-20% lower bulk modulus than conventional diesel fuel, and this difference in bulk modulus resulted in unintended retardation of fuel injection timing. Degrees of retardation was between 1.0-2.5 degrees in crank angle depending on the type of jet fuel and engine load. Correlation equation between the speed of sound and injection timing shift is also established and presented in this work.
Effects of a Delay Compensation Aid on Teleoperation of Unmanned Ground Vehicles

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Teleoperation of unmanned vehicles allows remote presence to hazardous or inaccessible environments. However, it faces many challenges due to the time delay between the input from a human operator and the corresponding feedback from the system. To tackle this, various types of delay compensation algorithms have been developed and evaluated. However, evaluation of these algorithms has primarily focused on task performance such as lane keeping accuracy and completion time. How such algorithms impact human operators’ cognitive workload has been largely overlooked. The present study, therefore, aims to examine the effects of a delay compensation algorithm based on a model-free predictor on human operators’ workload.

A human-subject experiment was conducted where participants teleoperated an unmanned ground vehicle using a gaming steering wheel in a driving simulation with and without the delay compensation aid while performing a secondary task. Participants’ trust toward the aid was measured using an established survey. Workload was measured by subjective rating, physiological measurement and secondary task performance. Preliminary results show that the delay compensation aid reduces human operators’ workload.
Trip-Based Graph Partitioning in Peer-to-Peer Ridesharing

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Ridesharing systems connect drivers who use their personal vehicles to travel with riders who are in need of transportation. Since each driver/ride may have several potential matches, to achieve a high performance level the ridesharing operator needs to make the matching decision based on a global view of the system that includes all active riders and drivers when proposing ride-matches. Consequently, the ride-matching problem that needs to be solved can become computationally expensive, especially when the system is operating over a large region, or when it faces high demand levels during certain hours of the day. This work proposes a methodology to decompose the matching problem into multiple sub-problems with the goal of reducing the overall computational complexity of the problem as well as providing a high quality solution.
Optimization of Smooth Isotropic Pair Potentials for the Self Assembly of Complex Structures

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The synthesis of complex materials through the self-assembly of particles at the nanoscale provides opportunities for the realization of novel material properties. However, the inverse design process to create these materials is uniquely challenging. Standard methods for the optimization of isotropic pair potentials tend toward overfitting, resulting in solutions with too many features and length scales that are challenging to map to mechanistic models. Here we demonstrate how to effectively regularize the optimization of pair potential functions toward smooth and simple solutions by taking advantage of the unique properties of Fourier space. Such simpler functions are not only more readily realized experimentally, but we can show that they are also critical for robust self-assembly processes.
Self-Consistent Computation of the Directional Shear and Young’s Moduli in Small Molecular Organic Semiconductors

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Recent advancements in large-area patterning of small molecular organic semiconductors on flexible substrates with high fidelity have extended the use of these materials to flexible electronic devices such as wearable sensors, organic LEDs, and organic solar cells. However, in order to maintain the electronic integrity of organic semiconductors subjected to long periods of continuous and sometimes arbitrary bending moments, fundamental understanding of elastomechanical properties such as the shear and Young’s moduli are needed. Here we present a computational evaluation of the directional shear and Young’s moduli of the family of high performance small molecular organic semiconductors with tetracene backbone, i.e. tetracene, rubrene, and tetra-thiatetracene (TTT), using molecular dynamics (MD) simulations and density functional theory (DFT). We find that MD simulations performed at the COMPASS molecular mechanics level do not reproduce the intermolecular separations and orientations of dimers in the experimental crystal structure, leading to values that are inconsistent with elastomechanical properties calculated using DFT (which are usually consistent with experimental values). We attribute this to improper accounting for the quantum nature of non-bonded interactions, which are usually excluded in the semi-classical (continuum) force field (i.e. COMPASS), highlighting the significance of quantum effects on the elastic properties of small molecular organic crystals. By systematically modifying the intermolecular potentials in COMPASS to account for quantum effects on non-bonded interactions, we aim to determine a new force field that can self-consistently describe the role played by supramolecular interactions (synthons) on the directional shear and Young’s moduli in small molecular organic semiconductors.
Engineering Energy Flow in Multimetallic Plasmonic Photocatalysts

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It has been demonstrated that plasmonic metal nanostructures (Ag, Au and Cu) illuminated by low intensity visible light can drive photochemical transformations. However, the main obstacle to expanding the utilization of this technology in catalysis is the fact that typical plasmonic metals exhibit inherently low chemical reactivity. Catalytic metals (Pt, Pd, and Ru) are highly active for a wide variety of chemical transformations, but do not interact with strongly with light (i.e. they are non-plasmonic). Efforts to combine plasmonic and catalytic metals in a single nanostructure have been limited and the physical mechanisms governing energy transfer between plasmonic and catalytic metals remain unclear. Herein, we demonstrate that multimetallic core-shell nanoparticles with a plasmonic metal core (Ag) and catalytic metal shell (Pt) can selectively channel the energy of visible light into catalytically active sites on the surface of the nanostructures. The core-shell architecture serves as a model system to effectively decouple the optical and catalytic functions of the hybrid material, allowing the physical mechanism of energy transfer to be determined. The ability of these particles to perform photochemical transformations is demonstrated via the preferential oxidation of CO in the presence of excess H₂, where we show the reaction occurs solely on the Pt surface.
Dead Lithium: Mass Transport Effects on Voltage, Capacity, and Failure of Lithium Metal Anodes

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Improvement of the performance of Li metal anodes is critical to enable high energy density rechargeable battery systems beyond Li-ion. However, a complete mechanistic understanding of electrode overpotential variations that occur during extended cycling of Li metal is lacking. Herein, we demonstrate that when using a Li metal electrode, the dynamic changes in voltage during extended cycles can be increasingly attributed to mass transport. It is shown that these mass transport effects arise as a result of dead Li accumulation at the Li metal electrode, which introduces a tortuous pathway for Li-ion transport. In Li–Li symmetric cells, mass transport effects cause the shape of the galvanostatic voltage response to change from “peaking” to “arching”, along with an increase in total electrode overpotential. The continued accumulation of dead Li is also conclusively shown to directly cause capacity fade and rapid “failure” of Li–LCO full cells containing Li metal anodes. This work provides detailed insights into the coupled relationships between cycling, interphase morphology, mass transport and the overall cell performance. Furthermore, this work helps underscore the potential of Li–Li symmetric cells as a powerful analytical tool for understanding the effects of Li metal electrodes in full cell batteries.
3D Nano-metallic Thin Films by Design

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Nanostructures, self-organized into periodic concentration modulations, have been reported with radically different two-phase morphologies, including vertical and lateral striations. To understand the origin of these morphologies, we study the organizing mechanisms of these architectures via phase decomposition during elevated temperature co-sputtering of immiscible metals using analytical electron microscopy. Based on structural and chemical analysis results, an evolution in self-organized, nano-metallic morphologies was observed according to the direction of phase separation. This was the result of the phase separation kinetics relative to the deposition rate during growth. Depending on the comparison between the rate of phase separation and the deposition rate, lateral, vertical, and randomly oriented concentration modulations in three-dimensions were obtained. A predictive capability over these self-organizing nano-metallic thin films will allow for unique designs needed for the advanced functionalities of the future.
Harnessing Immune System to Battle Cancer By Using Protein-Based Nanoparticles

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Cancer immunotherapy takes advantage of the body’s own immune system to fight cancer. Antigen-specific immunotherapy is realized by identification of cancer-specific antigens. Those antigens can be delivered to dendritic cells (DCs), which can initiate an immune response against the tumor by processing and presenting captured antigens to T cells. “Next-generation” vaccines or subunit vaccines are based on recombinant proteins or naked DNA; despite great promises, poor immunogenicity remains a big challenge. This issue can be addressed by using nanoparticles for co-delivery of the antigens and an adjuvant, which enhances the immune response.

Previously, antigens were loaded into particles or conjugated onto their surface. However, the delivery of antigens via a particle carrier requires either degradation of the particle to release the antigen, or post-modification of the particle surface for antigen conjugation. Both may result in insufficient antigen delivery. We address this issue by fabricating nanoparticles that are made of the protein antigen itself. By using electrohydrodynamic co-jetting, monodisperse nanoparticles made entirely from model protein antigen ovalbumin (OVA) are fabricated. Specifically, we fabricate OVA nanoparticles with 3 different crosslinker densities and two different sizes (200 nm and 500 nm). We find that DCs readily internalize and process the OVA particles, and OVA particle-treated DCs result in proliferation of cytotoxic T cells. Both, crosslinker density and size, are shown to affect the proliferation of T cells. To further boost the immune response, we utilize the OVA nanoparticles for co-delivery of CpG, a DNA-based adjuvant, which interacts with Toll-like receptors (TLRs) of DCs.
Reconfigurable Light Diffraction Response of Ellipsoidal Colloids by Electric Field Assisted Assembly

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It has been shown that colloids can self-assemble to various crystal structures which can potentially contribute to applications involving structural color materials. However, the fundamental relationship between real space crystal structure (microscopic-scale) and light diffraction response (macroscopic-scale) remain poorly understood. In this study, we use alternating current (AC) electric field assisted assembly to produce millimeter-scale ellipsoidal colloids arrays whose diffraction response is quantified by small-angle light scattering (SALS). This time-resolved SALS can probe the kinetics of positional and orientational ordering in anisotropic structures. The ordered colloidal structures are created with polystyrene ellipsoids of aspect ratio 1.8 (major axis 6.85 μm and minor axis 3.85 μm). Here, we show three different light diffraction patterns from low ordering phase (fluid), high orientational ordering phase (chain-like structure), to high positional and orientational ordering phase (close-packed structure). We also demonstrate potential methods to improve the quality of the assembled crystal by optimizing electric-field strengths, frequencies and colloids Debye lengths. This research can contribute to the understanding of optical properties of anisotropic colloidal crystals that showing structural color.
Influence of Softness on Binary Sphere Crystal Stability

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The self-assembly of nanoparticles is a promising route for the fabrication of new nanomaterials. In particular, experimental research shows that binary systems containing nanoparticles of two different sizes can self-assemble into a wide variety of superlattices with different crystal structures. Understanding how the interparticle forces govern the assembly is critical to our ability to design materials with desirable properties. Our understanding of how these forces govern self-assembly in binary sphere systems is currently limited, especially with regard to the influence of a nanoparticle’s soft ligand corona. The objective of this work is to analyze how the softness of the interparticle interaction influences the stability of different binary crystals through the use of repulsive isotropic pair potentials.
Direct methane conversion to ethane and ethylene by oxidative coupling

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There is significant interest in converting methane (the major component of natural gas) into valuable chemicals due to its abundance and low cost. Current multi-step industrial methods of converting methane to valuable chemicals are energy-intensive and uneconomical for use with “stranded” small-scale sources of methane. Consequently, methane from such stranded sources is typically flared which contributes to greenhouse gas emissions. Direct methane conversion processes such as the oxidative coupling of methane (OCM) can help mitigate this problem. In OCM, methane reacts with oxygen at high temperatures (650-900°C) in the presence of a catalyst to produce ethane and ethylene (C₂), which are both key feedstock for the petrochemical industry. However, OCM is yet to be commercialized due to the low C₂ yields obtained, particularly in conventional packed bed reactors (PBRs). In this work, we have used reactor modeling studies to demonstrate that a reactor with distributed oxygen feed (i.e. an O²- conducting solid oxide membrane reactor) can give much higher C₂ yield compared to a PBR. A practical design for these membrane reactors would include an active OCM catalyst, preferably O²- conducting, integrated with an O²- conducting membrane. Using a PBR, we have tested several O²- conducting materials in OCM to evaluate their applicability as catalyst/membrane in OCM membrane reactors. From our reactor tests, we identified specific perovskite oxides as potential catalyst/membrane materials for application in practical OCM membrane reactors.
The localization of charge carriers in organic semiconductors is closely related to structural disorder, making the ability to carefully control this disorder important to the performance of organic materials in flexible electronic and optoelectronic applications such as wearable sensors, organic LEDs, and organic solar cells. In small organic molecular semiconductors, weak van der Waals interactions cause substantial coupling of charge carriers to low frequency collective vibrations of the surrounding lattice, leading to short-lived electronic transport channels with localization lengths on the order of the lattice spacing. The intrinsic carrier mobilities in these materials systems are thus highly sensitive to the nature of bonded and non-bonded interactions, and can inherit the directional anisotropies of elasto-mechanical properties such as the shear and Young’s moduli, which critically govern the electronic/spatial overlap of π-molecular orbitals and thus charge transport. Here, we numerically study the role played by externally and internally induced strain on carrier localization/delocalization in a family of high performance small molecular organic semiconductors, benzothieno[3,2-b][1]benzothiophene (BTBT). We show that local anisotropic pressures induced by these stressors can tune the elasto-mechanical properties along the π-π stacking direction of BTBT, which in turn impacts the dominant mechanism that is responsible for carrier localization, dynamic lattice disorder. We generalize these observations in terms of the ensuing softening/hardening of longitudinal and transverse optical phonon modes and provide simple design rules for enhancing carrier mobility in small molecular organic semiconductors by engineering local strains that suppress dynamic lattice disorder.
Working towards a Multivalent Battery by Studying the Effects of (de)localization of d-electrons on Ion Transport in Chevrel Phase Mo$_6$S$_8$

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Multivalent ion technologies offer a means to increase theoretical capacity and energy density by merely doubling, even tripling the number of electrons stored per ion. Exploration of these technologies is limited by the current body of knowledge present, which is limited by the materials that can efficiently intercalate the higher valence ions. Chevrel Phase Mo$_6$S$_8$ has been shown to be the only material that charge and discharge multivalence ions such as Mg$^{2+}$ and Ca$^{2+}$ effectively, leading to a viable rechargeable Calcium or Magnesium battery. Though, there have been some studies and even construction of a low voltage magnesium battery using the Chevrel Phase material, it is currently not known how the intercalation mechanism works. This study will investigate how (de)localization of d-electrons affects ion migration of cathode materials. The candidate test subject would be the Chevrel Phase(CP) compound Mo$_6$S$_8$ due to its interesting properties and capabilities of intercalating multivalence ions with relative ease. Density Functional Theory(DFT) calculations will be performed with a GGA+U functional to vary the (de)localization and see how it affects ion transport and electronic properties of the material. This work will contribute to understanding other transport mechanisms in solids that can potentially be used for Li ion technologies as well. Understanding how this material effectively shields the higher charged ions during transport can lead to exploration of a new frontier in multivalent batteries. Mg, Ca, Al are far more abundant in the earth’s crust than Li leading to cheaper, energy dense alternative for energy storage technologies.
Workflow Design and Management with signac-flow

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Foremost among outstanding technical hurdles to be overcome in scientific computing are the efficient, effective management of data, and the construction of well-documented, easily reproducible workflows to generate data in predictable ways. We recently introduced signac to provide a light-weight solution for scientific data management. Here we present the signac-flow module to aid in the implementation and execution of workflows operating on signac managed data spaces. Provided a well-defined workflow consisting of atomic operations – such as the simulation of nano particle systems with molecular dynamics – signac-flow supports the execution of these operations on individual data points. By using signac to tend to the underlying data, signac-flow eases the definition and execution of complex workflows on vast data spaces. For computationally demanding workflows, signac-flow is designed to work well on high performance computing clusters. The commands required to execute specific operations on signac statepoints can be transparently generated, optionally grouped, and submitted to standard cluster scheduling systems. The execution status of operations is tracked to automate the submission of operations in the appropriate sequence and to ensure that no redundant operations are performed.
Spatiotemporal Evolution of Layer-by-Layer Assembled Oppositely Charged Polyelectrolytes Multilayer Thin Films

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Despite the numerous applications of polyelectrolyte (PE) multilayer films and coatings in the pharmaceutical industry and novel cancer therapies, a framework to model the dynamics of this process quantitatively is still lacking. We here deploy a stress-diffusion multi-fluid framework to integrate transient unidirectional migration of strongly-dissociating PE chains in the presence of gradients of electrochemical potential as well as of elastic stress with previously reported quasi-equilibrium descriptions of PE Layer-by-Layer (LbL) assembly. The significant role of chemical specificity of PE functional groups is accounted for by explicitly tracking the formation of the mean-field density of ionic pairs between the two segment types. Ionic pairs alter the local diffusion driving force, slow down mutual diffusion of chains and control the relaxation of elastic stress generated by the ingress of solvent. The film structure and the interface between PE multilayer and external solution is tracked continuously by numerically solving a set of coupled and nonlinear equations, namely the Poisson equation, Maxwell constitutive equation, solvent osmotic pressure equilibrium, flux equations derived from multi-fluid model as well as material conservation equations. Additionally, the Landau-Ginzburg non-local free energy density functional employed here allows for the structure of diffuse interfaces in the system to be resolved dynamically. The proposed model could drastically accelerate engineering of the structure and properties of multilayered coatings.
Comparison of Active Motion Induced by AC Electric Fields and Ionic Fields

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The non-equilibrium and self-propelling motion we see in nature, also known as active motion, can be synthetically induced by fields, including electric fields, light, and ionic fields from chemical reactions. Although we generally understand how individual fields induce active motion, there has not yet been a comparison between the active motions induced by different fields, especially with respect to the collective motions they generate. In this study, Janus ellipsoids made of polystyrene and half-coated along the major axis with platinum were exposed to either varying AC electric fields applied perpendicular to the substrate or varying ionic fields via different concentrations of hydrogen peroxide. The resulting active motion was observed using confocal laser scanning microscopy and quantified by image analysis. AC electric fields at high frequencies caused the ellipsoids to evenly disperse and stand up with their long axis parallel to the field while at low frequencies the field caused the ellipsoids to lie perpendicular to the field and cluster. When exposed to hydrogen peroxide, ellipsoids had one of three types of motion: spinning, ballistic trajectories, or a combination of spinning of ballistic trajectories. As the concentration of hydrogen peroxide increased, all three types of motion increased in speed. This study characterizes the different types of active motion, so as to enable better selection of active motion modalities in potential applications such as the self-assembly of artificial tissues, microrobotics, and active materials.
Typical materials science is top-down: processing influences structure, yielding properties. Yet, conventional processing often limits precise control over the structure-property relationship. However, advances in nanotechnology, such as DNA nanoparticle (NP) functionalization, allow for a bottom-up approach to materials design. By coating nanoparticle surfaces with DNA strands that terminate in unpaired bases, specifically engineered DNA sequencing can programmatically enforce nanoparticle bonding. But this enthalpic basis alone is insufficient to explain all aspects of DNA NP self-assemblies: entropic parameters like particle size and shape, as well as DNA flexibility and length all contribute to the equilibrium structure. Computer simulations of these systems allow us to screen candidate building blocks and probe the effects of interactions between particles more easily and efficiently by modeling rather than experimental exploration. Previously, our group successfully used a coarse-grained molecular dynamics model using the Discrete Element Method implemented in HOOMD-blue to simulate double-stranded DNA NP unary structures. In this work, we expand this implementation to binary structures and more flexible single-stranded DNA. We use this to model unpublished experimental results in a collaboration using cubic and octahedral nanoparticles, employing machine learning to track orientational order in these systems. We find that DNA flexibility and shape are critical to self-assembly in these systems and the DNA NPs may form plastic crystals before condensing into more ordered structures — a result previously not captured via experiment. In future work, researchers can use these results to engineer DNA NPs useful in plasmonics, photonics, and catalysis.
Growth of Nanoparticles in Reactive Systems

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Accurate simulations of reactive systems present foremost challenges to both our fundamental understanding and computational modeling capabilities. In this work, we present a computational approach based on kinetic Monte Carlo to describe the growth of molecular structures of in high temperature regimes, typical of flames. The new code named, SNAPS II, is based on an initial version summarized in Lai et al. Phys. Chem. Chem. Phys., 2014, 16, 7969, and it has been completely revisited to include a wide range of chemical networks and chemical descriptors for reactions. SNAPS II is used to study the formation of polycyclic aromatic hydrocarbon and particles in flames. Modeling results in terms of size distribution and particle morphology are compared successfully against experimental data, such as mass spectra collected in flames. SNAPS II in the future will be used to gather insights on chemical compositions and reaction pathways for different reactive systems.
High activity carbide supported catalysts for aldehyde water shift

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Recently, there has been significant interest in biomass conversion using H₂O as an oxidant, which can be facilitated by the aldehyde water shift (AWS) reaction. In the aldehyde water shift (AWS) reaction, an aldehyde is oxidized by H₂O and converted into the corresponding carboxylic acid and H₂. To date, studies of the AWS reaction has been limited to homogeneous catalysts. To continue the development of AWS catalysis, we propose the design of the heterogeneous catalysts, which in general offer higher stability and ease of application, and created the benchmark for the progression.

In this work, we explored the use of molybdenum carbide as the non-innocent support for transition metal. The areal AWS rates for the carbide-supported catalysts were 5-fold higher than for the analogous catalysts on metal oxide supports. Characterizations of these materials suggest that the mechanism for high AWS activity involves distinct sites for water dissociation and aldehyde oxidation.

Moreover, we reported that the AWS activities of carbide were phase-dependent. β-Mo₂C was intrinsically more active, with an observed turnover frequency (TOF) 3-fold higher than α-MoC₁ₓ. For the carbide supported metal catalysts, the differences in surface electronic structure on each phase impact the metal deposition and the resulting catalyst activity/selectivity. By depositing Cu on the carbide support, the TOF for α-MoC₁ₓ was elevated by 100% and the selectivity to AWS reaction was enhanced by 15%. The analogous enhancement was not observed for Cu/β-Mo₂C.

A full determination of carbide phase effects on AWS catalysis will be presented in the work.
FMR: Functional Materials Research
Solution-Grown Organolead Trihalide Perovskite Single Crystals for Radiation Spectroscopy

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The ubiquity of spectroscopic radiation detectors, used primarily for defense, non-proliferation, and medicine, is constrained by product cost and operational requirements. Currently, there is a tradeoff between detector cost and high energy resolution, with lower-cost scintillation detectors having poor resolution which limits their utility. There are high-resolution semiconductor detectors, but their expense and requirement for active cooling also limits their applications. Here, we demonstrate a semiconductor detector capable of high-resolution room temperature operation using methylammonium lead triiodide perovskite single crystals. The fair mobility (~150 cm\textsuperscript{2} / Vs), long carrier lifetimes (over 100 \mu s), and low density of defects (under \(10^{10} / \text{cm}^3\)), in addition to its high radiation absorption cross-section, make perovskite the ideal material for spectroscopic detectors. These crystals, grown by solution-based crystallization, have been measured to have energy resolutions of under 10% for an 81 keV \(^{133}\text{Ba}\) peak, comparable to existing room-temperature semiconductor detection materials such as bare cadmium zinc telluride (CZT) crystals. Furthermore, the simplicity of the crystallization method, and the relative abundance of its elemental precursors, results in a production cost up to 100 times lower than semiconductor detectors, and even ten times less than scintillation detectors. Crystallization control and surface treatment processes, also investigated in this work, promise to increase energy resolution up to and potentially beyond that of CZT, currently the leading semiconductor material in industry.
Post-synthetic Functionalization of Three-Dimensional Covalent Organic Frameworks

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Covalent organic frameworks (COFs) are an exciting new class of porous organic materials due to their crystallinity, high porosity, and chemical tunability, which allows for the modification of the particle structure towards different applications. Recent work has mainly focused on the synthesis and functionalization of two-dimensional COFs, while there is a dearth of studies on three-dimensional COFs, despite their higher porosity and surface area.

In this project, a three-dimensional imine-linked COF was synthesized and characterized as control. Several different reaction pathways were explored for introducing easily reacted functional groups such as vinyl and hydroxyl groups, which can later be utilized as interfaces for post-synthetic functionalization, to the aldehyde monomer. The functionalized aldehyde monomers were then utilized for the synthesis of a novel functionalized COF which can be considered a “blank slate”, serving as the starting point for tailored post-synthetic functionalization towards a variety of applications. The functionalized COF was characterized using nitrogen adsorption/desorption isotherms, scanning electron microscopy, and X-ray diffraction. Future work includes photopolymerization with methacrylate monomers to fabricate a thin film for gas separation and modification of pore structure for carbon dioxide capture.
Entropy-stabilized materials are stabilized by the configurational entropy of the constituents, rather than the enthalpy of formation of the compound. A unique benefit to entropic stabilization is the increased solubility of elements, which opens a broad compositional space with subsequent local chemical and structural disorder resulting from different atomic sizes and preferred coordinations of the constituents. As the magnetic and electronic properties of oxides are strongly correlated to their chemistry and electronic structure, entropy stabilization could lead to interesting and novel properties. Anisotropic magnetic exchange and the presence of a critical blocking temperature indicates that the entropy-stabilized oxides considered here are antiferromagnetic. Changing the composition of the oxide tunes the disorder and exchange bias and here we exploit this tunability to enhance the strength of the exchange field by a factor of 10x at low temperatures, when compared to a CoO heterostructure. Significant deviations from the rule of mixtures are observed in the structural and magnetic parameters, indicating that the crystal is dominated by configurational entropy. Our results reveal that the unique characteristics of entropy stabilized materials can be utilized to engineer magnetic functional phenomena in oxide thin films.
Near-Edge Optical and Phonon Properties of β-Ga$_2$O$_3$

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Many experimental and theoretical studies have been performed on β-Ga$_2$O$_3$, a wide-band-gap semiconducting material (4.5 eV at room temperature), for applications in high-power electronics and optoelectronics. This material is capable of emitting light despite having an indirect gap and has been touted as a rival to GaN for high-power electronic applications. However, a better understanding of its fundamental electron and thermal-transport properties is needed to facilitate its commercial deployment. First-principles calculations using density functional theory, density functional perturbation theory, and many-body perturbation theory are used to elucidate these fundamental properties. Our calculations show the direction-dependence of light absorption, intrinsic deep-UV light emission, and the phonon dispersion. We further determine the overall and the individual-mode Grüneisen parameters to understand the anharmonic phonon-phonon interactions and the low thermal conductivity of this material. Our results for the electron-phonon coupling matrix elements provide atomistic understanding into the mobility and dielectric breakdown properties. We have identified a particular polar-optical phonon mode that limits the mobility at room temperature. We further apply the calculated matrix elements to estimate the breakdown field as a function of crystallographic direction. Our theoretical characterization sheds light on the microscopic origins of the intrinsic light emission, electron mobility, thermal conductivity, and breakdown field, and guides experiment for the development of materials for superior high-power electronics performance. This research was supported by the National Science Foundation through Grant No. DMR-1534221 and the GRFP through Grant No. DGE 1256260. Computational resources were provided by the DOE NERSC facility under Contract No. DE-AC02-05CH11231.
Systematic nanoparticle drug delivery analysis in high-grade serous ovarian cancer

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Current nanoparticle fabrication methods have several drawbacks: most are not scalable, do not inherently produce monodisperse nanoparticles, cannot accommodate multiphasic nanoparticle synthesis or do not enable independent manipulation of nanoparticle parameters. These drawbacks limit new drug delivery technologies from systematically understanding nanoparticle behavior \textit{in vivo}, and from being expanded to commercially available cancer therapies. In order to meet these challenges, we have developed a novel nanoparticle synthesis technique, called Wettability Engendered Templated Self-assembly (WETS), that uses layer-by-layer dip-coating of patterned wettability substrates to fabricate discrete, uniform polymer particles. With this method, monodisperse single phase or multiphasic polymer particles can be fabricated in a variety of planar geometries, and spherical morphologies. Each phase can independently encapsulate a different therapeutic or diagnostic agent, which eliminates any negative interactions between the various agents. Further, WETS methodology enables the independent manipulation of nanoparticle characteristics, including size, shape, morphology and composition over a broad spectrum, which makes it ideal for systematic cancer drug delivery studies. Single phase and biphasic nanoparticles composed of poly(lactic-co-glycolic acid) (PLGA) and poly(ethylene glycol) (PEG) will be fabricated and studied for their cellular internalization, biodistribution and co-delivery of paclitaxel and carboplatin \textit{in vitro} and \textit{in vivo} using high-grade serous ovarian cancer (HGSOC) cell lines in 3D spheroids and spheroid xenograft models. Through these experiments, an optimal nanoparticle size, shape, composition and drug loading will be identified for treatment of HGSOC.
Influence of conjugated polymer morphology on electronic properties at the polymer/conductor interface

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Understanding charge carrier transport at the semiconducting polymer/conductive substrate interface is vital for successful implementation of semiconducting polymers in electronic devices. Band bending, or the change of energy band offsets due to local reorganization of charge carriers, occurs at semiconductor/conductor interface when the Fermi levels of the two materials in contact align. The degree to which band bending occurs at the conjugated polymer/conductive substrate interface depends on several factors, including the electronic structure of the conjugated polymer and the number of charge carriers present. Here, we look to specifically probe the impact morphology has on the band bending effect of poly(3-hexylthiophene) (P3HT) films fabricated using both conventional spin-casting and the novel matrix assisted pulsed laser evaporation (MAPLE) technique on indium tin oxide (ITO)/poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) substrates. A stronger band bending effect, as studied with Kelvin probe force microscopy (KPFM), is observed in MAPLE-deposited samples than in the spin-cast analogs. With modeling, the charge transfer between the conductive ITO/PEDOT:PSS substrate and the MAPLE-deposited P3HT sample, resultant in the band bending we measure, can be explained by a broadening of the density of states (DOS). This broadening likely originates from the highly-disordered structure of MAPLE-deposited P3HT. Temperature dependence of the out-of-plane carrier mobility further corroborates the observed broadening of the DOS. Our work indicates a strong connection between molecular structure, electronic states, and bulk transport in conjugated polymer films.
Investigating the role of acidity in oxidation catalysis using model metal-oxide catalysts

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Keggin type polyoxometalates (POMs) such as phosphomolybdic acid (H₃PMo₁₂O₄₀) and its derivatives constitute model metal-oxide catalysts, as they have consistent well-defined structure with a variable composition. Dispersing POMs on an inert, high-surface-area support allows for the preparation of catalysts with uniform and tunable active sites that can serve to bridge the gap between practical and fundamental catalysis studies of oxide materials. The acid and redox properties of POMs can be tuned by changing the heteroatom (P or Si), framework atoms (Mo or W), cations (H⁺, Na⁺, etc.), or the support. While generally it is held that acid catalysis by Bronsted acid sites (H⁺) and oxidation by redox sites (Mo-O-Mo) are independent, there are many examples where this is not the case and the two parallel pathways are not independent. Here we will use POMs dispersed on silica as a model system to investigate the role of acidity in oxidation catalysis on oxides.

The nature of POM active sites was probed using methanol, an ideal probe molecule for bifunctional acid-redox catalysts, as parallel pathways of dehydration to dimethyl ether and oxidation to formaldehyde probe the acid and redox properties of POMs respectively. The active sites were quantified by titration with 2,6-Di-tert-butylpyridine (DTBP) during reaction with methanol. Cation exchange, POM coverage variation, and various pretreatments were used to prepare a series of POMs dispersed on silica with a 0 – 2 H⁺/POM, and these catalysts were used to elucidate the role of Brønsted acidity in oxidation and dehydration over a model oxide catalyst.
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 μm 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.
Correlating the Interface Resistance and Surface Adhesion of the Li Metal-Solid Electrolyte Interface

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Li metal anodes have long been recognized as the key to the high energy density batteries that future electric vehicles will require. Solid state electrolytes have demonstrated the potential to enable stable cycling of metallic Li anodes by acting as a physical barrier to dendritic growth. However, little is known about the mechanics of the Li-solid electrolyte interface. This study combines electrochemical and mechanical characterization to correlate interface kinetics with adhesive strength. Cubic garnet with the Li₆.25Al₀.25La₃Zr₂O₁₂ (LLZO) formulation was selected as a model solid electrolyte based on its high conductivity and stability against Li metal. Symmetric Li-LLZO cells were tested using electrochemical impedance spectroscopy to determine the interfacial resistance, $R_{\text{int}}$, and the adhesive strength of the Li-LLZO interface, $\sigma_{\text{adh}}$, was measured using a unique tensile test in an inert atmosphere. It was determined that the $R_{\text{int}}$ is directly correlated to the adhesive strength of Li on LLZO. At the highest $R_{\text{int}}$ in this study, 330k$\Omega\cdot$cm$^2$ the $\sigma_{\text{adh}}$ was 1.1kPa and at the lowest $R_{\text{int}}$ in this study, 7$\Omega\cdot$cm$^2$, $\sigma_{\text{adh}}$ was 8MPa. Furthermore, by optimizing the surface chemistry the wettability of LLZO was enhanced resulting in $\sigma_{\text{adh}}$ exceeding the ultimate tensile strength of Li metal. The relationship demonstrated provides a deeper understanding of the mechanical properties of the Li-electrolyte interface, which will play an important role in the design of batteries employing metallic Li anodes.
IOF-2: Industrial, Operations, and Financial Engineering Session 2
A Stochastic Programming Approach to Determine Decision Boundaries for Medical Diagnosis

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We use stochastic programming to determine decision thresholds for medical diagnosis risk models under uncertain data samples from a fixed population. These thresholds maximize sensitivity and specificity under constrained false positive and false negative rates. We show that sample average approximation solutions for these models are consistent estimators. We apply our method to concussion assessment and show that our thresholds dominate single decision thresholds under multi-criteria evaluation.
Effects of reliability levels and reliability information calculation methods on trust, dependence and task performance

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Existing studies have shown that the disclosure of automation reliability information, as one way to increase the transparency of the system, can facilitate trust-reliability calibration and improve human–automation task performance. However, few studies have addressed the question: how to calculate reliability information of the automation? The goal of this research is to investigate the effects of reliability levels and reliability information calculation methods on operators’ trust, dependence and task performance. We conducted a human subject experiment with 60 participants. Each participant performed a compensatory tracking task and a threat detection task with the help of an imperfect automated threat detector. Reliability information of the automated threat detector was calculated using different methods based on the signal detection theory and Bayesian probability. The results revealed that when overall reliability of the automated threat detector was 90%, positive/negative predictive values of the automation significantly helped participants to calibrate their trust in and dependence on the detector, which led to the shortest reaction time for detection task. This research indicates that users should be made aware of system reliability, especially of the positive/negative predictive values to engender appropriate trust in and dependence on the automation. The findings of this research can be applied to the interface design of automated decision aids.
Design of Multimodal Closed Queuing Networks for Transportation-as-a-Service

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Transportation-as-a-Service (TAAS) requires the service provider to integrate multiple modes of transport into seamless trip chains. In a trip chain, the smooth transfer from one mode to another is critical (ride-hailing, bike-sharing, public transport, etc.), which requires designing the transport hubs strategically and controlling service providers in a multi-modal system dynamically. In this work, we propose a scheme for network design on closed queuing networks. The objective is to minimize the operating costs, including costs for establishing hubs and routing, penalty for losing customers, and loss (negative profit) for finishing trips. The dynamic model also includes a matching mechanism to combine trips via carpooling. We are able to find the optimal pricing and matching policies under mild assumptions.
Quantitative Models for Managing Multi-Node Replenishment Logistics in the Food Supply Chain

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Most of the work done in the Food Supply Chain (FSC) field focuses on production control, leaving unaddressed a number of significant issues which relate to the logistics of replenishing food retail outlets. The main goal of this study is to develop an optimization model that integrates both inventory and routing decisions in order to minimize transportation and inventory holding costs, while meeting service level and capacity constraints. The resulting model will be a practical tool for decision-makers; it will allow them to simultaneously address the following key decisions: (1) The quantity of inventory to deliver; (2) The time periods in which to visit each outlet; (3) The ideal route for each delivery trip; and (4) The number of trucks needed for each time period. Using the inventory routing problem as a base, a simplified integer programming model was developed to gain insight into the complexity of the problem. Variations to this “starter model” were also developed to incorporate other factors of the FSC such as variable truck fleet size and multiple product types. Numerical tests involving the inventory holding cost and the transportation cost were performed on the starter model in order to analyze the results and assess the scalability of the model. The preliminary results obtained from this test suggest that the starter model can handle large, simple instances of the problem and it has the potential to serve as a foundation for key extensions such as multi-stop deliveries, storage capacity limitations at the outlets, and inventory perishability.
Statistical prediction of hand-load carrying strategy and load level from wearable inertial sensor data

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Carrying heavy hand loads frequently and for long durations is a known risk factor for low back disorders. While minimizing the frequency and intensity of manual load carrying is ideal, such tasks are common and unavoidable in non-routinized work such as in construction, firefighting, and patient care. In such jobs measuring longitudinal exposures to load carrying is an important step for managing and mitigating the incidence of low back disorders. Biomechanical adaptations due to the magnitude and position of hand loads are known to affect gait and movement patterns. Leveraging this knowledge, the objective of this study was to develop and validate a statistical prediction algorithm that uses body-worn inertial sensor data for classifying load carrying strategy and load level. Ten men participated in a laboratory experiment carrying a hand load in three common strategies (viz., lateral one-handed and two-handed, and anterior two-handed carry) at four levels of box weights each (viz., no load, 2.27 kg, 50% and 75% of the participant’s maximum acceptable weight of carry). Gait parameters calculated from the sensor data recorded at the upper back, low back, thigh, and shank along with individual anthropometry and strength measures were used as inputs to a statistical prediction model. A random Forest algorithm implemented in a two-stage hierarchy correctly classified 81.3% of the carrying strategies and load levels. Preliminary results demonstrate the potential for combining wearable instrumentation with statistical prediction to quantifying the biomechanical exposures from load carriage in non-routine work settings.
Aperture Control for VMAT Planning Systems

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The goal of VMAT is to deliver a prescribed dose of radiation to malignant tumors while trying to avoid the delivery of toxic doses to healthy organs. A multi-leaf collimator sits on a gantry and rotates around the patient’s body shuttering radiation through a dynamically changing aperture. Research shows that irregular aperture shapes in VMAT treatments can lead to inefficient and inaccurate deliveries. Since Accuracy studies and measurements suggest that “the majority of errors are concentrated on aperture edges.” We propose a new edge penalty function. We incorporate this new penalty into the conventional VMAT optimization planning model framework by incorporating aperture shape controls. This penalty function is combined with the dose-based treatment quality objective in the treatment optimization model, resulting in plans with larger apertures with more regular, rounded shapes. Our study achieves similar solutions in terms of dose volume metrics. We show how this penalty can be seamlessly incorporated into a typical column-generation model for VMAT treatment optimization, and discuss implementation and preliminary results. We describe a new column generation solution method for the proposed model. Finally, the algorithm is tested on a representative retrospective case. The relative weight of the two components of the optimization objective function (dose-based treatment quality metric and aperture shape penalty) is varied, and the quality of resulting treatment plans is compared to explore the tradeoffs.
Development of a Computational Driver Performance Model for In-vehicle Direct/Indirect Manual and Speech Interactions

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To maximize drivers’ safety and convenience while interacting with in-vehicle technologies, a variety of in-vehicle information systems (IVISs) using direct and indirect input devices have been developed. Direct input devices (e.g., touchscreens on the center console, voice interfaces) do not require any translations between actions of the device and the operator, whereas indirect input devices (e.g., steering wheel-mounted controls with a dashboard-cluster) require the translations between the device and the operator. Along with developing these IVISs using advanced automotive technologies, it is also necessary to evaluate the usability of the IVISs before they are commercialized. Traditional methods for evaluating the usability of the products include end-user tests in the laboratory setting, heuristic evaluation, and survey. However, these methods typically involve creating physical prototypes, recruiting human subjects or evaluation experts, as well as coordinating the usability experiments; thus, they require costly and time-consuming efforts to conduct. On the other hand, cognitive modeling methods generally use the simulation of real human behavior and performance based on scientific and engineering theories and knowledge; therefore, they do not require physical prototypes, usability experience expertise, and human subjects for the usability tests. In this study, I introduce a computational cognitive model study for in-vehicle direct/indirect interaction systems’ usability test. The model was developed using the Queueing Network cognitive architecture to predict task completion time and workload. The model was able to generate results similar to human experimental data: task completion time (R² = 88.1%, RMSE = 2.40s), workload (R² = 68.2%, RMSE = 1.46).
Adaptive Submodular Ranking

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We study a general stochastic ranking problem where an algorithm needs to adaptively select a sequence of elements so as to “cover” a random scenario (drawn from a known distribution) at minimum expected cost. The coverage of each scenario is captured by an individual submodular function, where the scenario is said to be covered when its function value goes above some threshold. We obtain a logarithmic factor approximation algorithm for this adaptive ranking problem, which is the best possible (unless P=NP). This problem unifies and generalizes many previously studied problems with applications in search ranking and active learning. The approximation ratio of our algorithm either matches or improves the best result known in each of these special cases. Moreover, our algorithm is simple to state and implement. We also present preliminary experimental results on a real data set.
PEN: Power and Energy
Transfer-Power Measurement: A Non-Contact Method for Fair and Accurate Metering of Wireless Power Transfer in Electric Vehicles

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By 2040, electric vehicles (EVs) will consume 1,900 terawatt-hours of electricity every year worldwide; even a 1% error in metering will cost energy consumers and providers $1 billion. With plug-in methods, utility-type meters can be placed at the outlet of EVs chargers to accurately measure energy transfer. However, wireless power transfer (WPT) is emerging as the pre-eminent way to charge EVs because of a growing consumer emphasis on convenience and perceived safety, but there appears to be no fair way to measure power transfer. In this work, transfer-power measurement (TPM) is introduced. TPM employs non-contact sensing elements to measure magnetic field from wireless power transfer and calculate the real power propagating through space. TPM provides fair metering because individual losses from the transmitter and receiver are disaggregated. Not only will this provide fair metering, but will also disaggregate individual Tx and Rx efficiencies, which can then inform provider and customer decisions and behaviors for financial benefits. Signal and data processing as well as a calibration method are discussed. Experimental results demonstrate a fair method of metering the real transfer power with low estimation error. Errors from misalignment are analyzed with respect to the size and position of the sense coils to improve the sensitivity of TPM. Fair metering incentivizes businesses and individuals to make choices that conserve energy and advance technology by providing more information and by properly assigning the financial loss.
A Non-Uniformly-Sampled Digital Controller for Constant-On-Time Valley-Current-Mode (NUS-COTCM) Buck Voltage Regulation Modules (VRMs)

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This work introduces a new method for controlling Voltage Regulator Modules (VRMs) that potentially offers the fastest closed-loop transient response in comparison to existing methods. Together with the relentless pursuit for more powerful communications and microprocessors, the demand for VRMs that are faster, more accurate, and more flexible is inescapable. Constant-on-time buck converters have been appealing because of light-load efficiency performance and in current mode, fast transient response. Digital controllers offer a number of advantages including control flexibility (e.g. nonlinear control), lower quiescent power, and robustness to component variations. For variable switching converters, the challenge of high sampling frequency is combined with the disadvantage of slow transient response for linear controllers. Here we present a new perspective in sampling where the sampling events are kept in phase with the switching events, which are in general non-periodic. A consequence of this event synchronization is the absence of intermodulation effects and a very relaxed anti-aliasing filter for the switching ripple with the opportunity to avoid switching transients by either a delay or anticipation in sampling.
Critical Parameter Values for Marginal Recovery from Parameter-Dependent Disturbances

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Consider a system of ordinary differential equations subject to a parameter-dependent finite time disturbance. The goal is to identify parameter values for which the system is marginally able to recover from the disturbance to a desired stable equilibrium point (SEP), called critical parameter values. These critical parameter values form the boundary in parameter space between values for which the system is able to recover to the SEP, and values for which it is not. The system state when the disturbance clears is called the post-disturbance initial condition, and it is a function of parameter. Under generic assumptions, a critical parameter value is a value whose corresponding post-disturbance initial condition lies on the boundary of the region of attraction of the desired SEP. It is proven that, under the assumptions above, the boundary of the region of attraction varies continuously with small changes in parameter value and admits a simplifying decomposition. This theory motivates an algorithm for numerically computing critical parameter values. The algorithm is illustrated on a simple power system where the disturbance is a fault on a particular transmission line.
Approximation Methods for Scheduling Battery Energy Storage for Multiple Services

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With increasing use and applications of Battery Energy Storage (BES), research is needed to improve methods for battery optimization for multi-tasking applications. Stochastic Dual Dynamic Programming (SDDP) has proven to be a computationally efficient method for solving large-scale multi-period convex optimization problems. However, when the battery is not perfectly efficient, the storage complementarity constraint leads to a non-convex formulation. Our contribution is to apply a Lagrange Relaxation (LR) method to obtain a convex relaxation of the BES multitasking problem and combine it with SDDP, a method formerly implemented on the hydrothermal operation planning problem. We use the subgradient method for selecting Lagrange multipliers to obtain a tight approximation of the cost function. Our preliminary results show that the LR method improves the approximation over a regular convex relaxation.
Quantifying energy efficiencies of buildings providing ancillary services

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As the power system rapidly integrates new generation technologies such as wind and photovoltaic solar with the goal of reducing environmental impacts, the challenges in meeting reliability goals will require new and creative solutions. The use of current infrastructure and demand side resources, such as building HVAC (Heating Ventilation and Air Conditioning) systems, present an attractive option for providing these grid solutions.

In these buildings, the system operator can use the HVAC systems to provide Ancillary Services (AS) like energy balancing and voltage control. A recent study showed that buildings providing such services tend to consume more energy, resulting in a low effective round trip efficiency. One of the major challenges in quantifying these efficiencies is accurately estimating the baseline operation of the HVAC system.

This research presents results of experiments conducted at three buildings on the UM campus. The building thermostats were globally reset to vary the power consumption such that there is a net-zero energy exchange with the grid, all the while trying to take advantage of the building’s thermal inertia to cause minimal occupational discomfort. We present accurate baseline estimation methods to quantify the additional energy consumption of these buildings and benchmark the results to previous works. The research also analyzes reasons behind the cause of the inefficiency, more specifically the effect of the building thermodynamics and control actions of the HVAC equipment. This would give a better understanding of the operation and efficiency of commercial HVAC systems, and improve their environmental impact on the power system.
Cost, timeline, and technology pathway of climate cure with direct air capture versus timely emissions abatement

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We evaluate the private costs, technological transformations, and net CO2 emissions to achieve sector-specific CO2 emission target in the U.S. electricity sector by 2050 when direct air capture (DAC) technology is available to cure excess emissions in the future. Results show that while DAC makes achieving emissions target feasible beyond 2025, this expanded timeframe for climate action extends only till about 2030 considering 1% of GDP as a cutoff value for abatement costs, and till 2035 if the GDP cutoff is 2.5%. The total abatement cost for a cure would be 3-10 times costlier than that of prevention through a timely transition to low-carbon alternatives, assuming climate action is initiated between 2025-2030 for the cure and 2015-2020 for prevention, respectively. The corresponding carbon removal rate for the cure would be about 1.4-3.0 Gt/year compared to 0.6-0.8 Gt/year through 2050. Should we need to cure with DAC we need 9-15 years of a preparatory period to expand total capacity, in addition to rapidly decarbonizing the grid by pre-maturely retiring inefficient fossil capacity and increasing low-carbon alternative. Compensating for additional emissions within a shorter timeframe leads to increased removal rate and cost for the cure. However, contrary to past studies, our systems-level analysis shows DAC can be deployed starting 2038 in a least-cost fashion, tolerating about 23% of natural gas capacity while fossil fuel carbon capture and sequestration technologies are outcompeted by a combination of renewable energy and DAC, suggesting the importance of zero or negative emissions in a carbon-constrained world.
Addressing Synchronization and Oscillations under Market-based Coordination of Distributed Energy Resources

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Transactive or market-based coordination strategies have recently been proposed for controlling the aggregate demand of a large population of distributed energy resources (DERs), such as air-conditioners, electric vehicles, storage devices. Such schemes offer operational benefits such as enforcing distribution feeder capacity limits and providing users with the flexibility to consume energy based on the price they are willing to pay. However, this work demonstrates that they are also prone to load synchronization and power oscillations. A transactive energy framework has been adopted and applied to a population of thermostatically controlled loads (TCLs). A modified TCL switching logic takes into account market coordination signals, alongside the natural hysteresis-based switching conditions. Studies of this market-based coordination scheme suggest that several factors may contribute to load synchronism, including sharp changes in the market prices that are broadcast to loads, lack of diversity in user specified bid curves, low capacity of distribution feeders, and the form of user bid curves. To address these issues, Markov transition equations that can express the aggregate dynamics of DERs under market-based coordination have been developed. By incorporating these in a model predictive control (MPC) setting, DERs can be controlled effectively and their synchronization can also be avoided.
Impacts on the Local Power Network when Residential Loads Provide Energy Balancing Services to the Regional Network

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This work is a study on the effects that load control for balancing services has on the physical constraints of a distribution network. A simulation study is conducted across a range of scenarios and prototypical distribution networks. Network constraint violations, such as overvoltages and blown fuses, are recorded and compared to a no-control baseline simulation. Notably, the simulation results show that no instantaneous constraints are violated due to load control. We find that the mean aging rate of the transformers decreases in 24 of 25 simulations, though in 21 simulations a majority of transformers experience increased aging rates. Overall the results indicate that load control for balancing services is unlikely to cause emergency-level issues on a distribution network. However, longer term impacts, such as increased aging of certain transformers, may warrant a control design that manages particular network constraints.
Multiple Access Wireless Power Transfer

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The internet of things is leading to a world of massively interconnected devices with limited battery power limiting the functionality of these devices. This huge explosion is thus creating a need for scalable architectures for multiple access wireless power transfer. The existing single frequency methods suffer from complexity of control and compensation techniques or the limited availability of spectrum and device ratings. Direct-sequence spread-spectrum wireless power transfer (DSSS-WPT) offers a solution that is immune to external disturbances, has relaxed tolerance for passive components and has lower electromagnetic interference problems. DSSS-WPT allows for abstraction of current and voltage waveforms to ternary codes thereby facilitating the power transfer analysis using the relationships between transmitter and receiver codes. The popular techniques of code division multiplexing (CDM) can now be applied for scaling wireless power transfer to possibly hundreds of devices. We present the implementation of CDM for WPT using direct-sequence spread-spectrum modulation. The power transfer analysis is done by abstracting the voltage and current sequences to ternary codes(+1, -1 and variable zero durations) and simple cases for doing multiple access wireless power transfer using CDM are presented.
Water-Power Distribution Network Coupling for Optimal Pumping to Reduce Energy Costs and Promote Resilience

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As the power grid’s penetration of renewable generation increases, net load forecast errors will increase due to the intermittent nature of renewables, requiring more active resources that can balance real-time supply and demand. Currently, the water distribution network acts as a passive load on the electricity distribution network; water utility companies pump water demanded by consumers as needed. Pumping water in high-demand times can be financially taxing to the water distribution network as well as impose a significant load on the electricity network. The goal of this research is to treat the water network as a demand response resource; the pumps, reservoirs, and storage tanks that make up the water distribution network are capable of spatio-temporally shifting their electricity demand. We are developing an optimization algorithm that schedules pumping to minimize energy costs by leveraging water storage and consumer flexibility. It will also schedule the storage in such a way that pumps will be able to help balance real-time net load forecast error. The challenge is that the joint water-electric network is a nonlinear, nonconvex stochastic system. We are exploring a variety of methods to solve the optimization problem including convex relaxations and Nash Bargaining Games. Our algorithm will improve the resiliency of both the water and power distribution network.
Designing a Better Battery with Artificial Neural Network

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Simulation-based battery design encounters the difficulty of high computational cost. This work develops a systematic approach based on the artificial neural network to dramatically reduce the computational burden of battery design by several orders of magnitude. Two neural networks are constructed using the finite element simulation results from a thermo-electrochemical model. The first neural network serves as a classifier to predict whether a set of input variables is physically feasible. The second neural network gives specific energy and specific power. Both neural networks are validated using extra finite element simulations out of the training data. With global sensitivity analysis using the neural network, we quantify the effect of input variables on specific energy and specific power by evaluating large combinations of input variables, which is computationally prohibitive for finite element simulations. Among all parameters the applied C-rate has the largest influence on specific power, while the electrode thickness and porosity are the dominant factors affecting specific energy. Based on this finding, we generate a design map that fulfills the requirements of both specific energy and specific power. This work highlights the value of neural network in handling the non-linear, complex and computationally expensive problem of battery design and optimization.
The Impact of Load Models in an Algorithm for Improving Voltage Stability via Control of Demand Response Resources

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Increasing communication and control capabilities will allow future power system operators to exploit large quantities of responsive demand. This work discusses ongoing work that employs fast-acting demand response resources to improve voltage stability via virtual spatial shifting of loads (i.e., altering the locational distribution of power consumption in one time period with a payback of the energy in a following time period). We use a previously proposed iterative linearization algorithm to determine loading patterns that maximize a voltage stability margin, namely, the smallest singular value (SSV) of the power flow Jacobian matrix. Proper representation of loads is particularly important in power system stability analyses. Accordingly, this work studies the impact of load models on the algorithm. Specifically, we extend the algorithm to enable inclusion of composite load models consisting of both “ZIP” components and a steady-state squirrel-cage induction machine (IM) model. We then investigate the impact of different load models on both the stability margin and the loading pattern. Using the IEEE 14-bus system as an illustrative example, the results show that the type of load model affects the nominal system's SSV, the maximum-achievable SSV, and the optimal loading pattern. The maximum-achievable percent change in SSV is larger using IM models than using ZIP models. We also discuss the difficulty in interpreting the stability margin when the system undergoes structural changes resulting from the use of different voltage-dependent load models.
Wireless Power Transfer for Implantable Medical Devices Using Piecewise Resonance to Achieve High Peak-to-Average Power Ratio

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Wireless power transfer is emerging as the pre-eminent powering technology for implantable medical devices. Efficiency, simplicity, and reliability are the key goals for receivers in vivo. We use piecewise resonant wireless power transfer (PR-WPT) to achieve these goals. A high peak-to-average power ratio (PAPR) waveform is generated by a current-mode class D amplifier operating at 6.78 MHz. A 4th-order passive filter is matched to the fundamental and third harmonic voltages of the transmitter, using harmonic elimination for the waveform and closed-form impedance analysis. A full-bridge Schottky rectifier converts the matched voltage into dc. Experiment demonstrates the proof of principle and simulation results show that the piecewise resonant methods can increase the dc output voltage by up to 30%, hence improving the rectifier efficiency. Potential applications for PR-WPT systems are discussed. Low power and relatively high voltage is the promising market for piecewise resonance wireless power transfer systems.
SICC: Signal and Image Processing, Computer Vision and Communication
Optimal Estimation of Information Measures and their Applications

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We propose a direct estimation method for information measures such as Renyi and f-divergence and mutual informations, based on a new graph theoretical interpretation. Suppose that we are given two sample sets X and Y, respectively with N and M samples, where \( \eta := \frac{M}{N} \) is a constant value. Considering the k-nearest neighbor (k-NN) graph of Y in the joint data set (X,Y), we show that the average powered ratio of the number of X points to the number of Y points among all k-NN points is proportional to Renyi divergence of X and Y densities. A similar method can also be used to estimate measures of divergence and correlation. We derive bias and variance rates, and show that for density functions with continuous and bounded derivatives of up to the order d, our estimator achieves the parametric MSE rate of O(1/N). Our estimators are more computationally tractable than other competing estimators, which makes them appealing in many practical applications such as change detection, learning graphical models, finding the error of classification, feature selection, etc.
Differential Privacy of ADMM-based Distributed Machine Learning Algorithms

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Alternating direction method of multiplier (ADMM) is a popular method used to design distributed versions of a machine learning algorithm; this enables decentralized learning over a network of nodes where data originates from different parts of the network but are used for a common collective learning objective. In such a setting, each node performs certain computation using as input its local data; results from the local computation procedure but not the raw data are then exchanged among neighboring nodes in an iterative fashion. During this iterative process the leakage of data privacy arises.

Dynamic differential privacy was proposed in prior work to examine the privacy property in such an iterative process using classical definition of differential privacy; this is done specifically for ADMM-based distributed algorithms for a class of regularized empirical risk minimization (ERM) machine learning problems. However, it only considers each node and each iteration of ADMM in isolation and only gives the privacy loss of every single iteration. If consider the sufficiently large numb

In this work, we consider all nodes and all iterations and propose a novel perturbation method for ADMM iterative process. By increasing the penalty parameter geometrically and at the same time adding a decaying gamma distributed random noise to penalty term, it turns out a bounded privacy loss can be obtained during the infinite number of iterations.
Predictive Models for Transitions in Brain States

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Brain states manipulate behavioral responses and are altered by the pathological condition of the brain. Their transitions capture underlying electrophysiological and neuromodulator activity and can be used to build closed loop controls for brain-machine interfaces and to control neural activity. However, predicting a transition with high temporal precision is not a trivial issue and hasn’t yet been done with high accuracy. We have investigated different features in EEG and intracranial local field potential recordings to figure out the instantaneous brain state and explore their predictive nature. Our algorithm uses spectral, bispectral, entropy and waveform shape analysis to build a predictive model applying machine learning techniques. We use adaptive thresholding to make the algorithm robust under variability across subjects. Preliminary results show predictive changes in features on a scale of 1-2s. We are currently testing and improving the algorithm based on rodent and human electrophysiological recordings. A potential application for this is in predicting seizures or drowsiness in drivers of semi-automated vehicles.
Personalized PageRank Estimation for Many Nodes: The Impact of Clustering on Complexity

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Personalized PageRank (PPR) is a measure of the importance of a node from the perspective of another (we call these nodes the target and the source, respectively). PPR has been used in many applications, such as offering a Twitter user (the source) recommendations of who to follow (targets deemed important by PPR). Computing PPR is infeasible for massive networks like Twitter, so efficient estimation algorithms are necessary. In this work, we propose strategies for estimating PPR of many source/target pairs.

We begin with the problem of PPR estimation for a single pair, introducing an enhancement to the state-of-the-art estimator for this task. Using this algorithm as a primitive, we then propose methods for estimating PPR of many pairs. These methods leverage the common underlying graph to avoid repeated computations that may occur when each pair is treated separately, thus accelerating the estimation task.

Analytical and empirical results show that our proposed methods offer complexity reduction when compared to existing methods. Furthermore, the complexity reduction scales with quantities that describe the degree of clustering of the sources and targets. Thus, at a high level, our work shows that many pair estimation is “easier” when the nodes of interest are clustered.
Acoustic localization of distributed coherent and incoherent sources using SEMWAN with subarray smoothing

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Accurate estimation of the location and level of remote acoustic sources from recorded acoustic signals is attractive in many applications. In wind tunnel tests, where noise sources are commonly distributed and incoherent, high resolution array signal processing techniques like the spectral estimation method with additive noise (SEMWAN) have been useful for source localization when background noise measurements are available. However, for many continuously distributed systems, such as a simple vibrating plate, the assumption of incoherent sources is incorrect, and techniques like SEMWAN may yield spurious results. In this presentation, results are reported for the use of SEMWAN alongside a subarray smoothing technique to formulate the coherent source localization problem as an incoherent source localization problem. Simulations comparing localization performance for distributed coherent and incoherent sources are shown. Results from a proof-of-concept experiment using multiple sources and a 15-element linear receiver array are also evaluated against simulation. Performance comparisons are made between SEMWAN, MUSIC, and conventional beamforming techniques in addition to showing the effects of subarray smoothing.
WaterGAN: Unsupervised Generative Network to Enable Real-time Color Correction of Monocular Underwater Images

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This work reports on WaterGAN, a generative adversarial network (GAN) for generating realistic underwater images from in-air image and depth pairings in an unsupervised pipeline used for color correction of monocular underwater images. Cameras onboard autonomous and remotely operated vehicles can capture high resolution images to map the seafloor; however, underwater image formation is subject to the complex process of light propagation through the water column. The raw images retrieved are characteristically different than images taken in air due to effects such as absorption and scattering, which cause attenuation of light at different rates for different wavelengths. While this physical process is well described theoretically, the model depends on many parameters intrinsic to the water column as well as the structure of the scene. These factors make recovery of these parameters difficult without simplifying assumptions or field calibration; hence, restoration of underwater images is a non-trivial problem. Deep learning has demonstrated great success in modeling complex nonlinear systems but requires a large amount of training data, which is difficult to compile in deep sea environments. Using WaterGAN, we generate a large training dataset of corresponding depth, in-air color images, and realistic underwater images. This data serves as input to a two-stage network for color correction of monocular underwater images. Our proposed pipeline is validated with testing on real data collected from both a pure water test tank and from underwater surveys collected in the field. Source code, sample datasets, and pretrained models are made publicly available.
 Accelerated diffusion-weighted magnetic resonance imaging using a low-rank tensor model

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Purpose: To develop an algorithm that accelerates the acquisition of diffusion-weighted imaging (DWI), in support of more extended or dense sampling of b-values for fitting of higher-order diffusion models and extraction of new biomarkers.

Method: The k-space data was retrospectively undersampled to achieve an acceleration factor of 8. To remove artifacts resulting from undersampling, we regularized the reconstruction using a low-rank tensor model, based on the fact that imaging coils and intra-subject decay signals across b-values are highly correlated. A phase constraint was further introduced to limit the large phase variations between b-values, which may otherwise invalidate the low-rank assumption. We first estimated phase maps from the fully sampled center of k-space. The phase-corrected k-space data was then organized into a 3D tensor and projected onto a low-rank subspace using multilinear singular value thresholding. A projection-onto-set algorithm was applied to iteratively enforce the low-rank property and data consistency.

Result: Reconstructed images using both simulated and patient data were observed to be free from aliasing and showed improved signal-to-noise ratio (SNR) as compared to conventional parallel imaging technique. The improvement of SNR on simulated data was 20.3%, with a relative rooted-mean-square error of 7.1%, as compared to the noise-free ground truth; the improvement of SNR on patient data was 27.7%.

Conclusion: Accelerate DWI by sparse k-space sampling and regularized image reconstruction is feasible, and has the potential to allow new b-value sampling scheme for image analysis using higher-order diffusion models.
Click Here: Human-Localized Keypoints as Guidance for Viewpoint Estimation

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We motivate and address a human-in-the-loop variant of the monocular viewpoint estimation task in which the location and class of one semantic object keypoint is available at test time. In order to leverage the keypoint information, we devise a Convolutional Neural Network called Click-Here CNN (CH-CNN) that integrates the keypoint information with activations from the layers that process the image. It transforms the keypoint information into a 2D map that can be used to weigh features from certain parts of the image more heavily. The weighted sum of these spatial features is combined with global image features to provide relevant information to the prediction layers. To train our network, we collect a novel dataset of 3D keypoint annotations on thousands of CAD models, and synthetically render millions of images with 2D keypoint information. On test instances from PASCAL 3D+, our model achieves a mean class accuracy of 90.7%, whereas the state-of-the-art baseline only obtains 85.7% mean class accuracy, justifying our argument for human-in-the-loop inference.
Feature Evaluation for EMG-Based Load Classification

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Human-machine interfaces (HMI)s used for rehabilitation or assistive purposes often have pattern recognition-based myoelectric control. To make this technology applicable in the real world, the control needs to be as robust as possible. Feature selection is a necessary step to find relevant data to improve robustness of a classifier and to reduce processing time with a lower-dimensional data set. Feature selection is highly task specific, and many different electromyography (EMG) feature selection strategies have investigated upper or lower limb myoelectric control applications. However, many of these applications are for static tasks and there is a lack of evaluation of features for dynamic tasks. This study presents a feature selection process for maximizing the accuracy of classifying a lifted weight from lower back muscle activity data, collected while subjects perform a dynamic lifting task. Twenty-six time-domain features are evaluated using a common strategy called min-redundancy max-relevancy (mRmR). The optimal features presented and validated here serve as a compact feature set recommended for myoelectric control applications for low-back lift-assist exoskeletons.
Sparse Coding with Memristor Networks

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We report the experimental implementation of sparse coding algorithms in a bio-inspired approach using a 32 × 32 crossbar array of analog memristors. This network enables efficient implementation of pattern matching and lateral neuron inhibition and allows input data to be sparsely encoded using neuron activities and stored dictionary elements. Different dictionary sets can be trained and stored in the same system, depending on the nature of the input signals. Using the sparse coding algorithm, we also perform natural image processing based on a learned dictionary.
A Convex Clustering Formulation Using the Similarity Matrix

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We consider the problem of clustering given data drawn from a finite K-mixture in high dimension. Our approach uses the similarity matrix of the data and an optimization based on the Ky-Fan K-norm of the similarity matrix. We show that under certain separation assumptions on the mixture centroids, the optimization when given the true similarity matrix returns the true clustering. In practice, we do not have access to the true similarity matrix. However, we demonstrate in synthetic experiments that our method far outperforms Kmeans even when we only have a single empirical estimate of the similarity matrix.
SSEC: Systems, Software Engineering and Computer Science
Performance characterization for a taxonomy of threading models applied to mid-tier servers

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Online Data Intensive (OLDI) applications like web search, online retail, and online advertisement comprise a significant fraction of datacenter applications. Meeting soft real-time deadlines in the form of Service Level Agreements (SLA) determines end-user experience and is hence of paramount importance for this application class.

The distributed system configuration for several OLDI applications comprise user-facing front-end servers communicating with mid-tier servers, which then query bucket servers and assimilate bucket server responses to provide a response to the user’s query. Therefore, the software design of mid-tier servers imposes significant ramifications to performance characteristics of such OLDI applications.

We present several software design choices for mid-tier servers in the form of taxonomy of threading models, in order to identify the influence of different threading models on performance characteristics such as saturation throughput, end-to-end response latency, and CPU cost per query for such applications. We use this performance characterization to show that different threading models are better suited under conditions like low and high system load, based on the performance metric considered. Hence, we propose a threading model auto-tuner that tracks load levels and tunes between different threading models based on the load detected, and the performance required. We implement the taxonomy of threading models in a custom large-scale distributed high dimensional search application called Imagen, which we will make open-source.
Localization, Approximations, and Nonlinear Consensus for Distributed Non-convex Optimization with Applications to Resource Allocation

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Distributed optimization has found its various applications in communication networks, sensor networks, signal processing, and data science. Methods for distributed convex optimization are widely investigated, while those for non-convex objectives are not well understood. The first non-convex distributed optimization framework over an arbitrary interaction graph was first proposed by Scutari et al., which iteratively applies a combination of local optimization with convex approximations and local averaging. We generalize the existing results in three ways. In the case when the decision variables are separable such that there is partial dependency in the objectives, we simplify the algorithm so that nodes only keep local variables instead of the whole vector of variables. In addition, we relax the assumption that the objectives’ gradients are Lipschitz continuous by means of successive proximal approximations. Interpreting Scutari’s algorithm as a two time-scale stochastic approximation, we consider nonlinear projections onto the consensus plane, which can speed up the convergence. We discuss many ways to apply our algorithm framework to the resource allocation problem in multi-cellular network. Simulation results show the superiority of our methods over naive single cell methods.
Foofah: A Programming-By-Example System for Synthesizing Data Transformation Programs

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Data transformation is a critical first step in modern data analysis: before any analysis can be done, data from a variety of sources must be wrangled into a uniform format that is amenable to the intended analysis and analytical software package. This data transformation task is tedious, time-consuming, and often requires programming skills beyond the expertise of data analysts. In this work, we develop a technique to synthesize data transformation programs by example, reducing this burden by allowing the analyst to describe the transformation with a small input-output example pair, without being concerned with the transformation steps required to get there. We implemented our technique in a system, Foofah, that efficiently searches the space of possible data transformation operations to generate a program that will perform the desired transformation. We experimentally show that data transformation programs can be created quickly with Foofah for a wide variety of cases, with 60% less user effort than the well-known Wrangler system.
Effective Premium Discrimination for Designing Cyber Insurance Policies with Rare Losses

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Cyber-insurance like other types of insurance is a method of risk transfer, where the insured pays a premium in exchange for coverage in the event of a loss. As a result of the reduced risk for the insured and the lack of information on the insurer’s side, the form is generally inclined to lower its effort, leading to worse state of security, a well-known phenomenon called moral hazard. To mitigate moral hazard, a widely employed concept is premium discrimination, i.e., an agent who exerts higher effort pays less premium. This, however, relies on the insurer’s ability to assess the effort exerted. In this work, we study two methods of premium discrimination that rely on two different type of assessment: pre-screening and post-screening. Pre-screening occurs prior to entering into a contract and can be done at the beginning of each contract period; the result of this process gives the insurer an estimated risk on the insured, which then determines the contract terms. The post-screening mechanism involves at least two contract periods whereby the second-period premium is increased should a loss event occur during the first period. Prior work shows that both pre-screening and post-screening are generally effective in mitigating moral hazard and increasing the insured’s effort. The analysis in this study shows, however, that the conclusion becomes more nuanced when loss events are rare. Specifically, we show that post-screening is not effective at all with rare losses, but pre-screening can be an effective method when the agent perceives them as rarer than the insurer does; in this case pre-screening improves both the agent’s effort level and the insurer’s profit.
A new locally tree like object: Erlang Weighted Tree

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Different random graph models have been proposed as an attempt to model individuals’ behavior. We study the asymptotics of a new proposed model, in which the individuals want to connect to each other based on the cost (benefit) of the connection. More precisely, node wants to connect with the first members of its ordinal preference, based on the cost of the connections. A connection will be established if and only if both sides agree to make that connection. We prove as the number of nodes goes to infinity, the model converges to a new locally tree-like object which we call Erlang Weighted Tree (EWT). EWT also models nodes with -dimensional attributes obtained from a spatial Poisson process where node wants to connect to closest nodes in. This connection allows us to use this generative model in two applications. The first is the generation of road transportation networks. The second is in distance-preserving low dimensional embedding of high-dimensional node attributes that is commonly observed in data science settings (including in social networks). In addition to understanding the sparse graph setting (where has finite mean) comprehensively, we also interpret the pruning process as obtained via cardinal preferences, which then allows us to study both cardinal and ordinal preferences with more general generative schemes.
Closing the Gap between Structured Codes and Random Unstructured Codes for Communication Networks

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The conventional technique of deriving the performance limits for any communication problem in information theory is via random unstructured coding involving so-called Independent Identically Distributed (IID) random codebooks. Stepping beyond this conventional technique, Körner and Marton proposed a technique based on identical random linear codes (structured codes). It was shown that this technique outperforms all techniques based on (random) unstructured codes in certain multi-terminal problems. A structured code (linear code, group code or lattice code) is completely structured in the sense that the size of equals the size of . A code used in random coding in Shannon ensembles is completely unstructured in the sense that the size of equals . There is a gap between the completely structured codes and the completely unstructured codes. Is there a spectrum of strategies involving partially structured codes or partially unstructured codes that lie between these two extremes? In this work, we will introduce a new class of code ensembles called Quasi Group Codes (QGC) whose closedness can be controlled. The parameters of a QGC can be chosen such that the size of can be any number between and . The PtP channel capacity and optimal rate-distortion function are achievable using QGCs. In addition, coding strategies based on QGCs will be introduced which improve upon the previous strategies based on unstructured codes, linear codes and group codes.
On a structural theory of fault detection for affine systems

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Structural analysis provides methods to examine systems with much less information and detail, as well as dealing with the indeterministic fault scenarios. Here we introduce the notion of detection for structural systems which is shown to be a prerequisite of Detectability for the numerical systems of such structures. We define structure for matrices and provide a graph theoretical representation of structure. We define and characterize “Structural Detectability” for discrete time invariant affine system-fault pairs and provide the sufficient and necessary conditions on the structures of system and fault defining matrices. We provide a manner to approach fault detection and sensor placement problems for systems with vaguely known relations, unknown parameters, tabular or approximated system dynamics, with unknown or vaguely known fault values, using the analysis of “Structural Detectability”.

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A Descending Price Auction for Matching Markets
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This work presents a descending-price-auction algorithm to obtain the maximum market clearing price vector (MCP) in unit-demand matching markets on m items by exploiting combinatorial structures. With a shrewd choice of goods for which the prices are reduced in each step, the algorithm only uses the combinatorial structure, which avoids solving Linear Programing (LP) problems and enjoys a strongly polynomial time runtime of $O(m^{4.5})$. Critical to the algorithm is determining the set of under-demanded goods for which we reduce the prices simultaneously in each step of the algorithm. This we accomplish by choosing the subset of goods that maximize a skewness function, which is solved in time $O(m^{2.5})$ using a simple algorithm based on ideas from the Hopcroft-Karp augmenting paths algorithm for finding maximal matching in bipartite graphs. As a by-product of the proof of our algorithm, we provide a novel combinatorial characterization of the maximum MCP, and an interpretation of the maximum MCP using buyers' externalities, which is the analogue of the Clarke pivot rule in the VCG mechanism. We finish by considering a 3-by-3 matching market with asymmetric buyers, and a Bayesian Nash equilibrium (BNE) in this market that is shown to achieve an expected revenue higher than the expected revenue of the VCG mechanism.
dsNN: Improving Energy Efficiency with Data Specialized Neural Networks

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As designers push for higher accuracy and more functionality, larger and more energy consuming neural networks (Nns) are becoming dominant. To reverse the energy trend, we take a counter-intuitive approach to investigate ensemble methods. Traditional ensemble methods use a group of weak learners operating collectively to create a strong learner that is capable of achieving higher accuracy and supporting a wider range of functionality. However, ensembles often suffer from high energy consumption due to the inherent inefficiencies of activating multiple, often redundant, learners. We adapt the traditional approach by creating a data heterogeneous multi-NN system. In contrast to traditional ensembles, data heterogeneous multi-NNs divide the data space into subsets with one specialized NN for each group of data. For each invocation, a selector identifies the input subset and activates the corresponding NN. To demonstrate the feasibility of data heterogeneity, we develop a systematic methodology to replace NNs with a set of automatically generated data specialized neural networks (dsNNs) to create an energy-efficient learner. By invoking only one dsNN for each input instance and reducing the interference between different input behavior patterns, our technique provides lower energy consumption while maintaining output accuracy. A multi-dsNN system comprised of two dsNNs is implemented and evaluated across six benchmarks. Results demonstrate that on average, multi-dsNNs reduce energy consumption to 32%, 38% and 35% and increase performance by 3.2×, 2.2×, and 2.0× on ARM Cortex-M4 Microcontroller, Kryo 280 octa-core Mobile CPU and Adreno 540 Mobile GPU while achieving 100% of the baseline accuracy.
Scalable Control of Cyber-Physical Systems

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The defense of computer systems (cyber security) plays a crucial role in their efficient/normal operation. One class of cyber security problems concerns the security of networks of computers (cyber networks), which are typically very large. In this work, we present a scalable approach to development of defense policies for the security of cyber networks. We consider a situation where the defender has imperfect observation of the attacks, defends the system dynamically, and is conservative in his defense.
Long term effects of pair programming

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Engineers often work in teams, both in industry and in academia. In particular, computer programming in partnerships is useful for practicing engineers and students alike. This study investigates the long term effects of pair programming on student performance. This quantitative analysis examines 2,468 students in an introductory computer science sequence at a large, public research institution. The data set comprises two academic years and includes partnership participation, project and exam scores, withdraw rates, time between courses, GPA, and gender information. In the results, a positive relationship is observed between partnering in an introductory course, and higher project scores in a future course where all students worked alone (N=1,003). Students with the lowest GPAs experienced the greatest benefits. Additionally, results with a large population of students confirm the observations of previous research, showing that partnerships are associated with an overall positive grade impact during the course in which the partnership takes place (N=2,468).
TCB: Tissue, Cellular, and Biomedical Engineering
Matrix Elasticity Defines Cell Migration Modes in Aligned Fibrous Microenvironments

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To understand how the extracellular matrix (ECM) affects cell migration, we implemented a recently established synthetic material system that models fibrous ECMs and affords independent control over mechanical and architectural features. Using this system, we sought to decouple the effects of alignment and stiffness on cell migration in fibrillar matrices. We found that increasing matrix alignment, independent of stiffness, increases the speed and persistence of cell migration via contact guidance. Interestingly, varying the stiffness of aligned matrices resulted in a biphasic response with respect to cell migration speed. Towards identifying the cause for these variations in speed, high spatiotemporal imaging revealed that stiffness defined the magnitude of matrix deformation resulting from cell generated traction forces. Specifically, at intermediate stiffnesses, cells were able to recruit and stretch fibers, storing elastic energy in the local matrix, which upon release resulted in rapid forward translation of the cell body. Furthermore, this phenomenon was found to be actomyosin contractility dependent, as inhibiting or enhancing myosin activity decreased or increased the frequency of rapid migratory events, respectively. This work characterizes a previously undescribed migration mechanism whereby the cell’s ability to physically reorganize its local microenvironment by stretching matrix fibrils considerably alters the mode and speed of migration. Given the ubiquity of fibrous, collagenous tissues within the body, an understanding of how matrix structure and mechanics guide cell migration could improve approaches to promote cell migration to wound sites or inhibit cancer cell dissemination through the surrounding tumor stroma.
Quantitative Single-Cell Analysis of Cancer Drug Response

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Targeted cancer therapies that block driver oncogenes often have substantial short-term effects, yet the development of resistant cancer cells leads to tumor relapse and is a major barrier to durable therapies. This highlights an urgent need for a better understanding of mechanisms associated with drug response and resistance in tumor cells. The current standard to assess drug response is to measure cancer cell viability at a fixed time point upon drug treatment of various doses. Metrics extracted from these dose-response curves, such as IC$_{50}$ and E$_{max}$, are then used to compare cellular response across different drugs or cancer cell lines. This approach, however, does not capture drug response dynamics; gives little insight about the mechanisms of drug action and unable to differentiate drug response in a subset of cells from the population. Here, we presented a quantitative framework to characterize both the dynamics and heterogeneity of drug response in BRAF melanoma cells treated with various doses of vemurafenib at a single-cell level, utilizing long-term time-lapse live-cell microscopy, which allow dynamic tracking of single cell fates (e.g. proliferation and apoptosis) with time. Quantitative metrics extracted from these dynamics, such as the kinetic rates of cell division or death, or time to the maximal rate of apoptosis, not only provided richer biological information about how cells respond to drug compared to conventional dose-response metrics, but also captured diverse drug-resistant phenotypes at a single-cell level. Informative drug response characterization will help us define the mechanisms resulting in residual tumors, enabling evidence-based precision medicine.
Bacterial MscL in Mammalian Cells for Novel Mechanobiology Applications

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Mechanobiology, a relatively young field centered on how external physical forces on cells or tissues and their intrinsic mechanical properties can influence physiology and disease, has already become a pillar in cell biology. Indeed, cells experience a myriad of external, mechanical stimuli. Mechanosensors on the cell surface interfacing with the external environment and others within the cell, can sense, transmit, and amplify these inputs. This results in intracellular chemical signaling that leads to altered gene expression, protein expression, and finally, altered cell behavior and function. This process is mechanotransduction. Mechanotransduction occurring at the cellular-scale, has perceptible, large-scale implications such as the ability for organisms to sense sound and touch, proper organ system function, providing key external cues for organism development, and disease. This has motivated researchers in recent decades to make breakthroughs in mechanobiology. Though these milestones cover a vast range of systems, all have focused on investigating or capitalizing on native, endogenous mechanotransduction. This work proposes moving into a relatively unexplored frontier in mechanobiology: exogenous mechanotransduction, by demonstrating a novel approach towards achieving signal transduction and mechanically driven behavior in cells through the introduction of exogenous mechanosensory components.

We demonstrate how the functional expression of the E. coli mechanosensitive channel of large conductance (MscL), which is gated through membrane tension, in mammalian cells endows new capabilities of (1) delivery of large, impermeable biomolecules into live, mammalian cells as a response to mechanical perturbation; (2) novel interaction with other native mechanosensory networks; and (3) altered cell migration in physiological applications.
Role of Fiber-Mediated Mechanical Cell-Cell Communication in Endothelial Cell Network Formation

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Vasculogenesis is the differentiation and formation of a vascular network from individual endothelial cells (ECs), and occurs during both early embryonic and postnatal vascular development. Vasculogenesis can be mimicked and studied in vitro using network formation assays. While the biochemical aspect of network formation has been well studied, the role of ECM mechanical and topographical cues is less understood. We hypothesize that the cellular extension and alignment required for network formation is mediated by the structure and mechanics of the ECM and subsequent cellular force generation and transduction through the system. Thus, we have engineered a synthetic electrospun fibrous material with controllable mechanics that supports network formation in vitro. To first confirm that this process was mediated by cell contractility, we utilized pharmacologic inhibitors to abolish actomyosin-generated forces, which led to the abrogation of fiber recruitment and inhibition of network formation. We also modulated force distribution through the fiber matrix by individually modulating fiber stiffness, density, and interconnections. We found that independently increasing all of these properties led to decreased force transmission through the matrix and subsequent inhibition of network formation. These results suggest that long range mechanical communication between individual cells is necessary for network formation, and supports the claim that fibrous microenvironments amplify cell-generated force propagation. This information further demonstrates the regulatory role of the physical microenvironment on multicellular morphogenetic processes and suggests that the incorporation of fibrous structure into scaffolds could improve vascularization of constructs for tissue engineering and regenerative medicine applications.
Fluid Shear Stress Induces Chemoresistance, Proliferation, and Mechanotransduction Phenotypes in Breast Cancer Cells

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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 breast cancer cells suspended in agarose-collagen hydrogels. Finite element modeling was used to determine the shear profile within the bioreactor. The effect of shear was characterized with immunohistochemistry for 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, a selective Cox-2 inhibitor, 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 mechanotransduction, invasion, and chemoresistance in breast cancer cells. This work is supported by the DOD OCRP Early Career Investigator Award W81XWH-13-1-0134 (GM).