Abstract Booklet

9th Annual Engineering Graduate Symposium

Friday, November 14, 2014

College of Engineering, University of Michigan, Ann Arbor
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From the Chairs

We, on the behalf of the planning committee, would like to welcome you to the 9th edition of the annual Engineering Graduate Symposium (EGS ’14), which is a premier event for graduate students in the College of Engineering (CoE). This event is aimed at establishing collaboration and communication from different disciplines, as well as facilitating interactions between current graduate students, prospective students, faculty members, and corporate sponsors.

This year, we arranged our technical sessions a bit differently. We tried to identify session themes that would bring together related posters from different departments. We hope this structure will foster students’ awareness, and perhaps even some scientific collaborations!

The planning committee for this event is comprised of representatives from all departments / tracks in the CoE, who review the submissions in their respective areas of expertise. This enables graduate students to share their research and accomplishments as well as review the research currently being conducted by their peers. In addition to the technical program, the symposium hosts special sessions and tours for prospective graduate students invited from top schools nationwide, introducing them to the broad research portfolio of the College of Engineering.

We look forward to meeting you and welcoming you!

Best regards,
Cheng Zhang and Karen Schroeder
Symposium Co-Chairs
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Abstracts – Morning Session
ACS: Atmospheric and Climate Science
A-Train Based Analysis of Frontal Cloud and Precipitation Structures: A Case Study

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Extratropical cyclones (ECs) are an important factor in regulating Earth’s energy balance and provide a considerable amount of precipitation in temperate climate zones. Preponderant amount of moisture present is transported through the warm conveyor belt (WCB), an airstream of ascending moisture that rises from the boundary layer to the upper troposphere. Previous research has shown that when WCBs strengthen, there’s a positive correlation of rain rate within ECs, experiencing nearly 100% efficiency at precipitating all poleward transported moisture. Given the large impact that ECs and their WCBs have on general atmospheric circulation, it’s important to conduct research to better understand the relationships between water vapor content, storm dynamics, frontal processes and the associated precipitation distribution. The week of Thanksgiving Day in 2006, an EC formed off the coast of Florida and slowly travelled along the eastern seaboard for approximately five days. Copious WCB transport of water vapor resulted in coastal flooding in the Carolinas and an inch of snow in portions of Georgia and South Carolina. Multiple overpasses of this long lived and nearly stationary cyclone were obtained from NASA’s A-Train satellite constellation. When combined with winds from an operational numerical analysis, this project was able to use data from the A-Train to observe and understand the evolution of the WCB cloud and precipitation structure. Our results demonstrate the value of an analysis that combines satellite and numerical model data, providing insight into the relationships between mesoscale cloud and precipitation features and cyclone scale dynamics and thermodynamic environment.
Investigating the impacts emissions have on indirect aerosol effects in convective clouds in the southern Great Plains.

Stacey Kawecki\textsuperscript{1}, Allison Steiner\textsuperscript{1}, David Stensrud\textsuperscript{2}, Larissa Reames\textsuperscript{3}, Geoffrey Henebry\textsuperscript{4}, Sam Pennypacker\textsuperscript{5}.

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Concentrations of anthropogenic air pollutants such as ozone and atmospheric aerosols are magnified in urban areas. Aerosols have direct, indirect and semi-direct effects on the atmospheric radiation budget and the formation, presence and persistence of clouds in the atmosphere. Depending on environmental factors such as vertical wind shear and relative humidity, aerosols can either suppress or enhance convection. We isolate the effects of urban emissions on convective events in the Southern Great Plains with WRF-Chem. Understanding convective events in the Southern Great Plains in the spring can provide insight into thresholds for whether convection is suppressed or enhanced in a region dominated by strong vertical wind shear, regular severe weather events, and varying levels of urbanization. While anthropogenic effects in this region are relatively small, we focus on the urban areas of Kansas City, MO, Oklahoma City, OK, and Wichita, KS, which represent moderate to high, low to moderate, and low levels of pollution respectively. To isolate the chemical effects of urban pollution on convective cloud dynamics and microphysics, we produce month long simulations in May 2013 using the WRF-Chem model using three emissions scenarios: the first simulation (BASE) includes the physical and chemical effects with prescribed dust and normal emissions. The second simulation uses prescribed dust and scales emissions by a factor of two and the third simulation prescribes dust and scales emissions by a factor of one half. Together, these simulations show the role of dust and anthropogenic pollution on regional severe weather events.
Investigating key BVOC vertical distributions and oxidation in atmospheric boundary layer in 2011 DISCOVER-AQ campaign

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² National Center for Atmospheric Research, Boulder, Colorado.

Biogenic Volatile organic compounds (BVOC) play crucial roles in the formation of ozone and secondary organic aerosols in the atmosphere. Using 2011 DISCOVER-AQ P-3B ground-based and aircraft observations, we categorize three distinct weather systems, including fair weather, convective precipitation and high temperature systems, and investigate their role in the vertical distributions of isoprene and its oxygenated products. At the Fair Hill and Aldino sites, isoprene has a large vertical concentration gradient, ranging from around 1.5 ppbv on average at the surface up to less than 0.1 ppbv at about 5 km. Methyl vinyl ketone + methacrolein (MVK+MACR), HCHO and methanol exhibit weaker vertical gradients, suggesting a more well-mixed atmosphere corresponding with their longer chemical lifetimes. Under high temperatures (> 90 F) and convective precipitation systems, elevated concentrations of all the species are observed throughout the vertical profiles. We plan to simulate these events using the NCAR Large Eddy Simulation (LES) model including a gas-phase chemical mechanism of isoprene oxidation to understand and improve simulations of the vertical distributions of key VOC species and their oxidation role in atmospheric composition.
A Coupled-Path Retrieval Algorithm for the Hurricane Imaging Radiometer (HIRad)

Mary Morris\(^1\), Christopher Ruf\(^1\)

\(^1\)Atmospheric, Oceanic and Space Sciences Department, University of Michigan

HIRad is a passive C-band radiometer that operates at 4, 5, 6, and 6.6 GHz. From HIRad's observations, surface wind speed and rain rate are retrieved over a wide swath of about 70 km with 1 – 5 km resolution. HIRad is capable of measuring wind speeds of 10-85 m/s and rain rates of 5-100 mm/hr. A situation unique to HIRad creates a need for a more rigorous, geophysically-based retrieval algorithm. HIRad’s observing geometry is such that the downwelling atmosphere in one viewing direction can be the upwelling atmosphere in another. This unusual condition introduces new complications to the retrieval algorithm that estimates surface wind speed and rain rate from the brightness temperature (TB) observations using an inversion of the forward radiative transfer model (FRTM). Using an iterative least squares estimator, surface wind speeds and rain rates are retrieved simultaneously at all viewing directions with the coupling between viewing directions fully accounted for by the FRTM. Flights over Hurricanes Earl and Karl during GRIP (Genesis and Rapid Intensification Processes) provided observations for developing a coupled-path precipitation retrieval algorithm for HIRad. However, other high-resolution imagers could potentially employ this coupled-path algorithm method.
Measuring snow grain size with the Near-infrared Emitting Reflectance Dome (NERD)

Adam Schneider1, Mark Flanner1
1Atmospheric, Oceanic & Space Sciences, University of Michigan

Because of its high visible albedo, snow plays a large role in Earth’s surface energy balance. This role is a subject of intense study, but due to the wide range of snow albedo, variations in the characteristics of snow grains can introduce radiative feedbacks in a snowpack. Snow grain size, for example, is one property which directly affects a snowpack’s absorption spectrum. Previous studies model and observe this spectrum, but potential feedbacks induced by these variations are largely unknown. Here, we implement a simple and inexpensive technique to measure snow grain size in an instrument we call the Near-infrared Emitting Reflectance Dome (NERD). A small black styrene dome (~17 cm diameter), fitted with two narrowband light-emitting diodes (LEDs) centered around 1300 nm and 1550 nm and three near-infrared reverse-biased photodiodes, is placed over the snow surface enabling a multi-spectral measurement of the hemispheric directional reflectance factor (HDRF). We illuminate the snow at each wavelength, measure directional reflectance, and infer grain size from the difference in HDRFs measured on the same snow crystals at fixed viewing angles. We validate measurements from the NERD using two different reflectance standards, materials designed to be near perfect Lambertian reflectors, having known, constant reflectances (~99% and ~55%) across a wide range of wavelengths.
APS: Applied Physics, Photonics, and Solid-State Devices
Self-Powered, Integrated Sensors Based on Efficient Photovoltaic Conversion

Kanika L. Agrawal¹ and Max Shtein¹
¹Department of Materials Science and Engineering, University of Michigan

Autonomous sensing of metal ions and biological species in remote environments with high reproducibility and sensitivity has the potential to enable many new applications. However, the large power draw of such devices limits their operational lifetime while prior demonstrations have typically incorporated the power source as an additional component, making the assembly bulky. We propose and demonstrate a sensing scheme in which the presence of ionic analytes disrupts (or triggers) the flow of electrical current between two electrodes, with the electromotive force provided by absorbed ambient light. This concept is implemented using the classical dye-sensitized solar cell structure consisting of cis-bis(isothiocyanato)bis(2,2′-bipyridyl-4,4′-dicarboxylato)-ruthenium (II) sensitizing dye (N3) and the iodide/triiodide redox shuttle. We demonstrate that the presence of Ag⁺ ions causes an appreciable change in the device characteristics, with a detection limit of 1 µM and provide an in-depth analysis of the underlying sensing mechanism. The ionic target species can also be generated using an auxiliary release mechanism so as to allow for indirect detection of biological analytes. This detection approach may enable a new class of highly miniature, low cost sensors for continuous, environmental and health monitoring.
The quest for “universal” low-energy and non-volatile semiconductor memories, spanning the entire spectrum of storage hierarchies, continues unabated. Charge-based conventional SRAM and DRAM devices are prone to data loss (volatility), high leakage energy, and timing errors due to process variations, while magnetic hard disks are subject to slow speed, poor reliability due to mechanical moving parts, and excessive power-hogging. Nonvolatile magnetic memories, exploiting the quantized electron spins to define the binary states, have been proposed to overcome the above limitations. Though the improved state-of-the-art spin-transfer torque (STT) magnetic memories require significantly lower write currents, yet they cannot keep up with the aggressive CMOS technologies scaling below 20 nm feature size. In order to extend the horizon of magnetic memories in sub-20 nm regimes of CMOS scaling, the Write currents in spin-based magnetic memories must be lowered further by over two orders of magnitude. In this work we show that piezoelectricity along with the Villari effect can be combined to assist magnetic switching at significantly lower energy by eliminating the static current flow during the Write operation. New Straintronics Random-Access Memory (STR-RAM) is discussed from different perspectives: materials suited for piezoelectricity and the Villari effect and the structure of the memory cell; 3-D micromagnetic modeling to illustrate the switching dynamics of the device; energy barrier and noise immunity under process variation; a novel Write protocol needed for inversion of memory bits; and power, performance, and area advantages.
Exciton-polaritons or polaritons in microcavities have been an area of intense research over recent years. These Bosonic quasiparticles, which are formed by the strong interaction of confined light modes and exciton states within the microcavity, can provide coherent emission without population inversion. This leads to the concept of the polariton laser, which is a next generation coherent emitter having a threshold density two orders of magnitude lower than that of an equivalent photon laser. The main obstacle towards the realization of commercially viable polariton lasers had been linked with the absence of an electrically pumped polariton laser which can operate above cryogenic temperature, if not at room temperature. In this work we present the first reported electrically pumped polariton laser which can operate at room temperature. The reported device is a GaN-based microcavity diode, in which current injection and optical feedback are in the orthogonal directions. Instead of the conventional vertical cavity surface emitting structure used for polariton lasers, a novel edge-emitting geometry is incorporated here, which minimizes series resistance of the diode and at the same time maintains strong optical feedback within the microcavity. Based on the same device structure, a GaAs-based electrically pumped polariton laser operating at 155 K is also presented. The polariton lasing threshold of these GaN- and GaAs-based polariton lasers are 169 A/cm$^2$ and 90 A/cm$^2$ respectively. Both the devices also show conventional photon lasing, at much higher threshold current densities of 44 kA/cm$^2$ and 32 kA/cm$^2$ respectively.
Measurements of the betatron spectrum around the K-edge of thin foils

Keegan Behm¹, Tony Zhao¹, Jonathan Wood², Jason Cole², Anatoly Maksimchuk¹, Victor Yanovsky¹, Stuart Mangles², Alexander Thomas¹, Karl Krushelnick¹

¹Center for Ultrafast Optical Science, University of Michigan
²Imperial College of London, London, UK

Simulations performed by colleagues at the Imperial College of London show temperature dependent absorption of thin metal foils near the K-edge. In order to experimentally measure the absorption of x-rays in these thin foils, it is necessary to have a diagnostic that can spectrally disperse x-rays. In the single photon regime, we have used a CCD camera to characterize the betatron spectrum from a LWFA. This however, limits the x-ray flux to the foil and may not be sufficient for accurate measurements of absorption at the Kedge. Therefore, curved Mica and HOPG crystals have been used to measure parts of the betatron spectrum at higher x-ray fluxes around the Kedge of different foils. The ability to measure absorption in the betatron spectrum due to the Kedge of thin foils will allow us to perform time resolved opacity measurements on a pump-probe experimental set up.
Multi-Bit Data Storage in MoS$_2$ Transistors
Via Plasma-assisted Doping Processes

Mikai Chen$^1$, Sungjin Wi$^2$, Hongsuk Nam$^3$, Xiaogan Liang$^4$

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$^4$Mechanical Engineering, University of Michigan

MoS$_2$ and other emerging layered semiconductors provide new opportunities in electronics, i.e., for new multi-bit memories with desirable data storage density and computing speed. In this work, we report that MoS$_2$ transistors fabricated via plasma-assisted doping process can serve as low-cost, non-volatile, highly durable memories with a multi-bit data storage capability. We have demonstrated data storage applications of binary and 2-bit (4-level) data states suitable for year-scale, as well as 3-bit (8-level) states for day-scale. Our Kelvin force microscopy (KFM) results indicate that the multi-bit memory capability is attributed to plasma-induced doping of the top MoS$_2$ layers that can spontaneously form a memory transistor structure with multi-level data states, similar to a floating gate structure. In addition, our research suggests that the programming speed of such memories can be improved by using nanoscale-area plasma treatments. This work provides a critical nanomanufacturing capability for low-cost and potentially upscalable multi-bit memory solution.

Acknowledgment. This work is supported by NSF grant CMMI-1232883 and ECCS-1307744. The authors would like to thank the staff of Electron Microbeam Analysis Laboratory as well as the staff of Lurie Nanofabrication Facility for their contribution to this work.
Effects of Chirped Pulses in Stimulated Brillouin Scattering

Mark Dong¹, Herbert Winful¹
¹EECS, University of Michigan

We investigate the phenomenon of stimulated Brillouin scattering (SBS) and how the pulse areas and frequency chirps affect the three wave interaction. The basis of this investigation is sending in two optical pulses, a forward propagating signal wave at the highest frequency and a backward propagating SBS wave at the stokes frequency. The beating of these two waves will generate a third acoustic wave in the medium. We ran several numerical simulations as part of this study.

Under the quasistatic approximation of no stokes wave depletion, we find that the pulses behave analogously to the quantum two-level equations when an atom interacts with a radiation field. Unchirped pulses follow the area theorem of McCall and Hahn where the acoustic wave's amplitude is proportional to the sine of the area of the stokes wave, so that a $\pi/2$ pulse will generate a maximum acoustic wave. However, we have also found that by chirping the input pulses, the area theorem will no longer hold and the final amplitude of the acoustic wave becomes much less sensitive to the area of the stokes beam. As long as the chirp rate is comparable to the pulse area, the acoustic wave will be efficiently generated for a wide range of total pulse areas ($\text{area} > \pi/2$). The biggest advantage here is no longer having to engineer precise pulse areas when generating SBS for optical storage or buffering applications.
Nanoscale Dielectric Coatings Enhance Near-field Radiation

Yashar Ganjeh††, Bai Song††, Seid Sadat††, Dakotah Thompson†, Anthony Fiorino†, Víctor Fernández-Hurtado‡, Johannes Feist‡, Francisco J. García-Vidal‡, Juan Carlos Cuevas‡, Pramod Reddy†,‡, Edgar Meyhofer†

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†These authors contributed equally to this work.

Thermal radiation plays a major role in energy conversion, thermal management, and data storage. Recent experiments on thermal radiation between bulk materials demonstrate heat transfer enhancements in nanoscale gaps, however, whether such enhancements can be engineered with nanoscale films thinner than the penetration depth of radiation remains unknown. Here, we conduct first, direct near-field radiation studies with a novel ultra-sensitive calorimeter and demonstrate increases by several orders of magnitude in radiative heat transfer—even for ultra-thin dielectric films (50 nm)—at spatial separations comparable to or smaller than the film thickness. These surprising results are explained by analyzing the mode shape-dependent transmission characteristics of cavity surface-phonon polaritons. Our findings have important implications to a variety of future energy conversion and heat transfer nanotechnologies.
Solution-processed Yttrium-Scandium Oxide Alloys for High-k Dielectric Thin Films

Wenbing Hu, Bradley Frost, and Rebecca L. Peterson
Department of Electrical Engineering and Computer Science, University of Michigan

High-k dielectrics are needed for gate insulators in high-mobility (i.e. Ge-channel) MOSFETs [1] and thin film transistors (TFTs) [2], [3]. Rare-earth scandates (ReScO$_x$, Re being Y, La, Gd, or another lanthanide), including YScO$_x$ are prominent candidates for these applications due to their large band offsets to silicon, high dielectric constants, and a high crystallization temperature, i.e. a wide stable temperature range in amorphous phase [1], [4], [5]. Previously, rare-earth scandates have been deposited by e-beam evaporation, pulsed laser deposition, and atomic layer deposition. Here we describe successful fabrication of high-quality insulating layers of Y$_{2(1-x)}$Sc$_x$O$_3$ (x varied from 0 to 1) via spin-coating inks with Y and Sc precursors. The stoichiometry in the films closely follow that in the inks. The films are smooth and have an optical band gap >5.6eV. All films are good insulators, with a DC resistivity of >10$^9$ Ω·cm. The frequency response shows capacitive behavior with a relative dielectric constant >9. The alloyed films generally show a lower leakage current density ~10$^{-7}$ A/cm$^2$ at ~0.3MV/cm and a higher breakdown field up to 3.5MV/cm.

Graphene nanoelectronic heterodyne sensors for high speed and high sensitivity vapor detection

Girish Kulkarni1, Karthik Reddy1, Xudong Fan2 and Zhaohui Zhong1

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2Biomedical Engineering, University of Michigan Ann Arbor

Fast and reliable on-site vapor monitoring for defense, industry, homeland-security and environmental applications place stringent requirements on speed, sensitivity, size and stability of electronic vapor sensors. Nanoelectronic devices provide an ideal platform for vapor sensing due to their extremely large surface-to-volume ratios, high carrier mobility, high compatibility and ease of on-chip integration with modern electronic technologies. Nearly all existing nanoelectronic sensors are based on charge detection where molecular binding changes the charge density of the sensor and leads to sensing signal. However, intrinsically slow dynamics of interface trapped charges and defect-mediated charge transfer processes significantly limit those sensors’ response to 10s – 1000s of seconds, which is a bottleneck for studying the dynamics of molecule-nanomaterial interaction and for rapid and sensitive vapor monitoring applications. Here we report a fundamentally different sensing mechanism based on molecular dipole detection enabled by a graphene nanoelectronic heterodyne sensor. The dipole detection mechanism was confirmed by a plethora of experiments with vapor molecules of various dipole moments. Rapid (~0.1 s) and sensitive (~1 ppb) detection of a wide range of vapor analytes was achieved, representing orders-of-magnitude improvement over state-of-the-art nanoelectronic sensors. Further, we demonstrate rapid heterodyne detection of a mixture of vapor analytes with comparable performance to commercial flame-ionization-detector, highlighting the compatibility of our device with portable real-time vapor analysis systems. Our work not only provides a fundamental understanding of molecule-nanomaterial interaction at high frequencies, but also leads to a platform technology for highly integrated, rapid, and sensitive biological/chemical sensors.
Electronic Cooling in Epitaxial and CVD Graphene

Momchil T. Mihnev$^{1,2}$, Charles J. Divin$^{1,2}$, Torben Winzer$^3$, Faris Kadi$^3$, Ermin Malic$^3$, Andreas Knorr$^3$, John R. Tolsma$^4$, Allan H. MacDonald$^4$, Seunghyun Lee$^1$, Che-Hung Liu$^1$, Zhaohui Zhong$^1$, Claire Berger$^5$, Walt A. de Heer$^5$, and Theodore B. Norris$^{1,2}$

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Recent rapid progress in graphene research has been fueled by a wide spectrum of promising applications in nanoelectronics and nanophotonics. The realization of ultrahigh-speed graphene-based devices requires understanding the high frequency response and the hot-carrier behavior of graphene synthesized by various methods. Using ultrafast time-resolved THz spectroscopy, we systematically study the dynamic THz response in a wide variety of graphene samples including multilayer epitaxial and CVD graphene. We report here comprehensive experiments by varying the graphene quality and the degree of disorder, the Fermi level, the number of graphene layers and their stacking orientation, the substrate temperature, the carrier temperature, and the type of underlying substrate to determine the dominant mechanisms responsible for carrier cooling for different graphene material parameters and under different experimental conditions. We also develop a microscopic theory within the density matrix formalism and a theory of hot-carrier equilibration based on interlayer energy transfer via screened Coulomb interactions that accurately reproduce the observed THz dynamics and electronic cooling.
Next-Generation 2-Dimensional Nanoelectronic Biosensors

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Field-Effect-Transistor (FET) based biosensors have focused the spotlight of attention because of their fast and label-free detection technique. Firstly, FET biosensors using bulk materials such as Si were introduced to detect biomolecules. However, due to the low sensitivity of those biosensors, there has been a great deal of effort to find a proper channel material for higher sensitivity. 1D structures, Si nanowires and Carbon Nanotubes have been found as a solution to substitute for the 3D bulk materials, but also have difficulty in fabrication. Naturally, 2D materials have attracted a lot of attention as they can achieve high sensitivity as well as large-area production. Recently graphene based FET biosensors have been widely studied, though they have limitation from lack of a band gap. Now people are interested in MoS\(_2\), which is 2D layered material with attractive electronic, optoelectronic, and mechanical properties. Especially, monolayer and few-layer MoS\(_2\) films have a large direct bandgap that is suitable for semiconductor-related applications such as thin-film transistors, chemical sensors, and light emission devices. In our project, back-gated MoS\(_2\) FETs are functionalized by Anti-TNF-α antibody. The device characteristic curves of the antibody-attached FETs are measured, and TNF-α droplets in DI water with different concentrations are prepared for specific antibody-antigen binding. The TNF-α solution is dropped on the device area and stabilized for 20 min followed with DI water rinse and N2 blow dry. Then the device characteristic curves of the antibody-antigen-attached FETs are measured. These preparation and detection processes are performed from lower to higher concentrations.
Coherent Pulse Stacking in Fiber Chirped-Pulse Amplification Systems

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We demonstrate a new technique of coherent pulse stacking (CPS) for increasing pulse energies from femtosecond chirped-pulse fiber amplifier systems based on time-domain combining of a sequence of amplified chirped input pulses into a single chirped output pulse. Coherent pulse stacking is achieved by tailoring the amplitudes and phases of a burst of pulses which are launched into a Gires-Tournois interferometer (GTI) traveling-wave cavity, so that they destructively interfere at the partially-reflecting front mirror and are stored as a single pulse inside the cavity, until the final pulse in the burst constructively interferes with the intra-cavity pulse at the front mirror and thus extracts all the stored energy from the cavity into a single output pulse. With several GTI cavities more than 100 pulses can be stacked.

In a proof-of-principle experiment, a five-pulse sequence of ~500ps stretched pulses is coherently stacked in a GTI cavity, yielding a theoretically predicted 2.56 times peak-power enhancement factor. Properly tailored five-pulse bursts are produced from a 122-MHz repetition-rate mode-locked pulse train using an amplitude modulator and a phase modulator positioned after the pulse stretcher. These pulse bursts are amplified into microjoule-millijoule range prior to stacking using an amplification chain with a final 55-μm Chirally-Coupled-Core (CCC) fiber amplifier. Comparison between measured autocorrelation traces of compressed stacked and unstacked pulses shows no observable pulse distortions.

CPS opens a path to extracting all stored energy from a fiber CPA with negligible nonlinear distortions. This can enable much higher pulse energies from FCPA and coherently-combined FCPA array systems.
Effects of Lattice Mismatch and Period Length on Thermal Transport and Phonon Density of States in Silicon and Germanium Hetero-structures

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Many of electronic devices are made of double-layer or multi-layer hetero-structures of different materials with considerable lattice mismatch. Due to lattice mismatch between the two materials usually a residual strain will remain in such structure after fabrication. This residual strain could change the physical properties of the material including their thermal properties. In addition to the strain effects, the size effects could also change the intrinsic thermal properties of materials in such small structures. Usually because of different phonon spectra of the materials, we see a reduction in thermal transport in multi-layered structures comparing to the pure materials. This thermal transport bottleneck in multilayer structures causes local heating in the device. Thermal degradation is one of the reasons for failure of multilayer structures which could be caused by local heating in the devices.

In this study we have used molecular dynamics simulations to study the strain relaxation profile in the Si/Ge structures and its effects on thermal transport in such structures. We have also studied the changes in the phonon spectra of superlattices with different period lengths. We have observed a minimum in the thermal conductivity of superlattices with respect to the superlattices’ period length which correlates with strain relaxation length of the Si/Ge hetero-structure. We have also seen new phonon modes in both materials at period lengths smaller than the period length where the minimum occurs. These modes are identical in both silicon and germanium and thus help transfer more heat through the interface.
Investigating the Crystal Structure of ZnSnN$_2$ Thin Films using Surface X-Ray Diffraction

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In recent years, Zn-IV-N$_2$ compounds have seen increasing interest as potential replacements for indium-based materials used for photovoltaic and solid state lighting applications. While a lot of research has gone into the growth and characterization of ZnGeN$_2$ and ZnSiN$_2$ compounds, little is known about the structure of ZnSnN$_2$. Using the surface x-ray diffraction technique, we investigate the crystal structure of ZnSnN$_2$, a member of the group of elements termed earth abundant materials. Density Functional Theory measurements predict that it crystallizes in the orthorhombic phase with an energy gap of 2eV but only a wurtzite structure has been previously observed experimentally using reflection high energy electron diffraction and soft x-ray measurements. We present initial findings from surface x-ray diffraction studies on ZnSnN$_2$ films grown on (111) Yttria Stabilized Zirconia (YSZ) substrates and show that the films indeed crystallize in a single crystal hexagonal symmetry. Pole figure measurements performed on one of the films show that ZnSnN$_2$ films grown on YSZ substrates may crystallize in the orthorhombic phase but work is still ongoing to prove the existence of this orthorhombic phase.
Polarization-controlled Single Photon Emission from Site-controlled InGaN Quantum Dots

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Single photon emitters based on semiconductor quantum dots (QDs) are promising candidates for quantum light sources in quantum information technologies. Controlling the polarization of single photon emission is essential and yet challenging task for quantum information processing and polarization encoding. Here we present a polarization-control scheme that utilizes elliptical QD geometry to produce predefined linear polarization without applying polarizers or photonic cavities. Elliptical QDs were fabricated by a top-down approach, which enables precise control of QD position and shape. Polarization-resolved micro-photoluminescence measurements were performed to characterize the polarization properties of both QD ensembles and single QDs and revealed that the emission was linearly polarized along the elongated direction. Polarization-controlled single photon emission was demonstrated from two single elliptical dots that have orthogonal polarization angles and degree of linear polarization over 0.9. Direct evidence of the correlation between QD geometry and polarization properties was found by comparing SEM images and photoluminescence results of several single QDs. The aspect-ratio dependent degree of polarization agreed very well with simulation results. Finally, QDs based on different semiconductor materials were also compared theoretically, with InGaN QDs being the most sensitive to asymmetric geometry and achieving the highest degree of polarization. Both experimental and theoretical results indicated the great potential of InGaN elliptical dots as highly polarized single photon emitters.
Spin Measurements in ZnO: A Study in Blue

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“Spin” in semiconductors is of interest not just from the viewpoint of fundamental physics but also for potential applications such as all optical ultrafast switching, laser diodes and quantum computing. As the lower limits of scaling are reached and current semiconductor technology is headed towards the quantum regime it becomes vital that we understand most aspects that govern the “information carriers” in this domain. This would prove crucial to address quantum mechanical issues at this level and could be the lifeline of charge based systems. On a different front, a spin based computational paradigm might arise as a technology in itself. Our aim is to work towards such ends. In this regard, we study the spin relaxation mechanisms in wide band gap semiconductors. We studied spin mechanisms in zinc oxide using Time Resolved Kerr Rotation as well as Resonant Spin amplification – two exotic techniques used in opto-magneto spectroscopy. We identified a higher spin coherence at low temperatures in these materials than which is expected and attribute it to contribution from impurities. Such a mechanism has not be observed before in these materials. In addition to this, we were also able to observe spin behavior that matched theoretically expected models and helped explain bands in zinc oxide. These experiments provide new insights towards understanding spin, which could go a long way in helping us to manipulate and understand spin in other material systems.
Indoor Photovoltaics for mm-Scale Wireless Sensor Nodes

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Indoor photovoltaics is a possible candidate for powering mm-scale wireless sensor nodes. We calculate the fundamental (detailed balance) limit on the efficiency and power density of indoor photovoltaic cells assuming full absorption of photons above the band gap, perfect carrier extraction, and no non-radiative recombination. We find that the optimal band gap for indoor photovoltaics is ~1.9 eV, with efficiencies up to 60%, owing to the narrow visible spectrum typical in most indoor lighting. In addition, we report the experimental efficiency and power density of a commercial Si, fabricated GaAs, and fabricated Al₀.₂Ga₀.₈As cell under AM 1.5 irradiation and white phosphor LED illumination. Dark current and shunt resistance were shown to have a critical effect on the efficiency and power densities of the cells under the low-illumination conditions that are characteristic of indoor lighting. The GaAs and Al₀.₂Ga₀.₈As cells each provide a power density of approximately 100 nW/mm² at 415 lux, sufficient for perpetual operation of present-day low-power mm-scale wireless sensor nodes.
CRM: Control, Robotics, and Mechatronics
Customizable Brushless DC Motor Controller for Modular Robots

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To enable new research directions in the control of modular robots, we are developing our own BLDC motor controller for use in such modules. This would allow us to explore non-standard approaches to control of individual actuators and even entire robots. We have chosen to implement the control strategies to generate the appropriate three-phase voltages using an ARM Cortex 4 microcontroller. The end goal of this research is to have a module with a brushless DC motor, microcontroller, encoder, power supply, and other peripherals contained within. This module would be designed in a “rugged” way so it would be able to operate outdoors in the rain, or in locations with extreme temperatures. Most commercially available robot modules are unable to do that. By creating and programming the module ourselves, complete control over the system is retained.
Viability in a Passivity-based Hopper

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Stable gaits exhibited by passive dynamic legged systems can provide highly desirable templates for legged robotic systems, as such gaits do not rely on actuators and can be energy efficient. However, even if such a stable gait were to be found, the question of its robustness remains open. We know that a sufficiently large disturbance will render any legged system in a state from where recovery is impossible, while - by definition - a stable system can recover from small disturbances. In order to differentiate between recoverable and unrecoverable disturbances, we need to go beyond a linear first-order approximation of stability and describe the complete viability kernel. Here, the viability kernel of a system is defined as the set of all states that don’t lead to inevitable failure.

In this work we investigated what is arguably the simplest system that can exhibit running: the spring-loaded inverted pendulum (SLIP) in two dimensions. Due to the low dimensionality of the system, an exhaustive search through the state space is feasible. As such we identified all states from where falling can be avoided. Even for such a simple model, a complex sequence of steps is sometimes required to avoid falling, which, combined with the fact that an exhaustive search is prohibitively expensive, means that it is unlikely that any realistic controller will lead to optimal robustness. We further investigated the performance of some approximate controllers and found that good, but not optimal, robustness can be achieved by a simply policy.
Perfect (“deadbeat”) Feed-forward Rejection of Uncertainty in Contact Events

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Uncertainty in contact events is a natural phenomena in both legged locomotion and robotic manipulation tasks - going from a loaded to unloaded state occurs when a limb or grasper comes into contact with the ground or target. Contacts may occur at unexpected times or states, which may accompany significant actuator or force limitations - the system is responsible for bearing a load, as well as controlling its state. Systems with such contact events are frequently modelled using “hybrid dynamical system”: ordinary differential equations whose vector fields are only piecewise continuous, allowing each piece to describe distinct behavior. While it would be a reasonable supposition to conclude that rejecting the influence of unpredictable contacts would require some knowledge or measurement of such disturbances, we demonstrate that proper choice of a feedforward controller allows deadbeat rejection of variation in the hybrid transition event. We present the theoretical result and a recipe for reducing the control problem to feedforward execution of a particular behavior. We then demonstrate a simulation of the method being used on a non-conservative Spring Loaded Inverted Pendulum (SLIP), an extension of a commonly explored model of legged locomotion.
A Novel Method for Self-Sensing Soft Fluidic Actuators

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Soft Fluidic Actuators have the potential to work in wet, messy environments, with compliant joints and in non-traditional robots. Unlike traditional actuators, they do not require the sliding seals or careful alignment. Unfortunately, the encoders they are used with often do. This has precluded their adoption into the environments and morphologies to which they are uniquely suited. We have developed a method for embedding force and position sensing into the structure of these actuators. This allows them to sense their own tension and degree of contraction just as biological muscles do. By replacing the typically non-conductive reinforcing fibers with conductive fibers, we’re able to measure strain and changes in alignment through changes in resistance and inductance. These electrical properties can be used to deduce the force and length of the soft, muscle-like actuator. We have applied this technique to Mckibben Muscles (Pneumatic Artificial Muscles), a popular class of soft fluidic actuator. Our results suggest our method can provide contraction information with sub-millimeter resolution. We also present analytic and finite-element models for the design of the self-sensing fiber structures. Our hope is that this work will open the door to new forms of compliant robots with actuators that can sense their own state without external transducers or encoders.
Empirically, many experimental data sets for rhythmic biomechanical systems have the property that cycles can be brought to excellent correspondence by rescaling time. In particular, one stride of an animal gait is very similar to any other stride of the self-same animal – just at a time varying rate. We present an algorithm that guarantees, under suitable assumptions, the elimination of this time rescaling, allowing measurements from multiple cycles to be combined for improved accuracy. Our algorithm assumes each of these biomechanical systems can be modeled by a mathematical oscillator – i.e. an attracting limit cycle of a differentiable dynamical system together with the dynamics in the stability basin of the limit cycle. Our result applies to two different cases: (1) the time-rescaling is a right-continuous function of bounded variation, and (2) the time-rescaling is the solution to a Stratonovich stochastic differential equation with purely additive noise.
A nonlinear model predictive control (MPC) algorithm is proposed for obstacle avoidance in high-speed, large-size autonomous ground vehicles (AGVs) that perceive the environment only through the information provided by on-board sensors. The mission of the AGV is to move from its initial configuration to the goal configuration safely with collision-free trajectory and guaranteed dynamically safety. As a starting point, the scenario where the vehicle moves on a flat surface at a constant speed is considered. The nonlinear MPC algorithm generates steering commands for completing the mission while enforcing safety constraints. The first safety constraint is avoiding obstacles. This is fulfilled by restraining the position of the AGV inside a safe region established from real-time sensor data. The safe region is partitioned into multiple sub-regions that can be specified without using piecewise functions. The second safety constraint is ensuring dynamical safety. This is translated into avoiding single tire lift-off, which is implemented by limiting the steering angle within a range obtained using a 14 DoF vehicle dynamics model. At each sampling time, at least one multi-phase optimal control problem (OCP) is formulated and solved on-line. The fact that the optimal trajectory traverses the sub-regions sequentially with different position constraints from region to region makes the problem a multi-phase OCP. The multi-phase OCP is transcribed into a nonlinear programming (NLP) problem using the \( hp \)-pseudospectral method, and solved using the interior-point method. Simulations of an AGV approaching multiple obstacles show the effect of the proposed algorithm.
Ground Proximity Detection and Warning for UAV

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A UAV, commonly known as drone, is an aircraft without a human pilot on board. The flight operation of the UAV is either controlled by an operator in the ground station or by the pre-programmed on board systems. They are designed for applications like aerial mapping, disaster and crisis management, environmental monitoring and surveillance operations. Hence, they can function with ease in environments which are difficult for manned systems to operate. Presently, manned aircrafts are equipped with ground proximity warning systems (GPWS) which are systems designed to alert pilots if their aircraft is in immediate danger of flying into the ground. Contaminated environments, very high and low altitude terrain and certain ecosystems pose danger to human life. So, the use of UAVs is inevitable in these places. Currently, there is a huge demand for implementation of systems like GPWS to enhance the performance and durability of the UAV. So, this paper proposes a Ground Proximity detection system for a UAV. It aims to discuss a warning mechanism to send out an audio and visual warning when the distance between the UAV and the terrain is below a threshold range. Also, it aims to implement wireless communication to transmit the distance between the UAV and the obstacle to the base station wirelessly. Finally, this paper intends to discuss about plotting a real time graph at every instant of the operation and save the results for future investigation and research.
Composite Adaptive Internal Model Control and Its Application to Boost Pressure Control of a Turbocharged Gasoline Engine

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Internal Model Control (IMC) explicitly incorporates the plant model and its approximate inverse, and offers an intuitive controller structure and calibration procedure. In the presence of plant-model uncertainty, combining the IMC structure with parameter estimation through the certainty equivalence principle leads to adaptive IMC (AIMC), where either the plant model or its inverse are identified. This paper proposes a composite AIMC (CAIMC), which explores the IMC structure and simultaneous plant dynamics and inverse dynamics identification to achieve improved performance of AIMC. A “toy” plant is used to illustrate the feasibility and potential of CAIMC. The advantages of CAIMC are later demonstrated on the boost pressure control problem of a turbocharged gasoline engine. The design of the CAIMC assumes that the plant model and its inverse are represented by first-order linear dynamics. The unmodeled dynamics and uncertainties due to linearization and variations in operating conditions are compensated through adaptation. The resulting CAIMC is applied to a physics-based high order and nonlinear proprietary turbocharged gasoline engine model. The simulation results show that the CAIMC can not only effectively compensate for uncertainties, but also auto-tune the IMC controller for the best performance.
Resilient Monitoring Systems: Protecting Critical Infrastructures against Cyber-Physical Attacks

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Cyber-Physical attacks on critical infrastructure systems such as power plants, water distribution networks, power grids, etc., by adversarial organizations are intended to disrupt the normal flow of goods and services, with potentially catastrophic consequences – both physically and economically. It is imperative, therefore, to design monitoring systems that, in the presence of attacks, accurately ascertain the condition of the infrastructures, thus helping operators to minimize the disruption of normal operation. Such monitoring systems are termed as resilient. In this work, we design and analyze the performance of a five-layer resilient monitoring system, which is applied to the sensor network of a simplified power plant model. It is shown that the system offers effective protection against cyber-physical attacks on the various components of the power plant.
Simultaneous Identification and Torque Regulation of Permanent Magnet Synchronous Machines via Adaptive Excitation Decoupling

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Parameter identification and output regulation are generally conflicting objectives. However, in the case of certain overactuated systems, there is an opportunity to achieve these objectives simultaneously. This project explores a simultaneous identification and adaptive control design methodology for overactuated systems which is applied to the torque regulation problem for permanent magnet synchronous machines. Excitation and control inputs to the system are first designated. The excitation input is then treated as a disturbance which is decoupled from the regulated output via an excitation decoupling control law. Machine parameters are estimated with a normalized gradient-based algorithm, and necessary conditions for parameter convergence are established. Simulation results confirm the necessary conditions for parameter convergence, as well as the effectiveness of the resulting closed-loop torque regulator.
Battery State of Health Monitoring via Health-relevant Electrochemical Feature Estimation

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The objective of this research is to develop a noninvasive method to estimate battery state of health (SoH) via health-relevant electrochemical features. Battery state of health estimation is a critical part of battery management because it allows for balancing the trade-off between maximizing performance and minimizing degradation. In this research, a health-relevant electrochemical feature, the side reaction current density, is used as the indicator of battery SoH. An estimation algorithm is required due to the unavailability of the side reaction current density via noninvasive methods. Under the assumption of no State of Charge (SoC) estimation error present, Retrospective-Cost Subsystem Identification (RCSI) is used to estimate the side reaction current density via identification of an unknown battery health subsystem that generates the side reaction current density. Simulations show that estimation can be made for constant current charge and discharge cycles with different C rates. A current profile for an electric vehicle (EV) going through Urban Dynamometer Driving Schedule (UDDS) cycles is also used as the excitation signal during estimation. When a persistent SoC estimation error present, a modification of RCSI, the Two Step Filter, is developed to identify the SoH subsystem and estimate the persistent SoC error simultaneously. Simulations using linearized battery model show promising results in battery health subsystem identification, side reaction current density estimation and persistent SoC error estimation.
FAT: Fluid Dynamics, Acoustics, and Thermal Science
Numerical Investigation of Bubble – Turbulence Interaction

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Bubbly flows are common in engineering and nature and are in many cases turbulent. Common examples include boiling in nuclear reactors and along propellers in naval applications. The bubbly flows exhibit complex dynamics including bubble interactions with the turbulence, other bubbles, and rigid structures. Due to the large range of relevant spatial and temporal scales as well as difficulties with measurements of fluid properties, theoretical and experimental investigations are challenging. Thus Computational Fluid Dynamics (CFD) is used to study the physics of such flows. Even with CFD it is impractical to use high fidelity numerical simulations that incorporate all of the relevant physics. Instead the goal of this work is to isolate the bubble and turbulence interaction and investigate the dynamics of individual gas bubbles in a turbulent flow, particularly in problems where the bubble response to the turbulent fluctuation is violent. Successful implementation of a code to simulate turbulent bubbly flows requires multiple steps, beginning with choosing and applying an appropriate numerical method. The work presented is a preliminary application of the Ghost Fluid Method, which is a sharp interface method that will allow us to clearly resolve the bubble interface at all times in order to understand the bubble response to turbulent fluctuations. This method is applied to multiple one and two-dimensional problems including the Sod shock tube problem and shock-bubble interactions in order to quantify its performance in simulating multi-fluid flows. This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program.
Probing Thermal Transport in Single Atomic and Molecular Junctions

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Atomic and molecular junctions (AMJs), in which an atomic chain or organic molecule bridge two electrodes, represent the ultimate limit of the electrical circuits and have been intensively studied as an ideal testbed of quantum transport theory. Recent work has successfully probed electric, thermoelectric and heat dissipation phenomena in AMJs. However, thermal transport in AMJs remains poorly characterized owing to experimental challenges. Probing the thermal transport in AMJs not only pave the way to the fundamental understanding of the energy transport in atomic scale, but also provide fruitful insight into the future molecular devices. In this work, we employ custom fabricated scanning probes with integrated Picowatt-resolution calorimeter to investigate the thermal transport across a single atomic and molecular junction. We design experiments to answer two important questions about thermal transport properties of AMJs: i) Is thermal conductance in metallic atomic-junctions quantized at room temperature?; ii) Is thermal conductance of molecular junctions independent of the junction length?
Hall-effect thrusters (HETs) are electromagnetic in-space propulsion devices that produce high specific impulse (1000s of seconds), but low thrust (10s of mN). Traditionally they are built with a single annular channel. HETs are typically used for station keeping and attitude control, but higher power devices may be used as main propulsion systems, as planned for the Asteroid Redirect Mission. Designing higher power HETs poses several challenges. A solution explored by the Plasmadynamics and Electric Propulsion Laboratory (PEPL) was to nest multiple channels (NHTs). First the 10 kW class X2 dual channel thruster was developed by Liang, followed by the 100-kW class X3 triple channel device developed by Florenz. Both have shown performance gains when operating multiple channels simultaneously as opposed to independent single channel tests. The unexpected improvements were more significant than could be explained by variations in the facility background pressure. This indicates that a beneficial form of coupling between the channels is taking place, and in order to better understand this phenomenon a series of simulations will be performed. The initial study is focused on simulating the operation of each channel of the X2 independently to validate the modeling approach by comparing to experimental measurements. The next step will be to create a dual channel simulation and concentrate on the channel interaction. For the current test conditions, computed thrust is matched to within 3% of the measured value. Moreover, it was determined that the facility background pressure does not influence the inner channel at the current operating point.
Energetic composite materials are used as propellants, explosives and fuel cell components. They can be engineered to tailor energy-release rates and sensitivity to shocks and impacts. Due to the extreme conditions (high temperature, high pressure) that result from rapid detonation of energetic particles, laboratory experiments are seldom equipped to handle these events. Advancements in computational methods and algorithms make it possible to simulate and peek inside extreme detonation events at multiple length and time scales with accuracy. The SOD shock test problem for the explosive HMX is presented. A one-step second-order Taylor-Galerkin formulation is used to solve the compressible Euler equations with discontinuous initial conditions. During the test, multiple species exist and it is assumed that the unreacted explosive and reaction products in partially reacted regimes are in both pressure and temperature equilibrium. A Newton-Raphson method is coupled with the formulation to ensure that these highly nonlinear equations of state reach equilibrium.
High-Fidelity Hydrodynamic Optimization of 3-D Morphing Hydrofoil

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From recent studies, it has been understood that active shape-morphing can lead to an increase in efficiency of lifting surfaces. In the present study, the objective is to find the optimal shape of an active shape-morphing hydrofoil as a function of operating conditions (i.e. speed and angle of attack) for high Reynolds number flow. An in-house compressible flow solver coupled with a gradient based optimizer, was used to achieve the objective. With this high-fidelity hydrodynamic optimization tool, the optimization problem can be solved efficiently for a large number of design variables. The idea is to reduce the drag coefficients at different operating conditions, while maintaining a required lift coefficient. In this research, a preconditioner was designed to solve the Euler equations for nearly incompressible flows, i.e. for Mach numbers of the order of 0.01. In addition, constraint was added to avoid hydrodynamic cavitation, which could lead to unwanted noise, vibration, and erosion. For a tapered NACA0009 hydrofoil of aspect ratio 3.33 at Reynolds number of $5.38 \times 10^6$ and Mach number of 0.03, reduction in drag coefficient of 24\% was achieved for the given lift coefficient of 0.5. If the hydrofoil is fitted with active shape morphing mechanisms such as smart materials or internal mechanical actuators, results show that an actively controlled hydrofoil (or any control surfaces) can be optimized for minimum drag throughout the operation while maintaining the required lift and satisfying additional performance requirements. This will result in much improved performance at off-design conditions, such as during hard turns, surfacing, and/or crash-stop maneuvers.
Channel Interaction in a 100-kW Class Nested-Channel Hall Thruster

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The Plasmadynamics and Electric Propulsion Laboratory has built a three-channel, 100-kW class Nested-Channel Hall Thruster known as the X3. It has seven operational modes consisting of each channel operating individually, all three channels operating simultaneously, and the various combinations of two. Preliminary operation has used xenon and krypton propellants and has achieved a maximum total discharge power of 61 kW. The test points are gathered into sets, where each set contains seven test points representing seven operational modes of the thruster at a constant current density. The current density at each test point was achieved using the propellant flow rate.

In this preliminary testing, significant channel interaction during multi-channel operation has been observed. There are two phenomena of particular interest. First is a propellant-sharing mechanism, in which the propellant necessary to achieve the desired current density of a multi-channel configuration is less than the sum of the propellant for each channel running individually. This effect is especially pronounced for the three-channel mode, showing a propellant savings of up to 26%.

Additionally, power spectral densities of the discharge current from high-speed current probes show a tendency of the breathing mode (the frequency at which the discharge current oscillates) of each channel to converge to a single frequency during multi-channel operation. This is again especially pronounced in the three-channel configurations. This behavior suggests an interaction of the plasma by a yet-unknown mechanism. Both phenomena will be studied with full thruster diagnostics and with simulations.
Wake entrainment of large bubbles

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The production and convection of bubbly populations in the vicinity of surface ships has received considerable study. Researchers have examined the sources of the bubbles in the flow, their interaction with the ship-induced flow around the hull, appendages, and propulsor, and their persistence in the ship wake. In many instances, a practical goal is the management of the bubbly flow in the wake of the ship. This includes control of the bubble size distribution, their spatial distribution, and their interaction with the time-varying flow of the wake. We will present results from a series of laboratory experiments conducted to examine the interaction of small (order 10 to 100 micron) bubbles with large (order 1 to 10 mm bubbles) bubbles and bubble models in both laminar and turbulent flows. A vertical water channel has been constructed that permits the detailed examination of bubble-bubble interactions. The downward flow of the free-stream can be maintained at roughly the magnitude of the large bubble’s terminal velocity, making the large bubble nearly stationary in the laboratory frame of reference. Then, the trajectory and interaction of the small bubbles with the large bubble can be examined and the entrainment properties of the wake determined.
Experimental Investigation of Atmospheric Ventilation on a Surface-Piercing Hydrofoil

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Modern high-speed marine vehicles rely upon high-lift devices for propulsion and, in some cases, dynamic lift, respectively provided by propeller and hydrofoils. Such lifting surfaces are often operated at or very near the fluid free-surface, making them vulnerable to atmospheric ventilation. Ventilation involves the entrainment of atmospheric air into low-pressure regions of flow, creating large air-filled voids or cavities. The transition between wetted and ventilated flows can occur suddenly and violently, resulting in large dynamic load fluctuations that threaten the stability, control authority, and structural integrity of vehicles that rely upon ventilation prone systems. Unfortunately, ventilation is inherently complex, and knowledge of its attending physics is incomplete. A novel experimental program is underway at the University of Michigan towing tank to study ventilation on a yawed surface-piercing strut. Characteristic flow regimes are identified and stability regions are established for each regime inside of parametric test-space. Unsteady transition mechanisms are shown to be responsible for changes between stable flow regimes. Each observed transition mechanism is categorized and broken down into distinct stages, which are driven by different physical processes. Scaling laws are proposed that match experimentally-observed transition boundaries. The completion of this work provides improved insight into ventilation’s underlying physics, ultimately advancing the ability of designers and operators to anticipate, mitigate, or take advantage of ventilation.
Aeroelastic Simulation of Highly Maneuverable Supersonic Munitions

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Directly solving fluid-structure interaction problems with a high level of fidelity is generally time consuming and resource-intensive. Beginning phases of vehicle system development require many iterations which implies a reduced order model with minimal loss of fidelity may be more appropriate. The fluid-structure interaction of a vehicle in supersonic flight is considered and the order of this system is reduced to enable time marching simulations of the vehicle in flight. In particular, the flexible vehicle is modeled similar to the AIM-9 sidewinder air-to-air munition currently in use with the exception of no control surfaces towards the nose. In this work reducing the span and overall box size of the vehicle is explored with the use of direct attitude control systems similar to those seen previously on the Standard Missile-3. The structural system of equations is reduced from over 9,000 degrees of freedom to 2 by projecting the system onto the vehicle free vibration mode shapes. The aerodynamic analysis has been simplified by using shock-expansion theory locally with piston theory for an unsteady correction. The full system of equations including flight dynamics are integrated in time using a framework that has been developed at the U-M. Time simulations of the vehicle undergoing high-g maneuvers have shown the vehicle flexibility having a large effect on the performance and overall trajectory compared to a rigid vehicle. The resulting reduced order model and framework provide greater understanding of highly maneuverable supersonic vehicles and a tool to enable controls research of flexible supersonic vehicles with alternative control systems.
Reduced Order Modeling of a Hypersonic Munition

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High speed weapons systems, particularly hypersonic munitions, operate in a high-energy environment characterized by strong fluid, thermal, and structural interactions which can compromise strike accuracy. The lack of ground test facilities which can generate the flight environment of interest forces the primary course of investigation be through computational simulation. However, the state of the art simulation tools are prohibitively computationally expensive to perform rapid structure and controller design studies.

Model reduction techniques were applied to a hypersonic munition on terminal trajectories to capture the aerodynamic, thermodynamic, and structural dynamic system evolution and couplings. The General Purpose Optimal Control Software (GPOPS-II) was used to determine a set of terminal trajectories which maximized impact velocity or range and minimized target error. Shock, Prandtl-Meyer expansion, and piston theory were combined to create an approximate flow solution over the munition outer mold line which was then compared to Fully Unstructured Navier-Stokes 3-Dimensional (FUN3D) computational fluid dynamics solutions. Proper orthogonal decomposition of the thermal state of the munition was conducted leading to 15 thermal degrees of freedom rather than approximately 28,000 contained by the original Abaqus finite element model, while sacrificing negligible system energy. Free vibration mode shapes are derived using the Lanczos algorithm and used to generalize the structural dynamics equations of motion, reducing the number of structural degrees of freedom to 8 from the original 130,000. The combination of these reduced models was used to perform a six degree of freedom flight simulation of the munition during the terminal phase of its trajectory.
Nozzle-free liquid micro-jet by homogeneous bubble nucleation for drug injection and printing

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Liquid micro-jets are used in many applications ranging from needle-free drug injection and high-resolution printing to material machining. Typical methods for producing liquid jets rely on an injection nozzle that defines the jet diameter. However, to obtain a fine feature size, nozzle-based approaches are required for reducing the nozzle size, which make them vulnerable to nozzle clogging. Moreover, the clogging issue becomes even worse when liquid is functionalized with different types of particles. We demonstrate a nozzle-free liquid micro-jet that is produced by cavitation following homogeneous bubble nucleation. High-speed imaging reveals that liquid jets emerge from water surface when the micro-bubbles (100 µm) collapse at the air/water interface. The bubbles are generated by a nanosecond-long pressure pulse that is produced by pulsed excitation of a carbon nanotube (CNT)-polymer composite, an optoacoustic transmitter that can convert light into sound. Because the negative pressure amplitudes (> 60 MPa) are significantly amplified by shockwave scattering at the air/water interface (a pressure-release boundary), the bubble nucleation falls into a homogeneous nucleation regime, thus forming a controlled liquid jets with a diameter of ~ 30 µm (1/3 of bubble diameter) and a speed of ~ 250 m/s. By using such nozzle-free approach, we will introduce a few applications, e.g., colored liquid injection into a tissue-mimicking material (agarose gel) and material printing.
Building a simple, accurate Lagrangian hydrocode

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Lagrangian hydrocodes play an important role in the computation of transient, compressible, multi-material flows. This work is aimed at developing a simple cell-centered Lagrangian method for the Euler equations that respects multidimensional physics while achieving second order accuracy. Algorithms that acknowledge the multidimensional physics associated with vorticity transport and acoustic wave propagation are needed in order to increase accuracy and prevent spurious mesh distortions. As such, one-dimensional Riemann solvers and spatial gradient limiters, which are common to traditional Godunov-type schemes, have been abandoned. Instead, we employ multidimensional vertex fluxes that automatically define the mesh motion and temporal physics-based limiting via flux-corrected transport (FCT). This research began by analyzing Vorticity Preserving Lax-Wendroff-type methods in the context of the linear acoustic equations. This family of methods can be written in terms of vertex fluxes and they exactly preserve vorticity, making them well suited for an extension to Lagrangian hydrodynamics. Work in the acoustic test environment focused on isotropy improvements and the development of a new temporal flux limiting strategy for use in a FCT algorithm. Results are presented which summarize this phase of research. The lessons learned from the acoustic work are now being extended to Lagrangian algorithms for the Euler equations in two spatial dimensions. Key areas of focus include estimation of the Euler vertex fluxes, eliminating spurious grid rotations, and designing a temporal flux limiter. Numerical results from the Sedov and Noh problems are presented to illustrate current successes and ongoing challenges.
A novel computational study of the combustion characteristics of syngas fuel

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Syngas (generally a mixture of H\textsubscript{2} and CO) can be produced from a variety of feed stocks and has potential to reduce carbon emissions in the stationary power sector. However, syngas fuel presents stability and safety challenges to gas turbine operation. In this work, the effects of thermal inhomogeneities on syngas auto-ignition are studied computationally at conditions relevant to gas turbine operation. The effects of thermal inhomogeneities are directly relevant to combustion stability and are investigated using one-dimensional numerical simulations with detailed chemical kinetics. Parametric tests are carried out for a wide range of thermodynamic conditions ($T = 850$-$1100$ K, $P = 3$-$20$ atm) and two fuel/air compositions ($\Phi = 0.1$, $0.5$). Effects of bulk thermal gradients and localized thermal hot spots are studied. In the presence of a thermal gradient, the propagating reaction front transitions from spontaneous ignition (strong) to deflagration (weak) mode as the initial mean temperature decreases. The critical mean temperature separating the two distinct auto-ignition modes is computed using a predictive criterion and found to be consistent with the front speed and Damkohler number analyses. The hot spot study reveals that compression heating of end-gas mixture by the propagating front becomes more pronounced at lower mean temperatures, significantly advancing the ignition delay. The present study reveals that the thermodynamic conditions of high pressures and low temperatures are sensitive to the presence of thermal fluctuations. The results inform the gas turbine combustion community on desirable and undesirable operating conditions.
Drag reduction by mitigating flow separation at the rear end of the ground vehicle is the major interest area. Current work is focused on performing numerical simulations of wall-bounded turbulent flows with passive vortex generators (VGs) to reduce flow separation. All the simulations are performed using a large eddy simulation (LES) technique in OpenFOAM®. The incompressible Navier-Stokes equations are solved using PIMPLE algorithm with homogenous dynamic smagorinsky sub-grid stress model. The algorithm was tested on various grid resolutions by simulating turbulent channel flow and the results are in good agreement with those published by Moser et al. Simulations were performed with a cube as a VG placed along the centre plane of a channel to observe some basic features such as, the horse-shoe vortex formed in front of the cube, the vortex shedding behind the cube and the region of influence of the VG. Simultaneously, flow over a backward facing ramp was simulated to understand the large region of flow separation over the ramp and downstream of the ramp. To mitigate separation a cube is placed as a low profile passive VG along the centre plane at two different positions on the surface upstream of the ramp. Further study on optimal configuration is being conducted, however, analyzing the x-component of the mean velocity profile along the ramp and further downstream it is certain that separation is mitigated. Future study will include simulating flow characteristics with multiple VGs and flow over a canonical car shape.
Towards the Accurate and Efficient Simulation of Transitional, Hypersonic Flows using a Hybrid Particle-Continuum Method

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Analysis of hypersonic flows requires consideration of multiscale phenomena due to the range of flight regimes encountered, from rarefied conditions in the upper atmosphere to fully continuum flow at low altitudes. The global Knudsen number, which is defined as the ratio of the freestream mean free path of a gas to a characteristic length scale of a vehicle or phenomenon of interest, describes the level of rarefaction of the flow field. At transitional Knudsen numbers, there are likely to be localized regions of thermodynamic nonequilibrium effects that invalidate the continuum assumptions of the Navier-Stokes equations. Accurate simulation of these regions, which include strong shock waves, boundary and shear layers, and low density wakes, requires a kinetic theory-based approach where no a priori assumptions are made regarding the velocity distribution function or internal energy distribution functions of the constituent molecules. The focus of the present research effort is the continued development of the Modular Particle-Continuum method, a hybrid approach where the Navier-Stokes equations are solved numerically using computational fluid dynamics (CFD) techniques in regions of the flow field where continuum assumptions are valid, and the direct simulation Monte Carlo (DSMC) method is used where strong thermodynamic nonequilibrium effects are present. With such a hybrid approach, numerical solutions of transitional, hypersonic flows are obtained with increased physical accuracy relative to CFD alone, and improved numerical efficiency is achieved because the more computationally expensive DSMC method is restricted to those regions of the flow field where it is necessary to maintain physical accuracy.
IOF: Industrial, Operations, and Financial Engineering
Reducing Patient Delays in an Outpatient Infusion Center

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Patients receiving chemotherapy in outpatient infusion centers often go through a variety of processes prior to receiving their infusion. Patients may go through a combination of getting blood work done in the lab, visiting their physician in the clinic, and having the pharmacy prepare their drugs all before receiving their infusion treatment. We use collaboration with nurses and physicians in the clinical environment, data collection and analysis, simulation, and optimization techniques to develop ways to improve the patient experience and reduce delays in this complex series of activities.
Impact of New Prostate Cancer Biomarkers in a Screening Setting

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Newly developed prostate cancer (PCa) biomarker tests have the potential to improve the approach to early detection of this disease; however, optimal use of these biomarkers and their impact on long-term health outcomes is unclear. A partially observable Markov chain was used to simulate patients' progression through PCa states to mortality from PCa or other causes. Patients periodically received one or more biomarker tests according to predefined screening strategies that use combinations of serum prostate specific antigen (PSA), urine PCA3 score, TMPRSS2(T2):ERG score, and the Mi-Prostate Score (MiPS) models (which combine these biomarkers to generate individualized all and high grade prostate cancer risk estimates). Monte Carlo simulation was used to estimate the number of screening biopsies and metastatic cases per 1,000 men and quality-adjusted life years (QALYs). Screening strategies based on MiPS were superior to PSA alone or PSA combined with PCA3 or T2:ERG. A MiPS strategy prioritizing high grade disease detection simultaneously reduced the number of screening biopsies by 23% and the number of metastatic cases by 11% compared to a PSA alone strategy. The best-performing PSA and MiPS strategies increased expected QALYs by 0.074 and 0.103, respectively, compared to no screening. New biomarkers with risk thresholds optimized for identification of high-grade cancer can reduce the number of screening biopsies and metastatic cases compared to PSA alone, while also increasing quality-adjusted survival. These data support prospective clinical validation trials using rationally selected thresholds in order to design more efficient PCa early detection strategies.
Stochastic Optimization to Reduce Patient Wait Times in a Chemotherapy Infusion Center

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In an effort to improve the quality of cancer care delivery and infusion center operations, we formulate a stochastic large-scale integer program that creates a patient appointment schedule under uncertainty of treatment times. We assume that the order of arrival of patients is known and has to be preserved when deciding their appointment times. The objective is to minimize a trade-off between expected patient wait times and expected overtime. Solving exactly this optimization problem would require a prohibitive computational time, so we develop a heuristic algorithm to find approximate solutions that we evaluate via computation of lower bounds on the optimal objective value. We then evaluate different sequencing strategies to find easy-to-implement rules to order patients appointment times during the day.
Enhancing hand function assessment by using low cost motion capture and pressure mapping system

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Hand injuries affect our ability to manipulate objects. Clinicians and occupational therapists have long used test assessments such as Jebsen-Taylor Hand Function Test (JTT), to provide information about discomfort, the ability to perform basic tasks, and as a measure of disability in RA patients. However, JTT scored is based only on the time to complete a task and is not sensitive to the ways that patients may alter their behavior. This study aims to supplement the JTT with force and Range of Motion (RoM) measurements to understand how people compensate for the effects of Rheumatoid Arthritis (RA) and their ability to grasp and manipulate work objects. Youth and Older control groups were used as a basis for comparison of RA patient performance. Results of the JTT itself illustrated how RA patient can perform some tasks more quickly than control groups. However, when including RoM measurements during the JTT assessment, there were significant differences between the RoM of RA patients and both young and older control groups. For example, hand displacement results for the RA participants were significantly greater than those of the older control. This demonstrates that the integration of motion capture analysis with the JTT gives a more comprehensive assessment for hand function.
Incorporating Nurse Absenteeism into Long Term Staffing with Demand Uncertainty

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Increased nurse to patient ratios are associated with both increased costs and improved patient care. Thus, it is critical from both a cost and patient safety perspective that nurses be utilized efficiently and effectively. To address this, we propose a stochastic programming formulation for nurse staffing that accounts for variability in the hospital census and nurse absenteeism, day-to-day correlations among the unit census levels, and costs associated with three different classes of nursing personnel: unit, float, and temporary nurses. The decisions to be made include: how many unit nurses to employ, how large a float pool of cross-trained nurses to maintain, how to allocate the pool nurses on a daily basis, and how many temporary nurses to utilize daily. Preliminary results using data from a large University hospital suggest that the proposed model can save the hospital hundreds of thousands of dollars annually as opposed to the crude heuristics the hospital currently employs. Nationally, this would project to billions of dollars of savings.
Optimal patient care resource allocation based on patient mortality risk and acuity

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Our research has examined patient admission policies, with an emphasis on studying intensive care units (ICUs) and intermediate care units (IMCs). The main hypothesis of our research is that we can optimize the ICU and IMC patient admission policy to get the neediest patients into the ICU and IMC. This will improve patient outcomes by reducing patient complications and mortality as well as reducing unplanned transfers to the ICU. Reducing transfers is important as transfers often require a physician handoff. Unplanned transfers from a non-ICU bed to the ICU are especially harmful, as in this case the patient needs immediate transfer or else their condition will deteriorate rapidly. In order to optimize the system, we propose the following admission policy. Mandatory patients (i.e. those who require treatment specific to the ICU or IMC) are always approved for admission to the relevant unit. All other patients, who we are calling discretionary, may be approved for admission to an ICU or IMC based on their respective Mortality Risk scores. We will use a threshold-type policy on these discretionary patients. Our methodology derives separate thresholds for ICU admission and for IMC admission using a concrete Mixed Integer Programming (MIP) model. The intuition here is that high risk patients would benefit most from ICU care, but would also benefit from IMC care, and that less risky patients would benefit from IMC care without requiring the extra level of care given by ICU admittance.
Retail supply chain network design under operational and disruption risks

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Supply chain network configurations play crucial roles in creating competitive advantages for businesses operating in an uncertain environment. Accordingly, designing stable and resilient networks to cope with various operational and disruption risks is of vital importance. In this paper, the concepts of robustness, responsiveness, and resiliency are incorporated in a decision problem addressing supply network design and supply facility location at a strategic level for a retail chain. A deterministic mixed integer linear programming model (MILP) is first developed and then it is extended by scenario generation and disruption profiling. Furthermore, a multiple set-covering model (MSCM) is proposed to make the designed network more resilient against disruptions. A hybrid solution methodology including a possibilistic programming and a robust scenario-based optimization technique is also developed to make the model more responsive to variations in parameters and robust in the case of disruption events. Finally, the appropriateness and applicability of the model is demonstrated through randomly generated examples and a real case study in retailing. The results show that using very detailed models is necessary when it comes to real-world complex problems where simple deterministic models can be very elusive.
An Efficient Multi-unit Auction for Selling to Newsvendor-type Cost Retailers

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A supplier with a supply shortage must make difficult decisions for how to allocate the limited supply to their buyers. When those buyers are retailers who have a set sales price but face random demand, the quantity desired by each retailer will depend heavily on the price they must pay to get that quantity. Because of this inverse relationship between price and demand, we consider a supplier who implements an ascending price auction to allocate the goods. We devise an efficient discrete auction similar to Ausubel (2004) such that the goods are allocated to the retailers with the highest marginal values.
Allocating scarce resources in a Patient Centered Medical Home (PCMH)

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We consider here a two stage stochastic allocation problem which assigns resources to teams in a PCMH, in particular, the number of hours of Primary Care Physician (PCP) needed to meet the patient demand on a team. In the first, the planning stage, a preliminary assignment of PCP hours to each team is made. Then after observing demand for these hours, in the second stage an adjustment is made to the preliminary hours assigned to each team and, if necessary, the overtime needed to balance the total supply and total demand. We use real options theory to get a fair and consistent adjustment during the second stage. The concept of fairness involves the pricing of the disruption and then making the adjustments through optimization so that the price of disruption for different teams is the same; and the concept of consistency is obtained by pricing the real options. We discuss several ways we can achieve this consistency. This model can be extended to included other specialties as well, like nurses.
The number of heavy vehicles in the United States of America has increased by 70% from 1975 to 2010. Meanwhile truck drivers suffered a higher number of fatalities than any other occupation, accounting for 13.6% of all work-related deaths. Truck drivers are five times more likely to die than the average worker on their duty, making this 3.5-million profession the most dangerous job in the country. The unsafe actions of drivers are a contributing factor in about 70% of the fatal crashes involving trucks. As appealed by Occupational Safety and Health Administration, ‘more public awareness of how to share the road safely with large trucks is needed’.

Heavy trucks were involved in about 82,000 police-reported lane change crashes annually, accounting for 23 percent of all police-reported heavy-truck crashes. However, because of the sparsity of critical events under naturalistic driving conditions, few statistical studies have been conducted on lane change behaviors. In this study, the IVBSS database was used to analyze the behaviors of heavy vehicles drivers, which consists of 601,844 miles of driving. 640 mandatory and 2,035 discretionary lane change events were extracted. Gap acceptance and lane change execution were investigated as two major contributors for lane change safety. Mann-Whitney-Wilcoxon test was used to analyze the non-parametric data distribution. Results show that mandatory lane changes are on average 4.5 times more likely to have critical gap conditions than DLC and over a 10% reduction of elapsed time in the lane line crossing stage.
NRS: Nuclear Engineering and Radiological Sciences
Estimating Critical Boron Concentration via Correlated Sampling Monte Carlo

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Nuclear power plants use boron in the coolant to regulate reactor criticality. Plants begin operation with boron concentrations on the order of 1300 parts-per-million and taper the boron concentration as the fuel depletes. Engineers calculate the critical boron concentration (CBC) as the fuel depletes to predict core refueling intervals. Current CBC estimation tools deterministically calculate the criticality coefficient at multiple boron concentrations. As one-step full-core Monte Carlo calculations become computationally affordable, an elegant Monte Carlo method for calculating CBC is desirable.

Correlated sampling (CS) can calculate CBC by simultaneously modeling several boron concentrations. To implement CS, the Monte Carlo code samples neutron tracks from a “reference” model. The tracks are tallied in “modified” models with a weight derived from the differences between the model and the reference. The modified models’ solutions form a set of calculated $k$ values at different boron concentrations. The $k=1$ intercept of the interpolant polynomial is the CBC estimate.

The CS code must account for differences in the fission source among the modified models. A correction using first-order perturbation theory is possible, but limits the solution's accuracy for large modifications. Alternatively, the track weights may persist from generation to generation. Although this approach is accurate, it results in increasing sample variance as the number of generations increase.

This project demonstrates CBC-estimation for a pincell problem using CS implemented in OpenMC. Because this model does not have significant model-to-model variation of the fission source, assembly- and core-scale test problems are planned.
Use of Stilbene Scintillators for Nonproliferation Applications

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The current shortage of helium-3 has led to the exploration of organic scintillators as possible alternates to helium-3 for their fast timing properties and dual gamma ray-neutron detection capabilities while implementing pulse-shape discrimination (PSD) to distinguish between the two particles. Stilbene has traditionally exhibited excellent PSD compared to other organic scintillators, and a new stilbene composition was recently developed by Lawrence Livermore National Laboratory and commercialized by Inrad Optics that can be grown to sizes of 5 centimeters or larger in diameter. The goal of this research is to utilize the new stilbene scintillator in nonproliferation applications that test its ability to act as an alternate to helium-3. PSD capabilities were tested in both cross-correlation measurements and extreme conditions while subject to a high-gamma field; these results were benchmarked to the EJ-309 organic liquid scintillator with proven PSD capabilities. Pulses were acquired using the CAEN DT5720 digitizer and processed using a data processing algorithm that rejects double pulses and applies PSD to each detector. Results show that the new stilbene was still capable of excellent PSD, comparing favorably to EJ-309, while utilizing minimal shielding.
Flux and Reaction Rate Kernel Density Estimators in OpenMC with Physically-Based Bandwidths

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Monte Carlo simulation methods typically compute flux and reaction rate profiles on a user-defined grid or histogram. The accuracy depends on the resolution of the grid, but the tallies can suffer from large uncertainties when a very fine grid is used. Recently, another estimation technique has been applied to Monte Carlo radiation transport simulations: the Kernel Density Estimator (KDE). KDEs are capable of calculating flux and reaction rates at multiple points. KDEs allow a single event to contribute to the score at multiple tally points, and the uncertainty at those points is independent of the number of tally points used in the simulation.

Previous research has shown the effectiveness of KDEs at estimating density profiles in one-group and continuous-energy problems with simple geometries. Recently, KDEs have been shown to exhibit inaccuracies at material interfaces when estimating flux or reaction rates in a 1D lattice of fuel pins. To mitigate this problem, an energy-dependent bandwidth based on mean-free paths rather than distance is introduced. The bandwidth is a smoothing parameter for KDEs analogous to the bin width in a histogram tally. Results obtained using the mean-free path based bandwidth are compared to those obtained using a fine-mesh histogram for a 1D and 2D representation of a lattice of fuel pins containing one or more strong absorbers. The results show that the physics-based bandwidth is capable of accurate estimates of fluxes and reaction rates in 1D, while errors in the 2D results suggest the need for a spatially-adaptive bandwidth.
CFD-grade Experiments of Thermal Striping in Nuclear Reactor Coolant Branch Lines and CFD Validation

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Thermal fatigue is a mechanism that leads to cracking in pipes which branch from nuclear reactor primary coolant piping and are primarily dead-ended. This phenomenon is a pressing issue for light water reactors, as well as advanced reactors cooled by liquid salts or metals. The main flow (hot) creates a secondary flow swirl which propagates in the branch line (cold). In the branch line below where the flow swirl transitions from turbulent to laminar, thermal stratification occurs. The interaction of the hot flow swirl and this stratified layer causes the hot and cold boundary to fluctuate, inducing thermal fatigue in the branch line walls.

Predicting the fluctuations of the hot and cold boundaries by means of analytic/empirical models has historically proven to be challenging, due to the complexity of the involved fluid dynamic interactions. At the same time, the assessment of the predictive capabilities of high fidelity computational fluid dynamics (CFD) methodologies (such as Large Eddy Simulations) has been hindered by the lack of sufficiently detailed experimental data.

The present project will produce a database of CFD-grade experimental data characterized by high spatial and time resolution providing:
   a) greater physical insight into the fluid-dynamic phenomena responsible for inducing thermal fatigue in branch lines;
   b) a sound basis for the validation of associated CFD models;
   c) enhanced predictive capabilities of structural analysis codes used to analyze crack propagation;
   d) greater design efficiency and lower failure probability of reactor piping.
Experiments on the OMEGA EP laser to study the material dependence of the two-plasmon decay instability

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Lasers interacting with under-dense plasmas drive laser-plasma instabilities (LPIs), which can convert a non-negligible fraction of the laser energy into hot electrons (>50 keV). In direct-drive inertial-confinement fusion implosion experiments, these hot electrons can preheat the fuel, reducing compression efficiency. Additionally, hot electrons interacting with high-Z materials in the target chamber can produce high-energy x-rays that interfere with diagnostics. Understanding the production of hot electrons in laser-produced plasmas is important to control and mitigate these effects.

For long-scale-length plasmas, two-plasmon decay (TPD) is a major LPI responsible for generating hot electrons. The convective gain of the instability is proportional to the length scale of the plasma electron density and inversely proportional to the electron temperature. Therefore, it has been predicted and demonstrated by preliminary experiments that hot electron production can be controlled through varying these parameters by increasing plasma Z [1,2]. Additionally, TPD may be saturated by further decay processes that depend on ion-acoustic wave damping, and therefore, plasma Z [3].

We have performed experiments on the OMEGA EP laser to thoroughly study the Z-dependence of the TPD instability, through varying the material with which the lasers interact. Hard x-ray diagnostics were used to measure hot electron production and optical diagnostics were used to measure plasma density profile for each material. Preliminary results will be presented, showing the general Z-dependence of hot electron production and electron density scale lengths.
Solid State Nuclear Track Detectors (SSNTDs) are dielectric materials that sustain damage when exposed to radiation. This damage is localized along the travel paths of radiation through the material. Damage paths can be made visible under a light microscope by chemically etching the exposed material with a strong acid or base. Damage tracks are counted and analyzed to learn about the radiation source that caused them. The type of radiation striking the material can be determined based on the geometry of the damage track relative to the energy of the original particle. SSNTDs are especially useful for measuring relatively rare events such as spontaneous fission, or for measuring extremely small sources when the decay rate is very low because very long exposure times can be reached without the need to power the detector.

This project focuses on detecting and measuring radiation particles from $^{250}$Cf which is unique compared to previous SSNTD studies. Generic polycarbonate and Makrolon™ were tested as SSNTDs. Both are sensitive to fission fragments but not alpha radiation. Small plates of these materials were exposed to sources containing $^{250}$Cf, which self-fissions, and then etched with hot 6M NaOH. The plates were examined under a light microscope to look for fission tracks.

Results show Makrolon™ is better than generic polycarbonate as an SSNTD. Makrolon™ provides clearer track resolution than generic polycarbonate. A general procedure has been developed for using Makrolon as an SSNTD for fission fragments.
Design of Future Neutron Transport Code through a New Code: NTS

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The neutron transport code describes the neutron physics of a reactor, and the fast improvement in computer science in the past decade opened new ideas. This research introduces some design ideas for the future neutron transport code through the demonstration of a code called Neutron Transport System (NTS). These efforts are made with a hope of benefiting future neutron transport codes.

The prevailing method in practical reactor simulation is the Method of Characteristics (MOC). It seems MOC is the only practical method without approximation of geometry. Maybe this is not the final answer. The SN method can also be adapted to solve the problem without geometric approximations. In this research work, the NTS code demonstrates this approach. The advantages include reducing storage requirements and better results.

In the University of Michigan, there is a MPACT code for reactor simulation. The input file format is probably incompatible with other codes. The NTS comes to resolves this issue through providing an interface compatible with MPACT input file. The design concept of NTS allows it to be exported to other code such as the open source code developed by MIT, the OpenMOC.

The User Interface is a key part in the design of NTS. It demonstrates some ideas how to input a complex reactor geometry intuitively through a graphics interface. This could help reactor designers reduce workloads and debugging efforts.
Performance of a EJ309 organic liquid scintillation detector pedestrian radiation portal monitor prototype at the 2nd SCINTILLA benchmark campaign

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The University of Michigan has developed a pedestrian radiation portal monitor (RPM) prototype incorporating eight 7.62 cm diameter by 7.62 cm length EJ309 organic liquid scintillation detectors. Pulse shape discrimination allows the RPM to distinguish gammas and neutrons and the RPM triggers an alarm on user-defined net gamma and neutron count rate thresholds (five $\sigma$ over background). The system can reliably alarm on $^{137}$Cs, $^{57}$Co, $^{60}$Co, $^{241}$Am, $^{133}$Ba, highly enriched uranium (HEU) and weapons grade plutonium (WGPu) (source strengths vary from ~5-50 $\mu$Ci) at 75 cm source to RPM distance and source speeds of 1.2, 2.2 and 3 m/s. It can also neutron alarm with high probability on a moving ~20,000 n/s $^{252}$Cf source shielded by up to 8 cm of high density polyethylene. The SCINTILLA project is a consortium of European research laboratories and companies with a vested interest in alternative RPM designs, especially in light of the $^3$He supply crisis. The benchmark campaigns at the European Commission’s Joint Research Centre in Ispra, Italy, provide developers of prototype RPMs an opportunity to test their designs on static and moving sources in a purpose-built facility for their gamma and neutron response characteristics, and their susceptibility to false alarms. Our team tested the pedestrian RPM prototype in Italy in February 2014 and is testing a vehicle RPM in November 2014.

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A plutonium metal sample was measured by a fast-neutron multiplicity counter for characterization of spontaneous fission neutron anisotropy and for verification of MCNPX-PoliMi calculations. Accurate neutron angular distribution models are important to properly simulating fast neutron coincidence measurements for nuclear nonproliferation and safeguards. A majority of prompt neutrons are emitted from fully accelerated fission fragments; those neutrons carry momentum from the fission fragments, and thus an anisotropic neutron angular distribution is observed in the laboratory reference frame. The fast-neutron multiplicity counter was used with pulse shape discrimination techniques to produce neutron-neutron cross-correlation time distributions from spontaneous fission in a lead-shielded 0.84 g $^{240}$Pu$_{eff}$ metal sample. Due to neutron anisotropy, the number of observed neutron cross-correlations varied as a function of angle between a detector pair and fission source. Fewer neutron correlations were observed at detector angles near 90 degrees, relative to higher and lower detector angles. Both the neutron correlations as a function of time difference and detector pair angle are compared with MCNPX-PoliMi calculations and show good agreement.

Key Words: Monte Carlo, safeguards, measurement, plutonium
Comparison of Calibration Methods for Radioxenon Detectors

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The Comprehensive Test Ban Treaty bans all nuclear explosions on Earth whether for military or peaceful purposes. Since 1996, the treaty has been signed by 183 countries. To enforce the treaty, a verification regime was created that includes the International Monitoring System (IMS), which monitors the world for signs of nuclear explosions. Radionuclide stations measure the atmosphere for radioactive particles from nuclear explosions using equipment such as the Swedish Unattended Noble Gas Analyzer (SAUNA). These radioxenon systems are beta-gamma coincidence detectors which must be calibrated before analyses take place. The methods of calibration vary in complexity and in some instances require 4 xenon isotope samples. The extrapolation method has been presented as an alternative to the absolute calibration method but requires further analysis. A simulator was used to create the radioxenon samples analyzed in the calculations. The absolute calibration method uses the relationship between the coincidence measurements and the branching ratios to calculate efficiency. The extrapolation method assumes all counts are related by a function, \( F \), which can be extrapolated to obtain beta efficiency and total activity. Using the simulated data it was shown that the calculated beta efficiencies for both methods were within a 2\% difference of one another. The calculated activity as compared to the simulated activity was within a 5\% difference of the expected value. It could be shown that the extrapolation method is sufficient in calculating the beta efficiency of detectors with the analysis of more data sets.
An Azimuthal, Fourier Moment-Based Axial $S_n$ Solver for the 2D/1D Scheme

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The MPACT neutronics code, collaboratively being developed by the University of Michigan and Oak Ridge National Laboratory, has been developed to simulate light water reactor (LWR) cores. The mostly commonly used method in MPACT is based on the 2D/1D method, which solves the 3D neutron transport equation by coupling 2D-radial and 1D-axial transport sweepers, usually wrapped by a three-dimensional coarse mesh finite difference (CMFD) accelerator.

The radial and axial solvers are coupled through transverse leakage terms that describe the rate at which neutrons leave a region in a given direction. A typical approximation is to assume that the transverse leakage is isotropic and neutrons travelling in any particular direction have the same leakage rate. For many problems this is sufficiently accurate, but for more difficult problems, such as those with control rods, mixed oxide (MOX) fuel, or other characteristics that lead to higher flux gradients, simulating the angular dependence of these leakages becomes more important. However, modelling the angular dependence explicitly requires a considerable amount of memory and computational time.

The work presented here employs Fourier moments to approximate the azimuthal dependence of the leakage, while maintaining explicit polar dependence within the framework of an axial $S_n$ solver. This approach allows for a significant reduction in the computational resources required and allows the number of azimuthal angles to be increased without increasing burden of leakage representation. In the cases analyzed, only one or two Fourier moments seem necessary to accurately capture the azimuthal behavior at a 2-3x speedup and 10-20x reduction in the memory footprint, making azimuthal representation of the leakage much more computationally feasible.

Key Words: MPACT, 2D/1D, Fourier, axial, transport
The Long Term Effects of Dielectric Barrier Discharges Treatment of Tissues*

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The treatment of human tissues by atmospheric pressure dielectric barrier discharges (DBDs) has been shown to be beneficial to wound healing and skin sterilization.[1] These benefits depend strongly on the proper plasma dose, the time over which the plasma is applied. Characterizing the dose is difficult due to the variable conditions the tissue may experience. In this poster, we report on a computational investigation of the interaction of DBDs in context of tissues. These simulations were performed using nonPDPSIM, a 2-dimensional model in which Poisson’s equation, electron temperature equation and transport equations for charged and neutral species are solved. The tissues are often covered by a thin layer of liquid, typically hundreds of microns thick. This liquid layer processes the plasma produced radicals and ions prior to their reaching the tissue. The discharges are operated at -18 kV with 100 pulses at 100 Hz followed by a 10 s afterglow. Three discharge modes are investigated. First, repetitive streamer strikes on the same location at liquid surface, which results in very non-uniform radical fluxes to underlying tissues. Second, random streamers strike spatially randomly at liquid surface, which produces quite uniform fluxes. Finally, five picked locations are chosen for streamers, and the fluxes to tissues show both non-uniform and uniform characteristics.


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Magneto-Rayleigh-Taylor Growth and Feedthrough in Cylindrical Liners

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Cylindrical liner implosions in the Magnetized Liner Inertial Fusion (MagLIF) concept [1] are susceptible to the magneto-Rayleigh-Taylor instability (MRT). In MagLIF, a pulsed power machine (such as the Z-machine at Sandia National Laboratories) is used to drive a large axial current, initiating the implosion of a metal cylindrical liner onto a pre-heated (~ 250 eV) and pre-magnetized (~ 10 T axial field) fusion fuel. During the implosion process the exterior surface of the liner is initially MRT unstable while the fuel/liner interface is stable. As the fuel becomes sufficiently compressed the liner begins to stagnate and the inner surface becomes MRT unstable (as the direction of radial acceleration has changed). Initial MRT growth on the outer surface of the liner may also feedthrough to the inner surface and provide a seed for the latter’s MRT growth during the stagnation phase. Cylindrical liners are additionally susceptible to the other MHD instabilities, in particular the sausage and kink mode. Analytic estimates of the coupling and subsequent growth of MRT and the latter MHD modes are given. Feedthrough estimates are compared to 2D MHD simulations and experiments [2] including the influence of an externally applied axial magnetic field. Lastly, we consider the effect of a shock on feedthrough of MRT, particularly in seeded liners.

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References
SIP: Signal and Image Processing
Multi-modal data fusion is an increasingly common problem arising in fields such as economics, statistical signal processing, medical imaging, and machine learning. In such applications, we have access to multiple datasets of possibly different modalities, each of which describes some aspect of the system. Canonical Correlation Analysis (CCA) is a dimensionality reduction algorithm that transforms each dataset to a lower-dimensional space of maximal correlation with the other datasets. However, when the number of observations is less than the combined dimension of the datasets, CCA deterministically returns a perfect correlation between the datasets. To overcome this performance loss, it is common to use a regularized version of CCA (RCCA); however, previous numerical simulations show that the performance of RCCA increases with the regularization parameter.

Motivated by this unsatisfying observation, we present a new algorithm called LRCCA. We show that LRCCA is the limiting algorithm of RCCA obtained by setting the regularization parameter to infinity. The resulting algorithm is simply the SVD of the product of the two data matrices. To analyze the behavior of our algorithm, we use random matrix theory to asymptotically predict the value of the largest singular value of a rank-1 perturbation of a product of random matrices. This analysis yields a phase transition that is dependent on the dimensionality of the datasets, the number of observations, the relative SNR of each correlated signal, and the correlation between the datasets. We then compare this theoretical bound to the theoretical bound of Informative CCA (ICCA) and numerically explore parameter regimes where each algorithm is best.
Universal Phase Transitions of Spectral Algorithms for Community Detection

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Spectral algorithms are widely used venues for data clustering, particularly in the contexts of community detection of social network data. In this presentation we investigate the community detectability of two spectral algorithms, the spectral clustering method and the modularity method, under a general network model. We prove the existence of abrupt phase transitions with respect to the network parameters, where the network transitions from almost perfect detectability to low detectability at some critical threshold. These phase transition results provide fundamental performance limits of community detection and they are universal in the sense that we allow the communities to have different sizes. We also use the results to establish an empirical estimator from data that is capable of evaluating the reliability of spectral algorithms for community detection. The phase transition results are validated via simulated networks and real-world datasets.
Modern MAP inference methods for accurate and fast occupancy grid mapping on higher order factor graph

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Using the inverse sensor model has been popular in occupancy grid mapping. However, it is widely known that applying the inverse sensor model to mapping requires independent cell assumption that is not necessarily true. Even the works that use forward sensor models have relied on methods like expectation maximization or Gibbs sampling which have been succeeded by more effective methods of maximum a posteriori (MAP) inference over graphical models. In this paper, we propose the use of modern MAP inference methods along with the forward sensor model. We also introduce a class of higher order factors for on which inference methods like Belief Propagation and Dual Decomposition can be computed in linear time on neighborhood size rather than exponential in the general case. Our implementation and experimental results demonstrate that these modern inference methods deliver more accurate maps more efficiently than previously used methods.
Spectral correlation screening of Gaussian stationary processes

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We propose a framework for spatio-temporal correlation analysis of jointly Gaussian Wide Sense Stationary (WSS) multivariate time series. The goal of the proposed method is to be able to identify the important time series among a set of $p$ time series where for each time series a total of $N$ time samples are available. The proposed method is specifically useful when the dimension of multivariate times series $p$, and the number of time samples $N$ are relatively large and direct correlation analysis in the time domain could be computationally intractable. We use an independence property of Gaussian WSS time series in frequency domain to perform multiple inference for detecting important time series. We also present experimental results which show the accuracy of our theoretical results and also usefulness of the proposed framework.
Action Proportion for Action Recognition

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Action recognition "in the wild" is a very difficult task due to some problems such as camera motion, action style variation, and background clutter. Moreover, many action classes share similar motions and this property makes it difficult to find a unique discriminative representation by using traditional weakly supervised learning methods such as Multiple Instance Learning. For example, Kicking usually contains running, and these two action types share similar running motion. In order to find better action representation for solving these problems, we propose to "proportional multiple-instance dictionary learning" method to automatically mine the semantically meaningful video evidences. These video evidences are treated as proportions for each action type. In the experimental results, we can see our method can find discriminative evidences and generate effective representations for each action. Furthermore, by analyzing the proportion for each action class, our method is also scalable to large scale dataset.
Facial movement is modulated both by emotion and speech articulation. Facial emotion recognition systems aim to discriminate between emotions, while reducing the speech-related variability in facial cues. This aim is often achieved using two key features: (1) phoneme segmentation: facial cues are temporally divided into units with a single phoneme and (2) phoneme-specific classification: systems learn patterns associated with groups of visually similar phonemes (visemes), e.g. /P/, /B/, and /M/. In this work, we empirically compare the effects of different temporal segmentation and classification schemes for facial emotion recognition. We propose an unsupervised segmentation method that does not necessitate costly phonetic transcripts. We show that the proposed method bridges the accuracy gap between a traditional sliding window method and phoneme segmentation, achieving a statistically significant performance gain. We also demonstrate that the segments derived from the proposed unsupervised and phoneme segmentation strategies are similar to each other. This paper provides new insight into unsupervised facial motion segmentation and the impact of speech variability on emotion classification.
Modeling Pronunciation, Rhythm, and Intonation for Automatic Assessment of Speech Quality in Aphasia Rehabilitation

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Patients with aphasia often have impaired speech-language production skills, resulting in tremendous difficulties in tasks that require verbal communication. To facilitate rehabilitation outside of therapy, we are collaborating with the University of Michigan Aphasia Program (UMAP) to develop an automated system capable of providing feedback regarding the patient's verbal output. In this paper we introduce a robust method for extracting rhythm and intonation features from aphasic speech based on template matching. These features, combined with Goodness of Pronunciation (GOP) scores and our previous feature set, help our system achieve human-level performance in classifying the quality of speech produced by patients attending UMAP. The results presented in this work demonstrate the efficacy of our technique and the potential of this system for handling natural speech data recorded in non-ideal conditions as well as the unpredictability in aphasic speech patterns.
Localized Temporal Subspace Modeling for Dynamic Contrast Enhanced Liver MRI

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Dynamic Contrast Enhanced (DCE) MRI is an important diagnostic tool in radiation therapy for liver cancer. A sequence of MRI images capture the natural process of liver perfusion, as brightly visible contrast agent moves from the injection site through main blood vessels of the liver and into the capillaries of the malignant and benign tissues. Measuring pharmacokinetic parameters before and during the treatment help oncologists assess the efficacy of the radiation therapy and to design other aspects of care. Accurately and consistently measuring these pharmacokinetic parameters necessitates capturing the time dynamics of perfusion as well as accurate spatial information. To address the inherent tradeoff between spatial and temporal resolution, DCE-MRI requires acceleration techniques such as parallel imaging and compressed sensing. Applying additional prior knowledge about liver perfusion models and the slowly varying contrast agent time series to the reconstruction model further improves the conditioning of the image reconstruction problem. This work explores the benefits of modeling the temporal object as residing in the union of several spatio-temporal subspaces, including predetermined quadratic spline time bases, and temporal subspaces estimated from subspace clustering methods. In particular, we wish to exploit the property that spatially neighboring pixels, such as those belonging to similar tissue types, are likely to exhibit similar temporal dynamics. We propose computationally efficient variable splitting methods for solving the resulting non-differentiable cost functions. We compare the computation time and ability of our proposed method to estimate pharmacokinetic parameters in simulation to the performance of low-rank and compressed sensing-based reconstruction methods.
Joint Camera-Blur and Pose Estimation from Aliased Data

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A joint-estimation algorithm is presented that enables camera-blur and pose estimation in the presence of aliasing and additive noise. Specifically, a parametric maximum-likelihood PSF estimate is derived for characterizing a camera's optical imperfections through the use of a calibration target in an otherwise loosely controlled environment. The imaging perspective, ambient light-levels, target-reflectance, detector gain and offset, quantum-efficiency, and read-noise levels are all treated as nuisance parameters. The resulting non-linear objective function is shown to be identifiable up to a set of cardinality of at most 2. A point-wise bound on the PSF error associated with wavefront perturbations is used in conjunction with a new test for global convergence of the log-likelihood to find globally optimal solutions. The Cramèr-Rao bound is derived, and simulations demonstrate that the proposed estimator achieves near optimal MSE performance. The proposed method is applied to experimental data to validate both the fidelity of the forward models, as well as the applicability of the resulting ML estimator in context of both system identification and subsequent image restoration.
Consider the problem of estimating a one-dimensional threshold classifier with a constraint on the allotted sampling time. The current literature focuses on one of two objectives, either minimizing the number of samples taken or the total distance traveled. In the active learning setting, probabilistic binary search schemes have been shown to minimize the number of samples required, while when sampling is free, the minimum distance is obtained by traveling along a straight path. We show that between these two regimes lies probabilistic quantile search, where at each iteration samples are taken at some location $1/m$ into the posterior distribution of the threshold location. We derive a rate of convergence for such a search, as well as the expected distance traveled under the noise-free setting, and show a fundamental tradeoff between number of samples and distance. This tradeoff can be used to determine the optimal value of $m$, significantly reducing the total sampling time when compared to existing methods.
A joint classification and bias field estimation algorithm for synthetic CT generation

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Bias fields in magnetic resonance (MR) images negatively impact the ability of intensity-based classifiers to distinguish different tissue types and degenerate the quality of synthetic CT (“MRCT”) volumes generated from MRI scans. This study developed an integrated bias correction method and compared it with a pre-processing technique in support of synthetic CT generation. The integrated method performs classification and bias correction jointly by modifying the objective function of fuzzy c-means (FCM) classification to take the multiplicative bias field into consideration. The objective function is minimized iteratively followed by a Laplacian regularized least square fitting at each iteration. The pre-processing method is a commonly used algorithm (N4itk), and is applied to all MRI image volumes before FCM classification. Both methods were tested on (1) a synthetic dataset of T1-weighted and T2-weighted images with a known ground truth bias field, and (2) a patient dataset of T1-weighted, T2-weighted, fat, water and ultra-short echo time (UTE) images with computed tomography (CT) as reference images. Both tests showed that N4itk yielded differences in bias fields from multiple images that nominally should not have such variations. The integrated method resulted in smaller square errors in the single bias field from the synthetic dataset than the pre-processing one. While initial evaluation of MRCT generation indicated that the integrated and the pre-processing methods achieve comparable performance in terms of estimating the electron densities within the head, the integrated method may yield better computational efficiency as it performs bias correction and classification in a single run.
Model-based image reconstruction (MBIR) for X-ray CT produces high quality images from relatively low-dose scans, but the high computational cost of MBIR algorithms prevent them from being used ubiquitously in the clinic. Variable splitting with the alternating directions methods of multipliers (ADMM) provides rapidly converging algorithms by decomposing the challenging MBIR optimization problem into an iterated sequence of simpler subproblems. Variable splitting algorithms have achieved state-of-the-art performance in 2D, but replicating those successes in 3D has proved difficult. In this work, we consider a simple splitting algorithm that decomposes the reconstruction problem into a nonnegative denoising problem and a quadratic tomography problem. Unlike prior work, we solve the tomography problem with a novel duality-based approach that yields convergent algorithms similar to ordered subsets methods and iterated filtered backprojection. We show some promising experimental results running on a GPU.
Ensemble Estimation of Multivariate $f$-Divergence and Applications

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$f$-divergence is a measure of the difference between two probability distributions and is a generalization of entropy and mutual information. The problem of $f$-divergence estimation is important in the fields of machine learning, information theory, and statistics. While several non-parametric divergence estimators exist, relatively few have known mean squared error (MSE) convergence rates. For those estimators whose MSE convergence rates are known, the asymptotic distributions are unknown. By using the theory of optimally weighted ensemble estimation, we derive a non-parametric $f$-divergence estimator that can estimate many different $f$-divergences and related quantities, is simple to implement, performs well in high dimensions, and achieves the parametric MSE convergence rate of $O(1/T)$ where $T$ is the number of samples for each distribution. We further show that the asymptotic distribution of the estimator is Gaussian which enables us to perform divergence-based inference tasks such as testing the equality of pairs of distributions based on empirical samples. We show simulated results which verify our theory and then use the estimator to empirically bound the best achievable classification error (the Bayes error) of a classical machine learning data set.
Improved robust PCA using low-rank denoising with optimal singular value shrinkage

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We study the robust PCA problem of reliably recovering a low-rank signal matrix from an observed signal-plus-noise-plus-outliers matrix. We analytically characterize the extent to which outliers degrade the singular vectors of the signal-plus-noise-plus-outliers matrix, and we present a new result on the efficacy of soft-thresholding the observations to mitigate this degradation. Based on this theory, we reason that a recently proposed method for robust PCA that exploits outlier sparsity to improve low-rank estimation will produce suboptimal low-rank matrix estimates in the presence of noise. Next, we propose a new iterative algorithm for robust PCA that utilizes an optimal, data-driven low-rank matrix estimator (OptShrink). Finally, we show that the proposed approach yields superior background subtraction on a computer vision dataset.

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BARISTA: A fast algorithm for MR image construction with sparsity-promoting regularization

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Although MRI is an imaging modality with excellent soft tissue contrast, major hindrances in its wider adoption are high monetary costs and long scan times. Both of these factors can be mitigated by shortening the scan time. MRI scan times can be drastically shortened by using multiple receive channels and sparsity-promoting regularization, but this necessitates solving difficult optimization problems. Variable splitting methods based on augmented Lagrangian principles are the current state-of-the-art methods for solving these optimization problems, but their convergence speed depends heavily on parameters that are difficult to tune. We introduce B1-based, adaptive restart, iterative soft thresholding algorithms (BARISTA) as an alternative to variable splitting methods. BARISTA uses different parameters that are easier to tune, and in our numerical experiments we observed that it converged as much as three times faster than optimally-tuned variable splitting methods.
The Higher Order Singular Value Decomposition is a popular algorithm for uncovering structure from tensor data cubes. This algorithm has been successfully used in many signal processing, machine learning and data mining applications. In this work, we use recent results from random matrix theory to analyze the performance of the HOSVD algorithm relative to an SVD based alternative. In particular, we rigorously characterize the performance of HOSVD when applied to certain signal plus noise tensor models in the missing data setting. The analysis brings into sharp focus when and the extent to which the HOSVD improves estimation performance for Multi Modal Fusion applications. We illustrate the predicted performance improvement using numerical simulations and on a background subtraction application from computer vision.
Image Interpolation from Manhattan Cutset Samples via Orthogonal Gradient Method

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Cutset sampling is a new approach to image sampling where 2D data is recorded densely along intersecting lines. A special case of cutset sampling is Manhattan sampling, where data is sampled densely along evenly-spaced rows and columns. This work presents a new method for interpolating pixels from their Manhattan samples called the orthogonal gradient (OG) algorithm, which exploits the fact that pixels tend to be correlated along the direction orthogonal to the image gradient. Such an approach is enhanced by Manhattan sampling, where dense sampling along straight lines allows for better reconstruction of both sharp and soft image edges. In particular, the OG algorithm alternates between solving a constrained optimization problem, and changing the weights of the optimization problem according to the direction of the gradient of each new image estimate. The proposed method improves upon previous Manhattan interpolation algorithms, both qualitatively as well as in mean-squared error. Furthermore, unlike the previous algorithms, the OG algorithm can easily be extended to any sampling scheme.
A Regularized, Model-Based Approach to Conductivity Mapping

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Electrical properties of tissues can be calculated from magnetic fields measured using magnetic resonance imaging (MRI) techniques. Electrical properties are expressed as the complex-valued \(\kappa = \varepsilon - \frac{i\sigma}{\omega}\), where \(\kappa\) is the complex permittivity, \(\varepsilon\) is permittivity, \(\sigma\) is conductivity, and \(\omega\) is the angular frequency – in our case the frequency of the MRI scanner. Permittivity and conductivity can be calculated independently and are also useful separately. This work focuses on conductivity mapping, which has applications in MR safety and oncology. Conductivity mapping is useful in subject-specific RF power regulation in MRI scanners. It has also been shown that tissue conductivity increases by at least a factor of two in cancerous tissues.

The major challenge in mapping conductivity using MRI images is that it involves calculating the Laplacian of the transmit magnetic field, which drastically amplifies any noise present in the image. Current solutions involve spatially filtering images before and after reconstruction. In this work we present a novel model-based reconstruction approach with edge-preserving regularization. This method determines the conductivity map that best fits the acquired magnetic field maps in a least-squares sense. Additionally, we offer a method for mitigating edge artifacts that result from calculating derivatives near the edge of the object. Our approach improves the signal-to-noise ratio (SNR) and accuracy, measured as root-mean-square (RMS) error, of the conductivity maps. Electromagnetic simulations have shown up to six-fold SNR improvements and 45% reduction of RMS error for the proposed method with respect to the current method.
Robust Classification of LEO satellite transmissions with uncertain orbits: A Transfer Learning Approach

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During initial post launch stages for artificial satellites, while initial estimates and likelihoods are available for the resulting orbits, exact orbital estimates are unknown. Due to the proliferation and popularity of small satellites, the number of small satellites per launch is increasing. Since small satellite missions are typically high-risk with potential infant mortality, it is crucial to verify their operational behavior and their status early after launch. Also, for collision avoidance and prediction, precise orbit determination is useful. Radar systems lack the resolution to track these clusters of small satellites. Recent developments in machine learning enables integration of multiple classification tasks with similar marginal probabilities to produce one learning system. Using these developments, we propose a probabilistic modeling, a transfer learning approach towards classifying the RF transmissions of these satellites with a probabilistic knowledge of the orbits and resulting doppler shift in transmissions. The resulting classified feature points can be used for both accurate orbit determination and to verify operational status of these satellites.
Consistency and MSE Performance of MUSIC-based DOA of a Single Source in White Noise with Randomly Missing Data

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MUSIC is a popular algorithm for estimating the direction of arrival (DOA) in array signal processing applications. In this work, we analyze the performance of the MUSIC algorithm for a single source system, in the presence of noisy and missing data (when only a random subset of the entries in the data matrix are observed). We prove consistency of the DOA estimate when signal from a single source is impinging on low coherence arrays, and derive an analytic expression for the mean-squared-error (MSE) performance of MUSIC for the case of uniform linear arrays, in the large array and relatively large sample setting. Our analysis is mathematically justified in both the sample rich and deficient regimes. The expression for the MSE is a simple function of array geometry, signal-to-noise ratio (SNR), the fraction of entries observed, and the ratio of the number of sensors to snapshots. We derive a phase transition threshold which separates a regime where MUSIC is consistent from a regime where MUSIC is inconsistent. This threshold depends upon the SNR, the probability of observing entries in the data matrix, and number of sensors and snapshots in a simple manner which we make explicit.
Multi-sensor classification via Consensus-based Multi-view Maximum Entropy Discrimination

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In this paper, we consider a multi-sensor classification problem when only a limited portion of labeled multi-modal samples are provided with a large portion of unlabeled samples available. The problem is formulated under the multi-view learning framework, and a Consensus-based Multi-View Maximum Entropy Discrimination (CMV-MED) algorithm is proposed. By iteratively maximizing the stochastic agreement between multiple classifiers on unlabeled dataset, the algorithm could learn multiple strong classifiers simultaneously. We demonstrate that our proposed method can yield improved performance over previous multi-view learning methods in many real multi-view data set, including a multi-sensor footstep dataset.
Localization of a high frequency source in a shallow ocean sound channel using frequency-difference matched field processing

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Matched field processing (MFP) is an established technique for locating remote acoustic sources in known environments. Unfortunately, environment-to-propagation model mismatch prevents successful application of MFP in many circumstances, especially those involving high frequency signals. For beamforming applications, this problem was found to be mitigated through the use of a nonlinear array-signal-processing technique called frequency difference beamforming (Abadi et. al. 2012). Building on that work, this nonlinear technique was extended to MFP, where Bartlett ambiguity surfaces were calculated at frequencies two orders of magnitude lower than the propagated signal, where the detrimental effects of environmental mismatch are much reduced. In the Kauai Acomms MURI 2011 (KAM11) experiment, underwater signals of frequency 11.2 kHz to 32.8 kHz were broadcast 3 km through a 106-m-deep shallow-ocean sound channel and were recorded by a sparse 16-element vertical array. Using the ray-tracing code Bellhop as the propagation model, frequency difference MFP was performed, and some degree of success was found in localizing the high frequency source. In this presentation, the frequency difference MFP technique is explained, and comparisons of this nonlinear MFP technique with conventional Bartlett MFP using both simulations and KAM11 experimental data are provided. [Sponsored by the Office of Naval Research]
Supervoxel hierarchies provide a rich multiscale decomposition of a given video suitable for subsequent processing in video analysis. The hierarchies are typically computed by an unsupervised process that is susceptible to under-segmentation at coarse levels and over-segmentation at fine levels, which make it a challenge to adopt the hierarchies for later use. In this paper, we propose the first method to overcome this limitation and flatten the hierarchy into a single segmentation. Our method, called the uniform entropy slice, seeks a selection of supervoxels that balances the relative level of information in the selected supervoxels based on some post hoc feature criterion such as object-ness. For example, with this criterion, in regions nearby objects, our method prefers finer supervoxels to capture the local details, but in regions away from any objects we prefer coarser supervoxels. We formulate the uniform entropy slice as a binary quadratic program and implement four different feature criteria, both unsupervised and supervised, to drive the flattening. Although we apply it only to supervoxel hierarchies in this paper, our method is generally applicable to segmentation tree hierarchies. Our experiments demonstrate both strong qualitative performance and superior quantitative performance to state of the art baselines on benchmark videos.
Rotation-Invariant Local Radius Index: A Compact Texture Similarity Feature for Classification

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This paper proposes a new type of statistical texture similarity feature, called Rotation-Invariant Local Radius Index (RI-LRI), whose goal is to quantify texture similarity consistent with human perception. The original LRI extracts texture features by using simple pixel value comparisons in spatial domain and is designed for applications in which shifts can be tolerated but rotations should be penalized monotonically. Such applications include perceptual image compression and identical texture retrieval. However, when it comes to texture classification and other applications in which rotation-invariance is desired, a rotation-invariant version of LRI is needed. The proposed rotation-invariant LRI is well suited to such applications. When combined with frequency domain contrast information and the well-known Local Binary Patterns (LBP) feature, the proposed metric has comparable texture classification accuracy to state-of-the-art metrics, when tested on the Outex and CUReT databases. Moreover, it has a much lower dimensional feature vector and requires substantially less computation than other state-of-the-art texture features, such as those based on LBP.
SPS: Space and Planetary Sciences
Development of Novel Propellant Feed Systems for the CubeSat Ambipolar Thruster

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The development of propellant feed systems for the CubeSat Ambipolar Thruster (CAT), a low-power permanent magnet helicon thruster for nanosatellites, is discussed. CAT can operate with inert gas-, liquid-, or solid-storable propellants, which require different propellant feed systems. For inert gas propellants a 1.5U (1U is 10 cm x 10 cm x 10 cm) pressurized propellant feed system module for a 3U CubeSat is being developed. A laser sintered titanium tank has been designed to store propellant pressurized to 100 atm with a safety factor of 4.5. This tank can store up to 800 g of supercritical xenon, the industry standard propellant, providing the satellite with a $\Delta V$ of 1700 m/s. An off-the-shelf multi-stage pressure regulator from Beswick Engineering regulates the pressure to 0 - 30 psig upstream of a solenoid valve and static orifice. A combination of orifice size and pressure regulator setting yields a wide range of flow rates and inlet pressures, enabling a broad array of mission capabilities.

However, the high storage pressure required for xenon poses design challenges and increases mission risk. Alternatively, iodine has similar performance characteristics to xenon, but is stored as a solid at room temperature, reducing mission risk and system mass. Unfortunately, iodine is corrosive and reacts readily with commonly used spacecraft materials. To determine the severity of these reactions selected materials were dosed at atmospheric conditions. Within 48 hours aluminum and stainless steel specimens underwent visible physical degradation. Based on these results a solid-storable feed system is under development.
SCION: CubeSat Mission Concept to Observe Midlatitude Small-Scale Irregularities and Scintillation

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The SCintillation and Ionospheric Occultation NanoSats (SCION) mission concept is to deploy two low-cost CubeSat spacecraft that maintain a separation distance <1 km to measure scintillation and associated small-scale density irregularities in the mid-latitude ionosphere. Each spacecraft is equipped with a dual frequency GPS receiver to measure total electron content (TEC) and the S4 scintillation index along raypaths from the receiver to the GPS constellation. Scintillation causing small-scale density irregularities are increasingly observed in the vicinity of large TEC gradients associated with storm enhanced density (SED) regions. Detection of irregularities of the scale that cause GPS and VHF scintillation has previously relied on assumptions about their structural stability and drift speed. Space-based, multipoint observations would provide broad, regional coverage and disambiguation of temporal and spatial density fluctuations in order to detect small-scale irregularities without these assumptions.
Cyber-physical Systems for Exploration

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As a starting point for the integration of biosensors and vehicle health and status systems. Due to the numerous vehicles, varying Environment, Climate and Life Support Systems (ECLSS) between vehicles, challenges of modifying EVA prebreath while using 50% less volume of Oxygen due to unforeseen uplift constraints, remoteness of operations, constrained resources and communications, the value of cyber physical systems that integrate the real-time behavior of vehicles and crew prompted NASA to solicit automated man-in-the-loop systems.

The objective is to apply the cognitive domain-knowledge of manned spaced operations from prior professional experience and academic training across space systems engineering, bioinformatics, and biomedical engineering by exploring autonomous man-in-the-loop systems for crew performance and safety requirements.

Classification of risk for prediction, monitoring, and countermeasure implements prior developed methods to data mine EVA Decompression Sickness database and extended to Acute Mountain sickness; diagnostic rubric for space exploration radiation is suggested.

Generalized hypotheses are proposed and shall be explored during this project, including, but not limited to the following: i) Scientific hypothesis: the cyber physical system shall predict, detect, and monitor selected crew disease and dysfunction with the same level of accuracy as current methods. ii) Engineering hypothesis is the power, memory, speed and structures budget of the embedded system shall meet NASA Flexible Path requirements; iii) Operational hypothesis is the scientific accuracy and engineering requirements shall economize time, cost, and risk for implementation of cyber physical system for space exploration. Further study shall include spectral analysis for monitoring of fatigue and emotion.
MESSENGER Observations of Cusp Plasma Filaments at Mercury

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At Mercury, MESSENGER has documented ~1-2-s-long reductions in the dayside magnetospheric magnetic field with amplitudes up to ~90% of the ambient intensity. These field reductions which we have termed cusp filaments are observed from just poleward of the magnetospheric cusp to mid-latitudes. During these events, MESSENGER’s Fast Imaging Plasma Spectrometer (FIPS) measured H⁺ ions with magnetosheath-like energies. Minimum variance analysis of the Magnetometer (MAG) data indicates that the filaments are simple two dimensional flux tubes filled with magnetosheath plasma that has a diamagnetic effect on the local background field. Here we analyze filaments identified in 3 years of MESSENGER magnetic field and plasma data to determine the physical properties of these structures. Our results indicate that cusp filaments are common phenomena for all solar wind conditions. They occur over a range of magnetic latitudes from ~50 to 80°N, with durations of ~0.1—2.5s and magnetic field decreases of ~50—300 nT. If the filaments are associated with flux transfer events (FTEs) and move over the spacecraft at speeds comparable to the flank magnetosheath flow speed of 300 km/s, then these filaments have dimensions of ~30—750 km, which is larger than the gyro-radius of a 1 keV H⁺ ion, i.e., ~ 23 km. Correlation analyses show no obvious dependence of the duration or magnitude of the diamagnetic decrease on magnetic latitude. Overall, the MAG and FIPS observations analyzed appear consistent with an origin for cusp plasma filaments by the inflow of magnetosheath plasma associated with the localized magnetopause reconnection process that produces FTEs.
Where did Earth’s Post-Midnight High Energy Plasmasphere Go?

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The Van Allen Probes Helium Oxygen Proton Electron (HOPE) instrument measures a high energy tail of the thermal plasmasphere that has strong MLT dependence in the near Earth space. In our study, we statistically analyze a 16 month period of HOPE data, looking at quiet times with a Kp index of less than 3. The high energy plasmasphere tail is the upper 5\% of plasmasphere energies, consisting of ions between 1 - 10 eV. We calculated plasma densities over this energy range and see that there is strong depletion in O\textsuperscript{+} and H\textsuperscript{+} from 1-4 MLT and a similar but less dramatic density decline in He\textsuperscript{+}. Our results are compared with the Van Allen Probes Electric Fields and Waves (EFW) instrument spacecraft potential to rule out spacecraft charging. We conclude that the post-midnight ion disappearance is due to diurnal ionospheric temperature variation and charge exchange processes.
The Origin of Mid-Latitude Fast Solar Wind

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The solar wind has long been divided into two types: fast and slow. These types of solar wind have been differentiated by their velocity, heavy ion charge state ratios, and composition. The slow solar wind has a low velocity, high charge states, and higher Fe/O ratio while the fast solar wind has a high velocity, lower charge states, and lower Fe/O ratio. In reality the solar wind is more complicated than this. In addition to the bimodal nature there exists another population of solar wind. This wind has slow wind velocity and charge states but is compositionally similar to fast solar wind. In this presentation we present data from three Ulysses fast latitude scans using compositional data from the SWICS and SWOOPS instruments. We argue that we have discovered a new population of the solar wind which originates from the same region as the fast solar wind but has slow solar wind properties.
Heavy Ion Temperatures as Observed by ACE/SWICS

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Heavy ions in the solar wind as observed near Earth, especially in fast solar wind, tend to have thermal speeds that are approximately equal, indicative of a mass proportional temperature. Additionally, observations near 1 AU have shown a streaming of heavy ions (Z>4) along the magnetic field direction at speeds faster than protons. The differential velocities observed are of the same order but typically less than the Alfven speed. Previous analysis of the behavior of ion thermal velocities with Ulysses-SWICS, focusing on daily average properties of 35 ion species at 5 AU, found only a small systematic trend with respect to q^2/m.

Utilizing improved data processing techniques, results from the Solar Wind Ion Composition Spectrometer (SWICS) onboard the Advanced Composition Explorer (ACE) shed new light on the thermal properties of the heavy ion population at 1 AU. A clear dependence of heavy ion thermal behavior on q^2/m has now been found in the recent ACE-SWICS two hour cadence data set at 1 AU. Examining the thermal velocities of about 70 heavy ion species relative to alpha particles (He^2+) shows a distinct trend from equal thermal speed toward equal temperature with increasing q^2/m. When examined for solar winds of different collisional ages, the observations indicate the extent of thermal relaxation present in different solar wind types. We explore this collisional dependence with a model for the collisional thermal relaxation of the heavy ions as the solar wind propagates out to 1 AU. This model is used to subtract out the collisional effects seen in the ACE-SWICS data, providing an estimate for the temperature distribution among heavy ions at the corona to be compared to remote sensing observations that have shown that heavy ions are preferentially heated at the corona. We will discuss how this new analysis elucidates the thermal behavior and evolution of heavy ions in the solar wind, along with implications for the upcoming Solar Probe Plus and Solar Orbiter missions.
Heavy Ion Dropouts in the solar wind: Multi-spacecraft Observations and comparisons to 1D Hydrostatic Simulations

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Heavy ion dropouts in the solar wind are thought to originate from large, closed magnetic loops in the Sun’s corona (the outermost layer of the solar “atmosphere”). The distinctive, mass-dependent fractionation patterns of the dropouts requires that their source loops are relatively quiet and stable long enough (on the order of a day) to undergo gravitational settling. Therefore by studying the composition of heavy ion dropouts we are able to peer into the solar corona and glean information about the fine balance of physical processes. Additionally, the occurrence rates and magnetic profiles of dropouts suggest specific forms of magnetic reconnection are responsible for the release of the otherwise trapped plasma into the solar wind.

In this study we identify and compare dropouts observed by two different satellites, ACE and Ulysses, which together provide over 20 years of continuous observations at a variety of heliographic latitudes and radii. The resulting partial global view (or 3D view) enables us to identify coronal source regions and release mechanisms of heavy ion dropouts. We also discuss a physical model of gravitational settling which can be used to reconcile fractionation rates with the rate at which plasma must be escaping via reconnection. Our conclusions and results may contribute towards the ongoing refinement and validation of theories which predict the origin of “slow type” solar wind.
SEN: Sustainable Energy
Designing Tandem Systems for CO$_2$ Hydrogenation Based on Heterogeneous Catalysis

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The world’s growing demand for energy and materials and their strong dependence on fossil fuels encourage the utilization of alternative feedstocks for chemical synthesis. CO$_2$ is an attractive and abundant feedstock. The hydrogenation of CO$_2$ can produce a number of products, among which, methanol is an attractive first product, for its versatile use as a fuel and a chemical precursor. Recently, there have been reports of low temperature tandem systems for converting CO$_2$ to methanol using homogeneous catalysts; tandem systems possess the advantage of promoting the overall process by identifying the most selective catalyst for each sub-step. The use of heterogeneous catalysts for this type of reaction has been limited.

We explored the feasibility of using heterogeneous catalysts for CO$_2$ reduction to methanol and dimethyl ether. High surface area Mo$_2$C (~150 m$^2$/g) based catalysts exhibited high activity for converting formic acid or formate to methanol. The selectivity to methanol was enhanced, when nanoscale particles of Cu, active species for methanol synthesis, were dispersed onto Mo$_2$C. There also appeared to be a synergy between the metal and carbide. We also observed that these metal/Mo$_2$C catalysts were capable of converting CO$_2$ to methanol possibly via a formic acid intermediate. Finally, an extended tandem system was developed combining Cu/Mo$_2$C and a HZSM-5 zeolite for the co-production of methanol and dimethyl ether.

This work is supported by the NSF under the CCI Center for Enabling New Technologies through Catalysis (CENTC) Phase II Renewal, CHE-1205189.
Charge-Storage Mechanisms in Nanostructured Carbides and Nitrides for Energy Storage

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The need for sustainable high-power and high-energy-density storage devices is of significant interest in applications such as electronic devices and electric vehicles. In an effort to meet this need, supercapacitors are being developed. Currently available supercapacitors lack sufficient energy densities for a number of applications including use in electric vehicles and other load-leveling applications. The energy stored in supercapacitors depends on the material. The material currently used in commercial supercapacitors is activated carbon, which is relatively expensive and has limited capacitance. In this work, we proposed the use of environmental friendly high-surface-area transition-metal carbides and nitrides as electroactive materials for supercapacitor applications due to their low cost, high electronic conductivities, high surface areas (can exceed 200 m²g⁻¹), good electrochemical stabilities and high capacitances (up to 1340 Fg⁻¹). Despite efforts to date, the charge-storage mechanism of early transition-metal carbides and nitrides remains ill-defined. This presents a challenge to the full exploitation of these materials. Here we report a detailed investigation of the charge-storage mechanisms in early transition-metal carbides and nitrides in aqueous media, using x-ray absorption spectroscopy (XAS), small angle neutron scattering (SANS) and a combination of electrochemical techniques including cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and electrochemical quartz crystal microbalance (EQCM).
Solar Tracking Using Dynamic Kirigami Structures

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Conventional solar cell modules suffer coupling losses due to a decrease in projected area that scales with the cosine of the angle of the sun from its zenith. To increase the electrical power output from a given cell area, source tracking is often integrated with concentrator components, such as parabolic reflectors, Fresnel lenses, luminescent films, and more recently, microconcentrator optics. However, despite the rapid advancements in both semiconductor and concentrator technologies, solar tracking has remained costly, complex, bulky, and consequently prone to malfunction and wind-loading. To fully maximize power output and minimize module size, revolutionary new approaches to solar tracking are required.

Here we introduce a low-profile, dynamic tracking structure inspired by the ancient art of kirigami, a form of origami that allows cutting as well as folding to achieve the desired shape. We analyze the combined optical and mechanical properties of the proposed structure, and identify the appropriate dimensions and tracking procedures to maximize power generation over the course of a day. For an optimized kirigami structure, the output energy density is shown to approach that of conventional single-axis tracking. Finally, we demonstrate integration of the kirigami structure with thin-film gallium arsenide, and study the effect of recurrent tracking on electrical and mechanical response.
Thin-film GaAs solar cells on integrated mini-concentrators

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A key challenge in photovoltaic technology is to achieve cost-efficient energy harvesting. Among the various approaches, one with particular promise is based on GaAs thin-film photovoltaic cells enabled by epitaxial lift-off (ELO); a technology that has demonstrated the highest power conversion efficiencies to date. However, the cost reduction long promised by the ELO process is limited even if the wafer is recycled multiple times due to the expensive processing and materials cost. Here we demonstrate a method that can achieve solar energy conversion that costs only 3% compared to conventional substrate-based, and 14% of ELO-processed GaAs solar cells, respectively. This is enabled by a high throughput, non-destructive ELO (ND-ELO) wafer recycling process that provides an approximately ten times faster lift-off with ~90% process cost reduction compared with conventional ELO, combined with a rapid thermoforming process that generates inexpensive and light-weight integrated plastic concentrator arrays which costs only ~1% of total module cost. The low-profile, 2 dimensional concentrators are uniquely designed to be truncated over 90% from conventional compound parabolic concentrators (CPCs), and aligned with the solar path to maximize the yearly energy harvesting (in this work, by 2.8 times compared with planar solar cells), thereby replacing high concentration factor optics that demand expensive solar tracking paraphernalia. Moreover, the concentrators provide efficient light collection not only in direct, but also in diffuse light with only minor losses, and operating temperatures near room temperature are achieved under concentrated light by directly bonding the thin-film GaAs solar cells onto a heat-sinking metal layer. This represents a reduction in temperature of over 40°C when compared to substrate-based GaAs solar cells. These results represent a new and cost-effective plastic-based low-concentration solar module that enables light-weight, high efficiency GaAs-based solar cells to reduce the balance of systems costs compared with heavy, rigid modules that are also subject to wind loading damage and high installation costs.
The Effect of Nano-Crystalline Morphology on Organic Photovoltaics via Organic Vapor Phase Deposition

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Recent improvements in small molecular-weight organic photovoltaics (OPVs) have been realized by controlling the morphology of thin-films down to the nanometer scale. Organic layer morphology affects device efficiencies, operational lifetimes, and failure mechanisms. One method to effectively control the morphology of organic layers is thin film growth of organic vapor phase deposition (OVPD). By using inert carrier gas, OVPD provides extra energy for organic molecules to find an equilibrium morphological configuration as they adsorb onto the substrate, whereas evaporated molecules in conventional vacuum thermal evaporation (VTE) growth proceed ballistically from the source until they strike the substrate and have little opportunity for reorientation.

In this work, we demonstrate organic photovoltaic (OPV) cells based on a nanocrystalline mixed tetraphenyldibenzoperiflanthen (DBP):C\textsubscript{70} heterojunction grown by OVPD with a power conversion efficiency, PCE = 6.7±0.2\%, compared to 6.2±0.2\% for analogous, optimized devices grown by VTE. Due to the lower electrical resistance of the nanocrystalline layers formed via OVPD, the active region thickness can be almost four times those grown by VTE. The increased cell thickness ease manufacturing tolerances by reducing the occurrence of shorts due to pinholes often encountered in thinner cells. In addition, we show that morphological changes over time in the bathophenanthroline (Bphen) cathode buffer layer in these organic solar cells strongly impact device reliability, and that these changes are reduced when the underlying active region of the OPV is grown by OVPD as opposed to VTE. The enhanced layer stability leads to significantly improved device operational lifetime as well.
Highly Efficient Small Molecule Multi-junction Photovoltaic Cells

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Organic photovoltaic cells (OPV) have merged as one of the most promising candidates for the renewable energies of the next generation. Small molecule OPVs attract considerable interest due to its easy of process, ultrahigh purity and well-defined molecular structure. The power conversion efficiency, however, is still considerably lower than its inorganic counterpart. To improve the efficiency, we design and fabricate a novel multi-junction photovoltaic cell which can absorb photons in both the first and second optical maxima across the solar spectrum. Therefore, the quantum efficiency of multi-junction cell has greatly improved compared to single-junction cells, leading to a significant increase in power conversion efficiency. In addition, we developed an efficient algorithm to optimize the device performance of complex multi-junction cells based on Monte Carlo simulation. Our optimized OPV cell reaches a record-high efficiency of 12.6% under 1 sun illumination, representing a significant step towards the commercialization of OPV cells.
Abstracts - Richard and Eleanor Towner Prizes for Outstanding Ph.D. Research Poster Session
Auditory and Visual Identification of Wave-Particle Interactions in Heliospheric Time-Series Data

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A growing number of NASA satellites produce large and complex data sets that must be visually rendered in groups of sub-dimensions for effective navigation and analysis. Audification, a specific type of auditory data analysis, offers a promising method for the evaluation of heliospheric time-series. In this study participants were trained to audify solar wind time-series and complete two analysis tasks: visual analysis of a spectrogram, and multimodal analysis of a spectrogram paired with audio playback. The task involved the identification of Ion Cyclotron Wave Storm (ICWS) activity by locating regions containing increased power within a specific spectral bandwidth. Participant analysis was compared against an expert assessment and it was found that multimodal analysis displayed a higher sensitivity with no loss in precision; however, this higher sensitivity resulted in a large number of false positive identifications. To better understand the nature of these false-positives, a list of five regions selected by the majority of participants through multimodal analysis was provided to the expert for a follow-up assessment. The expert found that all five regions contained some level of Ion Cyclotron Wave activity, and though four of these regions did not meet ICWS criteria, one region contained an ICWS event that had been overlooked in the original expert assessment. This supports the hypothesis that auditory analysis can be helpful in identifying features in time-series data that may otherwise be overlooked. Additionally, 90% of participants in the study indicated that they found the audio to be helpful in the analysis task.
Quantum-confined group-III-nitrides for efficient and tunable light emission at visible and ultraviolet wavelengths

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Group-III-nitrides (AlN, GaN, InN) are technologically important semiconductors widely used in visible and ultraviolet (UV) optoelectronics. Applications include solid-state lighting, sterilization, water purification, photolithography, and optical data storage. Their electronic and optical properties can be tuned through alloying, but this approach can lead to dislocation formation and composition fluctuation, which negatively impact performance and efficiency. These problems are especially pronounced in alloys emitting visible light at green wavelengths—important for solid-state lighting, and in alloys emitting UV light above 4.9 eV—important for germicidal applications.

Using predictive first-principles methods, we explore nanostructuring and quantum confinement of group-III-nitrides to tailor electronic and optical properties while circumventing the problems arising in alloys. We demonstrate that quantum confinement in InN nanowires 1 nm in diameter results in efficient green and cyan light emission—precisely where alloys suffer efficiency loss. This finding illuminates a new approach to engineering visible-wavelength light emitters using nanostructured InN that avoids the efficiency-loss mechanisms encountered in alloys. We also study the effects of quantum confinement on the band gap of GaN-AlN quantum well superlattices. We show that single-monolayer GaN wells embedded in AlN barrier layers emit UV light above the 4.9 eV germicidal threshold without efficiency losses from alloying or the quantum-confined Stark effect. Furthermore, we elucidate the relationship between band gap and GaN-well/AlN-barrier thicknesses for tuning UV emission between 4.0 eV and 5.4 eV. This work provides a roadmap for designing highly efficient UV emitters tailored to specific photolithographic or optical data storage applications.
Proper management and disposal of municipal solid waste (MSW) remains to be an unresolved global problem. The amount of existing MSW disposed of in landfills in the past decades is staggering, while the generation rate of MSW is expected to keep increasing due to steady increase of population and prosperity worldwide. Approximately 250 million tons of MSW are generated on a yearly basis in the United States. More than 50% of the generated waste is landfilled and of which 60% consisted of paper, food and yard wastes which are biodegradable. These wastes are in general economically or technically unfeasible for recycling and incineration. One solution to sustainably handle the incoming and existing MSW is to design or retrofit landfills as bioreactors to promote biodegradation of MSW, enhance methane (CH4) generation, and optimize CH4 collection and conversion as an alternative energy source.

My doctoral research aims to study the coupled hydraulic-mechanical-biochemical processes taking place during MSW biodegradation and thus enhance energy recovery from MSW in landfills. Micro- (10-9m-10-3m) and meso-scale (10-3m-1m) laboratory studies and macro-scale (1m-103m) field investigation on MSW undergoing accelerated biodegradation have been conducted. Consequently, the resulting influence of enhanced CH4 generation and energy conversion on mega-scale (103-109m) solid waste management has been studied. A variety of testing and analytical techniques from multiple disciplines have been utilized, including molecular microbiology tools and high-throughput DNA sequencing, mechanical and geotechnical testing using a unique device developed at University of Michigan, state-of-practice field measurements, and various statistical tools for data analysis.
Vision-Based Articulated Machine Pose Estimation for Excavation Monitoring and Guidance

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Background The pose of an articulated machine includes the position and orientation of not only the machine base (e.g., tracks or wheels), but also each of its major articulated components (e.g., boom and stick). The ability to automatically estimate this pose is a crucial component of technological approaches aimed at improving both safety and productivity of many civil engineering activities. Purpose A computer vision based solution using planar markers is proposed in this research to enable such capability for a broad set of articulated machines that currently exist, but cannot track their own pose. Method Firstly, a planar marker is magnetically mounted on the end-effector of interest. Another marker is fixed on the jobsite whose 3D pose defines a local project coordinate frame. Then a cluster of at least two cameras respectively observing and tracking the two markers simultaneously is able to transfer the end-effector's pose into the desired local project frame, based on a pre-calibration of the relative poses between each pair of cameras. Results and Discussion Through extensive sets of theoretical analysis and field experiments, this approach is shown to be able to achieve centimeter level positioning accuracy within 10 meters range with only three ordinary cameras and a few planar markers, providing a flexible and cost-efficient alternative to other commercial products that use GPS and angular sensors. A working prototype has been demonstrated and tested on several active construction sites with positive feedback from excavator operators confirming the solution's effectiveness.
Within-cycle Profile Monitoring for Real-time Defect Prevention

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In discrete manufacturing, online sensing and data capture technology provides cyclic profile data that are important for process monitoring and defect prevention. Existing research on the monitoring of cyclic profiles is limited to between-cycle detection at the end of part completion based on the entire cycle of signals. In manufacturing processes with critical part quality and high cost, however, process changes require detection before a part is completed so that within-cycle adjustments can be triggered. This paper develops a wavelet-based profile monitoring method that is capable of making decisions within a profile cycle and guiding real-time process adjustments. The proposed within-cycle monitoring technique integrates real-time monitoring and within-cycle control opportunity for defect prevention. The optimal decision point is determined through the formulation of an optimization problem. The effectiveness of the proposed method is validated and demonstrated by simulations and case studies.
A direct kinetic (DK) simulation, in which kinetic plasma equations are solved in discretized phase space, is presented. Using the DK simulation, plasma oscillations are captured without any statistical noise that exists in particle simulations. In this study, two applications for the DK simulation are shown. First, the discharge oscillations of a Hall effect thruster, which is one type of spacecraft electric propulsion device, are discussed. [1,2] The results obtained from our numerical simulations agree with experimental data. Although it has been commonly considered that plasma oscillations occur due to insufficient neutral atom flow, for the first time it is shown from our simulations that the stabilization and excitation of such oscillations result from electron transport. A new theory of ionization oscillations that supports the results of numerical simulations is also proposed.[3] Second, the collisionless DK simulation, often called the Vlasov simulation, is used to model nonlinear plasma waves where some fraction of particles are trapped in traveling potential wells. These trapped particles can induce instabilities that may be deleterious for stimulated light scattering in inertial fusion confinement. The trapped particle bunching instability that is recently discovered by Dodin et al.[4] is modeled using the Vlasov simulation and a quantitative study is performed for the first time.[5] The growth rates of the instability obtained from the kinetic simulations are in good agreement with the improved theory.

A Multi-Physics Approach for Understanding Zirconium Hydride Precipitation and Growth in Zirconium

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The formation of zirconium hydrides in zirconium alloys is an important aspect of the microstructural evolution of fuel cladding in light water reactors. To maximize fuel performance and lifetime, a more in-depth and predictive understanding of hydrogen effects on the cladding is required than is currently modeled in fuel performance codes. I have developed a physics-based, quantitative mesoscale modeling and simulation framework to describe the behavior of hydrogen diffusion and hydride precipitation in α-zirconium, named Hyrax. Hyrax is developed from the open-source finite element framework MOOSE. Several numerical and algorithmic challenges were addressed in the process, and their solutions have been or will be contributed back to MOOSE and the scientific community. Hyrax incorporates phase field modeling, classical nucleation theory, heat conduction, and hydride/zirconium misfit strain. A CALPHAD-based free energy functional provides realistic energetics of the system and of hydride nucleation driving force. The temperature dependence, applied stresses, and hydrogen flux conditions have been incorporated into the CALPHAD free energy functional and other model components, enabling Hyrax to simulate a wide range of technically relevant operating conditions. The simulations reproduce the experimentally observed shift in the solubility limit of hydrogen in the α-Zr solid solution upon heating and cooling, and the results are consistent with the hypothesis that the hysteresis arises from elastic strain energy due to matrix/precipitate misfit. A simplified analytical formulation is proposed to describe the hysteresis in this system as a function of temperature, interfacial energy, and precipitate size.
Electrospinning of polymer fibers is a technique that has been in use for nearly a century, and has recently been a popular platform for creating tissue engineering scaffolds. However, the use of these fibers is quite limited due to the inability to precisely control the fiber architecture. Electrohydrodynamic (EHD) co-jetting is a method of creating compartmentalized polymer fibers which allows multiple surface chemistries, mechanical properties, polymer degradation, or drug loadings to be confined into separate continuous compartments in a single fiber. Utilization of EHD co-jetting combined with a newly developed method for patterning polymer fibers via an ultra-stabilized jet has been used to create hyper-porous polymer scaffolds of multi-compartmental fibers. The combination of multicompartmental fibers and the direct fiber writing process provides a platform for controlled anisotropy, geometries, pore sizes, surface functionalities, and mechanical gradients independently on a single 3D structure. These scaffolds provide a platform technology that can be used to modulate multiple parameters simultaneously and repeatedly to more accurately recapitulate a cell's native environment. To demonstrate the fiber scaffolds can produce viable engineered tissues, the scaffolds were used to culture human mesenchymal stem cells (hMSCs) into thick tissue-like sheets. The hMSCs were subsequently osteogenically differentiated, and were implanted into a calvarial defect in nude mice for eight weeks. This system was able to generate new bone across a 3 mm defect in the mouse's skull using differentiated hMSCs grown on the fiber scaffolds, without implementation of BMP or other osteogenic growth factors.
Development of novel nuclear fuel characterization methods with the differential die-away self-interrogation technique

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The Differential Die-away Self-Interrogation (DDSI) instrument is proposed for use in nondestructive assay of nuclear fuel. Safeguarding spent fuel requires characterization and verification of the fuel content, which may be a challenging task in light of the complexity of the item. The DDSI instrument could aid this effort by measuring quantities of interest to safeguards without the need for an external interrogating source, which is a scenario often preferred by the operators and inspectors alike. DDSI is a passive neutron coincidence counting technique that utilizes neutrons primarily from spontaneous fission in an assayed spent fuel assembly (SFA) to preferentially interrogate its fissile material content. Data are collected in list-mode in order to construct and utilize a Rossi-alpha distribution (RAD) for SFA characterization. High fidelity simulations have been performed to produce realistic RADs and analysis has shown the potential of the proposed DDSI instrument to accurately reflect several parameters of interest to safeguards.

Results obtained from the simulations have demonstrated the ability of the DDSI instrument to measure the SFA multiplication, determine the total elemental plutonium content, and detect certain pin diversion and replacement scenarios with high accuracy and without the need for an (α, n) source correction factor. The primary methods of analyzing the DDSI instrument response by utilization of the RADs are novel in neutron coincidence counting analysis, and the ability to measure multiplication without direct measurement of real triple coincidences or the need for an (α, n) correction factor has not previously been possible with traditional neutron coincidence counting.
Wettability Engendered Templated Self-assembly (WETS) for Fabricating Multi-phasic Particles

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Precise control over the geometry and chemistry of multi-phasic micro- and nano-particles is of significant importance for a wide range of applications including drug delivery, vaccines and inhalation biotherapeutics, biological sensors, optical devices, and nanomotors. Here, we have developed one of the simplest methodologies to fabricate multiphasic particles using surfaces with patterned wettability as a template. The developed technique, termed WETS (Wettability Engendered Templated Self-assembly) provides us with an unprecedented ability to manufacture, on a large-scale, monodisperse, multi-phasic particles (homogeneous particles, Janus particles, tri-phasic particles, and quad-phasic particles) of any size, shape or chemistry. Using the WETS process, we have fabricated multiphasic particles with a variety of different polymers, inorganic micro-particles, as well as nanoparticles. The fabricated monodisperse particles have dimensions ranging from 25 nm – 200 µm. We have also fabricated different amphiphilic Janus particles, possessing both a hydrophobic and a hydrophilic phase, in a wide range of shapes and sizes. Using such amphiphilic particles of different sizes and shapes as building blocks, we have also obtained and studied a diverse set of self-assembled structures at an oil-water interface. We have further demonstrated that here developed multi-phasic particles, can be utilized as multi-compartment drug carriers, that can be independently loaded with multiple drugs as well as functional nano-particles or organic molecules to aid in imaging and transport of the drug carriers to the targeted location.
Simplex Algorithm for Countable-state Discounted Markov Decision Processes

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Markov Decision Process (MDP) is the most popular model for sequential decision-making problems. We consider infinite-horizon MDPs with countably-infinite state spaces (which we call countable-state MDPs). Typical examples are inventory management and queuing control where there is no specific limit on the size of inventory or queue. A policy is defined as a decision rule that dictates which action to choose at each state. The goal is to find a policy that maximizes the expected total discounted reward. Previous solution methods for countable-state MDPs obtain a sequence of policies which converge to optimality but the sequence may not improve monotonically, i.e., a policy in the sequence may be worse than its preceding policies. We propose an algorithm that finds a sequence of policies that improves monotonically as well as converges to optimality. It is a simplex algorithm solving a linear program formulation of countable-state MDPs. In each iteration, the algorithm updates one state’s action, called a pivot operation. Since the problem has an infinite-horizon and a countably-infinite state space, it requires an infinite amount of data and an infinite number of computations to exactly evaluate how the total reward changes by a pivot operation. To be implementable, each iteration of our algorithm approximately evaluates candidate pivot operations using finite data and computations, and considers only a finite number of candidates. Despite these approximations, it is guaranteed that the obtained policies improve monotonically and converge to optimality. Experimental results for small inventory management problems are also presented.
Colorful, see-through photovoltaics

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Most current solar panels are made by complicated processes using high-priced semiconductor materials, and they are rigid and heavy with a dull, black appearance. As a result of their unappealing appearance and weight, they are not compatible with vehicle applications. Significant amount of effort has been put forth in developing colored photovoltaics (PV) in recent years. Owing to their attractive appearance, they can be integrated with interiors and exteriors of a structure, allowing a large area of architectures to be efficiently used for the power generation. Recently we introduced dual-function PV based on ultra-thin doping-free amorphous silicon (a-Si) embedded in an optical cavity that not only efficiently extract the photogenerated electric charges but exhibit distinctive color patterns with the desired angle invariant appearances. In order to create the desired optical effect, the semiconductor layer should be ultra-thin and the traditional doped layers need to be eliminated. We employed the charge transport/blocking layers to meet this demand. Owing to an insignificant propagation phase shift obtained when propagating through the ultrathin a-Si layer and an interesting cancellation effect with respect to the phase of light reflecting from the interface, our devices exhibit angle insensitive performance that can be retained up to ±70° for both s- and p- polarizations. We showed that the ultra-thin (6 - 31 nm) undoped a-Si/organic hybrid PV cells can transmit desired wavelength of light and that the majority of the absorbed photons in the a-Si layer contributed to the extracted electric charges benefited by the highly suppressed electron-hole recombination in the ultra-thin a-Si layer. Reflective colored PV can be made in a similar fashion. Light-energy-harvesting colored signage was demonstrated accordingly. Furthermore, a similar strategy has been applied to other PV material system (i.e., perovskite), successfully achieving colored, semi-transparent perovskite PV. The presented approach could open a new avenue to achieve decorative thin-film PV and energy efficient color display technologies.
From Behavioral to Topological Connectedness: A Study of Similarity in Network-Level Maliciousness

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Observations of malicious activities originated from different networks are often symptoms of their underlying security posture. The interconnectedness of today’s Internet also means that what we see from one network is inevitably related to others. This connection can provide insight into the conditions of not just a single network viewed in isolation, but multiple networks viewed together. Such understanding in turn helps us predict more accurately malicious activities from networks. In this study we examine how to measure the \{em similarity\} in the dynamic evolutions of malicious activities originated from different networks. We then investigate the relationship between such behavioral similarity and similarity in topological features. Specifically, we use statistical inferencing to evaluate the significance of a set of spatial features in explaining the observed behavioral similarity. In doing so we map relationships in a highly dynamic domain (malicious activities) to a relatively static one (spatial features). Statistical performances are also thoroughly analyzed. This proves to be useful in predicting future behaviors. In particular, our results can enhance the temporal prediction of malicious activities of a network with known historical information, and can also provide accurate prediction for a network with unknown historical information but whose spatial relationship with a few other networks is known.
Stochastic fuel efficient cruise control for vehicle speed

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Stochastic dynamic programming (SDP) is applied to generate control policies that adjust vehicle speed to improve average fuel economy without degrading, significantly, the average travel speed. The SDP policies take into account statistical patterns in traffic speed and road topography. Specific problems of fuel efficient in-traffic driving and fuel efficient vehicle following are considered within the SDP framework. Simulation results are summarized to quantify fuel economy improvements, and experimental vehicle results are reported for the fuel efficient vehicle following case. The properties of vehicle speed trajectories induced by SDP policies are examined. Particularly, in the case for fuel efficient vehicle following, the emergence of periodic control policies are examined and discussed. Vehicle speed trajectories generated using the periodic control policies produce periodic intervals of acceleration and coasting which result in a higher fuel economy, on average, when compared to implementing a conventional cruise control system set to an equivalent constant speed. Reported results for vehicle tests include a maximum of 11.58%, a minimum of -3.28%, and an average of 5.38% fuel economy improvement over the implementation of a conventional cruise control system set to an equivalent constant speed.
A Tale of Two Mechanisms: Incentivizing Improved Investments in Security Games

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In a system of interdependent users, all entities are affected by the security related decisions of one another. In particular, these users benefit from the improved health of the system when their neighbors invest in security measures; an effect known as positive externality. The externality of these decisions make security a public good, the optimal provision of which in a system of self-interested users requires regulation through external mechanisms. Ideally, these mechanisms are designed to incentivize the socially optimal levels of investment, while ensuring voluntary cooperation by all users, and avoiding the need for additional budget expenditure.

In this work, we first show that due to the non-excludable nature of security, no mechanism can achieve the three aforementioned goals simultaneously for all instances of a security game. We then compare two incentive mechanisms for improving security investment among users, namely the Pivotal mechanism and the Externality mechanism. We show that even though both mechanisms incentivize socially optimal investments, they differ in terms of budget requirements and participation. The Pivotal mechanism guarantees users' participation; however, although (weakly) budget balanced in many game environments, it runs a budget deficit in security games. The Externality mechanism on the other hand is a budget balanced mechanism, but fails to incentivize voluntary participation. We further identify some of the parameters affecting the performance of these mechanisms, by studying the specific class of weighted total effort security games.
Design of medical devices for global health: Empirical evaluation of user requirements elicitation and prioritization methods involving multiple stakeholders

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Involving stakeholders directly throughout the design engineering process can help to identify needs, elicit user requirements, and develop optimal solutions, particularly when the constraints are difficult to ascertain a priori. This study evaluates and discusses three user requirements elicitation and prioritization methods: open-ended, clustering, and discrete choice, to design a post-partum hemorrhage device for use in low-resource settings. We characterize each method’s ability to elicit and prioritize user requirements and product preferences from four stakeholder groups involved in health care delivery.

Open-ended, clustering, and discrete choice methods elicited user requirements and preferences of physicians, nurse-midwives, biomedical technicians, and public health officers (47 participants) in Ghana.

The open-ended response method effectively captured the general requirements of a design concept, yet resulted in predominantly generic requirements, whereas the clustering and discrete choice methods were more useful for inferring in-depth user requirements and eliciting stakeholder priorities. The clustering method revealed that usability and affordability were high-priority requirements among all four stakeholder groups. An individual difference scaling analysis (INDSCAL) was performed using the clustering method outcomes and it indirectly identified ease-of-use, availability, and effectiveness as the priority UR categories. Stakeholders ranked ease-of-use as the highest-priority user requirement, followed by performance, cost, and place-of-origin requirements using the discrete choice method. Given the significance of the ease-of-use requirement, an analytical framework based on sub-requirements was developed for quantifying stakeholder needs. Lastly, we discuss the relative merits of the three elicitation approaches and their implications for use with different stakeholder groups.
Tool wear characterization and monitoring for ultrasonic metal welding of lithium-ion batteries

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In manufacturing lithium-ion batteries for electrical vehicles such as the Chevy Volt, it is critical to create reliable interconnections between battery cells, module to module, and module to control unit. Such connections must possess reliable electrical conductivity and sufficient mechanical strength to ensure battery performance. Ultrasonic metal welding has been adopted for battery joining in lithium-ion battery manufacturing due to its advantages in joining dissimilar and conductive materials. Tool degradation, especially tool surface geometry change, has a significant impact on joint quality, and tool replacement, including horn and anvil, constitutes a major part of the production costs in lithium-ion battery manufacturing. Therefore, it is essential to develop an effective tool condition monitoring (TCM) system to balance product quality and production cost. However, it is very challenging to develop a TCM system for ultrasonic metal welding, because the tool surface geometry is highly complicated and the tool wear mechanism has not been thoroughly understood. Thus, conventional data-driven monitoring techniques cannot be directly applied for this spatiotemporal process. To address these challenges, this study (1) characterizes tool wear progression by comparing tool surface measurements in different wear stages; (2) designs an impression method to efficiently obtain tool surface measurement in plant environment; (3) develops a tool condition classification algorithm with application-dependent features which are generated from both space and frequency domain; and (4) proposes a tool wear progression model using the extracted features. The developed TCM system has been validated using measurement data from a battery plant.
Agent Aware Organizational Design

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As multiagent systems (MASs) such as distributed sensor nets or multi-robot systems increase in size, interconnectivity, complexity, and longevity, coordinating the agents’ reasoning and behaviors becomes increasingly difficult. One approach to address these issues is to use insights from human organizations to design structures within which the agents can more efficiently reason and interact. While prior work has largely focused on developing modeling languages to allow expert humans to specify an organizational representation for a MAS, we instead investigate how an automated organizational design process (ODP) can create computational organizations. By leveraging details about how the agents reason about their decisions we establish quantitative, principled metrics for organizational performance based on the expected impact that an organization will have on the agents’ reasoning and behaviors. Using these metrics, we characterize the organizational design problem as a search in the organizational design space. Unsurprisingly, our analysis of the design space reveals that creating a provably optimal organization is computationally intractable, and thus we develop techniques that improve the efficiency of our ODP via approximating the incremental impact of a proposed organizational influence. Our empirical results demonstrate that our ODP can create organizations that not only steer an agent into behaving in ways that mesh well with other agents’ behaviors, but also can simplify an agent’s reasoning about such behaviors.
Plasma Protein Corona Modulates the Vascular Wall Interaction of Drug Carriers in a Material and Donor Specific Manner

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The nanoscale plasma protein interaction with intravenously injected particulate carrier systems is known to modulate their organ distribution and clearance from the bloodstream. However, the role of this plasma protein interaction in prescribing the adhesion of carriers to the vascular wall remains relatively unknown. Here, we show that the adhesion of vascular targeted poly(lactide-co-glycolic-acid) (PLGA) spheres to endothelial cells is significantly inhibited in human blood flow, with up to 90% reduction in adhesion observed relative to adhesion in simple buffer flow, depending on the particle size and the magnitude and pattern of blood flow. This reduced PLGA adhesion in blood flow is linked to the adsorption of certain high molecular weight plasma proteins on PLGA and is donor specific, where large reductions in particle adhesion in blood flow (80% relative to buffer) is seen with 60% of unique donor bloods while others exhibit moderate to no reductions. The depletion of high molecular weight immunoglobulins from plasma is shown to successfully restore PLGA vascular wall adhesion. The observed plasma protein effect on PLGA is likely due to material characteristics since the effect is not replicated with polystyrene or silica spheres. These particles effectively adhere to the endothelium at a higher level in blood over buffer flow. Overall, understanding how distinct plasma proteins modulate the vascular wall interaction of vascular targeted carriers of different material characteristics would allow for the design of highly functional delivery vehicles for the treatment of many serious human diseases.
Hippo/YAP-mediated rigidity dependent motor neuron differentiation of human pluripotent stem cells.

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Human pluripotent stem cells (hPSCs) are invaluable resources for developmental studies, transplantation, and disease modeling. However, it is still largely unclear how dynamic cell-biomaterial interactions play a role in regulating hPSC self-renewal, pluripotency and differentiation. In this work, we leveraged a library of micromolded poly(dimethylsiloxane) (PDMS) micropost arrays (PMAs) that present the same surface geometry, but different post heights, to modulate substrate rigidity independent of adhesive effects and other material surface properties. Using the PMAs, we screened a broad range of substrate rigidities, and our results revealed that substrates with a rigidity less than 5 kPa could promote early neural induction of hPSCs by increasing gene and protein expression levels of Pax6 and Sox1 and decreasing expression levels of pluripotency genes. Moreover, soft substrates strongly promoted caudalization of neural progenitor cells by elevating the HOX genes expressions. As a result, the purity and yield of functional motor neurons (MNs) derived from hPSCs within 30 days of culture using the soft PMAs were improved two- and fifteen-fold, respectively, compared to conventional hPSC culture. Motor neurons derived on the PMAs displayed electrophysiological activities comparable to those from primary neurons in vivo. Mechanistic studies further revealed a multi-targeted mechanotransductive process in hPSCs involving Smad phosphorylation and nucleocytoplasmic shuttling, regulated by rigidity-dependent Hippo-YAP activities and actomyosin cytoskeleton integrity and contractility.

Together, our data suggest that substrate rigidity is an important biophysical cue influencing neural induction and subtype specification. Synthetic, microengineered substrates therefore can serve as an innovative platform for future large-scale culture of hPSCs.
The Role of Tissue Mechanical Properties in Histotripsy Tissue Fractionation

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Histotripsy is a therapeutic ultrasound technique that controls cavitation to non-invasively fractionate tissue. This technique, invented in our lab at the University of Michigan, is the only non-invasive, non-thermal ablation method currently available. Preclinical studies have shown many advantages that suggest histotripsy has the potential to transform the field of ablation therapy, with the first clinical trial currently underway. Histotripsy has been demonstrated to successfully fractionate many different tissues, though stiffer tissues (i.e. cartilage, tendon) are more resistant to histotripsy-induced damage than softer tissues (i.e. liver, prostate). In this work, we investigate the effects of tissue stiffness on the histotripsy process including the cavitation threshold, bubble dynamics, and stress-strain applied to tissue structures. Histotripsy pulses at varying frequencies (345kHz, 500kHz, 1.5MHz, and 3MHz) were applied to tissue phantoms and \textit{ex vivo} tissues with varying stiffness. Results demonstrate that the intrinsic threshold to initiate cavitation microbubbles is independent of tissue stiffness while bubble expansion is suppressed in stiffer tissues, leading to decreased strain and increased damage resistance. These findings were used to develop a selective ablation approach in which a target tissue (i.e. liver, tumor) is fractionated while stiffer tissues (i.e. blood vessels) are preserved. This strategy was tested in an \textit{in vivo} porcine model, with results demonstrating the porcine liver was completely fractionated while vital hepatic vessels remained intact and functional. Overall, this work improves our understanding of how tissue properties affect histotripsy and is essential to develop tissue-selective ablation strategies and guide parameter optimization to advance histotripsy therapy.
High Performance Plasmonic Photoconductive Terahertz Optoelectronics

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Photoconductive sources are extensively used for generation of terahertz radiation in time-domain and frequency-domain terahertz imaging and spectroscopy systems for various chemical sensing, product quality control, medical imaging, bio-sensing, pharmaceutical, and security screening applications. They consist of an ultrafast photoconductor connected to a terahertz antenna, which is pumped by a pulsed or heterodyning laser illumination for pulsed or continuous-wave terahertz generation. In spite of their great promise, the inherent tradeoff between high quantum-efficiency and ultrafast operation of conventional photoconductors has significantly limited the output power of photoconductive terahertz sources. Here, we present a photoconductive terahertz emitter that incorporates volumetric metallic nanostructures inside the device active area to offer record high optical-to-terahertz power conversion efficiencies. By use of volumetric metallic nanostructures the majority of photocarriers are generated within nanoscale distances from the photoconductor contact electrodes and drifted to the terahertz radiating antenna in a sub-picosecond time scale to efficiently contribute to terahertz radiation. We experimentally demonstrate 105 $\mu$W of broadband terahertz radiation in the 0.1-2 THz frequency range in response to a 1.4 mW optical pump, exhibiting a record high optical-to-terahertz power conversion efficiency of 7.5%.
Chiral Transmission to Self-Assembling Nanostructures from Circularly Polarized Light

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Chemical reactions affected by spin angular momenta of circularly polarized photons are rare and display low enantiomeric excess. Because of high optical and chemical activity, nanoparticles (NPs) signifies the possibility of converting spin angular momenta of absorbed photons into structural changes of nanoscale materials by self-assembling. However, such processes are currently unknown. Here, we demonstrate that circularly polarized light (CPL) strongly affects the nature of self-assembly of racemic CdTe NPs. In particular, illumination of NP dispersions with right- and left-handed CPL induces the formation of right- and left-handed twisted nanoribbons, respectively. Enantiomeric excess of such reactions exceeds 30% which is ~10 times higher than other CPL-induced reactions. In contrast, illumination with linearly polarized light and assembly in the dark led to straight nanoribbons. This observation of imprinting the polarization information of incident photons by NPs opens new pathways for the synthesis of chiral photonic materials and allows for better understanding of the origins of biomolecular homochirality.
Corrected Diamond Difference Method for Coupling the Method of Characteristics and Sn for 2-D/3-D Nuclear Reactor Simulations

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This work develops a new method for obtaining full-core, 3-D solutions to the Boltzmann transport equation in the context of nuclear reactors. The method operates by decomposing the spatial domain of the reactor along the axial direction into multiple slabs, each of which are treated with a pin-resolved 2-D Method of Characteristics (MoC) solver. Select data from the 2-D MoC solutions are then used to inform a novel formulation of the 3-D Sn equations, called Corrected Diamond Difference (CDD) to obtain a global, 3-D solution on a coarsened, pin-homogenized orthogonal mesh. The CDD method preserves the angle-dependent neutron streaming and collision behavior from the fine-mesh MoC calculations, and in coupled 2-D problems, produces results that are equivalent to the fine-mesh MoC solution. Employing CDD to the coupled 2-D/3-D problem ameliorates the accuracy penalty of operating on a coarsened grid for the 3-D Sn solution, and constitutes an accuracy improvement over contemporary methods.

The 2-D/3-D approach is implemented in the MPACT reactor analysis code and applied to the C5G7 reactor benchmark cases. The results demonstrate improved accuracy relative to comparable methods.
Probabilistic forecasting of space weather for solar wind transients

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Space weather studies how the Sun influences Earth’s space environment and the technological and societal impacts of that interaction – damage to Earth-orbiting satellites and threats to both astronaut safety and to reliability and accuracy of global communication and navigation systems, as well as electric power distribution grids. Geomagnetic disturbances (storms or substorms) that drive space weather impacts, such as ground-induced currents and radiation belt enhancements are usually caused by extreme solar wind transients that have strong southward directed interplanetary magnetic field (IMF Bs). However, current heliospheric models either do not predict or provide low-accuracy forecasts of this most geoeffective parameter – IMF Bs. We analyze the in situ plasma and magnetic field measurements of long-duration, large-amplitude IMF Bs intervals, and examine the probability distribution function of simultaneous geomagnetic activity indices. We found that different solar wind parameters are correlated with geomagnetic indices in different ways, but IMF Bs is still the key for driving geomagnetic storms and magnetospheric ultra-low-frequency (ULF) waves. The statistical profiles also show significant differences during the periods one day before the strong IMF Bs intervals for different solar wind transients. We suggest that strong IMF Bs-events could be predicted from the preceding characteristics of solar wind and IMF changes, and that probabilistic forecasting of geomagnetic activity occurrence should be more widely used in space weather forecasting.
Abstracts – Afternoon Session
AEP: Applied Electromagnetics and Plasma Science
Design of Low Complexity Integrated Phased Arrays

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A phased array is an array of antenna which is capable of beam forming and electronic steering by adjusting the relative phase and amplitude of the signal received or transmitted by each antenna element. The most distinguished feature of phased arrays is their spatial selectivity which makes them attractive for many telecommunication systems and radar applications. Owing to their spatial selectivity, phased arrays increase the channel capacity, alleviate multipath fading and co-channel interference, and reduce the required transmitted power in telecommunication system. Phased arrays also enhance cross range resolution and signal to noise ratio in radar systems. These unique features of phased array technologies are very useful in many commercial applications; however, their size, cost and complexity have prevented them to be widely utilized. A large portion of size and complexity of phased arrays is due to their phase shifters used to allow beam steering. The research described is intended to address the problem of size, cost, and complexity of phased arrays, mainly by significantly reducing the number of required phase shifters in array configurations. So far, the main goal of the research has been accomplished by devising new techniques to achieve phase shifting and beam steering such that the required number of phase shifters decreases. In the proposed approach, rather than using one phase shifter per each antenna element, only a single phase shifter is utilized for a sub array of four antenna. Then, the sub arrays can be modularly scaled to hundreds of elements in the whole array.
An Iterative Array Signal Segregation Algorithm for Interference Detection and Cancellation in Complex Multipath Environments

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A frequency domain Iterative Array Signal Segregation Algorithm (IASSA) is conceived to estimate the directions of arrival, magnitudes and phases of the signals impinging on the receiver using a uniform circular antenna array in conjunction with a neoteric radio. The proposed approach is able to detect the signals within a very wide dynamic range. This technique is utilized to spatially separate the low level communication signals of interest from the strong interfering signals without a priori knowledge regarding their directions of arrival. As the ultimate upshot, not only does this technique clean up the contaminated received signal at each antenna element but also it is able to segregate the contribution of the desired signal from each direction of arrival on each antenna element. By the virtue of this algorithm, a radio receiver is developed to mitigate the interfering signals in a complex multipath environment. For single stationary jammer, if a replica of the jamming signal due to multipath effect quite a way from the desired signals exists, the radio is able to cancel out the jamming signal even if other arriving jamming signals exist in close angular proximity to the desired ones. Based on a Monte Carlo analysis in some part of Manhattan, IASSA radio succeeds to nullify interference and bring to the weak communication signal in 70% of occasions.
Quasi-One-Dimensional Particle Code for Simulation of Magnetic Nozzle Propulsion Systems

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Magnetic nozzles are strong magnetic fields which guide the flow of plasma in electrode-less plasma thrusters. These magnetic fields generate thrust through interaction with the expanding plasma and also limit plasma contact with the surfaces of the thruster, thereby increasing lifetime and thermal insulation. The plasmadynamics in a magnetic nozzle is complex and many magnetic nozzle devices of interest operate in regimes in which the physics may not be well described by conventional continuum models. To address this need we have developed a novel quasi-one-dimensional particle-in-cell code to study magnetic nozzle physics from a kinetic perspective. Herein we present the development and validation of this code.

The code resolves a single spatial dimension along the axis of symmetry and three velocity dimensions. Two-dimensional spatial effects are included through virtual displacements of magnetized particles from the axis of symmetry and cross-sectional area variation due to approximate conservation of magnetic flux. The conventional Boris algorithm for pushing particles is modified to accommodate the one-dimensional axisymmetric coordinate system. The code was validated with a number of test cases which illustrate the ability to capture plasma instabilities and oscillations, complex potential structures, and magnetic mirror physics, which are necessary to study magnetic nozzles from a kinetic perspective. These test cases included modelling two stream instabilities, Landau damping, source and collector sheaths, and magnetic mirrors.
A Novel Frequency Beam Scanning Radar System at 240 GHz

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This paper presents and overview of the design, fabrication and characterization of a frequency beam scanning radar system operating from 230 GHz to 245 GHz. The radar antenna is designed using hollow rectangular waveguides with slot cuts placed on the H-plane of the waveguide wall. The slots in turn excite a linear patch array above it. The progressive phase shift between the slots is facilitated by meandered waveguide lines supporting TE_{10} mode. By changing the frequency, the propagation constant of the waveguide changes, which in turn will change the excitation phase of each slot and hence the antenna beam is steered. To provide the desired phase shift between the two consecutive slots while maintaining a small physical separation between them, the waveguide is meandered. This one-dimensional array forms a narrow beam width in the plane of slots while generating a wide beam in a plane perpendicular to that. In order to confine the beam in the elevation direction, the antenna aperture is widened by using slot-coupled patch arrays. This two-dimensional structure provides a two-dimensional confined beam.

The patches are positioned on top of the slots separated by a dielectric substrate. The center patch is fed by the slot on the bottom layer of the substrate, while the rest are series-fed through the center one.

One method to fabricate the antenna is the micromachining technique where the waveguide trenches are etched in silicon and then covered with gold. Next the slots are fabricated on a wafer and bonded to the other wafer to form the one-dimensional array. Finally, the patches are fabricated on a membrane which is then attached to the one dimensional array to form the complete antenna.

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Electron Transport in Underwater Plasma Treatment

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As an alternative to the traditional physical and chemical methods of water purification such as filtering, pressurizing, heating and UV irradiating, non-thermal plasma treatment techniques are proposed as an application to investigate electron transport in physical chemistry. One procedure is to continually apply nanosecond-pulsed air streamers to water in a closed loop whereas the other is a brute force approach that attempts to pulse the water with plasma jets. Both systems use electrons in the tail of the EEDF to dissociate water molecules and create radicals. The combination of radicals from the air and water and increased entropy is believed to depopulate undesirable compounds in water. Using the treatment results, a model for electron transport and electrical breakdown in water, or more generally liquids, will be suggested and explored.
Preliminary results of equation of state measurements using imaging x-ray Thomson spectrometer

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Understanding the equation of state of materials under shocked conditions is important for laboratory astrophysics and high-energy-density physics experiments. The goal of the experiments discussed here is to create a platform for equation of state measurements in shocked foams on Omega EP. The target of interest for these experiments is shocked carbonized resorcinol formaldehyde foam with an initial density of 0.34 g/cc. Lasers irradiate an ablator, driving a shock into the foam. Plasma conditions ahead of the shock, at the shock and behind the shock are diagnosed using the imaging x-ray Thomson spectrometer (IXTS). The IXTS is capable of spectrally resolving the scattered x-ray beam while imaging in one spatial dimension. Preliminary results from these experiments will be shown.

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An Experimental Investigation of Secondary Electron Emission and its Role in Low Temperature Plasmas

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The nature of plasma transport across the magnetic field in crossed-field (CF) devices such as Hall effect thrusters (HET) remains largely an unsolved problem. This can be further complicated by the presence of secondary electrons derived from the wall due to electron impact. The role of these secondary electrons in the operation of HET has been a subject of investigation in the recent past. Under normal operating conditions of a HET, several physical phenomena are occurring simultaneously and the interaction of the plasma with the channel walls of the thruster play an important role in its effective operation. These plasma wall interactions produce secondary electrons that have a non-linear coupling effect with the bulk plasma and affect the performance of crossed field devices by changing the sheath potential as well as the electron energy distribution. This influence is not yet fully understood in the community and thus the computational models are based on assumptions that are not highly accurate. Experimentally, there is no available data on the SEE yield in plasma and its effects to environments similar to that of a Hall thruster, which could be used to validate existing numerical models. Needed to understand these effects is a test-bed apparatus that could serve as a tool to validate and improve existing numerical models by providing the appropriate boundary conditions, secondary yield coefficients and variation of plasma parameters to aid future design of HET.

In this work, a benchtop apparatus is used to elucidate the role that secondary electrons play in regards to crossed field transport and energy flow to the walls. An electron beam is used to generate a secondary electron plume at the surface of various targets (Al, Cu, C, BN). The response of the plasma device to these secondary electrons is assessed by measuring changes to the potential distribution in the sheath of the irradiated target and the measured electron energy distribution function. The variation in the discharge voltage at fixed emission current is also determined which yields insight into its impedance. An attempt is made to relate phenomena and trends observed in this work with those in Hall thrusters.
An Efficient and Analytical Model for Indoor Wave Propagation at Low VHF

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In this presentation indoor wave propagation issues at low-VHF band are considered. The premise of low frequency communication is in low attenuation and low multi-path fading and their major drawback for mobile applications is in the size of the antenna. With the advent of antenna miniaturization methods techniques this limitation is being removed. On the other hand, a salient feature for wave propagation at this band is the fact that the size of objects is smaller or comparable to the wavelength and therefore high frequency methods such as ray-tracing can no longer be applied. In addition, full-wave methods such as FDTD at HF and low-VHF bands quickly lose their advantage for problems with large computational domains and in situations where statistical parameters of wave propagation are to be determined. Thus, in these situations, low frequency approximations such as Generalization of the Rayleigh-Gans approximations can be utilized to find the scattered field. In these computations accurate calculation of the dyadic Green’s functions is used to capture the electric field at desired receiving points. In an extension to this approach, we also consider more realistic scenarios in which buildings use metallic frames as reinforcement. It should be noted that the presence of these metallic structures which are mostly in the form of loop frames inside the walls, floors and ceilings may cause significant attenuation of low frequency signals especially in the lower VHF and HF bands.
High Sensitivity RF Energy Harvesting from AM Broadcasting Stations for Civilian Infrastructure Monitoring

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Wireless energy harvesting technologies have attracted much attention as a promising method to supply power to various devices. This research is focused on harvesting the EM energy in the ambient environment for powering distributed autonomous sensors. In general, such sensors are expected to have a long lifespan. Furthermore, they are often located in hard-to-reach positions where battery replacement is either not possible or is very costly. Radio frequency energy scavenging at AM bands is chosen to power such sensors due to non-line of sight and lower propagation losses.

A typical radio frequency (RF) harvester consists of an antenna, a rectifier and a signal conditioning circuit. A ferrite rod loop antenna is utilized and matched to the rectifier to provide the maximum power transfer. The rectifier’s efficiency is carefully studied as a function of captured RF power and load values. A sleep-and-wakeup circuitry consisting of a self-sensing triggering unit with ultra-low power consumption is employed to enhance the system’s sensitivity. Laboratory and field tests were performed to verify the performance of the scavenger under different environmental conditions. It is shown that the scavenger can work within 10 km away from an AM station under a RF power density of \( \sim 0.13 \, \mu\text{W/cm}^2 \).

Further research is being conducted at a higher power levels targeting commercial applications such as wireless charges for mobile devices and electric vehicles. Efforts are devoted to reducing the size and power consumption and improving the robustness and frequency stability of wireless power transmitters.
MF Band Compact Helical Antenna Design and Imaging Techniques for Hydraulic Fractures Detection

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In this paper we present a medium frequency (MF) band imaging system to estimate the subsurface hydraulic fractures. Hydraulic fracturing is a technique to create small fractures in subsurface rock layers by a mixture of pressurized water, sand, and especial chemicals, in order to release the trapped gas and oil in shale rock. As the use of hydraulic fracturing has grown, concerns about its environmental and public health impacts have also increased—one of the most significant concerns being the hazardous fluids that are injected into rock formations may cause water and soil contaminations. Thus, fracture mapping in gas and oil fields is important for determining the accurate parameters of fractured area and this would help for regulating the fracturing process and preventing the potential environmental damage while optimizing the production efficiency of oil and natural gas. In order to detect fractures at a distance of kilometers, we propose to use a lower frequency band such as MF band (300 KHz - 3 MHz) to reduce the signal attenuation. Compared with conventional high frequency mapping system, the penetrating distance can be increased to kilometers range. As the most challenging component design in the system, we propose a helical dipole antenna for the borehole imaging application. The proposed antenna is loaded with a ferrite-bundle and is optimized to achieve an ultra-compact size to fit within a volume of $\frac{\lambda_0}{1600} \times \frac{\lambda_0}{1600} \times \frac{\lambda_0}{40}$ while maintaining a relatively high efficiency of about 20%. The feeding network is designed to match the antenna input impedance with the frequency tunability. Based on the proposed antenna, radio-wave techniques for detecting fractured regions in subsurface rock layers are developed. Multi-hole and single-hole setups with different imaging algorithms are studied in the paper. Many methods such as beam-forming, adaptive null-generating and time-gating are performed to minimize the direct-link. Post-processing maps the conductivity contrast in the target area with a good resolution.
All-directions through the wall radar imaging using a synthetic array formed by a finite number of moving robots

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Through the wall radar imaging is used for mapping buildings’ interiors and detecting static or moving objects behind the walls. This technique has found many applications in rescue and search operations. Current approaches for through the wall radar imaging employ ultra wideband radars with large arrays of transmitting and receiving antennas to achieve the required range- and cross-range resolution. Due to limited space of buildings’ interiors, placing large antenna arrays inside the buildings to achieve high cross-range resolution is not practical in the most cases and as a result, current approaches usually perform imaging from outside of the buildings. Systems for mapping the buildings from outside can usually investigate the first floor of the buildings and their imaging capability decreases as the complexity of the building interior increases. This research introduces a new concept for all directional through the wall radar imaging using an ad hoc network of a limited number of mobile transceivers. In the proposed method, instead of using a large array of transmitting and receiving antennas, a limited number of transceivers mounted on moving robots are used. As robots move, reflected signal is sampled at different positions. By applying an appropriate beam forming technique to the samples of the received signal, a 360° view of the building interior can be obtained with a high cross-range resolution. The proposed method introduces higher mobility for the imaging system and as a result, enables imaging of buildings from inside which results in obtaining more accurate map of buildings’ interiors.
ATE: Automotive and Transportation Engineering
3-D crystal plasticity modeling for development of automotive lightweight materials

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The use of lightweight materials such as Aluminum (Al) and Magnesium (Mg) alloys in vehicles will significantly increase fuel efficiency and cut emissions. Validated constitutive models can allow automakers to use these lightweight materials without expensive die tryouts and new model development costs. CP-FEM (crystal plasticity-finite element method) modeling allows development of constitutive laws for new materials based on the initial crystallographic texture and uniaxial stress-strain data, thereby predicting the evolution of the yield surface in multi-axial tensile space for a real specimen. In this work, we have used a rate-independent 3-D crystal plasticity model to model face-centered cubic (FCC) metals such as Al. The underlying deformation mechanisms and modes of failure during operation of hexagonal close packing (HCP) metals such as Mg are not currently well understood. We have considered both crystallographic slip and deformation twinning to model and simulate the spatial distribution of the relative amount of slip and twin activities in a polycrystalline AZ31 Mg alloy. Thus, the present work will lead to advances in rapid computer-aided design of magnesium alloy manufacturing processes.
Hybrid Material Interfaces: Strength and Modeling

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With national attention to increase fuel efficiency, scientists and engineers are looking for solutions to this challenge. Weight reduction through lower density materials is a leading method to achieve this goal. Composites have been used extensively in the aerospace industry for decades for their superior strength-to-weight ratio and property control; however, it was not until recently that composites became cost-effective for the automotive industry. Another barrier for composite automotive components is the adhesion with non-composite materials such as steel. At an interface between dissimilar materials, fracture becomes an inherently mixed-mode problem, dependent on both opening and shear loading. Part of the challenge of this work lies in separating the two failure modes in order to accurately model failure of an arbitrary geometry of the same composite/adhesive/steel system. The poster will provide initial findings of opening and shear traction-separation laws; using the cohesive zone model of fracture, these two laws (along with a failure criterion) govern adhesive failure across the dissimilar-material interface.
Computational Modeling of the Electron Transfer Reaction at the Anode-Electrolyte Interface in Lithium-Air Batteries with Ionic Liquid Electrolytes

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Lithium-air batteries are very promising energy storage systems for meeting current demands in electric vehicles. However, the performance of these batteries is highly dependent on the electrochemical stability and physicochemical properties of the electrolyte. The unique properties of ionic liquids such as relatively wide electrochemical stability window and very low vapor pressure have made them promising candidates as electrolytes for improving the cyclic performance of lithium-air batteries. The local current density, which is an important parameter in determining the performance of lithium-air batteries, is directly proportional to the rate constants of the electron transfer reactions at the surface of the electrodes. In this study, a novel method, based on Marcus theory coupled with the Conductor-like Screening Model (COSMO) is presented to investigate the effect of dielectric constant of the ionic liquid electrolyte on the kinetics and thermodynamics of the electron transfer reaction at the anode-electrolyte interface that involves the oxidation of pure lithium metal into lithium ion. The free energies for all the species involving in the anodic reactions were calculated using density functional theory (DFT). Our results indicate that the electron transfer rate constant as well as the magnitude of the driving force for the anodic reaction decreases linearly with the inverse of the static dielectric constant of the ionic liquid. The presented results provide important insight on kinetics and thermodynamics of electron transfer reactions in lithium-air batteries that will help in the identification of appropriate electrolytes for enhanced performance of lithium-air batteries.
Pre-emptive Vehicle Motion Control for Post-Impact Vehicle Stability

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This study proposes a preemptive vehicle control strategy that takes into consideration post-impact vehicle stability. To reduce the risk of subsequent crashes after an initial collision with another car, sufficiently fast decision and control are desired for stabilizing the vehicle motion. As opposed to active steering systems for lane or path tracking, the proposed control system needs to assess the strength of impact from the other vehicle and predict the resulting vehicle motion. To achieve faster and more effective control responses, impact prediction and estimation schemes that are performed before and at an early stage of a crash are proposed. Based on the predicted or estimated collision strength, steering and braking control actions are taken to drive the vehicle motion to a desired final state. Simulations and analysis results of the proposed estimation and prediction algorithm are presented, followed by the demonstration that shows the usefulness of the proposed control algorithm.
Efficient Exhaustive Search of Power Split Hybrid Powertrains in the Configuration, Sizing and Control Design Space

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Planetary Gear (PG) power-split hybrid powertrains have been used in the production vehicles from Toyota and General Motors. Some of those powertrains use clutches to achieve multiple operating modes to improve powertrain flexibility and efficiency. Along with the flexibility associated with the PGs and clutches comes design complexity. To address this complexity, an automatic modeling and screening process is developed here, which makes it possible to exhaustively search through all configurations with all possible clutches and operating modes. By combining this process with Power-weighted Efficiency Analysis for Rapid Sizing (PEARS), a near-optimal and computationally efficient energy management strategy, the extremely large design space of configuration, component sizing and control becomes feasible to search through to identify optimal designs that have not been reported in the literature. The configuration adopted in the THS-II system used in the Prius MY2010 and Hybrid Camry has been chosen as a case study to adopt the developed methodology. Two designs are further investigated for comparison against the Prius: one uses all possible operating modes, and another sup-optimal design that limits the number of clutches to three.
Accelerated evaluation of automated vehicle systems based on microscopic traffic modeling

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Automated Vehicle technology is leading a revolution in transportation. It shows great potential to save fuel, reduce traffic accidents, ease traffic congestion, and increase mobility of the elderly and disabled. It is estimated that market for the related industries will reach $87 billion in 2030.

As the automation of vehicles keeps evolving, the systems have become increasingly complex, which makes the evaluation of automated vehicles very challenging. Current evaluation methods such as Test Matrix and Naturalistic Operational Test suffer from difficulties to identify critical test scenarios or years of road testing. In this research, a model-based evaluation approach was proposed to accelerate the evaluation of automated vehicles. Stochastic driver models were built to control the vehicles surrounding the automated vehicle, which could emulate the driving variance over time as well as human driving mistakes, based on statistical analysis of large scale driving database. By eliminating the normal driving situation, more challenging microscopic environment was created to accelerate the evaluation procedure. The Autonomous Emergency Braking systems of Volvo 60 and Infiniti M37S were modeled and evaluated in car-following situation. Results show that the overall evaluation time was reduced by over 100 times in simulation. Volvo 60 outperformed the Infiniti M37S for forward collision avoidance but had a slightly high crash rate for rear-end crashes from behind.
CEN: Civil Engineering
A Layered Thermo-mechanical Shell Element for Analyzing Heated, Thin-walled Structures

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The analysis of thin-walled structures exposed to various heating conditions is of particular interest in civil structures and naval vessels alike. Non-uniformly heated concrete slabs or steel decking in building fires and the panels of ships and aircraft experiencing extreme heating are typical cases in which thin-walled structural elements need to exhibit satisfactory performance at elevated temperatures. A new element was implemented based on general shell theory for finite element analysis (FEA) using an eight-node, isoparametric, doubly curved formulation. The element is a thermo-mechanical shell capable of coupled heat transfer and structural analysis. Previous work aimed to develop a novel thermal shell element for heat transfer analysis (Jeffers, 2013) and an efficient mechanical shell element formulation was selected (Yunus et al., 1989). The resulting coupled element is capable of simultaneous temperature-displacement analyses. The eight nodes of the shell element include four located at the corners and four along the mid-side with all eight lying at the mid-depth of the shell. The thermal shell element can have multiple layers, each containing a temperature degree of freedom (DOF) through the thickness of the shell at each node. The mechanical shell has six DOF at each node including three for translation and three for rotation in the global coordinate system. The work presented here shows the initial performance of the thermo-mechanical shell element capable of this coupled temperature-displacement analysis implemented as a user-defined element in Abaqus. Examples for various heating cases are presented with an emphasis on expansion to include more complicated heating scenarios in future work.
The Effect of Orthogonal and Radial Layouts of Shear Studs on Shear Behavior of Reinforced Concrete Slab-Column Connections

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Headed Shear Studs can increase shear capacity of reinforced concrete slab-column connections. There are two layouts in which the studs are often installed in the portion of slab around the column, orthogonal and radial. While the radial layout is suggested in Europe, the orthogonal layout is preferred by construction practice in the North America because of its less complicated installation. Few studies concluded that these two layouts were equally effective in providing shear strength to the connections, other experimental research, however, showed that the premature shear failure in the connections, which reinforced with shear studs placed in orthogonal layout, could be due to the large spacing between adjacent stud rails at the corner of the column. This raised red flag have to be studied thoroughly for the sake of public safety. This paper presents an on-going research, in which the effectiveness of the two stud layouts in slab-column connections has been evaluated. The evaluation has also taken into account unbalanced moment transferred at the connections. A three-dimensional finite element model has been developed in Abaqus to model slab-column connections. The 8 nodes continuum solid elements are used to model concrete and the 2 nodes truss elements represent rebars and shear studs. An extensive experiment consisted of 10 full scale reinforced concrete slab-column connections has been also conducting. The preliminary result from the finite element model shows that the model is capable of modeling reinforced concrete slab-column connections, and shear strength of the connections can be increased by shear studs.
Ground Motion Measurements near Impact Pile Driving

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Driving piles for foundation support is a common method used in the civil engineering field. Pile installation is a complicated, energy intensive process, which induces vibrations into the ground. These vibrations can be transmitted to nearby structures and underground utilities and threaten their integrity and serviceability. Problems of settlement due to pile driving induced vibrations have been experienced recently by the Michigan Department of Transportation (MDOT) during operations associated with replacement of deteriorating bridges. The presented research, which was supported in part by MDOT, attempts to characterize the ground motion field near the driven pile and to quantify the energy transmission from the driven pile to the surrounding soil. This is achieved by performing field vibration measurements at ongoing MDOT pile-driving project sites. The conventional practice for monitoring vibrations is by placing surface sensors on the ground at various distances from the center of the driven pile. For this project we were able, for the first time, to collect vibration measurements at various depths from the surface (up to 35ft deep) and at various distances from the driven pile (up to 0.5ft from the pile) by installing sacrificial sensors in the ground. The field testing setup and data will be presented and outcomes from the data analyses will be discussed.
Experimental Assessment of Post-Liquefaction Behavior of Gravelly Soils

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Soil softening and soil liquefaction have long been a significant aspect of seismic risk, including at sites with gravelly soils. However, the performance of gravelly soils during and after earthquake events is still not fully understood. A prototype large-scale Cyclic Simple Shear (CSS) device is utilized in this research to perform monotonic and cyclic shear tests of gravelly soils to evaluate the susceptibility of these materials to liquefaction during earthquake events. Post-liquefaction strength, which is a key input parameter in analysis of post-liquefaction stability, is also evaluated. Shear wave velocity is measured for each specimen by a custom-built bender element system, and will be used to correlate the laboratory results with field conditions. The influence of particle morphology on the gravelly soil shear behavior will also be evaluated using a custom-made device that rapidly determines the size and shape distributions of large specimens of coarse sands and gravels from a digital photograph (Translucent Segregation Table). Three gravelly soils (Pea Gravel, Limestone, and Natural Stone) with different particle sizes and gradations are tested. Preliminary relationships of undrained shear strength and shear wave velocity are presented.
Assessing the Impact of High Volume Groundwater Withdrawals on Headwater Streams

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Use of high volume hydraulic fracturing to extract natural gas from shale formations often requires consumption of several million gallons of freshwater over a short time period. Groundwater is a common source of freshwater for this activity and these intense withdrawals may negatively impact flow in groundwater-fed streams. The State of Michigan currently uses a Water Withdrawal Assessment Tool (WWAT) as a screening mechanism to assess the impact of high-volume water withdrawal wells associated with hydraulic fracturing activities on nearby streams. This tool was not originally designed to evaluate transient high-volume water withdrawal activities and as a result it may not accurately capture stream-groundwater interactions during these industrial water withdrawals. In this study, we developed a high-resolution groundwater flow model to investigate scenarios where these groundwater withdrawals occur in the vicinity of headwater streams. The study area is in Michigan’s northern Lower Peninsula where sandy glacial till is the dominant aquifer lithology and headwater streams are primarily groundwater-fed. The Michigan Department of Environmental Quality has recently approved several high-volume water withdrawal wells associated with hydraulic fracturing activities in this area. This study examines stream-groundwater interactions in the area under transient pumping conditions similar to those expected during the withdrawals and assesses the influence of well distance from the stream, withdrawal well density, pumping rate, and aquifer heterogeneity on base flow reductions to the Black Creek. The results will then be compared to those of WWAT to assess the adequacy of WWAT in screening hydraulic fracturing water wells in Michigan.
Numerical Modeling of Steel-Concrete Composite Floor Systems under Elevated Temperatures.

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In this study, a three-dimensional finite-element (FE) model of a steel-concrete composite floor system subjected to fire is developed using the commercial modeling package ABAQUS. The numerical model is based on the Cardington fire tests, which were a series of full-scale structural fire tests undertaken on an 8-story composite steel framed building from 1995 to 1996 at Cardington, Bedfordshire, UK. The model is validated against experimental data from Test 3 of the Cardington fire test series. The FE model presented here represents a highly non-linear problem with very large structural deflections and distortions, thus, issues arise from the ability of the implicit static solver in ABAQUS/Standard to converge to a solution when computing nodal displacements. The study found that ABAQUS is capable of capturing the highly non-linear response of steel-concrete composite floor systems under a fully developed fire, with some modifications of the concrete constitutive relations required to overcome undesirable numerical instabilities. A discussion of the possible reasons for these instabilities, as well as potential methods to overcome numerical instabilities are offered. Additionally, modeling details and the approach taken to construct the numerical model are provided, and a brief description of the subsequent usage of this model to study the structural response of these composite floor systems under traveling fires is given.
Dynamic Fatigue Model for Assessing Muscle Fatigue During Construction Tasks

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Due to physically demanding construction tasks, workers frequently suffer from muscle fatigue that may result in productivity loss, human errors, and injuries. Although previous research efforts quantified muscle fatigue using surveys, instrument, and mathematical models, these approaches may not be able to assess muscle fatigue prior to work under real condition due to the subjectivity of surveys, invasiveness in instrumental methods, and difficulties on reflecting dynamic workloads in mathematical models. To address these issues, we propose a dynamic fatigue model with computer simulation approaches, such as System Dynamics (SD) and Discrete Event Simulation (DES), to estimate localized muscle fatigue during occupational tasks. Specifically, SD, a differential equation-based continuous simulation, models physiological responses and feedback in muscle fatigue generation and recovery. Also, we use DES to represent workloads of tasks and time intervals of a worker’s force exertion and release (e.g., idling and resting time). As a result, workers muscle fatigue can be estimated prior to work integrating workloads and its time intervals.

The proposed model was validated comparing with existing models. In addition, experimental validation was conducted by measuring endurance times, one measurement of muscle fatigue, from subjects under the protocols that mimic construction tasks. The results show that the model provides robust estimation comparing to the results from existing models through Normalized Root-Mean-Square Deviation (NRMSD) measured from 0.2 to 0.68. Further, the model can be used to evaluate workers’ muscle fatigue prior to works and adjust schedule or demand to reduce the undesirable consequences from muscle fatigue.
On-Site Biomechanical Analysis During Construction Manual Tasks to Understand The Risk of Work-Related Musculoskeletal Disorders

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In the labor-intensive construction industry, workers are frequently exposed to manual handling tasks involving forceful exertion and awkward postures. As a result, construction workers are at about a 50 percent higher risk of work-related musculoskeletal disorders (WMSDs) than workers in other industries. A biomechanical analysis is one of the widely used methods to evaluate ergonomic stresses during occupational tasks. However, the use of biomechanical analysis has been limited in only laboratory experiments due to the difficulty of collecting motion and external force data required for biomechanical models under real construction. To reflect postural variations during construction tasks, an effective and practical means that enable us to conduct a biomechanical analysis is inevitable. To address this issue, we propose an on-site biomechanical analysis for construction manual tasks by combining vision-based motion capture and force estimation. Specifically, the vision-based motion capture extracts skeleton-based motion data from images while force estimation predicts external forces acting on hands and feet during performing tasks. These approaches provide non-invasive measures of motion and force data without interfering workers’ on-going tasks. To test the feasibility of the proposed methods, we conducted case studies on masonry works and ladder climbing activities. As a result, we found that the method has potential to broaden our understanding of the causes of WMSDs by estimating musculoskeletal stresses during construction manual tasks without any invasive measures. Ultimately, the method helps to evaluate physical demands, which allows practitioners to identify effective interventions to reduce detrimental results caused by excessive demands beyond workers’ capability.
A flush clamp is a unique connection that is used in U.S. automotive plants to hang conveyor platforms from the facility’s roof trusses without bolting or welding to the truss itself. The connection consists of two plates that are bolted to the member to be supported and bear on the bottom flange of the bottom chord of the truss. There is currently a lack of literature about the behavior of these connections, and no standard design procedure exists. This study seeks to determine critical failure modes for flush clamp connections and lay the groundwork to standardize a safe and efficient design procedure. Laboratory tests are used to consider connections with varied geometry and the effects of cyclic and monotonic loading. The results from these tests are used to develop and validate finite element analyses that can be used for further parametric studies. The data show that commonly used design procedures underestimate the connection strength by as much as 50% and typically assume an incorrect failure mode. A more systematic analysis of each connection component will produce a more accurate and efficient design. New installations of these connections are frequent, and reducing the level of conservatism in design can have a significant impact on material and fabrication costs.
Multi-scale Numerical Investigation of Time Effects in Sand

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Sands have been reported to experience changes in penetration resistance, small strain stiffness, and liquefaction resistance over time under sustained loads. These phenomena are particularly distinct after disturbances, such as dynamic in-situ compaction. A hypothesis of static fatigue indicates delayed fracturing of micro-morphological features at inter-granular contacts as a key cause of the time-dependent effects in sands. The micromechanical evolution of grain surfaces at contacts was studied using discrete element method (DEM) simulations. Grains were simulated as sets of multi-bodies joined by bonds described by the parallel-bond stress corrosion model (PSC), capable of simulating the time-dependent stress corrosion process of sand grains. This process is central to static fatigue of asperities at inter-granular contacts. Numerical loading tests and static fatigue tests of a single contact were simulated. A single inter-granular contact comprises of many sub-contacts or contact “points”, with a number of sub-contacts increasing during grain convergence. Contact stiffness and friction were shown to increase during static fatigue. Biaxial tests on a model of a sand grain assembly were then conducted, with different contact stiffness and friction. The results are consistent with the static-fatigue hypothesis.
Finite Element Study on Performance of Innovative HSS-to-HSS Moment Connections

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Abstract: Seismic steel moment frames can effectively resist lateral force and dissipate input energy by forming plastic hinges in the beams and allowing moderate deformation in their panel zone. Although the majority of current moment frames utilize wide flange beams and columns or hollow structural sections (HSS) columns with wide flange beams, there is interest in developing alternative connection-HSS based moment connections. Based on previous experimental tests, if properly detailed, HSS-to-HSS connections can achieve a stable hysteretic behavior with plastic hinging in the beam. This behavior satisfies current strong column-weak beam requirements. In this study, innovative HSS-based collar connections are considered. These connections consist of two steel collars that are slipped over the column member and the beam endplate to connect the beam to the column. To investigate the force transfer mechanism and size effects of the collar and beam endplate on column face plastification, a parametric study using finite element analysis is performed. Based on the performance of the connections, the feasibility and detailing requirements for use in seismic areas is ascertained.
Ductile Spray-applied Fire-resistive Material for Enhanced Fire Safety of Steel Structures

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Spray-applied fire-resistive material (SFRM) is one of the most widely used passive fire protection material in North America. However, SFRM is inherently brittle and tends to dislodge or delaminate under extreme loading conditions (earthquakes or impacts) and even under normal service conditions such as wind induced building movement. Such loss of fire protection material puts the steel structure in great danger under fire loading, especially under multi hazards (post-earthquake or post-impact fires). As an alternative to conventional brittle cementitious material, engineered cementitious composites (ECC) is a family of high performance fiber reinforced cementitious composites. ECC typically exhibits strain hardening behavior with very high tensile ductility (3-5%) under static and high rate loading. In this study, a new spray-applied fire-resistive material that combines the desirable thermal insulation property, ease of construction (facilitated by sprayability), lightweightness of SFRM and the enhanced ductility of ECC is developed as an alternative material to current SFRM through a parallel design process. The newly developed spray-applied fire-resistive ECC (SFR-ECC) exhibits density as low as 550 kg/m3 yet with tensile strength, tensile strain capacity and interfacial adhesion (to structural steel) of 1~2 orders of magnitude higher than those of conventional SFRMs. The tensile strength, tensile ductility and adhesion of SFR-ECC were also found to increase as the loading rate increases, ensuring the performance of such material under impact or earthquake loads. SFR-ECC with enhanced mechanical performance is expected to improve the overall fire safety of steel structure under both service and extreme loads.
DEM: Design and Manufacturing
Manufacturing System Design for Resilience

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Unexpected disruptive events always interrupt normal production conditions and cause production loss in manufacturing systems. A resilient system should be designed with the capability to suffer little production loss during the disruption, and settle itself to the steady state quickly after the disruption. In this paper, we define production loss ($PL$), throughput settling time ($TST$), and total underproduction time ($TUT$) as three metrics to measure system resilience, and use these measures to assist the design of multi-stage reconfigurable manufacturing systems. Numerical case studies are conducted to investigate how the system resilience is affected by different design factors, including system configuration, level of redundancy or flexibility, and buffer capacities.
Electrochemical discharge assisted micro-machining of non-conducting brittle material

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The desirable physical and mechanical properties and poor machinability of glass have driven many studies towards glass machining. Electrochemical discharge machining (ECDM), also known as spark-assisted chemical engraving (SACE) or electrochemical spark machining (ECSM), is a non-conventional machining technology that has shown potential in machining non-conducting brittle material. This research is intended to develop a micro-milling technology on non-conducting material under the name “electrochemical discharge assisted micro-milling”. It is a hybrid machining process combining electrochemical discharge machining (ECDM) and mechanical milling. Such hybrid machining process significantly increases the rate of material removal, especially in deep hole drilling and milling processes. Material removal mechanism in drilling process was investigated from both experimental and simulation approach, revealing the reason behind the restrictions in conventional ECDM and the merits of hybrid drilling. The research dedicates to comprehensive and fundamental studies of the proposed micro-end-milling process, including investigation of discharging activity and cutting force, tool design and optimization, and complex geometry fabrication.
Electrically assisted friction stir welding for joining dissimilar Al 6061 to TRIP steel

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Multi-material structure is an efficient solution for vehicle weight reduction in automotive industry. One of the typical desirable pairs is aluminum alloy and advanced high strength steel, which is hardly achievable using traditional fusion welding techniques due to their great differences in physical properties as well as the formation of brittle intermetallic compounds (IMC). As a solid state welding process, Friction stir welding (FSW) shows its superiority and our initial results showed that joint strength of 85% of the base aluminum alloy can be obtained under appropriate combination of process parameters. However, the associated large welding force during FSW results in severe tool wear and requires a high stiffness equipment. Besides, the processing window for achieving satisfactory joint is narrow. Electro-plastic effect, which describes the material softening phenomenon during plastic deformation induced by high density current, is therefore considered to facilitate material flow during FSW, especially for steel. This study first designed and manufactured an electrically assisted FSW testbed. Welding force can be shown to be effectively reduced under various process conditions. Micro-interlock features can be observed at Al-Fe interface, which is conceivably beneficial for enhancing joint quality.
Blast/Impact Frequency Tuning and Mitigation

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Blast-born Traumatic Brain Injury (TBI) is the signature injury in the current US military conflicts resulting from being near an explosion in despite of wearing Advanced Combat Helmet (ACH). Similarly, Mild Traumatic Brain Injury (MTBI), known as concussion, is a serious injury resulting from impact in most contact sports, including professional football. Both injuries manifest several physical, psychological and cognitive symptoms. Therefore, there is an urgent need to reconsider helmets’ designs. The challenge is to understand first the mechanics of brain injuries due to blast/impact and second the mechanics of how to mitigate effectively the damaging features of blast/impact using dissipative materials. In this PhD research, we focused on this challenge: First, using a simple dynamic model of the head subjected to blast/impact, we identified the damaging features of the blast/impact causing stress (acceleration) on the brain; second, we introduced a novel design concept called “blast/impact frequency tuning and mitigation”. This design involves a multilayered structure in which the outer layers tune the stress waves to match the critical damping frequency of the inner visco-elastic layer. As the high frequency stress wave travels through this visco-elastic layer, it undergoes multiple loading-unloading cycles which can result in significant energy dissipation over a short duration. This novel design concept improves drastically the performance of the helmets considered as a simple and innovative solution to prevent TBI and concussion. It can also address other brain injuries occurred as a result of vehicle crashes and accidents in skateboarding, hockey, baseball, biking and firefighting.
Refreshing Refreshable Braille Displays

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The availability of digital resources for the blind via text-to-speech technology has given them long-sought independence for educational and recreational reading. Using text-to-speech however does not promote a deep understanding of material. Therefore blind readers often prefer hard-copy braille or electronic braille displays. Hard-copy braille is following the same trend as written text, rapidly moving toward electronic distribution, so electronic braille displays are fast becoming the only option for access to braille text. But these displays are expensive due to the high cost of the piezoelectric-based braille cells (single characters) within. The search is on therefore for a low-cost braille display device. Many solutions have been proposed, some of which reduce the cost by limiting the number of characters displayed, even down to a single cell. In this paper, we demonstrate that reducing the tactile cues during braille reading results in a decrease in accuracy for a letter recognition task. In particular, we show that continuous slip between the skin and the reading surface improves letter recognition and further, that the improvement is magnified at faster reading speeds. Our findings suggest that single cell braille displays with no sliding contact are less effective for braille reading.
EBS: Engineering in Biological Systems
Development of Hemocompatible Polymeric Nanoparticles for Advanced Prostate Treatment

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Conventional micelles exhibit rapid release of the loaded cargo in the systemic circulation before reaching the target organs, which diminish their therapeutic value. Furthermore, the carrier should be nontoxic, non-immunogenic, and biodegradable. To address these limitations, we synthesized an amphiphilic triblock copolymer, poly(ethylene)-b-poly(acrylic acid)-b-poly(methyl methacrylate), which self-assembles in aqueous medium forming nano-sized micelles that can encapsulate Cabazitaxel (CTX) in the hydrophobic core. Cross linkage of the PAA blocks using an acetal linker forms an acid-labile shell, which stabilizes the formed micelles at physiologic pH but allows selective release of the loaded cargo in acidic environments such as the tumor tissue or acidic intracellular compartments like the endosome/lysosome. Due to nano-sized particles and PEG brushes, the particles do not interact with blood components. Meanwhile, the encapsulated model drugs Nile Red (NR) and CTX were significantly arrested in SCLM (shell-cross-linked micelles) at pH 7.4 with minimal burst release, while they are gradually released in acidic pH, as compared to NSCLM (non-shell-cross-linked micelles) and SCLM at pH 5.0. Moreover, CTX loaded NSCL and SCL100 had lower IC50 values, (2.66 nMs) than free CTX (3.3 nM). More importantly, the therapeutic effect of CTX loaded SCL50 is statistically different than free CTX. Furthermore, we did not observe BSA protein absorption on the particle surface comparing to G5 particles. The particles did not exhibit any hemolytic activity on red blood cells comparing to Triton-X100. The increased retention time of the particles augment the contact probability with the coagulation system. Hence, we further examined our micelles coagulation effect on platelet cells. Our particles did not show any coagulate effect on the platelet cells but the platelet activators coagulated the cells around 30%. Thus these results indicate that pH-sensitive, CTX-SCLM can potentially achieve tunable CTX release in tumor lesion, which can selectively kill tumor cells while limiting systemic side effects.
Fluorescence-activated Droplet Sorting System for Improving Enantioselectivity of Esterase towards Profens

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Protein engineering is the emerging biotechnology to develop useful and valuable proteins, and has shown remarkable promise in the last few years. Directed evolution has been proved as a powerful tool for the engineering of enzymes. However, the traditional screening platforms, based on monitoring mutant activity on agar plates or in microtiter plates, are suffered from relatively low throughput ($10^3$~$10^5$/d) and laborious. Using microfluidic droplets with perfect uniformity and combining them with on-chip detection and sorting, the highly integrated and automatic FADS system will bring great revolution for ultrahigh throughput screening of enzyme. In this work, we developed an on-chip multi-color fluorescence-activated droplet sorting (MC-FADS) system with high screening throughput (>1000/sec) and sensitivity (100ng/ml) for droplets of 12 pL in volume. By incorporating a microfluidic multi-color screening device, this system can provide a means to preferentially isolate droplets emitting fluorescent light of desired color. The use of this system for enzyme directed evolution combined with emulsion droplet assay permits isolation of one enantiomer of a chiral enzymatic product with high selectivity. The system will serve as a general tool for ultrahigh throughput multi-species screening of enzyme.
Intracortical Neural Probes with Self-Deployed Electrodes

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Motor neuroprosthetics aid paraplegic patients regaining independence by controlling artificial limbs with signals recorded from the brain. Clinical pilot studies on these devices are presently being employed. A key requirement for control of motor neuroprosthetics is the ability to record brain activity of freely behaving patients accurately enough to distinguish action potentials of single neurons. To date, only neural probes implanted into the brain can provide the required specificity. However, the high spatial resolution of these neural probes comes at the cost of a high degree of invasiveness; the host immune response inhibits recording over a patient’s lifetime.

This project pursues two technologies to mitigate the immune response to implanted neural probes and its impact on their performance. The developed neural probes consist of silicon or Parylene formed into millimeter-long, needle-like shanks with multiple microelectrodes. Following the first technology, individual electrodes are placed at the end of very fine and flexible needle extensions, supported by the shank. Before implantation the needles are locked into a protected position close to the shank using a starch based hydrogel. After implantation they slowly and gradually deploy away from the shank into healthy tissue, where they act like satellites, floating almost freely inside the brain tissue. This is expected to greatly extend their working life. A second technology uses Parylene, a flexible and biocompatible polymer. It allows improving the insertion of Parylene probe shanks by formation of sharp tips and mechanical robustness enhancement without significantly increasing its size.

This work was funded, in part, by the DARPA Hybrid Insect MEMS program under grant # N66001-07-1-2006. Portions of this work were performed in the University of Michigan’s Lurie Nanofabrication Facility.
Virus-like Capsules from Iron Sulfide Nanoparticles

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Nanoparticles synthetized from various materials have become effective tools in biological cargo delivery. However, cytotoxicity and biocompatibility of these particles remains important challenges in their applications. In order to address these challenges, we synthetized iron sulfide nanoparticles which can form virus-like capsules. Synthesis was performed in DI water at room temperature. At these conditions, we obtained uniformly distributed ~100nm size in diameter iron sulfide capsules according to transmission electron microscopy images and dynamic light scattering analysis. These capsules have strong potentials to be used in biomedical applications due to natural origin of iron sulfide. Studies have shown that iron metabolism occurs in the human body through multiple pathways including crucial role of iron-sulfur clusters in mitochondrial electron transport system. Additional advantages of using iron sulfide nanoparticles are potential low price and high availability compared to many other nanocarriers.

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Investigating reconstituted actin networks in cell-like vesicles

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The role of actin-regulatory proteins in governing the mechanical properties of actin networks have been studied over the past decade in order to gain a better understanding of the mechanical behaviors of different actin networks. These mechanical studies have been overwhelmingly conducted on actin networks in bulk solution. The recent advancement of droplet microfluidics technology has enabled us to encapsulate actin monomers/filaments and actin network components in lipid vesicles. With this development, advanced investigations on the spatial confinement of actin networks and lipid-membrane interactions become possible in cell-like environments. In our lab, using a glass capillary microfluidic device, we encapsulated various actin-network components inside double emulsions with ultra-thin volatile middle oil phase. After oil evaporation, lipid bilayer vesicles with different actin structures were formed. In addition, we recently developed a microfluidic pipette array device (\textmu FPA), which is able to trap and apply pressure difference on vesicles in designated aspiration arrays. By examining the protrusion length of vesicles into the micropipette under an optical microscope, various mechanical properties can be quantitatively determined, such as the cortical tension and Young’s modulus. This versatile platform allows us to study mechanical properties of the actin-membrane network under the interactions of different actin-regulatory proteins.
Elucidating Vaginal Microbial Interactions through High-Throughput Microfluidic Co-cultivation

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There is increasing evidence which suggests microbial communities of the human vagina, or the vaginal microbiome, play fundamental roles in women’s health and disease. For instance, Bacterial Vaginosis, is the most common vaginal infection in women of reproductive age in the United States and is caused by disturbances in the vaginal microbiome. However, the fundamental question of how the diverse microorganisms interact with one another and with their host functionally remains largely unanswered. The proposed research plan is to investigate microbial interactions of the vaginal microbiome using co-cultivation in microfluidic droplets. Ongoing work includes development of cultivation protocol and fluorescent labeling of Lactobacillus iners, a key member of the vaginal microbiome. Future research will be conducted to develop a droplet co-cultivation and analysis platform for elucidating the complex microbial interactions of the vaginal microbiome, which will have important implications for diagnosing and improving women’s health.
Surface-templated hydrogel patterns prompt matrix-dependent migration of breast cancer cells towards chemokine-secreting cells.

**Taisuke Kojima**<sup>1,3</sup>, **Christopher Moraes**<sup>2,3</sup>, **Stephen P. Cavnar**<sup>2,3</sup>, **Gary D. Luker**<sup>2,4,5*</sup> and **Shuichi Takayama**<sup>1,2,3*</sup>

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This poster describes a novel technique to fabricate spatially-defined cell-laden collagen hydrogels, using patterned, non-adhesive polyacrylamide-coated polydimethylsiloxane (PDMS) surfaces as a template. Precisely patterned embedded co-cultures of breast cancer cells and chemokine-producing cells generated with this technique, revealed matrix- and chemokine isoform-dependent migration of cancer cells. CXCL12 chemokine-secreting cells induce significantly more chemotaxis of cancer cells when the 3D extracellular matrix includes components that bind the secreted CXCL12 chemokines. Experimental observations using cells that secrete CXCL12 isoforms with different matrix affinities together with computational simulations show that stronger ligand-matrix interactions sharpen chemoattractant gradients, leading to increased chemotaxis of the CXCL12 gradient-sensing CXCR4 receptor-expressing (CXCR4+) cells patterned in the hydrogel. These results extend our recent report on CXCL12 isoform-dependent chemotaxis studies from 2D to 3D environments and additionally reveal the important role of extracellular matrix composition. The developed technology is simple, versatile and robust; and as chemoattractant-matrix interactions are common, the methods described here should be broadly applicable for study of physiological migration of many different cell types in response to a variety of chemoattractants.
Development of Targeted, Enzyme-Activated Nano-conjugates for Hepatic Cancer Therapy

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Liver (i.e. hepatic) cancer is currently the 3rd leading cause of cancer-related deaths worldwide, and continues to lack an effective therapy. The current work involves developing a therapeutic drug delivery system targeted to hepatic cancer cells (HCC) that is able to release a loaded drug controllably within those cells. Specifically, a chemotherapeutic agent, doxorubicin (DOX), is conjugated to generation 5 (G5) polyamido-amine (PAMAM) dendrimers via different aromatic azo-linkers that exhibit a controllable release profile of DOX within HCC. We have previously shown that the display of N-acetylgalactosamine (NAcGal) ligands on G5 dendrimers through a poly(ethylene-glycol) (PEG) brush results in selective recognition and internalization of the nanoparticles into HCC via the highly expressed asialoglycoprotein receptor. The present work details the successful synthesis and characterization of NAcGal-PEG-G5-L(x)-DOX nano-conjugates. Further, we have established that the nano-conjugates are able to selectively target and internalize into HCC (e.g. HepG2 and Hep3B cell lines) more efficiently than free DOX controls, via flow cytometry. This internalization correlated with cytotoxicity profiles that show NAcGal-PEG-G5-L(x)-DOX nano-conjugates to have comparably toxic effects towards HCC when compared to the free drug, and this toxicity can be tailored based on the linkage chemistry. These promising results indicate the ability for the nano-conjugates to target and controllably kill hepatic cancer cells, and thus offer significant potential as a novel drug delivery system able to achieve a high local dose of chemotherapeutic agents to tumor tissue \textit{in vivo} for hepatic cancer therapy.
Continuous-flow microfluidic blood cell sorting for unprocessed whole blood using surface-micromachined microfiltration membranes

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White blood cells (WBCs) constitute about 0.1% of the blood cells, yet they play a critical role in innate and adaptive immune responses against pathogenic infections, allergic conditions, and malignancies and thus contain rich information about the immune status of the body [1]. Rapid isolation of WBCs directly from whole blood is a prerequisite for any integrated immunoassay platform designed for examining WBC phenotypes and functions. However, such functionality is still challenging for blood-on-chip systems, as existing microfluidic cell sorting techniques are incapable of efficiently processing unprocessed whole blood on chip with concurrent high throughput and cell purity [2-4].

Herein we report a microfluidic chip for continuous-flow isolation and sorting of WBCs from whole blood with high throughput and separation efficiency. The microfluidic cell sorting chip leveraged the crossflow filtration scheme in conjunction with a high-porosity poly(dimethylsiloxane) (PDMS) microfiltration membrane (PMM). Wafer-scale fabrication of 1 cm × 1 cm PMMs with 4 µm pores and 10% porosity was achieved using our novel surface micromachining strategy [5]. The microfluidic chip realizes separation by using a crossflow that is perpendicular to the PMM to push undesired red blood cells (RBCs) to pass across the PMM and a continuous tangential main flow to carry away WBCs.

We validated the separation performance of the microfluidic cell sorting chip using two different sized microbeads with diameters of 3 µm (yellow) and 11 µm (blue), respectively. Fluorescent microscopic images illustrated the separation of microbeads under \(v_{\text{sample}} = 2 \text{ mL hr}^{-1}\) and \(v_{\text{sheath}} = 4 \text{ mL hr}^{-1}\). Before separation, the microbead mixture contained an equal amount of 3 µm (yellow) and 11 µm (blue) beads. After separation, 97.3 ± 0.5% of 3 µm microbeads were removed from the solution collected at the top outlet, whereas 96.9 ± 0.4% of 11 µm microbeads remained. We further examined the effect of \(v_{\text{sample}} \) and \(v_{\text{sheath}}\) on the separation of microbeads, and found that the flow rate ratio, \(v_{\text{sample}} / v_{\text{sheath}}\), rather than the magnitude of the flow rate, mainly determined the separation efficiency.

We further applied the microfluidic cell sorting chip for separation of WBCs from unprocessed porcine whole blood. Blood cells (including both WBCs and RBCs) collected from the top outlet were examined and counted under phase contrast microscopy. WBCs were identified by their relatively larger size compared to RBCs. With a sample throughput of 1 mL hr\(^{-1}\), which was 270 times greater than those demonstrated previously using microfluidic filtration devices [4], the microfluidic cell sorting chip could recover 27.4 ± 4.9% WBCs with a purity of 93.5 ± 0.5% . We conducted cell viability assays for WBCs before and after separation, with data showing that microfluidic cell sorting had no significant effect on WBC viability. By virtue of its separation efficiency, ease of sample recovery, and high throughput enabled by its continuous-flow operation, the microfluidic cell sorting chip holds great promise as an upstream component for blood sample preparation and analysis in integrated blood-on-chip systems.

References
Engineering *Escherichia coli* specialist strains for optimal co-culture enabled production of cellulosic isobutanol

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Use of synthetic microbial consortia can help to address some of the limitations of monoculture bioprocessing, including high metabolic burden on the cells and the need to optimize multiple pathways or functions in the same species. Design of synthetic microbial consortia, however, brings the challenge of identifying or engineering strains that can perform optimally within a mixed population. Previous study has shown that a mixed culture of *Trichoderma reesei* and *Escherichia coli* can co-exist stably and directly convert cellulose to isobutanol, a promising biofuel candidate [1]. However, isobutanol yield and titer will need to be increased for the process to be economically viable on an industrial scale. The increase in byproduct levels compared to monoculture fermentations and the instability of the plasmids encoding the isobutanol production pathway indicate that there is considerable room for improvement of the *E. coli* for function in the co-culture. Here I describe my ongoing work and future plans to develop *E. coli* strains that are better suited to isobutanol production when co-cultured with *T. reesei* on a lignocellulosic carbon source.

Iron Sulfide Nanoparticles for DNA delivery

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Gene therapy has been widely used in treatment a number of complex genetic diseases including cancer types. Efficient delivery of nucleic acids has become a significant barrier in their clinical applications. Nanoparticles incorporated with nucleic acids has emerged as an efficient gene delivery method. We synthetized iron sulfide nanoparticles with DNA from salmon testes in DI water at room temperature and at pH=8-10. We then tested the existence of DNA in UV-Vis spectroscopy by measuring the absorbance at 260nm and characterized the nanoparticles under transmission electron microscopy, scanning Auger microscopy and Auger electron spectroscopy. Our results indicate that synthetized nanoparticles in size of 1-5nm in diameter incorporate with DNA. Since iron sulfide is a natural material, it presumably has low cytotoxicity and high biocompatibility. Therefore, this method can be used as an effective delivery tool in gene therapy.

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Tracking the Transport of Intact DNA in Gene Delivery using FRET Labeled Beacons

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Gene therapy that can potentially diseases such as cystic fibrosis, sickle cell anemia and cancer is limited by the lack of safe and effective delivery agents (vectors). Our limited understanding of how polymer-DNA complexes, termed polyplexes, are internalized into cells, transported to the cell’s nucleus and then translated into functional proteins hinders the development of new vectors. It is well known that gene expression is due to a small fraction of the delivered DNA. A major limitation with present imaging techniques is that they cannot distinguish functional intact DNA from degraded DNA. We use a DNA nucleotide labeled with a dye pair that exhibit Forester Resonance Energy Transfer (FRET). This two color DNA construct emits with greater intensity in the red region when intact and emits with greater intensity in the green region when cleaved. Two color molecular beacon oligonucleotides containing a FRET dye pair are delivered using various polycationic polymers. Flow cytometry and confocal microscopy are used to quantify the intracellular degradation of the beacon.
Bioengineered Hydrogels Support Vascularization In Vitro and In Vivo

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The formation of functional blood vessel networks in engineered or ischemic tissues remains a scientific and clinical hurdle. In this work, a poly(ethylene glycol) (PEG)-based hydrogel system was adapted and utilized to generate vascular networks from encapsulated cells in vitro and in vivo. Hydrogels were formed via a Michael-type addition between vinyl sulfone-modified PEG and cysteine-containing protease-sensitive peptides. Variation of the crosslinking peptide allowed tailoring of the gel degradation rate, while crosslinking density and mechanical properties were tuned by altering gel solids content. Co-encapsulation of endothelial cells and supportive fibroblasts within the gels led to vascular morphogenesis that was robust to changes in crosslinking peptide identity, but attenuated in more crosslinked gels. Cell-laden PEG hydrogels, along with fibrin controls, were delivered intramuscularly to SCID mice after femoral artery ligation. PEG hydrogels supported the formation of perfused vasculature irrespective of crosslinking peptide identity and hydrogel delivery was demonstrated to aid in reperfusion to the ischemic limb. Substantial loss of gel mechanical integrity and vessel regression were evident in fibrin gels, but not the engineered PEG gels, 2 weeks post-implantation. In sum, these findings suggest bioengineered hydrogels hold promise as cell delivery vehicles to support vascularization for applications in tissue engineering and therapeutic angiogenesis.
Injectable Peptide Decorated Functional Nanofibrous Hollow Microspheres to Direct Stem Cell Differentiation and Tissue Regeneration

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Injectable microspheres are attractive cell carriers for tissue repair through minimally invasive procedures. To carry stem cells for tissue regeneration, the microspheres need to present the critical cues in the natural cell microenvironment to properly direct stem cell differentiation. In natural extracellular matrix (ECM), growth factors (GFs) and collagen nanofibers provide critical chemical and physical cues to support and regulate stem cells. However, there have been no reported technologies that integrate synthetic nanofibers and GFs into injectable microspheres. In this study, we synthesized an advanced injectable stem cell carrier, functional nanofibrous hollow microspheres (FNF-HMS), which are comprised entirely of biomimetic nanofibers and can covalently bind GF-mimicking peptides to modulate stem cell differentiation. Two different GF-mimicking peptides, Transforming Growth Factor-β1 mimicking peptide Cytomodulin (CM) and Bone Morphogenetic Protein-2 mimicking peptide P24, were conjugated onto the FNF-HMS to induce, respectively, the chondrogenic and osteogenic differentiation of rabbit bone marrow-derived mesenchymal stem cells (BMSCs). While no existing biomaterials were reported to successfully deliver CM to induce chondrogenesis, the developed FNF-HMS were shown to effectively present CM to BMSCs and successfully induced their chondrogenesis for cartilage formation in both *in vitro* and *in vivo* studies. In addition, P24 was conjugated on the newly developed FNF-HMS and was shown capable of retaining its bioactivity and inducing ectopic bone formation in nude mice. The results demonstrate that the novel FNF-HMS can effectively deliver GF-mimicking peptides to modulate stem cell fate and tissue regeneration.
IVM: Integrated Circuits, VLSI and Microsystems
High-Performance Miniature Inertial Sensors for Non-GPS Navigation

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Timing Units (TUs) and Inertial Measurement Units (IMUs) have been used as central elements of navigation for a variety of mobile engineering systems, including aircraft, missiles, and land and marine vehicles without the need for external references. Miniaturization of IMUs and TUs to chip-size timing and inertial measurement units (TIMUs) has always been desirable because of low manufacturing cost, high durability, low weight, small size, low energy consumption, and compatibility with integrated circuits.

Developing all the necessary components of a chip-scale TIMU in a small volume requires some major redesign of individual components and innovation in integration. There are many difficulties when fabricating the six inertial sensors and a clock simultaneously in a TIMU microsystem. First, there is a tradeoff between area limitation and sensor performance. Second, fabrication of all the vibratory sensors, e.g. gyroscopes and clock, in one package introduces significant dynamic coupling that would certainly affect the overall system performance. Third, environmental effects such as thermal and mechanical shock can damage the TIMU. In this poster, a robust multi-layer design for the TIMU is introduced. Cross coupling between sensors is investigated, and an optimum design for reducing this coupling is proposed. Effects of different physical phenomena such as radiation, atmospheric pressure, thermal stress and mechanical shock on this system are analyzed. Mechanisms that cause energy loss from the resonant devices in this system, such as thermoelastic dissipation, anchor loss, surface loss are also studied.
An 8.7 GHz Temperature-Compensated Gallium Nitride Micromechanical Resonator

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AlGaN/GaN high electron mobility transistors (HEMTs), with high breakdown voltage, high electron mobility and sheet density are promising candidates for high-power applications at RF, microwave, and mm-wave frequencies. The AlGaN/GaN integrated circuit technology can benefit from high-frequency and low-noise GaN oscillators, which can enable a monolithic all-GaN transceiver. In order to realize such oscillators, AlGaN/GaN HEMTs can be integrated with GaN micromechanical resonators as the frequency selecting components. The significantly higher quality factor (Q) of micromechanical resonators as compared to LC tanks results in improved phase noise of the oscillator circuit. In addition to noise performance, oscillators need to be stable in a wide temperature range (e.g., from -40 °C to 85 °C). Temperature compensation techniques have not been shown for GaN resonators to date.

In this work, a GaN bulk acoustic wave (BAW) resonator is presented, showing fourth-order thickness-mode resonance at 8.7 GHz with an extracted quality factor of 330 and a coupling coefficient (kt²) of 0.7%. The resonator is integrated with an AlGaN/GaN HEMT; the integrated resonator/HEMT structure is coated with a silicon dioxide passivation layer. It is shown that the 400 nm thick silicon dioxide layer reduces the temperature coefficient of frequency (TCF) of the GaN resonator from ~ -30 ppm/K to ~ -13 ppm/K. Using thicker oxide, the temperature-induced drift in GaN can be compensated. To study the applicability of the GaN resonator for use in harsh environments, the effects of temperature and input power on its performance are characterized.
Whole-Angle Mode Micromachined Fused-Silica Birdbath Resonator Gyroscope (WA-BRG)

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We present the fused-silica micromachined birdbath resonator gyroscope (µ-BRG) operating in the whole-angle (WA) mode. The key advantages of the whole angle mode operation is rotation angle measurement, large bandwidth, and full-scale range which is needed in detecting the motion of fast-moving objects. The µ-BRG is made with fused silica using a micro blow-torching process and has n=2 wineglass modes at 10.46 kHz with a small frequency mismatch (Δf = 10 Hz) and a decay time (τ) of 2.2 seconds. The WA-BRG achieves a stable angular gain (A_g) and a large full scale range (700 °/s).
Electrostatic Size Selective Nanoparticle Confinement in 2D Nanovoid Array in Aqueous Solution

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Using a combination of size-specific electrostatic interactions in ionic solution and a unique 2D dynamic nano-inscribing (DNI) patterning technique, we have created a single-step methodology to selectively confine and pattern nanoparticles on flexible substrates over a large area. The 2D void pattern coated with Al₂O₃ film will present positive surface charge, generating a sinusoidal electrostatic potential in ionic solution. Once presented oppositely charged nanoparticles, the electrostatic interplay of the surface charges on nanoparticles and the patterned substrate as well as the ionic environment will induce attractive interaction. This electrostatic interplay, as demonstrated in our experiments, can lead to efficient nanoparticles trapping and confinement. And under certain conditions, the confinement shows strong selectivity depending on the relative particle size and geometry of the pattern. A theoretical study of the interaction free energy based on FEA simulations shows that particles with the size selected by the void pattern experience the deepest potential well. Further studies on electrical double layer overlap between the charged particle and patterned surface, show that the difference in free energy arises from ionic redistribution and the associated entropy change. Also, by controlling the feature of the 2D void pattern, its electrostatic potential profile can be tuned to accommodate specificity, trapping and organization. The patterning methodology presented here enables continuous and large scale ‘direct-writing’ of 2D nano-patterns on flexible substrates. The application of single-step, selective, nanoparticle confinement could be extended to selective localization of charged biological objects.
A Generic Oven Control System for Commercial Inertial Sensors

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As the market size of inertial sensors has been increasing significantly, inertial sensors have evolved in their speed, accuracy, size, and power. One of the remaining problems, however, is the degraded accuracy of the inertial sensor due to the change in surrounding temperature, which causes a large bias drift of the inertial sensor. Being able to control the temperature of the inertial sensor is critical to minimize the bias drift and increase the accuracy of the sensor. Using an environment-resistant package (ERP), the proposed generic oven control system stabilizes the temperature of the inertial sensor within tens of m°C stability with the environment temperature ranging from -40°C to 70°C with the rate of the change of 1°C/min. The stabilized temperature decreases the bias drift of the inertial sensor, resulting in more accurate performance. The future plan for the generic oven control system includes the improvement in the temperature stability by reducing possible temperature noise sources, and the integration of the oven control system with the inertial sensors inside the ERP through the application-specific integrated circuit (ASIC) design.
Temperature-Stable Multi-Resonator System for Timing Applications

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There is promise in replacing the large quartz crystals with micromechanical resonators in oscillators for time reference and timing applications due in great part to their miniaturization and integration capabilities. However, the temperature induced shift in frequency for silicon micromechanical resonators needs to be mitigated across the industrial temperature range of \(-40\) to \(85\)ºC in order to meet target requirements for certain communication applications. This work presents a multi-resonator system using MEMS resonators able to produce a frequency output independent from temperature variations.

The multi-resonator clock system is composed of three MEMS oscillators in the Pierce configuration that use piezoelectrically actuated AlN-on-silicon ring resonators as their frequency setting element. Each of these three resonators has a unique second-order temperature dependence of frequency as a result of the introduction of oxide within the resonator body. Due to the nature of the response, the frequency as a function of temperature of the temperature-compensated resonators can be expressed as a second-order polynomial. The individual oscillator output frequencies go through multiplication and mixing in two stages in order to cancel out the linear and parabolic terms of the frequency output. Consequently, the final frequency output using this implementation is a product of temperature-independent constants, thus achieving a temperature-insensitive frequency output across a wide range of temperatures.

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A System for Transdermal Acoustic Energy Transfer using Reverse Electrowetting-on-dielectric by Gas Bubble Oscillation

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Medical implants often have limited battery capacity due to their volume and weight constraints, and thus require frequent recharging of the internal battery. Because wired connection to an implanted device through living tissues is not suitable, various contactless energy transfer (CET) methods have been considered. The most prevalent CET methods, including Electromagnetic (EM) wave-based CET and acoustic energy transfer (AET) using implanted piezoelectric material, have several disadvantages including biocompatibility and may not be suitable for transdermal energy transfer.

We propose a new system that can be used in place of EM-based CET and piezoelectric receiver-based AET systems for transdermal power transfer. Instead of using piezoelectric material on the receiver side, the proposed system uses a biocompatible acoustic-to-electric energy converter based on oscillating gas bubbles, silicon based high-aspect-ratio microfluidic variable capacitor structures, and a simple variable-capacitance-to-voltage conversion circuit. To the best of our knowledge, the system is the one of a kind AET system that does not require piezoelectric material in the receiver side.

We present the results from a preliminary experiment with a prototype of the envisioned device and a theoretical efficiency calculation based on an analytical model for the system. The results show that the theoretical efficiency of the proposed system is not as great as that of a traditional piezoelectric-pair-based AET system. An analysis of the limited efficiency and potential solutions to improve the efficiency of the system are presented.
RF Switching Applications Using Phase Change Material

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Phase Change (PC) materials refer to a class of chalcogenide compounds including germanium antimony telluride (GST) and germanium telluride (GeTe), which have the phase transition properties, showing greatly different resistivity at two states. The state transition between the amorphous (OFF) and crystalline (ON) states is achieved by thermal actuation, and the resistivity is different by several orders of magnitude. In our project, GeTe is chosen as the phase change material used for RF switching applications due to its low crystalline resistivity and high OFF/ON resistance ratio. We have come up with RF ohmic switch designs using GeTe with direct heating and indirect heating schemes. An insertion loss of less than 0.5 dB and isolation above 18 dB up to 20 GHz is achieved. The cut-off frequency based on the figure of merit is 4 THz. A comprehensive non-linearity thermoelectric modeling of the phase change switches has recently been developed further investigate the limiting factors of the power handling capability and enhance the performance. Future work of RF phase change switches will focus on improving the insertion loss and isolation, power handling and switch reliability.
Low-Power Ovenization of Fused Silica Resonators for Temperature-Stable Oscillators

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This work describes a thermally isolated fused silica platform that contains an ovenized fused silica oscillator for use as a timing reference. Microelectromechanical system (MEMS) resonators look to compete with the current market in quartz timing references by offering high quality, batch fabricated resonators at a lower cost and smaller form factor than the commercially available alternatives. Fused silica was chosen as the resonator material due to its excellent thermal and resonant properties, allowing for low power ovenization and high resonator performance. Since all resonant devices experience frequency drift from temperature due to material parameter changes, a method of compensation needs to be implemented to stabilize the device output. In this work, drift is compensated through ovenization by using a platinum resistance temperature detector (RTD) as a feedback mechanism. The RTD resistance shift is sensed from a whetstone bridge and used to power an on-platform heater, which maintains the resonator at a set temperature and therefore stable. The design, modeling, and fabrication of fused silica resonators and oscillators are described. A resonator with quality factors of 16,000 at 4.9 MHz and measured phase noise of $-138 \text{ dBc/Hz}$ at 1 kHz, which meets the requirements for the GSM cell phone standard, is shown. Additionally, the measured results of the entire ovenization system is presented, with an overall reduction in frequency drift from over 9000 ppm to just 11 ppm shown over the temperature range of $-40 ^\circ \text{C}$ to $+65 ^\circ \text{C}$ with a maximum heater power consumption at just 16 mW.
3D Fused Silica Birdbath Resonators with High Q and Long Decay Time Constants

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Fused silica resonators with 3D shell geometries are fabricated using a micro blowtorch method in which thin substrates are softened with a blowtorch and vacuum molded. This versatile technique enables fabrication of different geometries by simply changing the mold shape. The resonant frequency of these wineglass-mode resonators can be easily tuned by adjusting the mold diameter and substrate thickness. Since these resonators are intended for use in a vibratory rate-integrating gyroscope, resonant frequencies around 10 kHz are chosen to minimize sensitivity to lower frequency environmental noise while still achieving a long decay time constant to maximize bias stability.

These birdbath resonators are driven and read out electrostatically, requiring a thin metal film on the surface for capacitive coupling. We have experimented with different film stacks and also developed a method of laser Doppler vibrometry testing (LDV) of uncoated devices to help understand the effect of the metal film on performance. A metal-coated device with a ring-down time, \( \tau \), of 15.24 s \((Q = 1.19 \text{ million}, f = 10.163 \text{ kHz})\) has been measured electrostatically, while an uncoated device with \( \tau = 43.58 \text{ s} \) \((Q = 1.19 \text{ million}, f = 8.725 \text{ kHz})\) has been measured with LDV. Future work will focus on improving understanding of the energy loss mechanisms that limit the quality factor and systematically addressing them to lengthen the vibratory decay time constants.
Technology for Fabricating Dense 3-D Microstructure Arrays for Biomimetic Hair-Like Sensors

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This project focuses on the design, simulation and fabrication of highly-dense arrays of 3-D high aspect-ratio MEMS structures that can imitate biological hairs. Hair has many unique properties including high aspect ratios, local neural processing, robustness, and multiplicity of functions. A key feature of our arrays is the tall, 3-D structure which allows for spatially efficient integration of traditional MEMS resonators which use a large mass to bend a much smaller spring. The sensors can be combined in series or in parallel and can include local signal processing using underlying CMOS circuitry. Here we implement 2-axis capacitive acceleration sensor arrays. Each sensor consists of a proof mass atop a narrow post. The post acts as mechanical spring and the mass is surrounded by four silicon electrodes for capacitive sensing of deflection. The sensor is fabricated using a silicon-silicon wafer-level integrating microfabrication process. DRIE is used to define the small capacitive gaps while simultaneously etching more deeply to separate neighboring sensors. The device is modeled in COMSOL to maximize sensitivity within the available process windows. After DRIE the wafer is bonded to another silicon wafer which has been prepared with recesses and metal electrodes and routings. By taking advantage of high aspect-ratio DRIE, we have fabricated a new class of dense 3-D MEMS accelerometer arrays which offer improvements in performance and robustness, and can potentially provide multi-sensor functionality.
Vertically Stacked Fused Silica Platform for Inertial Sensing

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This project aims to develop compact, high performance timing and inertial measurement unit composed of fused silica 30X smaller than the volume of a penny. This platform is targeted towards applications where space is limited, yet performance is still desired, such as satellite guidance. The TIMU consists of three single-axis accelerometers and three single-axis gyroscopes along with a clock. Miniaturization is achieved via the bonding of multiple device layers together into a single stack as well as integrated packaging in the stack. Fused silica, high purity amorphous SiO\(_2\), is used as the structural material. Fused silica has several material advantages over silicon. Its electrically and thermally insulating nature allows reduced parasitics and improved thermal stability, while lower thermoelastic damping can lead to higher quality factor resonant devices over traditional silicon. To date, we have demonstrated seven working devices in a package smaller than 13 mm\(^3\) with 60 electrical feedthroughs. Current work focuses on improving device performance, through improved etching and gap narrowing.

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MCT: Material and Chemical Technology
Molecular Dynamics Study of Hydration in Dynamically Polymerized Amorphous Polyimide

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Hydration in polymers is important, as the presence of water influences the structural, electrical, and mechanical properties. Previous studies of the hydration of polyimide have only considered systems of fully polymerized, monodisperse polyimide chains and neglect any possible effects from residual monomers and the intermediate reaction step, poly(amic acid). Atomistic studies of polyimide were conducted using structures generated with dynamic polymerization technique. This technique allows tracking the evolution of the network structure and the effect of hydration as the system evolves.
Relationship between Polyelectrolyte Bulk Complexation and Kinetics of their Layer-by-Layer Assembly

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The effect of pH and salinity on bulk phase behavior and layer-by-layer (LbL) growth kinetics are investigated for oppositely charged polyelectrolytes with the goal of relating phase behavior to LbL growth kinetics. Depending on salinity, pH and mixing ratio, the complex formed in the bulk is either a precipitate or a gel-like coacervate and multilayers grow either linearly or exponentially with deposition time. In addition to primary Coulombic interactions, we observe that polymer-specific interactions have a profound effect on both bulk complexation and LbL growth of the polyelectrolytes. The overall strength of interaction between polyelectrolytes, as indicated by their phase behavior, has a non-monotonic affect on LbL growth rate, because stronger interactions increase the driving force for diffusion, but also reduce the effective diffusion coefficient of a polyelectrolyte molecule through LbL multilayer. As a result, there is little correspondence between coacervation and exponential growth on one hand, and precipitation and linear growth on the other. Salt concentration has a non-monotonic effect on LbL growth at pH 7, with exponential growth found over the range 15-60\% of the critical salt concentration ($C_{S_{C}}$) needed to transition from coacervation to a clear solution in the bulk, regardless of the physical chemistry of polyelectrolytes employed, whereas salt concentrations both below and above this range result in linearly growing films. Finally, we report a “universal curve” for the dependence of LbL growth rate, normalized by its maximum value, against salt concentration, normalized by $C_{S_{C}}$, which could be useful for designing conditions for optimal LbL growth.
Shape Allophiles Improve Entropic Assembly

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Self-assembly of nanoparticles and colloids shows great promise in the creation of new materials. Nature utilizes self-assembly as a powerful tool to organize matter, observed in nearly everything from the bubbles on top of a glass of beer to the assembly of virus capsids. While the use of DNA tethers, chemical functionalization, and external electromagnetic fields have been shown to effectively direct self-assembly, the effect of particle shape on self-assembly has received surprisingly little attention. Nature makes extensive use of shape-based interactions, such as the \textquotedblleft lock-and-key\textquotedblright mechanism of enzymes and protein recognition at the surface of a cell. We investigate a class of \textquotedblleft shape allophiles\textquotedblright that are complementary in nature, similar to puzzle pieces, as a method to stabilize desired phases via an increase in the Directional Entropic Force (DEF). We consider the melting and self-assembly of square-like systems. Through these studies we determine that shape allophiles are useful in obtaining and stabilizing desired phases.

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Crack channeling in non-uniform crack arrays in thin films

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Channel cracking is one of the most common types of failure in brittle thin film subjected to tensile stress. Cracks can propagate in parallel pattern perpendicular to the direction of applied tension; the crack growth rate depends on energy-release rate, intrinsic film properties, and environments. The crack propagated between two preexisting cracks in a triple-layered system with dissimilar materials was studied, which extended earlier analyses where periodic crack pattern was assumed. Finite elements computation shows that for such crack the most dominant factor of energy-release rate is its distance to the nearest neighbor crack, which was experimentally verified on a system with colloidal silica topcoat, acrylic resin mid-layer and polycarbonate substrate. The results of finite elements calculation were also used with experimental observation to construct a graph of how the crack velocity depends on energy-release rate in this system.
Molecular dynamics simulations are performed to compute properties of cured epoxy resins reinforced with carbon nanotubes. The current tools available allow building of energy equilibrated epoxies with cross linking conversion similar to those seen in structural epoxies. These structures can be tested virtually for the purposes of materials selection and design even before synthesis of the polymer. In this presentation, results from molecular dynamics simulations performed on nanotube reinforced cross-linked epoxy matrix will be shown. Simulations are carried out using CVFF force field in LAMMPS. Nanocomposites are created by adding functionalized and non-functionalized carbon nanotubes to the epoxy matrix. We develop means to build simulation cells, perform annealing to reach correct densities and compute thermomechanical properties via molecular dynamics that can be verified with experiments. These simulations allow the effects of the nanotube on the composite system to be isolated in ways not possible with experiments. The nanocomposites reinforced with carbon nanotubes showed improved mechanical properties and lower coefficient of thermal expansion.
Nucleophilic Attack of Organolithium at Tetrahedral Silicon in Alkoxy silanes. An Alternate Pathway

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The currently accepted mechanism for nucleophilic attack at silicon in tetra-alkoxy silanes has been suggested to involve formation of penta- and then hexacoordinated intermediates as supported by the apparent exclusive formation of R₃SiOR and R₄Si from nucleophilic attack by RLi and RMgX. Our recent discovery of a direct route from biogenic silica to tetraalkoxy-spirosiloxanes prompted us to revisit this reaction as a potential route to diverse silicon containing species with single Si-C bonds. To our surprise, reactions of both Si(OEt)₄ and Si(2-methyl-2,4-pentanediolato)₂, SP, with PhLi when run at –78 °C form pentacoordinated Si, e.g. LiPh Si(OEt)₄ and LiPhSP in equilibrium with the starting reagents with no evidence for formation of hexacoordinated species in samples quenched at low temperature with MeI or Me₃SiCl. However, ring open-oligomerized products are observed, and potentially useful for conversion to silsesquioxanes.
Investigating Environmental and Microstructural Effects on Small Fatigue Crack Growth Mechanisms in Ti-6242S

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Many aerospace components originally designed for $10^7$ cycles are exceeding their expected lifetimes and entering the very high cycle fatigue (VHCF) regime. Fatigue lifetime in the VHCF regime is primarily consumed by the cycles needed to initiate and propagate a microstructurally small crack. Although strains are nominally elastic, local cyclic plastic strain accumulation occurs at the micro-scale and drives crack initiation and early crack growth behavior. Furthermore, fatigue crack formation is extremely sensitive to the microstructural landscape and environmental influences. The effects of both microstructure and environment on fatigue damage accumulation mechanisms were investigated in the near alpha titanium alloy, Ti-6242S. An experimental methodology was developed which combines ultrasonic fatigue at 20 kHz, scanning electron microscopy, and Digital Image Correlation (DIC) techniques to study the evolution of full-field strain mappings at the micro-scale. Crack initiation and propagation behavior in relation to microstructural features, such as high angle grain boundaries, was correlated with cyclic strain accumulation as measured by in-situ scanning electron microscopy DIC techniques. The evolution of small-scale strain fields at crack tips and in the microstructural neighborhood of the advancing crack was examined. The influence of environment and the presence of microstructural features on strain localization, crack initiation, and early crack propagation will be discussed.
Predicting Deformation in Magnesium Alloy WE43

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The ideas of Integrated Computation Materials Engineering (ICME) are important for accelerated magnesium development. Materials theory and experimentation are integrally linked, and our experimental work not only validates theoretical models, but it provides essential insight into the mechanical behavior and microstructural phenomena of magnesium that material simulation cannot currently account for independently. By combining scanning electron microscopy with digital image correlation, we are able to quantify deformation and strain at the microstructural level with high accuracy. This gives a thorough description of plastic deformation under monotonic loading to failure, as well as gives insights into ductile failure criteria. Strain evolution has been measured for in-plane tension of magnesium alloy WE43, and statistical tools have been applied to predict plastic strain localization and microvoid formation. Fractography using both secondary and backscatter electron imaging has also been used to describe macroscopic and microscopic failure modes under tensile loading.
Superomniphobic surfaces display contact angles >150° with nearly all liquids. Such a surface has the potential to be self-cleaning, drag reducing, chemical shielding and stain repelling. Not only are these surfaces extremely rare, but the large majority are opaque. To extend the usefulness of liquid-repellant surfaces to applications such as windows, smartphone screens, LCDs or eyeglasses, the surfaces must be transparent. In this work, we design superomniphobic surfaces that are highly transparent while maintaining a contact angle hysteresis of <3° for all tested liquids. The surfaces are fabricated using a facile mold and spray technique. The flow field formed during spray-coating allows for highly controllable particle deposition. Such control facilitates the design of textured surfaces that repel organic solvents, alcohols, oils, acids and aqueous media. Nearly all known liquids simply bead up and roll off the surfaces with little-to-no tilt angle. The surfaces fabricated in this work are the first to maintain a high degree of transparency while allowing low surface tension liquids like ethanol and n-hexadecane to roll off with a contact angle hysteresis of <3°.
Understanding Electronic Band-Edge Properties of GaSbAs/GaAs Nanostructures through k.p theory simulations

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Gallium antimonide (GaSb) nanostructures embedded in gallium arsenide (GaAs) are theorized and have been found experimentally to demonstrate either type-I or type-II band type alignment. The ability of GaSb nanostructures to exhibit two band alignment types makes them versatile in applications such as LEDs, photodetectors, and charge-based memory elements. We present a systematic study of the mechanisms behind the band alignment type in order to understand the underlying physics behind the alignment transition and allow for prediction and optimization of electronic properties. We employ the eight-band k.p method to self-consistently solve the Schrödinger and Poisson equations with a commercially available software package (nextnano) to calculate the band structure including strain and polarization charges. Results obtained for GaSbAs/GaAs quantum wells show both type-I and type-II band alignment depending on strain and composition. Calculated band-edges are compared to published experimental results.
Microstructural Strain Memory and Martensite Ratcheting in Superelastic NiTi Under Low Cycle Fatigue

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When cyclically loaded in tension, superelastic Nickel Titanium (NiTi) undergoes a characteristic shakedown behavior which dramatically changes its hysteretic stress-strain response. As many uses of superelastic NiTi involve cyclic loading, a detailed understanding of the interaction between phase transformation and associated plasticity is necessary to predict the lifetime behavior of NiTi devices. Previous macroscopic studies have dealt with this phenomenon on a bulk material level, but its microstructural origin and small scale analogues remain largely uninvestigated. To that end, low cycle, low strain-rate fatigue tests were performed on superelastic NiTi sheet to examine the local damage and accumulation of plastic deformation that contribute to the evolution of its stress strain response. Local strain measured in situ with Scanning Electron Microscopy Digital Image Correlation (SEM-DIC) was matched with individual microstructural features—such as individual parent grains and grain neighborhoods—measured with Electron Backscatter Diffraction (EBSD). Martensitic transformation associated with superelasticity was inferred from the full-field strain maps captured each load cycle. Special attention was paid to the particular martensite variants and twinning modes that nucleate in the first cycle and their similitude to subsequent martensite transformation. Additionally, cyclic behavior such as martensite retention and ratcheting, strain memory of both martensite and austenite configurations, and damage accumulation are also considered.
Energy Dense Non-Aqueous Redox Flow Batteries by Ligand Functionalization

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A series of chromium and vanadium acetylacetonate (acac) complexes were synthesized and characterized for use in redox flow batteries (RFBs). The acac ligands were functionalized to significantly enhance the complex solubilities in non-aqueous electrolytes. Some of these materials offer a 6-fold improvement in theoretical energy density over those for state-of-the-art aqueous vanadium chemistries. Complexes bearing ligands with ester substituents had solubilities of up to 1.8 M, a significant improvement over other metal complexes that have been considered for non-aqueous RFB applications. While the character of substituents affected the solubility, for most of the complexes, the substituent on the acac ligand did not significantly affect the electrochemical properties. The most promising complexes were then tested in a static charge-discharge cell, and a flow battery prototype at high current densities. The flow cell results for a highly soluble vanadium acac complex yield coulombic efficiencies of ~95%. Overall, this work identified novel non-aqueous RFB chemistries that hold promise for the generation of high energy density RFBs. In addition, the results provide the basis for development of structure-function relationships that could lead to new and better performing energy storage chemistries in the future.
Renewable Hydrocarbons from Catalytic Hydrothermal Treatment of Fatty Acids

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The objective of this proposed research is to use hydrothermal catalytic cracking with zeolite to generate key industrial chemicals, such as benzene, toluene, xylenes, and fuel gas. The experiments will be conducted in aqueous streams rich in fatty acids, because several processes produce precisely this type of stream, and fatty acids can be converted from biomass easily. Zeolite catalysis is applied because these catalysts promote aromatization reactions, and aromatics are our targeted chemical products. This novel method and our initial results have been published in ACS Sustainable Chemistry and Engineering as a cover story. My studies will include further development of the technology, applying it to more industrial scaled continued flow reactor, analysis of reaction mechanism and kinetics.

The research will not only introduce this new method for production of renewable chemicals from fatty acids, but also provide a deeper understanding of the chemical reactions and the catalytic hydrothermal stability. If we could instead use renewable sources to generate chemicals that have a large demand from industry, such as xylenes, which are a bulk material for plastic production, and which we have already found in the initial experiments, it would lead to a renewable, long-term sustainable process trend for chemical production in industry. Additionally, biofuel is considered very expensive; if we could make valuable chemicals as byproducts from the same biomass, it would offset the biofuel cost. Finally, it would help to cut down on GHG emissions from current petroleum-based chemical production practices.
Spatial organization of nanoparticles in thin film copolymer/homopolymer hosts

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Polystyrene-\textit{b}-poly(2-vinylpyridine) (PS-\textit{b}-P2VP) diblock copolymers (BCP) form spherical micelles, wherein each micelle is composed of an inner core of the P2VP-block and an outer corona composed of the PS-block of BCP, in thin film PS homopolymer hosts. The spatial distribution of PS-grafted gold nanoparticles (PS-Au NPs) within this thin film BCP/homopolymer system is characterized by a morphological diagram of the curvature of the Au cores, $1/R_C$, vs. the degree of polymerization $N$ of the grafted PS-chains. The distribution is quantified by five basic regimes, largely dictated by competing entropic and enthalpic intermolecular interactions. The NP distributions range from predominantly residing at external interfaces (free surface and substrate) to primarily locating within the interfacial regions between micelle and the host chains. The phase behavior of PS-Au/BCP/homopolymer (PS) systems is necessarily more intriguing than PS-Au/homopolymer (PS) systems, as the relative roles of specific intermolecular interactions on local NP distributions become more apparent.
Predicting the properties of stem cell culture coatings using a Design of Experiments model

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Surface-initiated Atom Transfer Radical Polymerization (SI-ATRP) is a powerful tool to obtain polymer brushes of the desired chemical composition and thickness. Mathematical models with the ability to predict the properties of the polymer coating obtained through “grafting from” or surface initiated polymerization can complement experimental investigations by zeroing in on the best synthesis conditions to achieve the required attributes. Our study, being the first instance of a Design of Experiments study performed for a “grafting from” process, was employed to understand and predict the gel architecture of a model zwitterionic hydrogel. PMEDSAH (Poly[2-(methacryloyloxy) ethyl dimethyl-(3 sulfopropyl) ammonium hydroxide] serves a synthetic substrate for human embryonic stem cells and has the property of sustaining feeder-free and xeno-free stem cell proliferation. Moreover, the rate of stem cell propagation can be tuned by modifying the gel architecture. Our study was motivated by two objectives. Firstly, we wished to quantify the impact of experimental variables on the molecular weight as well as the self-association behaviour of the zwitterionic polymer chains, as measured by thickness and water contact angle respectively. Secondly, it was desired to develop and validate a predictive model that is capable for capturing both the ATRP reaction kinetics as well as the inter and intra-polymer interactions that determine the gel architecture of the coatings. A factorial design of experiments was implemented and statistically significant main effects and interactions were identified and interpreted. A model that described thickness and contact angle as a function of process variables was developed and validated experimentally.
Study of shear-induced coagulation of spherical colloids for arbitrary flow strength using Brownian dynamics method

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Brownian dynamics simulations are performed to study the binding kinetics in the dilute-sphere limit by considering interactions of two spheres under shear flow across the entire range of Peclet numbers, spanning both perikinetic (diffusion-controlled) and orthokinetic (flow-controlled) coagulation regimes. The dilute regime is attained by carrying out two-sphere simulations in periodic boxes of different sizes and aspect ratios and extrapolating toward the infinite box limit. Effects of particle type (Janus and uniform particles), shear rate, hydrodynamic interactions, and inter-particle potential are explored. We find that rectangular boxes with appropriate aspect ratios overcome a particle “shadow effect” that cannot be overcome with cubic boxes unless huge boxes are used. With rectangular boxes, we obtain converged binding kinetics for the whole Peclet number range, while cubic boxes of increasing size allow converged results only in the absence of flow. Results are computed using both realistic interaction potentials and by replacing the potential with a simple cut off gap distance at which binding is deemed to occur. Results agree with Smoluchowski predictions in the zero- and infinite-shear-rate limits, and with the high-Pe perturbation results of Feke and Schowalter [J. Fluid Mech. 133, 17-35 (1983)] at Peclet numbers above 100. Finally, we compute binding times for anisotropic Janus particles which have both repulsive and attractive faces.
Detection of Aminoglycosides by Regulation of Fluorescent Dye Aggregates on Liposome Surfaces

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Polymer-lipid co-assembled liposomes are attractive sensory materials due to their ease of fabrication, robustness, and compatibility with both traditional and emerging diagnostic platforms. In our newly reported system, cationic Rhodamine 6G (R6G) dye is H-aggregated onto anionic liposomes through electrostatic interactions, resulting in quenched fluorescence emission. In the presence of aminoglycosidic antibiotics, R6G is displaced from liposome surfaces and fluorescence is recovered. Using an array of liposomes each containing a different phospholipid, a unique pattern of fluorescence intensities is obtained in the presence of an aminoglycoside. This fingerprint is used to detect and distinguish aminoglycosides.
New Modeling Framework for Layer-by-Layer Assembly of Oppositely Charged Polyelectrolytes

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Layer-by-Layer (LbL) assembly of oppositely charged polyelectrolytes (PE) involves a complicated set of physical processes. Despite the numerous applications of PE multilayer films (PEM), there is still no quantitative model that describes salient features of this process such as chain complexation, and diffusion of both polyions etc. Previous models are either only thermodynamic in nature or otherwise based on severe assumptions about dynamics and thus fail to predict some of experimentally observed trends. A continuum description of LbL assembly, accounting for PE chain diffusion, complexation and network relaxation is reported here. By formulating the model as a moving boundary problem, the height of the PEM can be continuously tracked over time. PE complexation is incorporated into model by considering the ion pairing reactions whereby repeat units of oppositely charged PEs lose their counterions to join the PEM. Using a combination of Flory-Huggins and Flory-Rehner free energy model and Poisson equation to solve for the electrostatic potential profiles, we observe that diffusion of PE chains even into a neutral PEM network is markedly different from diffusion of neutral polymers into a network. As PE chains diffuse, counterions readjust themselves to minimize the net local charge, but fail to do so completely as they would have to pay a significant entropic penalty. Diffusion of PE chains predominantly driven by the electrostatic field induced by the entropy and instantaneous migration of counterions is characterized by pulse-like PE composition profiles.
Active fractal gels of Janus colloids

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We find that fractal gel networks of polystyrene colloids can be broken up by active motion of Janus colloids that have been incorporated into them. We synthesized Janus particles by electron beam deposition of platinum onto one micron carboxylate modified polystyrene particles. By adding the divalent salt magnesium chloride, an initially stable suspension of Janus colloids and polystyrene colloids, present in equal proportion, underwent aggregation to yield a fractal gel. The Janus colloids were activated by the addition of hydrogen peroxide. Changes in colloidal structure and dynamics were visualized by two channel confocal laser scanning microscopy (CLSM). By means of image analysis, we calculated the mean squared displacement (MSD) and radial distribution functions (RDF) of particles before and after addition of hydrogen peroxide. The MSD confirmed active motion of the synthesized Janus particles, and the RDF demonstrated how the addition of peroxide changed the gel structures by breaking the gel network up into clusters.
Design of heterostructured oxide nanoparticles by liquid-feed flame spray pyrolysis

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A common aim in contemporary materials science is engineering from the bottom-up, combining different materials at nanometer length scales. The combination of materials on the nano-scale often produces materials with unique optical, electronic, or catalytic properties. Liquid-feed flame spray pyrolysis (LF-FSP) is a combustion technique for the production of metal oxide and mixed-metal oxide nanopowders. In LF-FSP, solutions of metalloorganic precursors are dissolved in ethanol, aerosolized with O₂, and combusted, producing metal oxides nanopowders with the exact composition of the starting precursor solution. The nanopowders produced are unaggregated but lightly agglomerated, with typical average particle sizes (APSs) of 15-45 nm. In this study, we produced heterostructured particles in the TiO₂-WO₃ and TiO₂-CuO systems. The TiO₂-WO₃ particles formed in a core-shell structure, and the TiO₂-CuO particles formed multi-phase particles. The TiO₂-WO₃ particles were further reacted with Cu precursor to produce TiO₂-CuWO₄ core-shell particles. These materials were characterized and tested for their photocatalytic activity.
Assemblies of Anisotropic Nanoparticles in Spherical Confinement

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We present results for self-assembled clusters of anisotropic hard particles in spherical confinement, simulated via Monte Carlo. For a variety of particle shapes and number of assembling particles ranging from 2 to 100, we look at assembled cluster structure as a function of the number of constituent particles, and note that at certain “magic numbers” of particles the density of the cluster is markedly higher than that of similar clusters (a phenomenon that is mirrored in clusters of isotropic spheres¹). Our findings serve a dual purpose- on the one hand they represent locally dense assemblies of anisotropic hard particles, and as such are a means through which we can measure the role that local particle packing plays in the self-assembly process. A future study will compare these densest clusters to local structures that are found in the self-assembled bulk phase. On the other hand, as a more immediate application, our results also serve as predictive guidelines for experimentalists. It is now possible to confine nanoparticles and colloids via emulsion droplets, and to form particle clusters by evaporating those droplets². The clusters thus formed may be used for various applications depending on their structure and composition, or as building blocks for larger structures³. These results are initial indicators of the rich variety of symmetry and structure that is possible when building clusters with anisotropic particles.

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²DOI: 10.1126/science.1086189
³DOI: 10.1103/PhysRevLett.103.118303
Investigating the Chemistry of Early Transition-Metal Nitrides/Carbides for Hydrogenation/Dehydrogenation Reactions

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Hydrogenation and dehydrogenation reactions are critical steps in the synthesis and large-scale production of many important chemicals including those in the petrochemical industry. This research aims to investigate the use of early transition-metal carbides and nitrides, a class of catalytic materials, for selective hydrogenation reactions with a focus on understanding the chemistry and reactivity of hydrogen, an important reactant (hydrogenation) and product (dehydrogenation). These materials are interstitial compounds, providing a variety of different binding sites for hydrogen, and have been reported to have properties that are similar to platinum-group metals [1]. A greater fundamental understanding of the chemistry associated with hydrogen and the reaction mechanisms will aid in designing more active and selective systems and may garner more widespread use of this interesting class of materials. In this work, we employ molybdenum nitride (Mo₂N), a highly active interstitial compound, as the catalyst. Mo₂N was found to have two primary sites for hydrogen adsorption. Initial results suggest these two sites arise from a surface site, with hydrogen bound to a terminal surface Mo or N atom, and a subsurface site in which hydrogen intercalates into a tetrahedral or octahedral site. By preferentially populating these hydrogen sites, we were able to directly probe the reactivity of each hydrogen site. The density of one of these sites correlates with the selective hydrogenation of crotonaldehyde to crotyl alcohol.

MTR: Medicine and Translational Research
Peripheral nerves are a promising source for neuroprosthetic control signals, as the information carried downstream of cortex is increasingly functionally selective and thus easier to interpret. However, the clinical viability of current approaches is still hampered by low signal amplitude and interface instability. Here, we address these issues by demonstrating the successful implantation of a Regenerative Peripheral Nerve Interface (RPNI) in a monkey, and the design of a low-power, wireless neural recording system.

The RPNI is constructed by selecting individual nerves at an arbitrary level (e.g. individual fascicles) and suturing them into a small graft of unvascularized, denervated donor muscle. The graft then revascularizes, regenerates, and is reinnervated by the transplanted nerve, acting as a bioamplifier for the efferent action potentials. We transplanted three terminal branches of the median nerve into three separate muscle grafts taken from the same arm. Six months after implantation, we could record a 400-600µVp-p EMG signal from an RPNI. Using EMG power within 100-500Hz we could detect finger flexion with 97% accuracy within 150ms.

To complete the interface, we designed a low-power neural recording system consisting of off-the-shelf components: an Intan bioamplifier and an Atmel microcontroller and wireless transceiver. The system is designed expressly to generate low-bandwidth prosthetic control signals instead of higher-bandwidth research-oriented data. For 16 channels, the system draws only 7.5mW of power.

Together, the RPNI and low-power recording system represent a path towards clinical viability for generating stable, functionally specific prosthetic control signals from peripheral nerves.
Effects of Repeated Deep Brain Stimulation of the Pedunculopontine Tegmental Nucleus on Current Thresholds for Movement-Related Behavioral Responses

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INTRODUCTION: The pedunculopontine nucleus has been used as a target for deep brain stimulation in the treatment of movement disorders. Previous work has shown that stimulation of the pedunculopontine tegmental nucleus can evoke movement-related behavioral responses, including increased exploratory activity and evoked jumping responses in rodents.

METHODS: To assess the effects of PPTg DBS on stimulation evoked behavioral responses, a bipolar electrode was implanted within the left PPTg of each male Wistar rat (n=10) three days prior to beginning stimulation trials. Stimulation was performed in freely moving animals using biphasic stimulation (25 Hz, 100 µsec pulses). Animals were then randomly assigned to one of two treatment groups, the first group to undergo PPN DBS for 6 days (12 hours per day), and the second to serve as a control. On day 10, an assessment of current threshold for evoking behavioral responses was determined.

RESULTS: Analysis of stimulation currents between baseline and post-stimulation utilizing non-parametric one-way ANOVA analysis showed significant differences between DBS and SHAM groups (P< 0.05). DBS animals had an average increase of 322.5 µA (SEM: 130.7 µA) compared to SHAM animals with an average increase of 20 µA (SEM: 11.5 µA) in stimulation current that evoked a behavioral response.

DISCUSSION: DBS animals required greater current stimulation on the final day of stimulation compared to initial stimulation period suggesting that PPN DBS produces an inhibitory effect on measured behavioral endpoints that may be related to synaptic changes within the PPTg or secondary nuclei innervated by PPTg neurons.
Targeted starch nanoparticles for cancer therapy

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Nanoparticles as drug delivery vehicles have been well studied and characterized, and alternatives include polymer-based solutions, liposomes, and core-shell colloidal particles. We developed and characterized starch hydrogel nanoparticles as a targeted drug delivery vehicle using DNA aptamer ligands to deliver the encapsulated drug specifically to cancer cells as a proof-of-concept in vitro study. By using TEMPO-mediated oxidation of the starch hydroxyl moieties we formed carboxyl functionality, allowing for EDC-NHS linking with amine-modified ssDNA aptamers, in particular the guanine-thymine rich nucleolin-targeting aptamer AS1411. With fluorescence and confocal microscopy on HeLa cell-line cultures we demonstrated improved targeting using the aptamer ligand. We further observed high cellular internalization of the particles, suggesting an advantage of the starch carrier vehicle over other delivery systems. Loading doxorubicin into different starch nanogel particle compositions allowed for the effect of hydrogel cross-link density on the drug release profile to be measured. These studies indicated the potential of these particles to better control both the distribution and release of the drug. Last, a cell viability study demonstrated superiority of starch nanoparticles over free doxorubicin, as a cost-effective method of improving chemotherapy treatment.
Data-driven model comparing the effects of glial scarring and interface interactions on chronic neural recordings

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The ability to record single-unit activity with chronically implanted microelectrode arrays is hindered by low recording signal-to-noise ratio (SNR). Low SNR can result from glial scarring or interface interactions stemming from materials failures. The objective of this project is to quantify the effects of glial scarring and interface interactions on electrode impedance and unit amplitude using a data-driven model.

A finite element method (FEM) electric field model with detailed representation of a single Utah array electrode was developed to analyze impedance as a function of encapsulation thickness, encapsulation resistivity, and interface resistivity. Impedance measurements from four Utah arrays implanted in two monkeys for twelve weeks were reconciled with the model. A neuron cable model was then coupled with the FEM model to analyze amplitude as a function of the aforementioned parameters.

From the neural data, two arrays showed a statistically significant change in impedance (p < 0.05) while zero arrays showed a statistically significant change in amplitude. Histology at four months showed a scar thickness of 16 µm.

Impedance increased as a function of encapsulation thickness, encapsulation resistivity, and interface resistivity. Amplitude decreased as a function of encapsulation resistivity and interface resistivity, and increased/decreased as a function of encapsulation thickness depending on whether or not the neuron moved.

Impedance and amplitude were most sensitive to interface resistivity and encapsulation thickness, respectively. While scarring may still lead to inflammation and neuron displacement, our results suggest that large increases in impedance are more easily explained by interface interactions than glial scarring.
Secondary flows enhance mixing in a model of vibration-assisted dialysis

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Hemodialysis is an integral part of treatment for patients with end stage renal disease. While hemodialysis has traditionally been described as a diffusion-dominated process, recent in vitro work has shown that vibration of the dialyzer can enhance the clearance of certain solutes during treatment. We hypothesize that the addition of vibration generates secondary flows in the dialysate compartment. These flows, perpendicular to the longitudinal axis of the dialysis fibers, advect solute away from the fiber walls, thus maintaining a larger concentration gradient and enhancing diffusion. Using the finite element method, we simulated the flow of dialysate through a hexagonally-packed array of cylinders and the transport of solute away from the cylinder walls. The addition of vibration was modeled using sinusoidal body forces of various frequencies and amplitudes. Using the variance of the concentration field as a metric, we found that vibration improves mixing according to a power law dependency on frequency. We will discuss the implications of these computational results on our understanding of the in vitro experiments and propose optimal vibration patterns for improving clearance in dialysis treatments.
Fabrication of Multi-Functional Particles with Controlled Size, Shape, Surfaces, and Release Kinetics for Drug Delivery Applications

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In nature, the hierarchical organization of material has led to the creation of precisely structured entities that range from subcellular components to entire organisms. Within a single mammalian cell, for example, the specific compartmentalization of chemical and biological functions in separate organelles has resulted in more intricate functionalities as compared to less advanced prokaryotic life forms.¹ Inspired by this organization and resultant complexity, our lab has fabricated multicompartmental particles using the electrohydrodynamic co-jetting technique. In these particles, the internal and external architecture of the particles can be precisely controlled to incorporate different materials and unique properties in separate compartments. To date, our lab has focused on the design and engineering of the internal structure of these particles to include stimuli-responsive polymers, therapeutics, imaging agents, catalyzers, as well as other functional materials.² Herein we demonstrate the selective surface decoration of particles composed of three distinct regions using bio-orthogonal modifications. Each of these compartments contains a different functionalized poly-lactide from a library of polymers synthesized in our laboratory. The orthogonal functional groups in the polymers are used for the selective modification of each surface.³ Such particles with unique external geometries and surface patches have implications in several fields including drug delivery, tissue engineering, and self-assembly, a few examples of which will be discussed.

References:

PEN: Power and Energy
High performance vector control of Surface Mount Permanent Magnet machine (SMPM) and real time implementation issues

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Nowadays, electrical vehicle are getting increasing attention. Electrical machines such as Surface-Mount Permanent Magnet machines are used in electric cars because of their high performance and efficiency. Usually speed and current electrical machines are regulated based on Pulse width modulation (PWM). Performance and efficiency of the electrical machines and drives highly depends on the control method, sampling time, controller calculation time. Traditional filed-oriented control is used for current or torque regulation which are unstable at high speed regime implementation. A novel high performance torque controller is developed for torque regulation of the surface permanent machine with capability of working at high-speed regime. Real time implementation issues are investigated. For this aim, a discrete time simulation platform is developed to capture the issues of real time implementation.
Experimental Demand Response Employing Commercial Building HVAC Systems

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Expanding penetration of non-dispatchable renewable resources into the power system generation portfolio is forcing increased reliance on demand-side strategies to achieve generation/load balance. Commercial heating, ventilation, and air conditioning (HVAC) loads are potential candidates for providing such demand response (DR) services, both because the magnitude of the energy they consume is significant, and because this load has inherent temporal flexibility due to the buildings' thermal inertia. Several ancillary services markets have recently opened up participation to DR resources, provided they can satisfy certain performance metrics related to their ability to adjust load in accordance with a broadcasted signal. This work seeks to determine whether a group of collocated commercial buildings can adjust their aggregate HVAC load to track test waveforms and historical data from the PJM RegA regulation control signal. Using a reduced-order controller previously developed for a single ~30,000 m² office building, we conduct experiments to quantify the accuracy and latency of aggregate HVAC load modulation compared to the regulation signal. Additionally, we will seek to determine the penalty of providing this service, in terms of excess energy required compared to a counterfactual baseline. These experiments will help establish whether existing commercial HVAC system architectures are a practical candidate for DR participation.
Polyoxometalate application in Redox Flow Batteries

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Energy has been a key issue in this generation, with various energy resources, such as solar and wind power, being investigated. These renewable energy resources are attractive, but the method of storing the energy is one of the main problems. Redox Flow batteries designed to store energy in the electrolyte can address the energy storage problem. The energy is stored and released through the use of two electrolyte tanks with pumps. Polyoxometalates, with versatile, tunable properties, undergo multielectrons redox reactions which may meet the requirements of high performance Redox Flow Batteries. A high performance Redox Flow Battery should have an active species that undergoes a multi-electron redox reaction, with high solubility and wide cell potential. Therefore polyoxometalates are potential candidate active species in redox flow batteries.

Research conducted to date has focused on the electrochemical characteristics of different combinations of Keggin polyoxometalate ($\text{XM}_n\text{O}_{40}^{n-}$). The goal of the project is to select suitable polyoxometalate species that can be used for Redox Flow Batteries. Based on the preliminary results, metals substituted into the Keggin framework play a key role in altering redox properties of polyoxometalates. The results showed high coulombic efficiency (~90%), which reflected the reversible property of the polyoxometalate redox reaction. New polyoxometalate species and membrane investigation is needed to achieve higher energy density and an energy efficient battery. A flow cell study is planned to be tested to simulate the reaction in the real redox flow battery. We anticipate exciting results for polyoxometalates in redox flow battery applications.
Optimal Power Flow for Large Networks with Storage

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Algorithms for solving the optimal power flow (OPF) problem on large traditional power systems at a single time period are well established. However, there is an increasing need for integrating renewable sources and energy storage into electricity networks. Adding storage devices into networks introduces temporal coupling in the OPF problem, which greatly increases the complexity and size of the problem to be solved over a given optimization horizon. This work focuses on extending an AC-Linear Program (AC-LP) OPF method in two ways. First, non-ideal efficiencies of storage devices are considered. This requires including complementarity conditions to prevent simultaneous charging and discharging of storage devices, which ensures solutions are physically realizable. Second, two formulations of the alternating direction method of multipliers (ADMM) have been applied to decompose the multi-period OPF problem in time. These techniques reduce the size and complexity of the problem that must be solved at each time period in the optimization horizon. These methods have been implemented on networks ranging from 24 to 3000 nodes. The performance of the algorithms is compared in terms of convergence properties and quality/optimality of their respective solutions. The scalability of these methods with regard to both the number of nodes in the system and the number of storage devices added in the network is also assessed.
Gas Pressure Fluctuations about Optimal Steady State caused by Gas-Grid Coupling

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Wind turbines and solar panels introduce uncertainty in electric power generation. Recent downward trends in gas prices have led to increased penetration of gas-fired generators in the power grid. Such generators are often used to respond to fluctuations in renewable generation due to their ability to rapidly adjust their output. As gas-fired generators vary their generation they also vary their gas consumption, inducing fluctuations in the gas network. A perturbative solution to gas network flow dynamics is presented which determines the asymptotic distribution of pressure fluctuations about the steady state. The steady state operating point is chosen to be the configuration which minimizes the total cost of operation of the gas network. In the United States, sources of gas are often separated by hundreds of miles from large loads. Gas pressure falls with distance, so to prevent it from dropping too low it is necessary to install compressor stations, which locally boost the pressure. The primary operational cost in these networks is associated with the use of the compressor stations. The goal for the steady state is to minimize the total cost of compression while still maintaining feasible pressures. Previous work has been successful in solving for an optimal steady state on tree networks, and analyzing the pressure fluctuations about that steady state. Results are discussed for the Transco gas pipeline which extends from the Gulf of Mexico to New England. Current work to obtain approximate solutions for general networks will be presented.
Energy Cycling and Efficiency Improvement for Electrical Ship Propulsion Systems with Hybrid Energy Storage

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Shipboard electric propulsion systems experience large power and torque fluctuations on their drive shaft due to propeller rotational motions and waves. This research seeks new solutions to address the fluctuations by integrating a hybrid energy storage system (HESS) and exploring coordinated power management. An electrical ship propulsion system with the propeller and ship dynamics model, which captures the underlying physical behavior, is established to support the control development and system optimization. Given the fact that both high and low frequency contents exist in the power fluctuations, a combination of battery pack and ultra-capacitor bank is proposed. A model-based analysis is performed to evaluate the interactions of the multiple power sources when a hybrid energy storage system is introduced. To evaluate the benefits and limitations of different control strategies, a comparative study is performed in different sea conditions, and results show that the integrated energy management system strategy has advantages over other strategies in terms of many of the performance metrics. In the future, the flywheel system will be considered in this study. Our ultimate goal is to develop optimal system integration strategies and control solutions for electric drive systems with hybrid energy storage, and establish their feasibility and effectiveness through model-based analysis and experimental demonstration. Towards this goal, a combined analytical and experimental research will be pursued. The test-bed which is current under construction will be leverage for algorithm validation and verification. Optimization-based control design framework and the associated numerical challenges will be address.
Instanton Analysis: Understanding Wind-related Transmission Grid Vulnerability

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The prevalence of renewables in modern transmission networks has researchers and system operators asking: What happens when the wind changes, and could fluctuations harm the grid? The instanton problem formalizes this question. Although small changes in wind are typically harmless, it is possible for certain patterns of fluctuations across several wind farms to violate one or more network constraints. Out of all such troublesome patterns, the most likely is termed the instanton. Prior work has shown that the instanton may be found by optimizing over a physically accurate AC model of the system. With no guarantee of convergence, this method is unlikely to see use in a real-time operating environment. The DC power flow approximation, on the other hand, yields a convex instanton problem that may be solved quickly and efficiently, albeit with questionable accuracy. The DC approximation makes several assumptions to linearize the system; of these, the most significant is that all voltages are equal to 1 per unit (a “flat” voltage profile). Current work is focused on moving away from this DC approximation by accounting for voltage deviations and other realistic phenomena. If we are careful, we can improve solution accuracy while maintaining the convergence properties of convex optimization that are so important to system operators. The ultimate goal of the instanton project is to make successive improvements to the DC model until its results are effectively indistinguishable from those of full AC analysis.
Applying networked estimation and control algorithms to address communication bandwidth limitations and latencies in demand response

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Demand response can provide services to the power network; however, coordination of spatially distributed demand response resources generally requires coping with imperfect communication networks. This work investigates methods to manage communication constraints (e.g., delays and bandwidth limitations), faced by demand response aggregators who manipulate the on/off modes of residential thermostatically controlled loads (TCLs). We present two model predictive control (MPC) algorithms that exploit a priori knowledge of delay statistics. We also present three Kalman filter-based state estimation methods that handle measurements with heterogeneous delays that are known a posteriori. We simulate the closed loop system to quantify the error while the system tracks simplified power system signals of various frequencies. We find that the MPC algorithm incorporating the full delay distribution, versus only the mean delay, reduces the average tracking error 39%. Also, incorporating individual TCL models, identified on-line, within the state estimator versus only using a TCL aggregation model reduces the average estimation error 19%
Corrective Model Predictive Control in Electric Power Systems with Renewables and Storage

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In severe contingency situations, electric power systems run the risk of cascading failure leading to system blackout. Model predictive control (MPC) is able to direct the system to a safe operating point while avoiding cascading failure by rescheduling generation, curtailing controllable load and renewables, and utilizing energy storage. System flexibility is increased by exploiting the thermal characteristics of conductors to allow short-term line-flow overloads. MPC circumvents line tripping by ensuring conductor temperatures remain within an acceptable range. Performance of this process has been demonstrated on small test systems but has not been extended to large utility-scale systems that occur in practice. This work utilizes a 4600 bus model of the Californian power system to examine the behavior of this MPC-based corrective control strategy on a large system. Computational efficiency is increased through the use of sensitivity analysis to identify the most effective subset of control resources and the lines most at risk of overload. It is demonstrated that applying MPC on only these resources is sufficient for the safe operation of the entire system.
Multi-Area Energy Trading Process under Localized Externalities

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We discuss a multi-area energy trading process between non-strategic regional transmission operators (RTOs) possessing asymmetric information. We consider a physical network with finite capacity lines connecting the buses within and between RTOs. Each RTO knows the network topology, bus voltage angle constraints, and cost functions within its own region. Each RTO also knows the topology of the network connecting its own region to its neighboring regions and the bus voltage angle constraints of the buses of neighboring RTOs that are immediately connected to its own region. We apply the extended alternating direction method of multipliers (ADMM) to determine the optimal energy trades. Under the mild assumptions of convex and strictly increasing cost functions, we can exploit the structure of our problem and apply recent convergence results for the ADMM to establish a sublinear convergence rate for the energy trading process.
Contracts under Uncertainty for Electricity Markets

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We consider a contract design problem for strategic players in electricity markets. We assume that the seller's cost of production depends on the seller's privately known technology and a random variable (uncertainty) that realizes after the contract signing (e.g. wind speed for wind generation). We characterize an optimal contract for energy procurement. We show the optimal mechanism is a menu of contracts (pricing schemes) that the buyer offers, and the seller chooses one based on the seller's technology and expectation about the uncertainty. After the random variable realizes, an energy quantity and its associated payment are selected from the contract chosen by the seller. We investigate two cases: (1) a case when the realized uncertainty is commonly observed by both the buyer and the seller and (2) a case when the realized uncertainty is observed privately by the seller and not revealed to the buyer.
Battery State-of-Health Monitoring Using Incremental Capacity Analysis with Support Vector Regression

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With the wide spread use of energy storage systems, battery state of health (SOH) monitoring has become one of the most crucial challenges in power and energy research, as SOH significantly affects the performance and life cycle of batteries as well as the systems they are interacting with. Identifying the SOH and adapting of the battery energy/power management system accordingly are thus two important challenges for applications such as hybrid electric vehicles (HEVs), electric vehicles (EVs) and all electric ships (AESs). This research focuses on the identification of Li-ion battery capacity fading, as the loss of capacity is the primary concern for applications that use batteries for energy storage. While most studies on battery capacity fading are based on laboratory measurement such as open circuit voltage (OCV) curve, few publications have focused on capacity loss monitoring during on-board operations. An SOH monitoring scheme that is based on real-life battery charging data is proposed in this work. Through analysis of battery aging cycle data, a robust signature associated with battery aging is identified through incremental capacity analysis (ICA) using the support vector regression (SVR).

Moreover, this work aims to develop analytical and numerical frameworks that explore the sparsity of the SVR representation for model parameterization and adaptation. Using the SVR parameterization, we hope to reform the high dimensional optimization problem in kernel based learning into a parameter estimation problem which can be solved by standard estimation algorithms such as the least-squares method. The reformulation greatly improves the computational efficiency.
SCE: Systems and Communications
Finite Block-length Gains in Distributed Source Coding

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We propose a new coding strategy for the distributed source coding problem with general discrete memoryless sources. The coding scheme involves two layers of codes. The first layer code is of constant, finite block-length whereas the second layer contains codes of block-length approaching infinity. We observed previously that small block-length codes preserve the correlation between the sources more efficiently; however it is well-known that there is a rate-loss due to the application of small block-length codes in a point-to-point compression perspective. Consequently, there is a sweet-spot for the length of the first-layer code. Since the scheme involves using finite block-length codes, single-letter characterization of the achievable rate-distortion region for the coding strategy proves to be difficult. We propose a method to characterize an inner bound to the achievable rate-distortion region using single-letter distributions. It is shown that this region strictly contains previous known achievable rate-distortion regions for the distributed source coding problem.
The feedback capacity of a class of finite state multiple access channels

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For the discrete memoryless (DM) multiple access channel (MAC) with noiseless feedback Cover and Leung (CL) provided an achievable region that was later shown by Willems to be the capacity region for a special class of channels. In this paper, we investigate the generalization of the DM-MAC channel with state evolving as a Markov chain, with or without inter-symbol interference (ISI). The state is perfectly observed at the receiver and through noiseless feedback the state and output are also available at the transmitter with unit delay. For the case of no ISI, we provide an achievable region that can be thought of as the generalization of the CL region, and show that it is the capacity region of a special class of channels.

For the case where ISI is present such a single-letter achievable region is harder to find. To address this difficulty, we start from the general multi-letter capacity expression derived by Permuter, Weissman and Chen for MACs with state and feedback, and attempt a reduction towards a single-letter expression. This novel—in the context of MACs—approach is based on viewing the multi-letter optimization problem as a stochastic control problem and finding a sufficient “state” for control. The aforementioned reduction is not complete but it hints at a single-letter region that is proven to be achievable using typicality arguments.
Design of a passive compliant leg for a Hexapod robot

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When legged robots are required to perform tasks like running, the compliance of the legs becomes important. We have designed and constructed a passive compliant leg for a hexapod robot. Recent research shows that the performance of this robot design can be influenced significantly by leg compliance. Our design is such that we can independently study the effects of leg compliance in the vertical direction and in the fore-aft direction. By attaching a sufficient number of motion tracking markers to the leg structures, we gain the ability to study the complete kinematics of the legs. Our design prioritizes manufacturability, as the majority of leg components were fabricated from materials commonly available in hardware stores, without specialized machining tools.
Structured codes have been of great interest in recent years. Linear codes over algebraic fields have been studied extensively in the literature. Under certain constraints, codes with weaker algebraic structure (such as groups or rings) outperform linear codes. Nevertheless, it has been shown that for certain channels, group codes cannot achieve the symmetric capacity. Based on this observation we investigate codes with weaker structure than group codes. In this work, a novel structured code based on group codes is proposed. For a given group, the scheme involves two layers of codes. The first layer consists of a group code over a subgroup. The second layer contains a code over the transversal of that subgroup. It is shown that the scheme achieves the point-to-point symmetric capacity for any discrete memoryless channel. The coding strategy also achieves the optimal point-to-point rate-distortion. In certain multi-terminal communications settings, the proposed codes give gains over group codes. We illustrate this for the case of computation over MAC in channel coding and the distributed source coding problem.
A Supervisory Control Approach to Dynamic Cyber-Security

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An analytical approach for a dynamic cyber-security problem that captures progressive attacks to a computer network is presented. We formulate the dynamic security problem from the defender's point of view as a supervisory control problem with imperfect information, modeling the computer network's operation by a discrete event system. We consider a min-max performance criterion and use dynamic programming to determine, within a restricted set of policies, an optimal policy for the defender. We study and interpret the behavior of this optimal policy as we vary certain parameters of the supervisory control problem.
Can Less Be More? A Game-Theoretic Analysis of Filtering vs. Investment

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In this work we consider a single resource-constrained strategic adversary, who can arbitrarily distribute his resources over a set of nodes controlled by a single defender. The defender can (1) instruct nodes to filter incoming traffic from another node to reduce the chances of being compromised due to malicious traffic originating from that node, or (2) choose an amount of investment in security for each node in order to directly reduce loss, regardless of the origin of malicious traffic; leading to a filtering and an investment game, respectively. We shall derive and compare the Nash equilibria of both games for different resource constraints on the attacker. Our analysis and simulation results show that from either the attacker or the defender's point of view, none of the games perform uniformly better than the other, as utilities drawn at the equilibria are dependent on the costs associated with each action and the amount of resources available to the attacker. More interestingly, in games with highly resourceful attackers, not only the defender sustains higher loss, but the adversary is also at a disadvantage compared to less resourceful attackers.
A General Mechanism Design Methodology for Social Utility Maximization with Linear Constraints

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Social utility maximization refers to the allocation of resources in a way that maximizes the sum of agents’ utilities, under the system constraints. Such allocation arises in several problems in the general area of communications, including unicast (and multi-rate multicast) service on the Internet, as well as in applications with (local) public goods, such as power allocation in wireless networks, spectrum allocation, etc. When agents are strategic (selfish), an appropriate contract i.e. mechanism must be designed to obtain enough information to get the right allocation. Mechanisms that implement such allocations in Nash equilibrium have been studied but either they do not possess the full implementation property, or are given in a case-by-case fashion, thus obscuring fundamental understanding of these problems. In this work we propose a unified methodology for creating mechanisms that fully implement, in Nash equilibria, social utility maximizing functions arising in various contexts where the constraints are convex. To make the designed mechanism amenable to learning, three additional design goals are the focus of this work: a) the size of the message space scaling linearly with the number of agents (even if agents’ private information is their entire valuation functions), b) allocation being feasible on and off equilibrium and c) strong budget balance.
Synthesis of Supervisors for Centralized and Decentralized Discrete-Event Systems

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The synthesis of supervisors for discrete-event systems (DES) is an important research field in the study of cyber-physical systems. On the one hand, this problem arises in the study of complex automated systems where the behavior is inherently event-driven, as well as in the study of discrete abstractions of continuous, hybrid, and/or cyber-physical systems. On the other hand, working with discrete-event abstracted models is, in many cases, the most effective way of tackling control problems for many classes of complex cyber-physical systems. Due to the limited actuation and sensing capabilities in the plant, a DES in the real world is always partially-controlled/observed. Moreover, in large complex systems, due to the distributed nature, a decentralized approach is always the desired or the only way to implement the controllers. In this poster, we present novel synthesis methodologies to the centralized and the decentralized supervisor synthesis problems. We illustrate our synthesis methodologies with a vehicular electric power system (EPS) example.