Research Day 2016

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Annette Caldwell Simmons School of Education & Human Development

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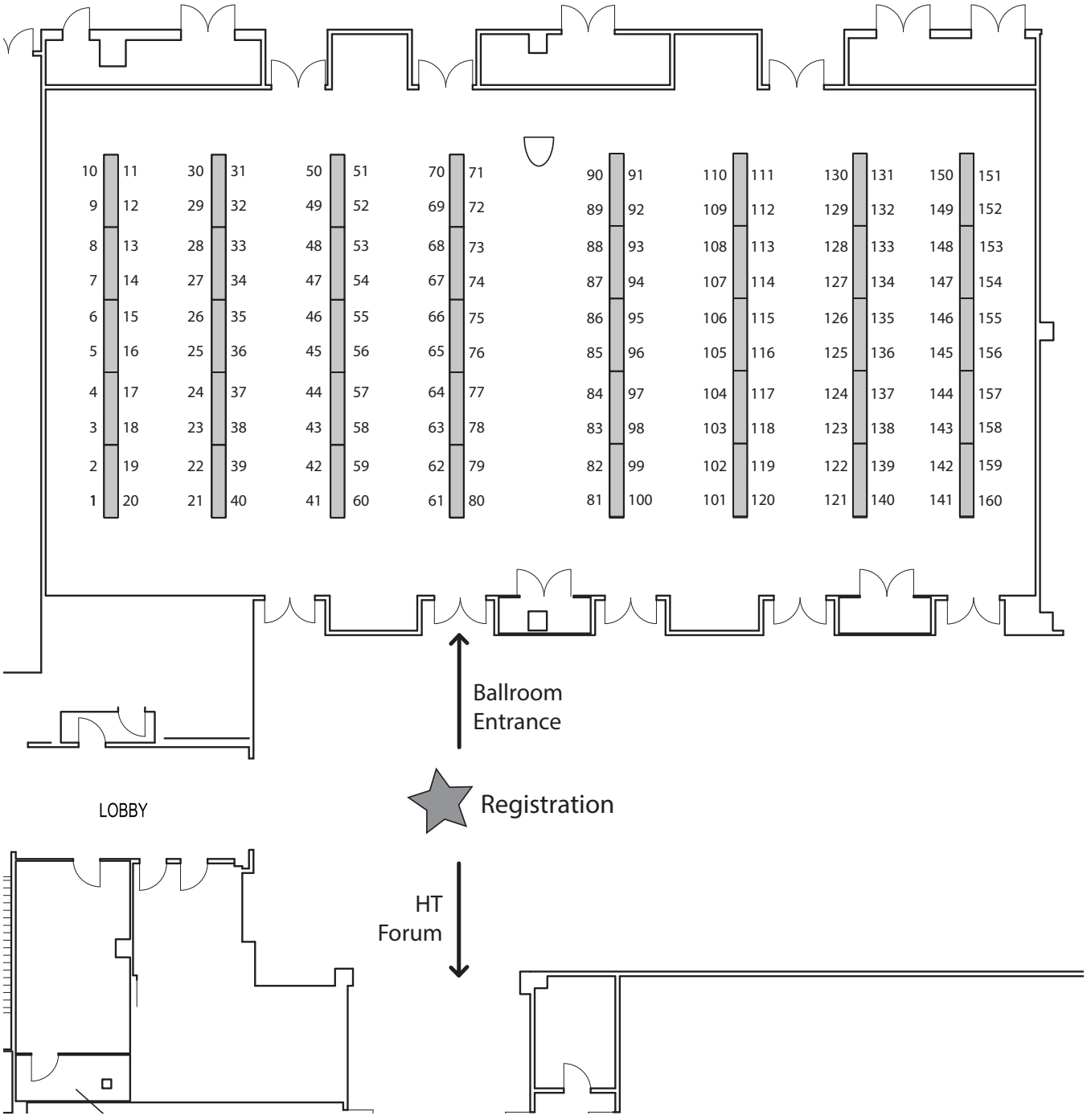
SMU | RESEARCH AND GRADUATE STUDIES



Map of Research Day: Ballroom and HT Forum

Applied Physiology & Wellness

Engineering

Civil and Environmental Engineering

Computer Science and Engineering

Electrical Engineering

Engineering Management, Information, and Systems (EMIS)

Mechanical Engineering

Natural Sciences & Mathematics

Biological Sciences

Chemistry

Geology/Earth Sciences

Mathematics

Physics

Statistical Science

Social Sciences

Anthropology

Economics

Psychology

Education

Humanities

Theology

UG = Undergraduate Student

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MULTIPLE SCLEROSIS PATIENTS EXHIBIT BLUNTED ARTERIAL BLOOD PRESSURE RESPONSES TO A WHOLE-BODY COLD STRESS STIMULUS

Multiple sclerosis (MS) is a neurological disease that disrupts nerve signal transmission and/or integration in the central nervous system. Our lab has previously demonstrated that MS patients have reduced resting sympathetic nerve activity. We tested the hypothesis that individuals with MS will have blunted sympathetic vascular responses to a whole-body cold stress compared to healthy controls (CON). Fourteen subjects (10 MS, 4 CON) were outfitted in a tube-lined perfusion suit and exposed to thermoneutral (34 °C water for 10 min), and cold stress (5 °C water for 3 min) conditions. Skin blood flow was continuously measured via laser-Doppler flowmetry and expressed as laser-Doppler flux (LDF), cutaneous vascular conductance (CVC), and percentage of maximal CVC after local heating (%CVCmax). Mean arterial pressure (MAP) was derived using an upper arm cuff. No differences in ΔLDF (CON: -2.83±3.76; MS: -3.73±4.29), Δ CVC (CON:-0.05± 0.06; MS: -0.05±0.06, p=0.89), and Δ%CVCmax (CON: -2.43±3.75; MS: -0.24, p=0.12) were observed between groups. However, ΔMAP was blunted in MS compared to CON (MS: -0.99±7.00; CON: 12.17±9.70; p=0.01). These data suggest individuals with MS exhibit reduced sympathetically mediated changes in blood pressure in response to a whole body cold stress. Interestingly, cutaneous vascular responses to a global cold stimulus are unaffected by the disease.

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DECREASES IN CORE TEMPERATURE AND SWEATING ONSET DURING WHOLE-BODY HEATING IN INDIVIDUALS WITH MULTIPLE SCLEROSIS FOLLOWING ADMINISTRATION OF 4-AMINOPYRIDINE

Multiple sclerosis (MS) is a progressive neurological disease that can result in heat sensitivity and thermoregulatory dysfunction. 4-aminopyridine (4AP), a voltage-gated K+ channel blocker, has been indicated to manage MS related symptoms. The aim of this study was to test the hypothesis that administration of 4AP would improve sweat function in individuals with MS during passive whole-body heating (WBH). Eleven individuals with MS participated in a randomized single-blinded crossover study design utilizing 4AP and placebo (PBO). Subjects were outfitted in a water perfusion suit and exposed to a normothermic (NT) baseline (34 °C) and WBH (48 °C; increase in core temperature of ~0.8 °C) condition. Core temperature (Tcore; telemetric pill) and sweat rate (capacitance hygrometry) were continuously measured. Baseline NT Tcore while on 4AP was lower compared to PBO (4AP: 37.3±0.2; PBO: 37.5±0.2 °C, p=0.002). Tcore at sweating onset was also lower on 4AP compared to placebo (4AP: 37.4±0.2; PBO: 37.6±0.3 °C, p=0.0006). However, sweat rate during heating (Δ from baseline) on 4AP was similar compared to PBO (p=0.49). These initial findings suggest 4AP may have benefits for people with MS by lowering Tcore at rest and sweating onset during heat stress. Thus, administration of 4AP may improve heat sensitivity in MS by expanding the range for Tcore increases prior to symptom worsening.

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IMPROVEMENT IN BRAIN BLOOD FLOW REGULATION DURING POST-CONCUSSION RECOVERY PHASE IS ASSOCIATED WITH REDUCED POSTURAL SWAY: A PILOT STUDY

Postural instability shown with concussion may be related to impaired cerebral blood flow regulation. The purpose was to examine if changes in cerebral autoregulation from acute injury to recovery phase after concussion is associated with changes in postural sway in athletes participating in contact-collision sports. Five NCAA Division I male athletes (21±2 yrs) with sports related concussion participated in the study. Arterial blood pressure (ABP) and middle cerebral artery blood flow velocity (MCAV) was collected on days 3 and 21 post-concussion. Dynamic cerebral autoregulation was estimated from beat-to-beat fluctuations in ABP and MCAV using transfer function analysis. Postural sway was measured from the deviation of the center of pressure during quiet standing with eyes closed on a

force plate. Multiple linear regression analyses were used to examine the association between changes in low frequency (LF, 0.07-0.2 Hz) phase and mediolateral range and variability on days 3 and 21 post-concussion. Improvement in LF transfer function phase from day 3 to day 21 post-concussion was associated with reductions in mediolateral range (β estimate= -19, p=0.02) and variability (β estimate= -4.3, p=0.04) of postural sway. Cerebral blood flow regulation is associated with alterations in postural control and may be useful as a potential vascular biomarker for recovery post-concussion.

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USING PHYSICS TO ISOLATE FOOTWEAR IMPACT FORCES

Running shoes were initially developed for protection and cushioning the impact forces between the foot and the ground. However some researchers contend that these shoes do not reduce impact forces, and may actually increase the risk of injuries. These issues remain unresolved because a quantitative method for extracting the impact portion of the total vertical ground reaction force (VGRF) measurements has not been available. Here, we test the ability of the Two-Mass Model; which, decomposes the total VGRF waveform into two impulses: 1) a high-frequency impact component corresponding to the motion of the shoe, foot and lower-limb, and 2) a low-frequency component corresponding to the motion of the remainder of the body's mass. We hypothesized that the total VGRF waveform would be accurately predicted ($R2 > 0.90$) regardless of shoe conditions. We measured VGRF waveforms across a range of speeds (3.0 – 7.0 m/s) in eight subjects in four different footwear conditions. Model-predicted waveforms were generated from measured lower-limb accelerations along with contact and aerial times. The Two-Mass Model accounted for running ground reaction forces in their entirety at two speeds across all footwear conditions ($R2 = 0.96 \pm 0.03$; range 0.92-0.98). We conclude that the Two-Mass Model provides an accurate method for isolating and quantifying footwear impact forces during running.

Commercial Viability:
Ground reaction force curves during running, walking and other activities (i.e. jumping, hopping, etc.) can be analyzed to obtain a variety of important variables. These include: impact forces, loading rates, maximum forces, applied impulses, and foot-ground contact times. These parameters are important evaluation tools for footwear analysts, physical therapists, coaches, orthopedic surgeons, podiatrists, and trainers. Accordingly, our experimental demonstration of model efficacy for predicting the impact properties of athletics shoes identifies obvious applications for design, individual customization and potentially the development of smart shoe sensing capabilities. Similar potential uses extend to orthotics, prosthetics, and exoskeleton design. Implementation in a shoe store, athletics performance facility or clinical site would involve a treadmill or runway and the instrumentation needed to acquire the limited motion data needed from the subject. The subject would run at the selected speed while his or her motion data is captured and used in conjunction with software that incorporates the model's algorithms in order to generate ground reaction force waveforms. The waveforms would be used to analyze and potentially customize the needs of the subject for footwear, orthotics, and/or gait retraining to improve performance and/or minimize injury risk, etc.

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SPATIAL AND TEMPORAL DISTRIBUTION OF HEAVY METALS IN COASTAL RED SEA SEDIMENTS OF JEDDAH, SAUDI ARABIA

Jeddah is the most industrialized city on the west coast of Saudi Arabia. In this study, the spatial and temporal distributions of heavy metals were obtained from near-coast Red Sea sediment cores in close proximity to Jeddah. Six elements (Cr, Cu, Mn, Zn, Pb, and Fe) from three impacted locations (Prince Naif Street, the Downtown area, and Al-Khumrah) and an upstream reference site (Salman Gulf) were analyzed via heavy acid digestion and inductively coupled plasma-mass spectrometry (ICP-MS). The average concentrations of Cr, Cu, Mn, Zn, Pb, and Fe in core sediments of all sites were 245.96, 251.82, 478.45, 623.09, 362.75, and 8506.13 mg/kg, respectively. The depth-resolved results showed that highest concentrations of Mn, Cu, and Pb were found in the top 15 cm of the core profile distributions compared to other depth sub-samples.

Heavy metal concentrations in core sediments seem to be increasing toward the area of the downtown and higher in the recent years. This indicates that this area has suffered from heavy metal pollution compare to other locations in the Red Sea.

Commercial Viability:
Heavy metal contamination due to anthropogenic activity should be taken into account to protect the Red Sea during future growth.

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ENHANCED METHANE GENERATION FROM MUNICIPAL SOLID WASTE

The solid waste generated in the world is expected to almost double by going from 1.314 billion tons in 2013 to 2.19 billion tons in 2025 according to a World Bank report. This introduces more challenges in our way of collecting, treating, and discarding municipal solid waste (MSW). More than half of the generated MSW in the United States is discarded in landfills. Natural anaerobic biological reactions can be managed in the landfill environment at the right conditions to result in waste reduction and landfill gas production (mainly carbon dioxide and methane). Methane is an important gas that can be captured and used for energy. The goals of this research are to investigate methane generation reactions by methanogens and the factors involved to maximize methane generation using experimental and modeling studies. The results of our research are aimed to improve the current practice with anaerobic digestion of MSW. The ongoing research is also addressing the solid waste problems while providing science-based solutions for cleaner, renewable sources of energy for the future.

Commercial Viability:
The study investigates experimental and modeling approaches for enhanced methane generation from municipal solid waste, while providing science-based solutions for cleaner, renewable sources of energy for the future.

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PARALLEL ALL-PAIRS SHORTEST PATH ALGORITHM: A NETWORK-DECOMPOSITION APPROACH

The all-pairs shortest path algorithms compute the shortest paths between all node pairs in the network. This paper presents a parallel algorithm for the all-pairs shortest path problem using a network decomposition approach. The algorithm decomposes the network into a set of independent augmented directed acyclic sub-networks that can be efficiently processed in parallel. The shortest path computation for each sub-network provides a subset of the all-pairs shortest paths in the original network. The superiority of the new algorithm is verified through comparing its performance against that of the parallel single-origin shortest path algorithm. The execution times are compared for hypothetical and real-world networks with different sizes. A percentage improvement in the execution time of about 50% is recorded for the transportation network of a large metropolitan area.

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DYNAMIC ANALYSIS OF TRAFFIC SIGNAL STRUCTURES

This research is focused on dynamic behavior of traffic signal structures and the accumulating fatigue due to the structure's dynamic response. The goal of this research is to better understand the relationship between obtainable diagnostic data and the structural health of the traffic signal structure. Theoretical baseline dynamic behavior (e.g. natural frequency and time history response) will be estab-

lished analytically and verified experimentally in laboratory conditions. The snap back test will be used to excite a scale traffic signal structure. Experimental data will be collected using accelerometers and strain gages. This data will be processed and compared to the analytical values. Once the behavior of the structure is fully understood the relationship between the fatigue life of the structure and the diagnostic data can be developed.

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MODELING THE COMPRESSIVE STRENGTH OF COMPRESSED EARTH BLOCKS BASED ON RESULTS FROM QUALITATIVE SOIL ANALYSIS

Compressed earth blocks (CEBs) represent a cost-effective material for construction of homes in low-income areas. CEBs are made by machine-compressing soil, water, and cement to form block units that resemble concrete masonry units (CMUs) in size. The challenges with CEB construction are that it is a largely unstandardized method of construction and that there is a large variability in the strengths that can be achieved due to the dependence on soil qualities. The current focus of this project is deriving a relationship between qualitative field soil analysis and quantitative laboratory soil analysis. The overall aim of this project is to use data fusion via neural networks to create a model that accurately predicts the strength of CEBs based on qualitative analysis of the soil used in production, with the end goal of developing a tool that allows designers in the field to accurately predict the strength of their designs.

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INVESTIGATING MECHANICAL RESPONSE OF FLUTED POINTS WITH GEOMETRIC VARIATIONS

This research project is an interdisciplinary effort between engineering and archeology and will investigate mechanical behavior of Paleolithic-era fluted points. Specifically, the effects of geometric variations on static and dynamic responses of fluted points are investigated. Using the finite element method (FEM) modeling software, ANSYS, a shell-element model was created with specified thickness and applied static loading. This model was analyzed to determine the static loading capacity of the point's material and geometry. Physical static loading tests on four obsidian points of similar geometry were conducted. Each specimen was loaded into the Instron 5582 tensile and compressive testing machine, held at the tip and base of the point. Static tests were performed under displacement control that ran until the specimen failed through cracking or the displacement reached ten millimeters. The results of these tests will be compared to the FEM model to validate numerical quantities from the ANSYS analysis.

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MAPPING OF CONTAMINANTS IN DEVELOPING WORLD AQUIFERS FOR ORIGINATION AND RISK ASSESSMENT

Hand pumps and groundwater wells are the primary water source for many families in developing countries. Water from these sources are typically only screened for bacterial contamination. For communities using these groundwater sources for extended time periods, chemical contamination becomes a significant issue. Our field team found several locations with concerning levels of groundwater species. Lab analysis used chromatogram and inductively coupled plasma mass spectrometry instrumentation to analyze samples. Appropriate remediation techniques are not always environmentally or economically viable for communities in these areas.

Spatially resolved mapping may be a cost effective solution. Risk maps can outline groundwater contamination distribution. ArcGIS can be used to generate chloropleth maps highlighting chemical spatial distribution. Using GPS points as the basis, the chloropleth map emphasizes chemical concentration values and other pertinent water quality parameters and the ArcGIS software interpolates between points to generate a spatial distribution map for each contaminant.

Commercial Viability:
In contaminated drinking water, appropriate remediation techniques are not always environmentally or economically viable. Creating spatially-resolved risk assessment maps using ArcGIS chloropleth mapping methods may be a cost effective solution.

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APPLICATION OF AN IMPROVED PROBABILISTIC NEURAL NETWORK IN STRUCTURAL IMPAIRMENT DETECTION

Structural systems are prone to impairment during their service life. Usually, structural impairments will change a structure's response and capacity. In order to obtain better agreement between the numerical and field-measured responses and evaluation of remaining capacity, a finite element model of the structure is modified and updated based on detected impairments. In many situations, damage is not visually detectable. In these cases, existing damage can be assessed based on measured responses (e.g. eigenmodes, frequencies, or static displacements). This problem can be described as an inverse static analysis problem. One of the approaches for solving this type of problems is to find all practical solutions and classify the measured responses to the most probable solution. In this research, an improved Probabilistic Neural Network is introduced and used as an expert evaluator for each part of structure. Each part has its own expert PNN which estimates the status of that member.

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PREDICTIVE CYBERSECURITY ANALYTICS FRAMEWORK

Numerous security metrics have been proposed in the past for protecting computer networks. However we still lack effective techniques to accurately measure the predictive security risk of an enterprise taking into account the dynamic attributes associated with vulnerabilities that can change over time. In addition zero day attacks exploiting unknown vulnerabilities presents a major challenge to both security vendors and enterprises alike. It is therefore critical to establish an effective cyber-security analytics strategy to minimize risk and protect critical infrastructure from external threats before it even starts. We present a novel security architecture which takes into account both the interrelationship between different vulnerabilities as well as temporal features that evolve over time such as vulnerability discovery rate and their lifecycle events. Our model is novel as existing research in attack graph analysis do not consider the temporal aspects associated with the vulnerabilities which can affect the overall network security based on how the vulnerabilities are interconnected to compromise the system. Gaining a better understanding of the relationship between vulnerabilities and their lifecycle events allow security experts to capture the current state of network security as well provide predictive insight into how the security will evolve over a given time period.

Commercial Viability:
A June 2014 report from cyber security firm McAfee places the annual global cost of cybercrime to be between $400 and $575 billion. According to GAO & Federal government, 59% of enterprises believe they have been attacked in the past year. The recent cyber-attack incident at Target Corp & Sony Pictures illustrates how security breaches can seriously affect profits and cause reputational risks. Hence security has now become a top management priority in many organizations and over the past years, corporations have consistently increased their security budget by an average of 20% annually.With a cumulative market valued at $65.5 billion (2015 – 2020), the U.S. Federal Cybersecurity market will grow steadily at about 6.2% CAGR.

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DEMOGRAPHIC GROUP CLASSIFICATION OF SMART DEVICE USERS

Interacting with smart devices is a common experience and is becoming an integral part of daily life for many people. Modern smart devices are equipped with a large variety of environmental and user input sensors. We hypothesize that a fusion of smart device sensor data can provide biometric data that allows for classification of user demographics such as age, gender, and native language. A smart device is instrumented with sensor data collection software and with user demographic classification software. An experiment is devised where data is collected for a sample group of users. The data is analyzed, and two classification algorithms are implemented based on the fusion of the different sensors. The classification methods are based upon decision tree and principle component analysis. The results of the experiment indicate that high accuracy is achieved for user demographic classification. Finally, we further discuss the applications and limitations of the study's approach.

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SELECTING COMMUNICATING WIRELESS SENSOR GRIDS

The field of wireless sensor networks (WSN's) is a rising technology which employs spatially distributed autonomous sensors to monitor physical conditions like sound, temperature, humidity and so on. We use a random geometric graph concept in computer science to model WSN's by placing a random set of points either in a planar region or over the surface of the globe. Our goal is to determine disjoint subsets of the sensors that each can serve as a backbone for monitoring the whole region. The presentation will show an interactive graphical demo of creating WSN's and three processes (ordering, coloring and relay coloring) which are efficiently used to determine well-connected backbones to achieve the goal. Our results are efficiently scalable from hundreds to tens of thousands of sensors. We typically are able to employ about 85% of the sensors in disjoint connected backbones where each one covers on average about 99% of the region. For each backbone, we have dynamic data collected and an interactive control feature to explore numerous options.

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THE PROM PROBLEM: FAIR AND PRIVACY-ENHANCED MATCHMAKING WITH IDENTITY LINKED WISHES

We present the Prom Problem which exemplifies a special class of matchmaking challenges. We also introduce the notion of identity linked wishes – wishes that involve specific identities and are valid if and only if all involved parties have that wish. A number of protocols over the years have highlighted the conflicting goals of anonymity and authentication in attempting to match users with common wishes and recent works have defined private and privacy-enhanced matchmaking with additional security goals. Yet prior protocols are insufficient in the context of the Prom Problem due primarily to the lack of fairness and vulnerability to a variety of attacks. We contribute a fair and privacy-enhanced matchmaking protocol supporting identity linked wishes with an untrusted matchmaker that satisfies essential security properties. In practical terms, our technology could have prevented most of the damage from certain data breaches such as the recent Ashley Madison hack which has allegedly resulted in blackmail, ruined careers, espionage, and even suicide. We have successfully tested a proof-of-concept implementation of our solution, are currently conducting performance tests, and are pursuing a patent. Future plans include a full-featured implementation with enhancements such as temporal and location-based constraints, decoys, and more.

Commercial Viability:
Our research could improve security and privacy for a number of practical applications involving identity linked wishes, the most obvious of which is matchmaking such as with match.com®, eHarmony®, OkCupid, and Tinder™. Examples of other potential commercial applications might include facilitating privacy-preserving negotiations in contexts like legislative bodies or corporate mergers and acquisitions.

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IMPLEMENTATION OF SWITCHING CIRCUIT MODELS AS TRANSFER FUNCTIONS

A transfer function is a mathematical function relating the output or response of a system to the input or stimulus. It is a concise mathematical model representing the input/output behavior of a system and is widely used in many areas of engineering including system theory and signal analysis. Binary Decision Diagrams (BDDs) are a canonical representation of Boolean functions. We implement a framework to build transfer function models of digital switching functions using BDDs and demonstrate their application on simulation and implication.

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DO CLASS DATA DEPENDENCIES SUPPORT THE PREDICTION OF CODE CHANGE PROPAGATION?

This poster addresses one question: how to predict software code change propagation (cochanges) through source code dependencies. In particular, we predict the impact of future software changes based on known changes and call/data dependencies between these changes and the rest of the software. Indeed, recent works have already shown the existence of dependencies between change propagation and call dependencies (methods calling one another). However, it has not been shown whether change prediction is also affected by data sharing within the source code (data dependency). We thus propose a new method and tool (COP) to predict code change propagation based on three types of data dependencies. The proposed approach has been evaluated on four open source systems and we demonstrate that data dependencies have a significant impact on change propagation prediction in that it improves prediction accuracy.

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ENHANCED SECURITY FOR LSIB ACCESS USING FPGA-BASED CONTROL IN 3D STACKS

The new IEEE Standard, 1687, is intended to enhance the accessibility of embedded instruments and data. This standard uses data shifted through the scan chain to open Segment Insertion Bits (SIBs) to provide access to additional test data registers (TDRs). To help prevent an attacker from systematically scanning data through the network to map it, a variety of Locking SIBs (LSIBs) have been previously introduced. LSIBs require additional key bits to be set to the correct values before the LSIB will open and provide access. Unfortunately, an attacker with access to licensed software may still be able to watch the data transmitted between the computer and the chip and use that information to reverse engineer the scan network unless appropriate measures are taken to hide the critical data. This thesis considers the enhanced security that may be provided if IEEE 1687 networks are used to protect information in a 3D stacked integrated circuit (IC) that contains programmable logic. Specially, it will investigate the ability of a Field Programmable Gate Array (FPGA) to contain the necessary programming to identify the status of the current LSIBs in a restricted network and to send data to other parts of the stack to allow an authenticated user to open and close those LSIBs.

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MAI-WRITER: DECREASE PROCRASTINATION WITH TECHNOLOGY

Research shows that procrastination creates negative feelings, reduced self esteem, and even causes health problems. Psychologists typically rely on accepted patient exercises to help mitigate these problems. For example, the time traveling technique is a strategy where patients anticipate their feelings after completing undesirable tasks. Unfortunately, these techniques rely largely on a human's ability to imagine realistic scenarios. Our research investigates how modern technology, like Natural Language Processing and Machine Learning, coupled with psychological theories such as Flow and Self-Determination theory can help users overcome procrastination. We target how technology can be used to help users write more regularly, since it is a common form of procrastination. This investigation could potentially open up the possibility of solving larger procrastination problems such as saving for retirement, gambling, or stopping smoking.

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IDENTIFYING IMPORTANT CELL-AWARE TYPE FAULTS FOR MANUFACTURING TEST USING MANDATORY ASSIGNMENTS AND EXCITATION CONDITION

In integrated circuit production, each circuit must be tested to identify circuits with manufacturing defects to prevent bad parts from being sold to customers. To perform these tests, input combinations of 0's and 1's are applied to the circuits. Defects are detected if incorrect logic values are observed at gate outputs. Ideally, all possible combinations would be applied to a circuit. However, this is impractical, so a small subset of input combinations is applied instead. The traditional model for testing is the stuck-at fault model for defects at gate inputs and outputs. However, this model can miss defects that occur inside of gates. Cell-aware faults models are used to detect internal faults. Aiming for 100% coverage of all cell-aware faults makes tests sets too long and impractical for large circuits. To solve this problem, we are developing new algorithms to determine which cell-aware faults actually cause errors in functional operation.

Commercial Viability:
Cell aware fault analysis can help improve testing procedures for integrated circuits that are put into commercial products.

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DIELECTRIC WAVEGUIDE FOR THZ COMMUNICATION

A holey waveguide with square cross section is designed, simulated, fabricated and tested. The dielectric waveguide is to be used in a 300Gbps communication system in THz range. The desired waveguide is going to carry information from 10 channels with frequency range of 160GHz to 380GHz. The in addition, it is required to support both vertical and horizontal polarizations. The mode propagation is simulated on commercially available Rsoft software in order to choose the best holey waveguide design that supports the frequency range and both polarizations. The waveguide was made with Cyclic Olefin Copolymer (COC), TOPAS due to low absorption loss (0.15 dB/cm to 0.2 dB/cm at 0.2THz to 0.3THz respectively). The effect of different parameters on fabrication process and final shape of the waveguide was studied and controlled. A functional characterization experiment is set up to determine the absorption loss, transmission loss, effective refractive index, acceptance angle of waveguide and mode profile in waveguide.

Commercial Viability:
A unique waveguide is designed as a bridge between a receiver and a transmitter in a THz communication system.

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RELIABILITY BLOCK DIAGRAM EXTENSIONS FOR NON-PARAMETRIC PROBABILISTIC ANALYSIS

Multi-Valued Reliability Block Diagrams (MVRBD) are introduced as a generalization of classical reliability block diagrams (RBD) commonly used in system analysis. MVRBD offer the advantage of allowing systems and subsystem components to be modeled with arbitrary hazard failure rate relationships. MVRBD are based upon a multiple-valued discrete switching algebra that is functionally complete with constants thereby affording a corresponding model to be formulated for any system that is capable of being modeled in a reliability block diagram form. The utility of this new model is that system failure and reliability analysis can be performed without restricting component hazard rate relationships to the binary case of either "failure" or "fully operational." The incorporation of any desired number of "degraded" states into the MVRBD model allows for non-parametric probability mass functions (pmf) to be used. Any arbitrary number of intermediate system states of "degraded" may be incorporated into the MVRBD model without significant increase in the complexity of the analyses methodologies.

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A HIERARCHICAL ELECTRICITY MARKET STRUCTURE FOR THE SMART GRID PARADIGM

This paper proposed a hierarchical structure for the electricity market to facilitate the coordination of energy markets in distribution and transmission networks. The proposed market structure enables the integration of microgrids, which provide energy and ancillary services in distribution networks. In the proposed hierarchical structure, microgrids participate in the energy market at the distribution networks settled by the distribution network operator (DNO), and load aggregators (LAs) interact with microgrids and generation companies (GENCOs) to import/export energy to/from the distribution network electricity markets from/to the wholesale electricity market. The proposed approach addressed the synergy of energy markets by introducing dynamic game with complete information for GENCOs, microgrids, and LAs. The proposed hierarchical competition is composed of bi-level optimization problems in which the respective upper-level problems maximize the individual market participants' payoff, and the lower-level problems represent the market settlement accomplished by the DNO or the independent system operator. The bi-level problems are solved by developing sensitivity functions for market participants' payoff with respect to their bidding strategies. A case study is employed to illustrate the effectiveness of the proposed approach.

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CROWDSOURCING FADING CHANNEL MODELS ACCORDING TO GEOGRAPHICAL CONTEXT

A number of channel models have been developed based on extensive measurements from sophisticated hardware at select locations. However, such a methodology makes comparison across different environments extremely challenging. Hence, we seek to build a comprehensive view of wireless channels across diverse geographical locations. In this paper, we create a channel classification framework from crowdsourced data around the world to understand the degree to which small-scale fading occurs in a broad range of environments. Using an Android-driven data set consisting of millions of signal strength measurements, we characterize a normalized signal-strength histogram in a given area according to its closest Nakagami distribution, which has been shown flexible in representing a wide array of wireless environments. Then, we consider the KL-distance from the histogram to the distribution to validate our approach. Finally, we consider which environments have similar Nakagami characteristics through analysis of our crowdsourced data to reveal similar settings across geographically diverse regions.

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USING GEOGRAPHICAL FEATURES TO REDUCE IN-FIELD PROPAGATION EXPERIMENTATION

Ensuring cellular coverage is an important and costly concern for carriers due to the expense of in-field experimentation (i.e., drive testing). With the ubiquity of smartphones, apps, and social media, there has been an explosion of crowdsourcing to understand a vast array of trends and topics at a minimal cost to the organization. While cellular carriers might seek to replace the expensive act of drive testing with the nearly cost-free crowdsourcing, questions remain as to: the accuracy of crowdsourcing, considering the lack of user control, the detection of when drive testing might still be required, and the quantification of how many additional in-field measurements to perform for a certain accuracy level. In this work, we use geographical features of a region to reduce in-field propagation experimentation by predicting the number of measurements required to accurately characterize its path loss. In particular, we study the path loss prediction accuracy of drive testing and crowdsourcing by taking millions of measurements in a suburban and downtown region. We then use statistical learning to build a relationship between these geographical features and the measurements required. In doing so, we find that the number of measurements collected to achieve a certain path loss accuracy over the entire region can be reduced by up to 58% in a high density drive testing scenario.

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ESTIMATION OF WIRELESS SIGNAL ATTENUATION IN URBAN AREA

The wireless signal propagating through the urban area is significantly affected by a lot of factors, such as buildings, foliage, vehicles and people. In the project, we use a ray-tracing based simulator to study the wireless signal attenuation in urban area, and the effects of those factors. A equation is given in the end to estimate the attenuation coefficient.

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JOINT BLUR IDENTIFICATION AND IMAGE SUPER-RESOLUTION

Blur identification is one of the crucial steps in Super-Resolution Reconstruction. The blur effect degraded the image by removing high frequency components. This work proposes a joint estimation scheme which can estimate the blur and sharp image simultaneously. Alternating minimization scheme is used, containing an image estimation and a blur estimation step. At each iteration, a temporary unnatural image is created using L0 norm reduction to mimic the original sharp image for blur estimation. A blur extend measurement step is introduced to control the blind estimation scheme, i.e. the de-blurring will stop when the blur extend does not change any more. This not only indicates a good convergence, but also save time for cases with easy removing blur. The proposed scheme does not assume a parametric for of blur and can be used extensively to all type of blurs, even when the blurs are different when the low resolution frames have individual blurs. Both synthetic and real data experiment results show the effeteness and robustness of the proposed method.

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MEASUREMENT OF SIGNAL STRUCTURE VIBRATION BY CAMERA ALGORITHMS

This research calculated the position of the camera under vibration by camera calibration with 3D corner points whose world coordinates are known. We also designed the corner tracking algorithm based on SIFT flow motion detection and sub corner detection. We will be working on the 3D vibration measurement of the targets with only one vibrating camera.

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INCREASING CAPACITY OF COMMUNICATION NETWORKS WITH OPTICAL VORTICES

The next generation of telecommunication technologies as a part of 5G is underway to support the increase in traffic demand. This study investigates the use of beams with orthogonal basis sets to increase the capacity of current optical networks. These beams are also known as Orbital Angular Momentum beams (optical vortices), which is basically a twisted beam of light. Beams can be twisted at different speeds and propagated along the same axis and since they are orthogonal they have very little cross talk. Taking advantage of these higher order modes of light rather than just the zeroth order Gaussian mode allows us to transmit multiple channels through fiber or free space using the same frequency. Aside from applications in optical communications this technology can also be applied to free space communication links such as microwave backhaul and can be a step towards fully software defined networks (SDN).

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CREATING A MOBILE PLATFORM FOR CERVICAL CANCER DIAGNOSIS

Cervical cancer is the third most common cancer worldwide and the leading cause of cancer mortality among women in developing countries. Developing countries often have neither the manpower, nor the infrastructure, nor the funds to implement pap smears and other cervical cancer screening techniques commonly used in developed nations. With this work, we present a mobile, low-cost hardware and software design that could allow an untrained nurse to screen patients for cervical cancer.

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FULL DUPLEX MAC DESIGN FOR WLAN

In this poster, we described the full duplex (FD) medium access control (MAC) protocol designed based on IEEE 802.11 standard for Wireless Local Area Network System (WLAN) according to the hard requirement that no modification is allowed on the client's protocol. We discuss about potential solutions to the problem of Multiple ACK collision using implicit multi-user MIMO technique and demonstrate the feasibility of our MAC protocol when implemented in various scenarios.

Commercial Viability:
Nearly all wireless communication devices today work only in half duplex mode, which means that they can either transmit or receive signals, but not at the same time. Full duplex communications are the next generation wireless solution to meet the increasing requirement of capacity in wireless networks. Full duplex communication means simultaneous transmission and reception from the same node and at the same frequency channel, which means a huge revolution for current wireless communication.

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ALL-IN-FOCUS IMAGE CAPTURE THROUGH SWIVELING LENS

A camera cannot produce an image that has everything from the near to the far in sharp focus. The lens produces a sharp image of a planar object only if the object is at a precise distance from the lens. Several computational approaches to produce an all-in-focus image have been proposed. For example, in one of the techniques, a complex pupil mask is placed at the aperture to render the computational impulse response of the imager invariant to defocus (within a limited volume). In another approach, known a focal stacking, multiple images formed by focusing the lens at several intermittent distances within a volume of interest are combined. In this work, we present a novel technique to produce an all-in-focus image by computationally combining images captured while rotating the lens. The main advantage of our strategy over the other techniques is higher SNR (compared to pupil mask approaches) and fewer number of images (compared to focal stacking). In this work, we have also developed a rather general imaging model using geometric optics that accommodates the lens and image planes to swivel about two independent pivots. We have verified the accuracy of the model through optical ray tracing. Using this new model, we have also found unique requirements under which our method to create an all-in-focus image by rotating the lens image will work.

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A MULTIPLE-VALUED LOGIC SYNTHESIS TOOL FOR OPTICAL COMPUTING ELEMENTS

Optical computing elements offer benefits over traditional CMOS-based electronic logic gates such as increased performance and reduced power. Using polarization to encode the information to be processed allows for the possibility of non-binary switching theory to be applied that further offers the benefit of reducing the number of required elements in an optical computing circuit. A methodology for synthesizing non-binary optical computing circuits is described and experimental results are provided that justify the approach.

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SEGMENTATION AND RECOGNITION IN VEHICLE DETECTION

Nowadays, vehicle detection plays a more and more important role in our daily traffic system. Fortunately, over the last decade, the segmentation and recognition has progress from its infancy to maturity. This Poster will present several popular method in segmentation and recognition which can be used in vehicle detection.

Commercial Viability:
It can be used in on road vehicle detection for the security reasons. Also, when it can be used in real time with the camera mounted in the vehicle, it can be used to avoid collision and become the basic of self-drive vehicle.

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COORDINATED EXPANSION PLANNING OF DATA CENTERS IN ENERGY AND CYBER NETWORKS

The growing tendency toward cloud computing rises the number and capacity of the data centers in cyber and electricity networks. The energy consumption of these centers increases the demand in electricity network, which in turn raises the cost and carbon footprint of supplying these loads. Data centers serve the clients in cyber networks with diverse requirements including processing, data storage, web services and other IT applications. The customers in cyber networks are required to be served within reasonable waiting times corresponding to service level agreements (SLAs). Hence capacity planning and allocation of such servers not only depends on the demand served in the cyber networks and the respective latencies and traffic flow but also depends on the energy consumption, price of electricity, and reliability of supply in the electricity networks. This paper addressed the interdependency of energy and data network in capacity planning and allocation of the data centers in data and energy networks. The objective in this problem is to minimize the installation and operation cost of the data centers subjected to the constraints imposed by the power and cyber networks. The expansion-planning framework is extended to address the uncertainties in the demand in power and cyber networks.

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A METHODOLOGY TO SUPPORT DECISION MAKING IN PROGRAM ORGANIZATIONAL ARCHITECTURAL FRAMEWORK (POAF)

A feasible program schedule and personnel allocation model may contribute to identifying the final shape of a program organization. If a program organizational design can be shown to be constructed such that it will satisfy the requirements without violating the constraints, then the design may be considered a feasible solution. This paper targets program organizations that are capable of designing and developing complex products. The approach in this paper builds upon the results of the Program Organizational Architecture Framework (POAF). We utilize constraint programming in order to extend the architecture framework and find a feasible design. Important decision variables and constraints are considered in this study. A hypothetical scenario of an ongoing program is presented to demonstrate that a given program organizational design is a feasible solution. This approach enables the program designers to support the decisionmaking process of implementing an effective program organizational design to manage a complex system and select the "best" program organizational structure

Commercial Viability:
Complex systems such as aircraft or space programs.

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FINDING OPTIMAL THREADS IN REAL-TIME SYSTEMS

Calculating the optimal number of servers (called threads in computer systems) of an M/M/c Queue can be costly and require historical information. However, upon investigation, the formulas for the M/M/c Queue can be reduced to O(n) complexity and the base values needed for the calculations can also be calculated real time.

Commercial Viability:
Applications which manage multiple threads for performing work, but also need to share system resources gracefully, can calculate needs of the application real time. Applications with multiple M/M/c Queues can spread its allocated resources over each queue as needed.

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EXTREME-POINT SEARCH HEURISTICS FOR GENERALIZED INTERVAL-FLOW NETWORK PROBLEMS

Generalized Interval-flow networks are a new extension of the classic generalized network formulation that adds a conditional lower bound constraint on the arcs. An interval-pivoting heuristic that exploits the quasi-tree-forest basis structure to explore extreme points is developed and computational testing is presented.

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A COMPARATIVE STUDY OF TABU SEARCH AND GENETIC ALGORITHM FOR SOLVING THE SERIATION PROBLEM

The seriation or sequencing problem is an important combinatorial optimization problem. The goal of seriation is to find a linear reorder for data objects in order to reveal structural information given a loss or a merit function. Seriation has been used to solve problems in many areas such as archaeology and anthropology, cartography and graphics, sociology and sociometry, psychology and psychometrics, ecology, biology and bioinformatics, and operations research. Metaheuristic algorithms have proven to be an excellent tool for solving combinatorial optimization problems performing local search and using operations to escape the trap of local optimality. Tabu search (TS) is a single point search short-term memory based approach while Genetic Algorithm (GA) is a population-based approach that imitates a biological system; both algorithms have been applied with great success to many difficult combinatorial optimization problems such as traveling salesman problem (TSP), vehicle routing problem, scheduling problem, and assignment problem. In this study, we investigate the use of tabu search and genetic algorithms to the seriation problem. We have implemented both algorithms and compare them in terms of both solution quality and runtime.

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SENSING, CONTROL AND PROCESS PLANNING FOR ROBOTIZED LASER-BASED 3D METAL PRINTING

The state-of-the-art manufacturing centers available for additive processes are predominantly characterized by self-contained 3-axis and powder-supported systems. Several challenges have been identified with respect to the additive manufacturing of metal components using these systems. The development of a robotically controlled 8-axis system targets solutions and/or improvements for limitations related to build volume, production time, material waste, process integration, and graded composition. This poster describes the current state of RCAM's hybrid system and highlights areas of development in regard to powder delivery, sensing and control of molten pool, and software development on path planning. Challenges regarding dimensional accuracy and material density are highlighted with solutions presented based on optical sensing and closed-loop control. The process monitoring approach presented incorporates a coaxially-mounted high-frame-rate CCD camera and infrared filters to isolate molten pool behavior. Image processing algorithms were developed to analyze the recorded molten pool state and ultimately maintain uniform deposition rate and quality. Path planning software were developed based on the characteristics of the 8-axis LBDMD system. This poster shows the printing process specific to a kind of complex part: revolved part.

Commercial Viability:
The commercial objectives of this research target a wide range of industries. These objectives are centered on the production of larger net and near-net components with minimal post-production requirements. Motivation is focused on large, low volume and mass customized parts which cannot be feasibly manufactured with additive manufacturing systems currently on the market.

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DIELECTROPHORETIC CAPTURE OF CANCER CELLS FROM BLOOD

Isolation of rare cells from dense suspensions is critical for many biomedical applications.. However, rare cells usually exist in very small quantities in dense suspensions, and building devices to capture them is a great challenge. In this study, we present a novel separator that uses dielectrophoresis (DEP) to isolate rare cells from dense suspensions where size based filtering is combined with DEP based flow field fractionation. As a model system, we used whole blood with spiked prostate cancer cells. As a first step, we dielectrically characterized blood cells populations and prostate cancer cells to obtain Clausius-Mossotti (CM) factors of the cells. Second, fluorescently labeled cancer cells were spiked into whole blood at known numbers and introduced into the DEP separator. Third, at each run separation efficiency and purity were calculated analyzing the number and types of cells at the outlets. Separation and isolation of live rare cells is important from a biotechnology point of view; therefore, a membrane integrity test was performed on isolated cancer cells using trypan blue exclusion assay. Lastly, effects of AC electrohydrodynamic flow, such as AC electrosmosis and electrothermal motion on separation yield was qualitatively discussed.

Commercial Viability:
It can be used as a diagnostic device (prognosis). The rare cells can be separated from blood and they can be used to develop a new drug for individual patient (Personalized medicine).

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MODELING OF ADVANCED COMBAT HELMET UNDER BALLISTIC IMPACT

The use of combat helmets has greatly reduced penetrating injuries and saved lives of many soldiers. However, behind helmet blunt trauma (BHBT) has emerged as a serious injury type experienced by soldiers in battlefields. BHBT results from non-penetrating ballistic impacts and is often associated with helmet back face deformation (BFD). In the current study, a finite element-based computational model is developed for simulating the ballistic performance of the Advanced Combat Helmet (ACH), which is validated against the experimental data obtained at the Army Research Laboratory. Both the maximum value and time history of the BFD are considered. The simulation results show that the maximum BFD, the time history of the BFD, and the shape and size of the effective area of the helmet shell agree fairly well with the experimental findings.

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MUTUAL CAPACITIVE SENSORS FOR TISSUE DIAGNOSTICS

Mutual Capacitance Sensors (MCSs) make use of the fact that the capacitance between two conductors (electrodes) can be altered by a third conducting object. The third conducting object decreases the charge hold between electrodes, and therefore the mutual capacitance between electrodes decreases depending on the electrical properties of the object. Among other projected capacitive touch technologies, MCSs are widely used in industry and especially in mobile phone screens Recently, we have tested a MCS array that was fabricated using standard lithography and lift-off techniques. We have tested the sensors sensitivity to different liquids filling a PDMS (polydimethylsiloxane) chamber that was placed on an intersection at the MCS.We have also utilized finite element model simulations to understand the MCS response.

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ANALYSIS OF TAPE-BASED TECHNIQUES TO SECURE ORAL ENDOTRACHEAL TUBES: A SIMULATION STUDY

When patients go into surgery, they are intubated with endotracheal tubes that are secured using either commercial devices or medical tape. Commercial devices are expensive, so adhesive tape is more commonly used. There are six main taping methods, and doctors generally choose their own personal favorite. Displacement of the tube can cause death. The taping methods are to secure the tube, however the strength of different taping methods varies, and doctors' personal preferences can endanger patients. This research focused on testing the taping methods in a controlled, lab environment. After strength tests and analyses, the strongest method was determined. A portable device was then designed, built, and tested to find the extubation force and displacement of an endotracheal tube in a hospital setting. This machine will be taken to UT Southwestern Medical Center to conduct more tests. These findings provide insight into a common problem in hospitals across the world.

Commercial Viability:
You know that when in the hospital, your life is in the hands of doctors, but they control more than you thought! How can you limit your risk of death?

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HOLLOW MICROSPHERE SENSORS FOR ADVANCED PROSTHETICS

Upon completion of our current avenue of research, we hope to use this technology to create implantable, biocompatible, electric field sensors capable of detecting electric fields small enough, and signals fast enough, to interpret nerve impulses in real time, without having to compromise the nerve bundle itself through surgery or other invasive means. This research is intended to lead to the development of micro-scale sensing units for advanced prosthetic devices and other brain-machine interface applications, in addition to other commercial and academic applications. Specifically, we are developing methods to allow commercially available and in-house fabricated hollow microspheres to support Whispering Gallery Mode (WGM) phenomena, in order to decrease minimum measurable signal duration and increase sensitivity of electric field sensors over that previously demonstrated by solid microsphere sensors, so that we can detect the electric impulse created by a firing nerve. Having already proven significant sensing capabilities with solid microspheres, we anticipate that a substantial sensitivity and bandwidth improvement will result from developing hollow microspheres for these and other similar sensing applications.

Commercial Viability:
Commercial Applications of this research include the development of sensing elements for advanced prosthetic devices and other brain-machine interface applications, among other commercial and academic sensing applications, such as temperature, force, pressure, and strain sensing elements.

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FIBER ENCAPSULATED ADDITIVE MANUFACTURING

Fiber Encapsulation Additive Manufacturing (FEAM) is a new 3-D printing technology in which a fiber (e.g., solid metal wire) and a matrix material (e.g., an insulating thermoplastic polymer) are co-deposited using a novel printer at build rates comparable to single-material 3-D printing processes. FEAM enables 3-D printing of electronic and electromechanical devices using low resistivity (1.7 μohm-cm), commodity conductors such as copper, rather than less conductive and far more costly materials, such as conductive inks.

The FEAM printhead allows wire to be stopped and started under computer control, and junctions between wires can be formed using electrically conductive polymer composites deposited by the system. Several simple devices such as a solenoid actuator, loudspeaker, inductive sensors, and membrane switches have been successfully fabricated using FEAM. By using an elastomeric polymer, flexible and highly stretchable interconnects have also been made. Applications of FEAM include soft robotics, wearables, consumer electronics, and military systems.

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IMPROVING THE WELD SURFACE QUALITY IN LASER WELDING OF ALUMINUM ALLOYS

The poster illustrates how to join thin aluminum panels with the high surface quality and desirable ultimate strength, and provides the optimal welding parameters.

Commercial Viability:
The project is supported by GM and results are beneficial to the whole automotive industry.

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A NON-CLASSICAL MODEL FOR CIRCULAR KIRCHHOFF PLATES INCORPORATING MICROSTRUCTURE AND SURFACE ENERGY EFFECTS

A new non-classical model for circular Kirchhoff plates subjected to axisymmetric loading is developed using a modified couple stress theory, a surface elasticity theory and Hamilton's principle. The equations of motion and boundary conditions are simultaneously obtained through a variational formulation. The new plate model contains a material length scale parameter to capture the microstructure effect and three surface elasticity constants to describe the surface energy effect. To demonstrate the new model, the static bending problem of a clamped solid circular Kirchhoff plate subjected to a uniform normal load is analytically solved by directly applying the general formulas derived. The numerical results reveal that the deflection of the clamped circular plate predicted by the current Kirchhoff plate model is smaller than that predicted by the classical elasticity-based model, but the former approaches the latter with the increase of the plate thickness.

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LASER CLADDING OF MARTENSITIC STAINLESS STEEL (AISI 420) WITH MO AND NI TO ENHANCE ITS CORROSIVE PERFORMANCE

Corrosion is the most frequent failure of mechanical components in diverse industries such as oil and gas extraction and mining. Surface coating of the components exposed to corrosive conditions with the high corrosion resistant material is a common solution to extend the lifecycle of the equipments. Laser cladding as a surface coating technology has been gaining interest in order to fabricate the protective coatings with fine microstructure, uniform chemical composition, and superior mechanical properties. In this study, laser cladding of martensitic stainless steel 420 with addition of Mo and Ni was performed in order to investigate the microstructure evolution, phase distribution, microhardness, and corrosion performance. It was found that the addition of Mo and Ni improved the corrosion resistance of 420 SS coating.

Marziyeh Badinloo; Elizabeth Nguyen; Jovelyn Castellanos; Winston Shu; Faisal Alzahrani; Kelly Cotchett; Abdul Yassine; Jody Barnhardt; Dylan Erwin; William Orr; Svetlana Radyuk (#51)
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THE EFFECT OF DEFICIENCY AND ENHANCEMENT OF HUMORAL IMMUNITY ON FLY LIFE SPAN

The innate immune responses become hyperactive and pro-inflammatory in older organisms. We investigated whether the increase level of anti-microbial peptides (AMP), a hallmark of Drosophila immunity, contributes to the aging process, or is a consequence of it. AMPs expression is regulated by NF-kappaB transcription factor Relish. We showed that the overexpression of Relish increased the AMPs levels in young Relish overexpressor comparable old control flies and resulted in shortened longevity. Induction of most AMPs clearly failed in the rel mutant, however life span was slightly extended in male rel mutants and not female. Downregulation of Relish in the fat body resulted in extension of life span in both sexes. Global overexpression of AMPs, Attacin, Defensin, Metchnikowin and Cecropin A1 exhibited significant decreases in life span in both sexes and life span was significantly shortened by the fat body-specific overexpression of Attacin A and Metchnikowin. Using TUNEL assay, the pro-apoptotic changes were particularly evident in the fat body in flies ubiquitously expressing CecA1, AttA, Def and Mtk, and these changes were comparable to those observed in old flies. Overexpressors of Attacin A1, showed significant increase in the caspase activity. The result of this study established causality links between high level production of antimicrobial peptides and longevity.

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PURIFICATION AND RECONSTITUTION INTO NANODISCS OF MOUSE AND HUMAN P-GLYCOPROTEIN

P-glycoprotein (P-gp) overexpression is often correlated with multidrug-resistance (MDR) of the cancer. The search for P-gp inhibitors as co-therapeutics to combat MDR has had little success so far. We used high-throughput in silico ligand docking studies and identified drug-like compounds that reversed MDR in human cancers. Biochemical screens were used to identify the first set of MDR reversing compounds. Interestingly, another 12 compounds were found that reversed MDR in cancer cells but were not recognized in the biochemical screens. One reason why the biochemical screens did not identify these compounds may be that the mouse P-gp homolog used in the biochemical test may be sufficiently different from human P-gp, making the mouse protein non-representative. We have since established methods to successfully incorporate (mouse) P-gp into membrane nanodiscs with high recovery yields and increase in activity and stability. We are currently trying to reconstitute human P-gp (MDR1), well known for its instability when removed from the membrane environment, into nanodiscs. Unfortunately, the MDR1-clone available in our lab exhibits low protein yield during purification, making it undesirable for further experimentation. To address this problem, we constructed an improved MDR1 clone and will employ the high protein expression PichiaPinkTM system to obtain higher protein yield.

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FUNCTIONAL RECONSTITUTION OF P-GLYCOPROTEIN INTO NANODISCS: BIOCHEMICAL AND BIOPHYSICAL EVALUATION

Multidrug resistance (MDR) proteins protect normal cells from xenobiotic attack by pumping a large range of toxins out of the cell. Unfortunately, over-expression in cancer cells increases efflux of therapeutic drugs rendering them ineffective. In order to re-sensitize multidrug resistance cancers to chemotherapy, we have found inhibitors of P-gp by in silico screening methods. To further investigate the mechanism underlying the inhibition, we have employed biochemical assays and electron spin resonance spectroscopy (ESR), and have established nanodisc technologies to incorporate and stabilize P-gp for our drug finding and mechanistic studies. A cysteine-less mutant of the mouse MDR3 P-gp (MDR3CL) has been incorporated into nanodiscs and showed several fold enhanced ATPase activities. The stability of P-gp in nanodiscs was also dramatically increased. Biophysical studies using ESR showed that P-gp in nanodiscs

as compared to micelles retains the maximum ATP binding value of 2.2 mole/mole, while the dissociation constant Kd was decreased to 40 μM. Enzymatic activity assays showed similar inhibition of P-gp in nanodiscs by potential inhibitors that were identified using P-gp in micelles. These results indicate that the performance of P-gp in nanodiscs was superior to that of micelles in terms of activity, stability and ATP binding.

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INHIBITION OF ABC-TRANSPORTERS BY IN SILICO IDENTIFIED SMALL MOLECULES

Multidrug resistance (MDR), characterized by simultaneous resistance to structurally and functionally dissimilar drugs, is a major obstacle to the successful treatment of cancers. MDR is frequently associated with overexpression of transmembrane efflux proteins belonging to the ATP-binding cassette (ABC) transporter superfamily including P-gp, MRP1, and BCRP. Normally expressed at tissue barriers, these proteins protect vulnerable cells from xenobiotic attack by pumping a wide range of toxins out of the cell. Unfortunately, this broad substrate range allows the majority of clinically relevant chemotherapeutic drugs to be effluxed by P-gp, MRP1, and BCRP. Treatment and prevention of MDR have been studied extensively for decades, and yet, there are still no effective FDA-approved therapies available. Using targeted molecular dynamics and massively parallel drug docking studies, we have screened millions of drug-like molecules and identified hundreds of compounds that are predicted to specifically inhibit P-gp. In this study, we expand our in vitro screening to evaluate 46 potential inhibitors identified by our in silico screening methods and report that over 30% of these compounds restored chemosensitivity to MDR human cancer cell lines. The best of these compounds will be further investigated to determine toxicity and specificity.

Commercial Viability:
With future chemical optimization, we are working towards developing powerful co-therapeutics to treat and prevent MDR in human cancers.

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RECOGNITION OF TARGET GENE TRANSCRIPTIONAL STATE BY EPIGENETIC REGULATORS

Polycomb group (PcG) proteins are conserved epigenetic transcriptional regulators that are involved in maintaining the transcriptional repression of silenced genes rather than initiation of repression. giant (gt), a PcG target gene, is a zygotic gap gene involved in the development of the head and abdominal regions in Drosophila. To identify whether the presence of repressive transcription factors or the transcriptional state of a target gene determines how PcG proteins recognize it as repressed, a genetic system in which gt is ubiquitously activated was constructed by producing Drosophila embryos that lack the gt repressor Hb and ubiquitously express a maternal gt activator, Cad. The TATA box, Inr region and DPE of gt fragment in pENTR-gtm were mutated, then the resulted gt fragment was transferred into the Pelican destination vector and the resulted expression vector will be injected into the embryos and transgenic lines will be generated. Males then will be crossed to females expressing gt ubiquitously. By comparing recruitment of PcG and other relevant proteins at the transcriptionally active endogenous gt locus with recruitment at the transcriptionally inert Pelican-gtm-Δ Inr ΔTATA Δ DPE transgene, we will test whether the binding of repressive transcription factors or the transcriptional state of a gene initially identifies a PcG target gene as repressed.

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MECHANISM OF TAKEOUT-DEPENDENT LONGEVITY IN D. MELANOGASTER

Overexpression of takeout specifically in the adult fly fat body extends longevity by ~40%. These flies exhibit defective male mating behavior and reduced female fertility (Chamseddin, Khan et al. 2012). In Manduca sexta, takeout has over 24% identity and 54% similarity to Juvenile Hormone binding protein (Sarov-Blat, So et al. 2000). When treated with methoprene (JH analog), the longevity and mating phenotypes observed in takeout overexpressing flies were reversed (Chamseddin, Khan et al. 2012). This might suggest that takeout extends lifespan by decreasing JH signaling. As takeout overexpressing male flies have reduced courtship behavior, it might be possible that takeout is able to regulate signaling pathways that are important for specific social behaviors. In animals, social behaviors are regulated through pheromones. Interestingly, in flies pheromone profile changes with corpora allata (site of JH production) knockout (Bilen, Atallah et al. 2013). This might indicate that JH plays a significant role in pheromone production. I hypothesize that takeout exerts its effect through modulation of Juvenile Hormone signaling, which in turn modulates pheromone production. Altered pheromone production may in turn change male mating and female fertility phenotypes. This will then ultimately lead to lifespan extension.

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THE HTLV-1 LATENCY-MAINTENANCE FACTOR P30II INHIBITS TAX-INDUCED NF-KAPPA B ACTIVATION AND PREVENTS ONCOGENE-INDUCED CELLULAR SENESCENCE

Human T-cell leukemia virus type-1 (HTLV-I) infects CD4+ T-cells and is linked to adult T-cell leukemia/lymphoma (ATLL). The viral transactivator, Tax, is important in the early stages of T-cell immortalization by HTLV-1. Tax functions as a regulator of cellular signaling pathways. HTLV-1 latency-maintenance factor, p30II, has been shown to negatively regulate retroviral replication at the transcriptional and posttranscriptional level. Tax is a potent activator of HTLV-1 gene expression through NF-kB-dependent signaling. Tax also represses the transcriptional activity of p53 and inhibits p53 functions through the activation of NF-kB signaling. Studies from our lab have shown that HTLV-1 p30II cooperates with c-Myc and enhances its oncogenic potential through activation of p53-dependent pro-survival genes. Stathmin gene- a member of microtubule-destabilizing proteins is negatively regulated by p53. Stathmin is known to interact with p65-RelA complex in pancreatic cancers. My studies have demonstrated that HTLV-1 p30II induces p53 and inhibits Stathmin expression. p30II also reduces Ser16-phosphorylation of Stathmin. We hypothesize that p30II may augment p53 pro-survival functions in HTLV-1-infected cells by inhibiting Tax-induced NF-kB activation, through a mechanism involving the phosphorylation of Stathmin and inhibition of Stathmin/p65 (RelA) molecular interactions.

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IN SILICO SELECTIVE SCREENING FOR INHIBITORS OF ABC TRANSPORTERS THAT MINIMIZES OFF TARGET TOXICITY

The ATP-binding cassette (ABC) class of transporters is involved in many diseases. Chemotherapy resistant, recurrent cancers commonly express ABCB1 P-glycoprotein transporter (P-gp) and ABCG2 Breast Cancer Resistance Protein (BCRP). At high levels of expression, both transporters lower the intracellular concentration of chemotherapeutics to a subtherapeutic level. The prokaryotic transporter MsbA is an essential ABC lipid A flippase homologous to the human multidrug resistance proteins. Currently used methods of computational screening for inhibitors lack discrimination against off target interactions and are dependent on the quality of the starting structure. To prevent inherent biases from single structures, simulations of a catalytic cycle using targeted molecular dynam-

ics was performed. Molecular dynamics simulations of MsbA and Cyt P450 3A4 were used to generate screening targets. Targeting the ATP binding domains and drug binding domains of P-gp, and related domains of MsbA and the active site of P450 allowed for selection of hit compounds that are specific to one region of the protein of interest and avoid off site interactions. Iterative screening on similarity subsets of the ZINC database was performed, with subsequent screens based on the diversity of hits found in initial screens.

Commercial Viability:
This method directly identifies potential treatments to resistant cancer and novel antibiotics.

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REVERSAL OF MULTI DRUG RESISTANCE IN CANCER CELLS.

Overexpression of ATP-binding cassettes (ABC) type transporters is associated with multidrug resistance (MDR) in tumors. P-glycoprotein (P-gp) and breast cancer resistance protein (BCRP) are two of the most studied drug transporters regarding to MDR and still no clinically approved drugs are available to inhibit these proteins. Using computational studies we have identified new compounds that can inhibit P-gp. Several of these compounds show successful MDR reversal in drug resistant DU144TXR prostate cancer cell line. Here, we study the three initially identified compounds (SMU-29, 34 and 45) in the P-gp overexpressing A2780ADR ovarian cancer cell line.

Commercial Viability:
Overexpression of P-gp was confirmed by western blot analysis in A2780ADR compared to parental, drug sensitive cell line A2780. Drug resistance of A2780ADR to vinblastine could not be reversed by the BCRP-specific inhibitor, novobiocin, or the MRP1 specific inhibitor, probenecid, indicating P-gp specific overexpression in these cells. Resistance of A2780ADR to the P-gp substrates, vinblastine and paclitaxel, was reversed by the three newly identified P-gp inhibitors. We also report preliminary results of developing a BCRP overexpressing MCF-7 breast cancer cell line through exposure to incrementally increasing concentrations of the BCRP substrate, mitoxantrone, to achieve drug resistance.

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MITOCHONDRIAL PEROXIREDOXIN 5 IS ESSENTIAL FOR REGULATION OF REDOX, IMMUNITY AND LONGEVITY

Drosophila under-expressing dPrx3 and dPrx5, the only mitochondrial peroxidases, have a dramatically shortened life-span and other aging-associated characteristics. Functional analysis of RNAseq data revealed a prominent cluster enriched for immunity-related genes, including a considerable number of antimicrobial peptides (AMP), whose activation is triggered via the Drosophila NF-kB immune pathways, Imd and Toll. Using qRT-PCR analysis we determined that the age-dependent changes in AMP levels in mutant flies were similar to those observed in controls when scaled to percentage of life span, or physiological aging. A similar age-related tendency has been observed in GSH:GSSG ratio and levels of protein sulfhydryls, suggesting links between redox and the immune pathways. To further clarify the role of Prx-dependent mitochondrial signaling, we expressed different forms of dPrx5, which unlike mitochondrial dPrx3 is found in multiple subcellular compartments, including mitochondrion, nucleus and cytosol. Ectopic expression of dPrx5 solely in mitochondria but not nucleus or cytosol partially rescued the shortened longevity phenotype of the double mutant and completely restored survivorship under oxidative stress conditions. The role of these different forms in regulation of immunity is currently under investigation.

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THE CONTRIBUTIONS OF MULTIPLE FACTORS IN PCG RECRUITMENT

Polycomb-group(PcG) proteins are conserved epigenetic transcriptional regulators that are capable of maintaining transcriptional repression through an indefinite number of cell cycles. giant(gt) is a gap gene in Drosophila and also a PcG target gene. Hunchback(Hb) is a repressor for gt. Previously we found that PcG takes over gt repression after Hb is degraded. We have generated a genetic system in which maternal hunchback Hb is expressed ubiquitously but no zygotic Hb expression is absent. Chromatin immunoprecipitation (ChIP) analysis of embryos at multiple developmental stages is being performed to determine the timing and locations of binding by transcription factors, PcG proteins, and deposition of histone modifications. In order to determine the roles played by individual proteins or protein complexes in establishment of PcG silencing, individual proteins will be knocked down using combinations of a maternal Gal4 driver and UAS- shRNA-expressing transgenes. Current work includes construction of necessary fly stocks and testing the effectiveness of individual transgenes. Immunostaining of embryos and ChIP experiments will be done to examine the consequences of PcG recruitment when losing each one of these proteins.

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THE ROLE OF CEREBELLIN-4 IN THE REGULATION OF NEURODEGENERATION

Huntington's disease (HD) is neurodegenerative disorder caused by an abnormal expansion of a polyglutamine stretch in the huntingtin protein (mut-Htt) and that is characterized by a selective loss of striatal neurons. Another member of the lab recently identified a protein, FoxP1, that is highly expressed in the striatum and which can protect cultured neurons from mut-Htt toxicity. To understand the mechanism by which FoxP1 protects against mut-Htt, we analyzed RNA-Seq data of gene expression changes in the striatum of FoxP1 conditional knockout mice recently published by another lab. I picked 6 genes reported to be differentially-expressed in the RNA-Seq analysis and analyzed their expression in neurons overexpressing FoxP1. I found that one of the 6 genes, cerebellin-4 (cbln4), is highly up-regulated in FoxP1-overexpressed neurons. To examine if clbn4 contributes to neuroprotection, I overexpressed it in a model of neuronal apoptosis utilizing cerebellar granule neurons. Preliminary results I have obtained suggest that overexpressing cbln4 can protect these neurons from apoptosis. In the future, I will check if cbln4 can protect neurons from mut-Htt toxicity. Then, I will try to find the mechanism by which cbln4 protects neurons. I hope my research will lead to the identification of molecules that can be targeted for the development of therapies for Huntington disease.

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THE DESIGN AND SYNTHESIS OF C6-SUBSTITUTED CARBAPENEM COMPOUNDS WITH IMPROVED EFFICACY AGAINST HIGHLY RESISTANT GRAM-NEGATIVE PATHOGENS

In 2050, scientists predict 10 million deaths due to highly antibiotic resistant strains of Pseudomonas aeruginosa, Klebsiella pneumonia, and Acinetobacter baumanni will develop. These strains process multiple resistance mechanisms, including the production of multiple beta-lactamases, including carbapenemases, decreased permeability, and up-regulated efflux, thus presenting the clinician with highly limited opportunities for successful treatment. All current commercial carbapenems have a C6 hydroxyethyl group. We will discuss our research methods of C6-modified carbapenems.

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RATIOMETRIC PH SENSITIVE CHEMILUMINESCENCE PROBE

A pH sensitive chemiluminescence probe has been developed and synthesized in the past several months. For this probe, the intensity of the light generated by the probe will increase with the pH of the ambient environment. Another property of this probe is with the existence of the pH sensitive dye SNARF-I, the ratio of red and green light will vary, which can provide more accurate quantification since the intensity of light will vary if we use the probe in vivo. The ratio of the light intensity at different pH will be reported. The ratio of light emission at the normal pH in human body, which is 7.4, is three fold then the ratio at pH 6.8, which is usually the pH of a tumor. I've also change the other factors, which can effect the ratio of the light. Fortunately, the other factors only minimally change the ratio. The correlation between different pH and the ratio of light can be applied to test different pH in vivo in the future.

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IN VIVO CHEMILUMINESCENT IMAGING AGENTS FOR NITROREDUCTASE AND TISSUE OXYGENATION

Tissue oxygenation is a important parameter of the tumor microenvironment and hypoxia can be a prognostic indicator of severity of cancer disease. Therefore, finding an easy way for detection and monitoring oxygen level and hypoxia is of great importance in cancer diagnosis and treatment. Here we report a reaction-based chemiluminescence imaging probe (HyCL-2), which responds to nitroreductase with ~170-fold luminescence intensity increase within 20 min, with high selectivity for nitroreductase versus other biological reductants. HyCL-2 has also been demonstrated to image exogenous nitroreductase in vivo in wild-type mice. Finally, HyCL-2 can image tumor hypoxia during oxygen challenge in tumor xenografts.

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EVOLUTION OF SEQUENCES AND STRUCTURES IN METALLO-B-LACTAMASE SUPERFAMILY

Metallo-β-lactamase (MBL) enzymes produced by gram-negative bacteria were identified to cause numerous antibiotics ineffective by breaking lactam structure. Although the wide usage of antibiotics for protecting human health has significantly accelerated the emergence of resistant strains, MBL resistance function against antibiotics is found to have first evolved beyond two billion years. Therefore, the understanding of the evolution of resistance is helpful to explain the mechanism of resistance generation and develop effective strategies to prevent the MBL antibiotics resistance. In our study, we compared those MBL coding sequences in gram-negative bacteria to explore the evolution of resistance, and found the genetic basis that influenced the resistance for antibiotics. In addition, we attempt to analyze the change of MBL structures caused by genetic mutations in evolution process to improve the understanding of the mechanism of resistance generation.

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SHORT LOV PROTEINS IN METHYLOCYSTIS REVEAL INSIGHT INTO LOV DOMAIN PHOTOCYCLE MECHANISMS

Light Oxygen Voltage (LOV) proteins are widely used in optogenetic devices, however universal signal transduction pathways and photocycle mechanisms remain elusive. Short-LOV (sLOV) proteins have been discovered in bacteria and fungi, containing only the photoresponsive LOV element, lacking signal transduction domains. Herein, we identify a family of bacterial sLOV proteins present in Methylocystis, of which sequence analysis demonstrates conservation with sLOV proteins from fungal systems that employ competitive dimerization as a signaling mechanism. Characterization of Methylocystis LOV proteins (McLOVn) confirms functional dimer formation and reveals unexpected photocycle mechanisms. Specifically, McLOVn photocycles are insensitive to external bases such as imidazole, in contrast to previously characterized LOV proteins. Mutational analysis identifies a key residue that imparts insensitivity to imidazole and affects the rate of adduct decay. The resultant data identifies a new family of LOV proteins that indicate a universal photocycle mechanism may not be present in LOV proteins. We focus on two experiments. 1) Eyring and Arrhenius parameters for adduct decay. 2) The effect of small molecule bases on adduct recovery. Previous research in other LOV proteins indicates that solvent access to the active site can be probed using small molecule bases.

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DETERMINATION OF THE INTRINSIC BOND STRENGTH OF TRANSITION METAL DIMERS

Diatomic transition metal molecules M2 have been repeatedly investigated in the last 4 decades in either model-based investigations or in a more quantitative approach targeting the bond dissociation energies (BDEs). One has described σ-, π-, and δ-bonding between the M atoms and has identified MM bonds with quadruple, pentuple, and even sextuple character. However, any MO or NO (natural orbital) bond order is limited by the definition it is based on whereas the BDE can say little about the intrinsic strength of a bond. We use the MM stretching force constant to determine the intrinsic bond strength because a stretching vibration probes the strength of a bond. Since the force constant is determined via the second derivative of the energy with respect to the bond length and thereby relates to an infinitesimal change in the geometry, it corresponds to a bond strength descriptor without changes in the electronic structure of M2. Stretching force constants are calculated because of the multireference character of many M2 molecules, either by CASPT2, NEVPT2, RASPT2 or MR-AQCC methods and augmented quadruple-zeta basis sets. Using the stretching force constants of suitable reference molecules with known bond multiplicity, a bond strength order (BSO) of M2 molecules is derived, which reveals that Mo2 and W2 are the molecules with largest intrinsic bond strength investigated so far.

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STRUCTURAL BIOCHEMISTRY OF A FUNGAL LOV DOMAIN PHOTORECEPTOR REVEALS AN EVOLUTIONARILY CONSERVED PATHWAY INTEGRATING LIGHT AND OXIDATIVE STRESS

Envoy is a photoreceptor protein found in fungus Trichoderma.reseei. It belongs to a subclass of PAS (Per-Arnt-Sim) family of proteins known as LOV (Light Oxygen Voltage) domains. They are prevalent in all kingdoms of life involved in regulation of various physiological processes. Envoy has evolved as a dual oxidative stress and blue-light sensor to regulate sexual reproduction, cellulase production and stress responses. It has 38% identity and 57 % similarity to the amino acid sequences of VVD. VVD is also an fungal photoreceptor protein involved in circadian regulation of Neurospora.Crassa. Similarity of sequences may suggest similar mechanisms of activation. Using a combination of solution biophysics and structural characterization we have demonstrated that ENV1 employs a divergent mechanism to incorporate oxidative stress and blue-light signaling into regulation of gene expression. Interestingly,

although the core circadian machinery in T.reesei is conserved with N. crassa,(VVD=ENV1, Blr1=WC1, Blr2=WC2), they differ on the level of fundamental chemistry and signaling mechanisms. Thus, even closely related species adapt integration of environmental variables into circadian regulation.

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THE PSEUDOLIBRATIONAL SURFACES OF THE (DEOXY)RIBONUCLESIDES

The strands of RNA and DNA obtain their flexibility to a large extend from the (deoxy)ribose rings. In this work, the ring puckering, ring deformation, and pseudorotation of the four ribonucleosides and four deoxyribonucleosides are investigated utilizing curvilinear coordinates to adequately describe their complex conformational processes. The latter are strongly coupled to changes in their H-bonding patterns. The ring systems undergo pseudolibrational and pseudoinversional processes. Changes in H-bonding are monitored using the local O…H stretching force constant as a reliable measure for the intrinsic strength of these interactions. Calculations were also carried out for a DNA dimer to show the applicability of the former studies to a larger system and describe the apparent differences between an X-ray structure and gas phase calculations.

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EFFICIENT SYNTHESIS OF CIRCADIAN CLOCK MODULATOR: DELTA CARBOLINES

Cryptochrome (CRY) is an important class of mammalian flavoprotein, which participates in various metabolic pathways including sleep-wake cycle, hormone secretion in an auto-regulatory manner. Biochemical studies have shown their involvement in regulating hepatic gluconeogenesis, hence could be a potential diabetes target. Recently carbazole scaffolds have been demonstrated to bind the active site of cryptochrome proteins, however, lacks critical H-bonding atoms that can facilitate recognition and binding. In contrast, carbolines, which contain two fused nitrogen rings, are important carbazole derivatives that introduce H-bonding characteristics to the carbazole scaffold. Notably, these carboline scaffolds have been targeted as potential drug molecules. Specifically, beta-carbolines occur widely in nature and have been studied as potential anti-cancer and anti-malarial compounds. Delta-carbolines are less common in nature and historically been viewed as having cytotoxic effects. To better understand the functional differences of carbazole, delta-carboline and beta-carboline scaffolds we sought out to prepare analogues varying in the nature of the core scaffold. In the process we have identified two-step robust formation of delta-carbolines via reactions of benzyne and 2-halo-aminopyridines, followed by microwave intramolecular cyclization.

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POLYPHOSPHAZENES AS AN ANTIMICROBIAL SURFACE COATING FOR BREAST IMPLANTS

Infection of implant site after reconstructive breast surgery is an increasingly serious problem for post mastectomy patients. The purpose of this ongoing work is to prepare antimicrobial inorganic polymers, specifically polyphosphazenes, and test their biocompatibility so that they may serve as infection-preventing surface coatings for reconstructive breast implants. Several methods are being explored for the synthesis of such polymers, with a focus on deprotonation-substitution derivation of the parent polymer through an aldehyde functional group. The precursor polymer has been developed and characterized, and reaction conditions for attachment of the antibacterial group are currently being investigated.

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HALOGEN BONDING - A HIGH-ACCURACY DESCRIPTION OF ITS UNIQUE FEATURES

Halogen bonding corresponds to a non-covalent interaction between electrophilic X2 or XY (X, Y = F, Cl, Br, I, At) and a nucleophilic heteroatom. Due to its unique features, this interaction is increasingly utilized in medicinal, supramolecular, and materials chemistry. Halogen bonding has been investigated in numerous quantum chemical studies. Despite of this, there are still a scarce number of high accuracy studies on halogen bonding. In this work, the strength and nature of 40 halogen-bonded complexes were analyzed and compared with 8 complexes formed by other types of non-covalent interactions. These interactions were investigated using as appropriate tools the local stretching force constant ka, the electron density ρ(r), and the energy density H(r). All calculations were carried out using the highly accurate CCSD(T) method. It was found that halogen bonding has a larger covalent character and can make stronger bonds than other types of non-covalent interactions, including hydrogen bonding, for both neutral and ionic species. DFT overestimates the strength of very weak halogen bonds and is unreliable when describing the strength of non-covalent bonds in ionic systems. These findings shed a new light on how to use halogen bonding in materials science.

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THREE-DIMENSIONAL IMAGE GENERATION BY A RHODAMINE-DERIVED OPTICAL SWITCH

A series of optical switches for the generation of three-dimensional images was synthesized from halogenated rhodamine derivatives via amide ring-forming substitution. Samples of each compound were irradiated using light from a fluorometer, and then the UV visible spectrometer was used to measure absorbance values to characterize the concentration, exposure time, wavelength dependence, and solvent effects of the compound. Optical displays were then generated within a solution of the optical switch at the intersection of a projected image in 532 nm light and ultraviolet light. Thus, we have been able to successfully create planar, two-dimensional images as well as symmetrical, three-dimensional images.

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A FACILE MODIFICATION OF POLY[ETHYL 2-(HYDROXYMETHYL) ACRYLATE] INTO POLY (ETHYLCYANOACRYLATE) USING HYPERVALENT IODINE

Alkyl cyanoacrylate-derived polymers are widely used as drug carriers, especially for cancer treatment, because of their biocompatibility and biodegradability under natural conditions. Alkyl cyanoacrylates have already found applications as super glue in surgeries because of their excellent adhesion to biological tissues and lack of toxicity. These monomers are highly reactive due to the presence of two electron withdrawing groups (-CN and -COOR) attached to the same carbon atom of the vinyl group, and as a result of the high reactivity, they cannot be polymerized under controlled radical polymerization conditions. We used an alternative method to convert poly[ethyl 2-(hydroxymethyl)acrylate], which is easy to prepare under controlled radical polymerization conditions to poly(ethyl cyanoacrylate) using (diacetoxyiodo)benzene as an oxidant, TEMPO as a co-oxidant, and ammonium acetate as a nitrogen source. The reactions were tested in three different solvents (DMF, acetonitrile, and DMAc), and DMAc was found to be the most useful reaction medium for the modification. 13C NMR spectroscopy was employed to monitor the progress of polymer modification.

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SPECIFIC, CELL-PERMEABLE FLUORESCENT PROBES IN THE IMAGING OF ENZYMATIC PATHWAYS IN LIVING CELLS

HNO, or nitroxyl, is a gaseous signaling molecule known to promote vasorelaxation, cardiac contractility, and antinociception. Here, we study its role as an inhibitor of the enzyme aldehyde dehydrogenase, an enzyme key in the conversion of acetaldehyde to acetic acid. We have developed two cell-permeable fluorescent probes, one specific for HNO and one for acetaldehyde, in order to visualize this pathway in living cells. In vitro studies also show that these two probes demonstrate excellent selectivity for their respective substrates, each providing a significant fluorescent turn on to their respective substrate.

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SYNTHESIS OF VIOLOGEN-CONTAINING BRANCHED POLYMERS AND THERMORESPONSIVE BRANCHED POLYMERS

Hyperbranched polymers (hb-polymers) can be synthesized through radical copolymerization of a monovinyl compound with a divinyl crosslinker in the presence of an efficient chain transfer agent. This project has two main focus areas. First, the synthesis of hb-polymers with viologen peripheral groups was carried out using oligo(ethylene glycol) methyl ether methacrylate (OEGMEMA) and crosslinker ethylene glycol dimethacrylate (EDGMA). The produced Br-capped hb-polymers were then reacted with 4,4'-bipyridine followed by alkylation with 1-bromodecane to afford the target viologen-capped polymers. The polymers were then combined with β-cyclodextrin to study the interaction (complexation) between the peripheral groups and the cyclic carbohydrate. Second, studies were conducted on the impact of branching on the thermal responsive behavior of polymers with lower critical solution temperature in aqueous solution. In particular, the two factors studied are the hydrophilic/hydrophobic nature of the crosslinker and the amount of crosslinker used. Both of these factors impacted significantly the thermal responsive behavior of the polymer.

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A DIRECT MEASURE OF METAL-LIGAND BONDING REPLACING THE TOLMAN ELECTRONIC PARAMETER (TEP)

The prediction of the catalytic activity of transition metal complexes is a prerequisite for homogeneous catalysis. The Tolman Electronic Parameter (TEP) was derived to provide this information. It is based on the CO stretching frequencies of metal-tricarbonyl complexes L-M(CO)3 with varying ligands L. It has been used in hundreds of cases. We show that the TEP is misleading as i) it is not based on mode-decoupled CO stretching frequencies and ii) a quantitatively correct or at least qualitatively reasonable relationship between the TEP and the metal-ligand bond strength does not exist. This is demonstrated for a set of 181 nickel-tricarbonyl complexes using both experimental and calculated TEP values. Even the use of mode-mode decoupled CO stretching frequencies does not lead to a reasonable description of the metal-ligand bond strength. A reliable descriptor replacing the TEP is obtained with the help of the metal-ligand local stretching force constant. For the test set of 181 Ni-complexes, a direct metal-ligand electronic parameter (MLEP) in the form of a bond strength order is derived, which reveals that phosphines and related ligands (amines, arsines, bismuthines) are bonded to Ni both by σ-donation and π-back donation. The strongest Ni-L bonds are identified for carbenes and cationic ligands. The new MLEP quantitatively assesses electronic and steric factors.

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THE PIVOTAL ROLE OF DI-COPPER CATALYSIS IN 1,3-DIPOLAR CYCLOADDITIONS: A REACTION VALLEY STUDY

Catalysis is one of the major chemical challenges of our time. Transition metal catalysis specifically has the potential to facilitate the synthesis of desirable chemicals. This work is a mechanistic investigation of homogeneous catalysis utilizing an off-mainstream methodology: Rather than investigating just the energetics of a catalyzed reaction, the potential energy surface is explored in the vicinity of the reaction path following it from its start to its end. In this way, the reaction valley is studied for the purpose of unraveling the coupling between vibrational and translational motions of the reaction complex, which is decisive for the mechanistic outcome. A dual level approach was used, based on Coupled Cluster theory for the energetics and a lower level method for the description of the reaction valley. Eight Cu-catalyzed 1,3-dipolar cycloadditions to acetylene are analyzed. Decomposition of the reaction path curvature into internal coordinate components allows the identification of chemical events, such as rehybridization and bond formation, as they occur along the reaction path. A di-Cu catalyst converts a one step mechanism to a two-step mechanism, where each step has a significantly lower barrier than the uncatalyzed reaction. Electronic reasons for the effectiveness of the Cu catalyst in the cycloaddition reactions will be discussed.

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ATP HYDROLYSIS MECHANISM IN P-GLYCOPROTEIN SYSTEM STUDIED BY QM/MM

P-Glycoprotein (P-gp) is a plasma membrane efflux pump that is commonly associated with therapy resistances in cancers and infectious diseases. There are two parts in Human P-gp. One is two nucleotide-binding domains (NBDs) and the other is two transmembrane domains (TMDs). The NBDs provide a location for adenosine triphosphate (ATP) to bind whereas the TMDs provide a binding site for drugs. ATP is an energy source for drug transport through its hydrolysis. Currently, ATP hydrolysis mechanism in this biological system is not well understood. Hybrid quantum mechanical and molecular mechanical (QM/MM) methods are applied to investigate the ATP hydrolysis mechanism in NBD of P-gp. In QM/MM methods, quantum mechanics (QM) are used to calculate the key part of a system, molecular mechanics (MM) are used to calculate remaining parts. In this system, the methyl-triphosphate fragment of ATP is treated as QM region. Some water molecules, ions and residues around ATP are also included. The remaining of the P-gp simulation system is treated as MM region. We will use CHARMM (Chemistry at HARvard Molecular Mechanics) and Q-Chem program to perform the calculation.

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SYNTHESIS OF SULFUR-RICH BRANCHED POLYMERS BASED ON ALPHA LIPOIC ACID DERIVATIVES

Sulfur-rich branched polymers have been prepared from 2-acryloyloxyethyl lipoate (AOELp), a monomer containing two radically polymerizable moieties: a cyclic disulfide and a vinyl group, which is synthesized by the esterification of 2-hydroxyethyl acrylate (HEA) and lipoic acid (LA). Since the cyclic disulfides are able to participate in radical ring-opening polymerization, they incorporate into the propagating polymer chain and leave the vinyl sites as pendants for crosslinking during the free radical polymerization. The branched polymers with disulfide bonds embedded in the backbones are thus formed by at least two consecutive cyclic disulfide radical ring-opening reactions or by the radical coupling of two sulfur-centered radicals. Alternatively, the disulfide bonds can cleave into two thiols upon suitable reducing agents, and produce a much branched architecture when treated with radicals or bases due to the coupling reaction between vinyl groups and thiols. These two different mechanisms highlight the application of the lipoate in the synthesis of sulfur-rich branched polymers and also the design of new biodegradable materials.

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THE 16 DIFFERENT TYPES OF H-BONDING IN WATER

Liquid water is considered as the original birthplace of all living creatures on earth. All its properties are intimately related to the H-bond network among the individual water molecules. Although water has been investigated a multitude of times with many different methods, it still bears its secrets. In this work, we demonstrate that vibrational spectroscopy is a powerful tool to investigate water clusters, which may function as useful models for liquid water. We identified 16 different types of H-bonding in liquid water as modeled by water clusters of 50 molecules and being optimized using the ωB97X-D/6-31G(d,p) level of theory. Utilizing local vibrational modes, the 16 types of H-bonding are quantitatively distinguished. Thermodynamic stability of a water cluster is given when the maximal number of 4-fold coordinated water molecules is reached.

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CHALCOGEN BONDING – FROM ELECTROSTATIC TO COVALENT INTERACTIONS

One understands as chalcogen bonding the interaction of a heteroatom Y possessing one or more electron lone pairs with an EX single or double bond where E = O, S, Se, Te, Po. Chalcogen bonding has similarities with halogen bonding and can be as strong as halogen bonding. Very often chalcogen bonding is supported by hydrogen bonding. It can be of electrostatic nature or, if there is a strong delocalization of the electron lone pair of Y into the σ*(EX) orbital, of covalent nature. Especially, the interaction of halogenide anions with XEH molecules can lead to strong covalent chalcogen bonds. In this work, the strength and nature of 50 chalcogen-bonded complexes were investigated utilizing coupled cluster and density functional theory at the CCSD(T)/aug-ccpVTZ and ωB97X-D/aug-ccpVTZ levels of theory. The intrinsic strength of chalcogen bonding was determined with the help of the E…Y local stretching force constant. For each bond investigated, the nature of the bond was determined by calculating the electron density ρ(r) and the energy density H(r) at the bond critical point and then using the Cremer-Kraka criterion of covalent bonding.

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THE DYNAMICS AND MECHANISMS OF B-LACTAMASES ABOUT ANTIBIOTICS RESISTANCE USING COMPUTATIONAL METHODS

β-Lactamases provide resistance to β-lactam antibiotics such as penicillins, cephamycins, and carbapenems by breaking the antibiotics' structures. We employed various computational methods to study β-lactamases dynamics and mechanisms related to antibiotics resistance. First, the elastic network models (ENMs) were used to characterize the global dynamics of β-lactamases through vibrational normal modes. Second, molecular dynamic (MD) simulations were carried out to sample the canonical ensemble of β-lactamases. Quasi-harmonic analysis will be carried out on MD simulations and compared with ENM results. Third, quantum mechanics/molecular mechanics (QM/MM) methods will also be applied to elucidate the catalytic mechanisms of selected β-lactamases.

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SYNTHESIS AND CHARACTERIZATION OF LINEAR HOMO- AND CO-POLYMERS CONTAINING PENDANT VIOLOGEN UNITS BY ATOM TRANSFER RADICAL POLYMERIZATION

A radically polymerizable viologen-containing compound, 1-propyl-1-[2-(methacryloyloxy)ethyl]-4,4'-bipyridinium hexafluorophosphate (Pr(MEOE)Vl), was synthesized and polymerized under traditional atom transfer radical polymerization (ATRP) conditions to yield well-defined linear polymers (poly(Pr(MEOE)Vl)) with multiple viologen pendant groups. Poly(Pr(MEOE)Vl) tended to aggregate in solutions in the absence of salts and disaggregate in solutions containing high concentration of salts such as NaCl. The aggregation phenomena were studied by diffusion-ordered NMR spectroscopy and dynamic light scattering. Fluorescence spectroscopy studies also showed that poly(Pr(MEOE)Vl) was highly fluorescent in aqueous solutions and the addition of NaCl quenched the viologen fluorescence. Upon reduction by hydrazine, the aqueous solution of poly(Pr(MEOE)Vl) became intensely purple due to formation of viologen radical cations followed by very fast dimerization; this process was studied by UV-vis spectroscopy. Poly(diethylene glycol methyl ether methacrylate)-b-poly(Pr(MEOE)Vl) were synthesized by ATRP by chain extension of poly(diethylene glycol methyl ether methacrylate)-based macroinitiators with Pr(MEOE)Vl. The macroinitiators were synthesized by low-catalyst concentration (ARGET) ATRP. The thermoresponsivity of the block copolymers was studied by UV-vis spectroscopy.

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THE SHARPLESS EPOXIDATION OF ALLYLIC ALCOHOLS WITH AN TITANIUM CATALYST – EXAMPLE FOR THE TRANSITION FROM HOMOGENEOUS TO HETEROGENEOUS CATALYSIS

The Sharpless epoxidation implies an enantioselective reaction to synthesize 2,3-epoxyalcohols in the presence of hydroperoxide, a titanium (IV) catalyst with a tartrate diester ligand, and secondary allylic alcohol. The oxidation to epoxides proceeds with good yield and an excellent enantioselectivity. We studied a number of Sharpless epoxidations to clarify the basic reaction mechanism and to explore the dependence of the reaction on the conformation of the starting reactant. Depending on the position of the allylic ligand below (barrier: 25 kcal/mol) or above the ring system (barrier: 19 kcal/mol) the reaction barrier changed along with the mechanism of the reaction. The catalytic activity is based on a ring system and it's substituents where the latter force the hydroperoxide into a central position with one O atom being easily positioned opposite to a rotating allyl group. The Sharpless catalyst mimics a surface in heterogeneous catalysis with a top or bottom approach possibility. The Ti -peroxide interactions labialize the OO bond and in this way reduce the barrier for OO cleavage, which without catalytic support would be above 40 kcal/mol.

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COMPUTATIONAL STUDY OF ALLOSTERY OF VIVID PROTEIN, A PAS/LOV DOMAIN IN CIRCADIAN CLOCK SYSTEM

Allostery is a ubiquitous process allows for protein function changes due to ligand binding. Developing allosteric drugs targeting key proteins in signaling pathways is becoming important revenues in drug discovery. However, the understanding of protein allosteric mechanisms is the major bottleneck in this effort. To make breakthrough, fully understanding allostery that is highly correlated with protein dynamics is inevitable. Recently, we developed a novel simulation method, named as rigid residue scanning (RRS), to systematically identify key residues for allostery. In this study, we employed RRS method to explore the allosteric mechanism of VIVID protein from Light-Oxygen-Voltage (LOV) domains in circadian clock system. In RRS method, an efficient rigid body dynamics integrator was applied to carry out MD simulations to systematically probe the effect of removing individual residue internal degrees of freedom on the whole protein dynamics. We also calculated entropies of individual simulations and applied RMSD clustering method to show the alteration between two states simulations. Several key residues including Ser63, Ala88, Val118 and Val168 were identified. In addition, the principle component analyses (PCA) combining with quasi-harmonic approximation were carried out to reveal the changes of dynamics in different parts of protein when each residue being held rigid.

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A GEOTHERMAL GRADIENT BASED CORRECTION TO BOTTOM-HOLE TEMPERATURES: DENVER BASIN

The purpose of this project is to make the numerous amounts of publicly available bottom-hole temperature (BHT) data usable in order to approximate temperatures at depths throughout sedimentary basins. BHT data was gathered from the National Geothermal Database from oil and gas well located in the states of Colorado, Wyoming, Nebraska, and Kansas of wells greater than 1 kilometer in depth. BHT data is often misleading due to the fact that the well bore is not at thermal equilibrium when the well is logged at its bottom. Given the height, width and breadth of sedimentary basins and the non-uniform crustal heat flow, previous 1D BHT correction models exclude regional variability in thermal regimes within the basin. This correction model normalizes the vast database of BHT points by its measurement depth to use the whole dataset while assuming that there is variation in equilibrium geothermal gradient throughout the basin. Over 55,000 BHT data points fell within the 1 kilometer or deeper threshold for this project. A correction was then developed from the difference in uncorrected geothermal and equilibrium geothermal gradients. This correction allows me to make a more accurate prediction of temperature at depth across the basin using the vast database of BHTs.

Commercial Viability:
Approximating temperature at depth within a sedimentary basin is a useful tool whether you are looking for the right thermal maturation window for hydrocarbons or temperature at depth for geothermal energy systems. The most abundant source of information for temperature at depth comes from bottom hole temperature measurements from oil and gas wells that are recorded shortly after the cessation of drilling fluid within the wellbore

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IMPROVING INFRASOUND DETECTION AND LOCATION CATALOGS IN THE WESTERN US USING ATMOSPHERIC MODELING

Automated infrasound catalogs are useful for documenting repeated sources as well as evaluating detection performance across a given network under time-varying atmospheric conditions. An automated process for detection, association, and location is tested using data from three infrasound arrays (BRP, FSU, and HWU). The adaptive F-detector (Arrowsmith et al., 2009) accounts for correlated and uncorrelated noise through modification of the conventional F-statistic to capture time-varying background noise and reduces false detections due to the presence of coherent noise. The Bayesian infrasonic source location (BISL) method updated by Blom et al. (2015) produces source location and time credibility contours from posterior probability density functions. For this work, propagation-based models have been calculated from the Ground-to-Space (G2S) atmospheric database. Infrasonic array data is tested over a two-year time period (1 November 2010 to 31 October 2012) and compared to a previously constructed catalog of infrasonic events within the western US (Park et al., 2014) to analyze changes in spatial and temporal confidence bounds of the source with the addition of propagation-based priors.

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PHYSICS-BASED MODELS OF ALEUTIAN VOLCANISM: A STUDY OF THE EFFECT OF SUBDUCTION ZONE DYNAMICS ON DEFORMATION SOURCE PARAMETERS USING INSAR, GPS, AND SEISMICITY

The Aleutian arc is composed of volcanoes affected by varying subduction zone dynamics. As the rate, angle, and material subducted transitions longitudinally, eruption and deformation styles between each volcano also evolve. Although remote, the Aleutians are situated along a major flight path between North America and Asia. Hazards posed by ash emissions from volcanic eruptions can

include loss of life and substantial economic loss to the airlines involved. Therefore, being able to accurately predict the onset and style of eruption would be extremely beneficial. InSAR, GPS, and seismic analyses, will allow the development of individualized physics-based models at five volcanoes in the Aleutians: Korovin, Okmok, Shishaldin, Augustine, and Spurr. These volcanoes require more precise characterizations for deformation source parameters than are currently available through simplified kinematic models. The need for more realistic physics-based models and investigations into the effect tectonic regimes have on these model parameters have presented themselves as the next challenges in the study of volcanic deformation. I will use a combination of Bayesian inversion and Markov Chain Monte Carlo algorithms to assess the dominant stresses involved at each volcano to improve our understanding of volcanic plumbing systems and tectonic deformation along the Aleutian arc.

Commercial Viability:
The Aleutian arc contains nearly 8% of the world's active volcanoes and more than 85% of historically active volcanoes in our nation. There has been an average of 3-4 explosive eruptions per year from the Aleutian arc. Monitoring these remote volcanoes is important as explosive eruptions produce ash clouds that pose serious hazards to aircrafts over the Aleutian arc, where ~10,000 passengers and millions of dollars in cargo fly across daily. The application of physics-based models to remote locations like the Aleutian arc is essential for efforts involving the mitigation of economic and personal loss.

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INSAR ANALYSIS OF FIRE-INDUCED SURFACE DEFORMATION OVER PERMAFROST IN ALASKAN BOREAL FORESTS

Permafrost plays a significant role in landscape stability, carbon cycling, and socioeconomic development, and is crucial for regulating the biological, hydrological, geophysical, and biogeochemical processes in cold regions including Alaska. The discontinuous permafrost zone is one of the most sensitive areas to climate warming because its active layer thickness is highly responsive to subtle temperature changes. Alaskan boreal forest widely overlaps the area of discontinuous permafrost. Wildfire is one of the most important agents affecting permafrost in the boreal forest. After wildfire, there is usually a subsequent increase in soil temperature and depth of thaw that accelerate surface deformations. With large-scale coverage features, InSAR is a useful tool for mapping deformations yet has some limitations in retrieving deformations over permafrost, especially in boreal forests, such as, scarcely-distributed good scatterers and decorrelation. Our study area is located in Alaska interior near the flood plain of Yukon River and was covered by boreal forest before experiencing wildfire in 2009. In this project, in addition to fire scar mapping using Landsat TM/ETM and SAR intensity images, advanced SAR analyses was conducted, using L-band ALOS PALSAR data, to quantify fire-induced permafrost degradation by producing improved deformation time-series based on SBAS algorithm.

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SPACEBORNE RADAR OBSERVATIONS REVEAL THE COMPACTION OF TAILINGS IMPOUNDMENT AND THE COUPLING BETWEEN HYDROLOGICAL AND SEISMOLOGICAL PROCESSES OF AQUIFER BASIN OVER SALT LAKE VALLEY, UTAH

Pore pressure transients in aquifer basin can induce ground deformation and modulate seismic behavior. We applied interferometric synthetic aperture radar analysis to map time-series deformation at the tailings impoundment and the aquifer in Salt Lake Valley from 2004. We show that the impoundment is sinking at >200 mm/yr. Geertsma's poroelastic model suggests a 200~300-m-radius disk reservoir beneath the southeast compaction source. Displacement maps also highlight an area southwest to the Salt Lake City bounded by faults, exhibiting marked seasonal oscillations with a net uplift of 15 mm/yr. The confined aquifer between the impoundment and Salt Lake City witnessed the majority of earthquakes. The number of earthquakes peaks in March, corresponding to the time of uplift summit. In addition, the cross-correlation with hydrological observations reveals that the seasonal deformation is modulated by water recharge and discharge simultaneously. Large seasonal oscillations reflect rapid redistribution of groundwater whereas long term uplift reflects net increase in pore pressure. The spatiotemporal correlation demonstrates that the hydrological and seismological processes are coupled. The complex kinetic chain associated with natural and human activities can greatly influence the Wasatch fault segments underlying Salt Lake City, which is probably overdue for another >M7 earthquake.

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STRESS DROPS OF THE AZLE, TEXAS, EARTHQUAKE SEQUENCE

This study describes the source properties of injection-induced earthquakes in Azle, Texas located in the Fort Worth Basin. The earthquake sequence in Azle was shown to be triggered by fluid injection. For this study of source characteristics, 57 earthquakes (≥ ML 2.0) were used. The epicentral distances of the observed waveforms ranged from 2 to 230 km with source depths from 1.6 to 7.8 km. Brune's earthquake source model was used to estimate source parameters. The source parameters such as moment, corner frequency and stress drop were estimated in both the time and frequency domains using P, SH, and SV waves. The results show that stress drops for these Azle earthquakes are lower than values observed for tectonic earthquakes by a factor of 10. The series of injection-induced earthquake in Azle was derived by high pore-pressure because of wastewater injection. The high pore-pressure and low stress drop could be a result of the change in effective stress on the existing fault as a result of the injected fluids. These results suggest a different interpretation with a past study in Cleburne, TX in the southern part of the Fort Worth Basin. Although the earthquakes in Cleburne are also inferred to induced-earthquakes, stress drops of these earthquakes show values of typical of intraplate earthquakes. We therefore need additional study to understand these differences.

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INVESTIGATING COMPLEX FAULT STRUCTURE AND STRIKE-SLIP RUPTURES FROM THE 2012 NORTHERN WHARTON BASIN EARTHQUAKE SEQUENCE

The multiple fault ruptures of the April 11, 2012 Wharton Basin earthquake sequence demonstrated great complexity of faulting within the Indian Ocean Basin near the 2004 Sumatra megathrust earthquake epicenter. The aftershock locations do not occur on one single fault plane but rather on multiple near-orthogonal fault planes. A new catalog of high-resolution earthquake locations paired with P-wave back-projection images improve the temporal and spatial mapping of energy released within the oceanic lithosphere during this unique earthquake sequence. Approximately 86% of analyzed events occur below the oceanic crust indicating significant deep rupture in the lithospheric upper mantle. The majority of aftershock locations appear to cluster around the edges of significant co-seismic slip or in low-slip areas when compared to fault-slip models derived from seismic and GPS data that showed most slip occurring within ~15 km depth in the lithosphere. This might suggest that aftershocks further from the main slip represent newly localized stressed areas where the fault did not slip completely. The largest fault slip occurs SE of the mainshock whereas peak short-period energy is located NW of it on a WNW trending fault. The cluster of events in the outer-rise trench near the aftershocks is inferred to be triggered events from the mainshock due to the lack of observed rupture energy.

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SEISMIC SOURCE CHARACTERIZATION OF SMALL-SCALE CONTAINED EXPLOSIONS UTILIZING NEAR SOURCE EMPIRICAL DATA

The seismic moment tensor is a general representation for both natural and manmade seismic sources. A linear relationship is established between observed ground motions and a set of Green's functions and this moment tensor. Green's functions describe the path taken from the source to the receiver and can be estimated using the one dimensional reflectivity approach. Data from the Source Phenomenology Experiment is used to estimate the seismic source for this series of 9 chemical explosions within a copper mine in Morenci, Arizona. The goal of this study is to assess the uniqueness of the source representation constraining the effects of yield, depth and geology. In this particular study the P wave velocities are well constrained but the accompanying shear wave velocity is less constrained. In order to assess the effects of source depth and shear velocities on the moment tensors, Green functions were computed for different source depths as well as different shear wave velocities, holding the P-wave velocity constant. The compensated linear

vector dipole and explosion components of the new Green's functions are compared to quantify the possible effects of source depth and shear wave velocity on the source representation. Source type plots are used as a graphical display to more clearly understand how the seismic sources are represented.

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NELE: NOISE CHARACTERIZATION OF THE NORTHERN MISSISSIPPI EMBAYMENT

Seismic hazard models require knowledge of shallow sediment structure in order to accurately estimate strong ground motion. The New Madrid Seismic Zone is embedded within the northern Mississippi Embayment (ME) sediment basin and the existing sediment model (Dart, 1992) has not been updated with new data since its publication. Here the thickness of the unconsolidated sediments is estimated using continuous seismic noise data recorded on 150+ seismic stations deployed over the last 5 years in the ME. Data comes from the Northern Embayment Lithosphere Experiment (NELE), which consisted of 4 consecutive 6-month deployments of broadband stations, a single 2-year deployment of 51 broadband stations, and from the Earthscope Transportable Array (TA). Noise was characterized using Probability Density Functions of Power Spectral Densities (PDFPSDs), which make use of overlapping, long-term noise windows to compute PSD estimates for each of the 3 components at each station. Using a combination of maximum power in the PDFPSDs and horizontal/vertical techniques I was able to estimate sediment thickness below each station. The results of the new method are compared with the existing Dart model and appear approximately 300 meters deeper at all points across the embayment and are anywhere from 0 to 100 meters deeper outside the embayment. The source of the discrepancy is being explored.

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DEPOSITIONAL FACIES AND POTENTIAL BOUNDING SURFACES ALONG AN ERG AXIS TO ERG MARGIN TRANSECT, PERMIAN CEDAR MESA SANDSTONE, UTAH

The Permian (Wolfcampian) Cedar Mesa sandstone in southeastern Utah is a 300m thick erg system spanning 8000km2. This study characterizes the variation in depositional facies of the Cedar Mesa sandstone along 7 measured sections spanning 80km through southeast Utah. Outcrop data indicates that the Cedar Mesa is comprised of two primary facies associations. Aeolian facies are dominated by large-scale trough cross-bedded or wind-rippled sandstones with minor finer-grained interdune deposits. Fluvial facies consist of small (< 0.5m) planar cross-bedded, current rippled and bioturbated sandstones and pedogenically-altered mudrocks. The vertical transition from fluvial to eolian facies is sharp and in outcrop facies are often continuous on the order of 600 meters. Occasionally fluvial facies occupy aeolian interdunes as well as interfinger with dune deposits, suggesting coeval deposition. Towards the erg margin, Aeolian deposits are thin and fluvial facies comprise nearly 40% of the section indicating a complex depositional environment with fluvial influence. In the erg axis, fluvial facies become discontinuous and less abundant while aeolian facies become thicker with well-developed deflationary surfaces. Abundance of hiatal surfaces decreases from erg margin to erg axis. Across the erg, deposits tend to be trending towards a relatively wetter environment through time.

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CHARACTERIZATION OF THE 2015 M4.0 VENUS, TX EARTHQUAKE SEQUENCE

On May 7, 2015, a M4.0 earthquake occurred in Johnson County, TX, south of the Dallas-Fort Worth metroplex. It is the largest event recorded to date in the Fort Worth (Barnett Shale) Basin, which is an active shale gas production area that has been associated with induced earthquakes. Beginning on May 11, 2015, a temporary seismic network was deployed to monitor the aftershock sequence.

Currently, there are 13 stations in the Venus area being operated by SMU and 4 stations throughout Johnson County being operated by the University of Texas. To date, we have located over 150 events that define a 5 km long normal fault striking 35°NE and dipping ~40°. Events occur in the Precambrian granitic basement at depths of 4-6km. These locations are near the bottom of the Ellenburger Group (~3.5km in depth), which is an Ordovician carbonate platform overlying the basement and is often used for wastewater disposal. Five large volume injection wells operate within 10km of the earthquake sequence and inject very near, if not through, the Ellenburger-basement contact. Here, we characterize the Venus, TX earthquake sequence and present evidence of a causal link between wastewater disposal and seismicity in Johnson County.

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ANCIENT ATMOSPHERIC CARBON DIOXIDE FROM COOLER LATE OLIGOCENE AND WARMER EARLY MIOCENE TIMES, ESTIMATED FROM FOSSIL LEAVES

Plants use atmospheric carbon dioxide to produce their own food via photosynthesis. Recent variations in the concentration of atmospheric carbon dioxide (pCO2) have been shown to affect this process, and are correlated with anatomical and physiological changes seen in leaves. These include changes to stomatal frequency and size, which can be measured on leaf fossils. Thus, fossil leaves can be used as proxies for Earth's atmospheric carbon dioxide history. This study tests the link between pCO2 and global temperature for two time slices shown by marine isotope records to document warming in the past, and is important for understanding current climate change.

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APPLYING DATA PROCESSING TO REVEAL GEOLOGICAL PROCESSES IN JOSHUA TREE NATIONAL PARK

The stratigraphy of Joshua Tree National Park contains complex igneous and metamorphic relationships at different depths. The Proterozoic host rock contains Cretaceous magmatic intrusions (consisting of granite and granodiorite) with increasing mafic compositions at greater depths. Exploration of the complex relationships between igneous and metamorphic rocks in this area requires synthesizing different datasets at many scales. In order to analyze and describe the arrangement of host rock and magmatic units, field (measurements and digital images) and geochemical data will be collected this year. My work aims to compile data with geographical information system software in order to strategize a way to reveal petrological, geochemical and structural relationships. Preliminary assessments of Little Morongo Canyon and Long Canyon reveal similar structural and compositional trends that can be utilized in creating a stratigraphic column of the region. My objective is to use data processing and imagery to help identify more trends and relationships from well characterized outcrops that best represent the petrology of the canyons.

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NONLINEARITY, DISORDER, AND UNCERTAINTY QUANTIFICATION IN DISCRETE NONLINEAR SCHRÖEDINGER EQUATION

The study of optical waveguides arrays has drawn a great deal of attention in the field of nonlinear physics during the past few years since they provide spatially inhomogeneous structures for guiding light. Of particular interest are disordered photonic crystals and optical lattices in which the propagation of light is affected by the phenomenon of Anderson localization. We explore the dynamics of

localized wavepackets in the presence of disorder and nonlinearity applied to discrete lattices, starting with the discrete version of 1-D nonlinear Schrödinger equation (DNLSE). We investigate numerically whether there is localization when varying the strength of the nonlinearity and the effect of disorder in the on-site energies of the lattice. We use symplectic integration methods to study the asymptotic behavior of wave packet spreading in DNLSE. Furthermore, we explore the localization of light considering a model with parity and time-reversal (PT) symmetry. For a particular layout of the optical lattice, we show that there exists a parametric transition region from broken to unbroken PT symmetry.

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CYCLIC-PARALLEL TREECODE FOR COMPUTING ELECTROSTATIC INTERACTIONS ON MOLECULAR SURFACES

We study the parallelization of a Cartesian grid based treecode algorithm for evaluating electrostatic potentials for charged particle systems where N particles are located on the molecular surfaces of biomolecules such as proteins. When the well-separated condition is satisfied, the treecode algorithm uses a far-field Taylor expansion to compute $\mathcal{O}(N\log{N})$ particle-cluster interactions to replace the $\mathcal{O}(N^2)$ particle-particle interactions. The algorithm is implemented in MPI by creating identical tree structure in memory on each processor. We designed a cyclic scheme uniformly distributing spatially closed target particles to processors, which drastically improves the load balancing between processors. We also optimized the parallel efficiency by modulating treecode parameters such as Taylor expansion order p, maximum particles per leaf N_0, and maximum acceptance criterion θ. In addition to efficiently computing the N-body problem of charged particles, our approach can potentially accelerate GMRES iteration for solving boundary integral Poisson-Boltzmann equation.

Commercial Viability:
Treecode method is a part of TABI (treecode-accelerated boundary integral) Poisson-Boltzmann solver. The TABI is a general tool to compute electrostatics on all proteins with structure information from protein data bank (up to 107,086 protein structures). There are other two PB equation solvers, which are finite difference method and finite element method. These are two primary methods used in PB solvers, such as APBS (Adaptive Poisson-Boltzmann Solver), which has more then 20,000 active users. On the compare with APBS, we find that TABI is more efficient when higher accuracy is required, and TABI uses less memory than APBS for comparable levels of accuracy. TABI is also parallelization friendly. Cyclic-parallel treecode method is based on TABI's parallelism, and improves the parallel efficiency of TABI.

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THRUST SENSOR BASED NONLINEAR PID MOTOR CONTROL FOR QUADCOPTER APPLICATIONS

Quadcopter unmanned aerial vehicles (UAVs) are the current focus of much research and development. These flying robots have strong potential for a wide variety of applications. However, they face significant and complex aerodynamic disturbances which interrupt controlled, stable flight. Currently, quadcopter brushless direct current (BLDC) motors are run in open loop, and the task of compensating for motor control error lies either with the pilot or, in autonomous systems, with upper-level attitude or altitude control loops or elsewhere in the system. This project presents a novel nonlinear proportional-integral-derivative (PID) BLDC motor controller that incorporates thrust feedback from a force sensor installed on the motor mount. This work includes a Lyapunov stability analysis which proves the design is globally asymptotically stable. It also includes a custom MATLAB/Simulink model of the derived system, with simulation outputs and analysis that demonstrate the design's stable and precise setpoint tracking and robustness. Lab experiments tested the system's response both with and without the controller, and illustrated the thrust sensor based design's ability to maintain a desired propeller thrust in the presence of perturbations that caused thrust deviations in the traditional system of nearly 50%.

Commercial Viability:
This thrust sensor based motor controller for quadcopters is commercially viable, since there is a market need for improved stability, autonomy, and robustness to external forces for quadcopters. The sensor and associated circuitry are lightweight, low power,

and flyable. The controller software can be incorporated into existing quadcopter motor controllers. It computes the control algorithm in real time and greatly improves the system's thrust setpoint tracking, which enables a significant improvement in quadcopter control.

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A DOUBLE ABSORBING BOUNDARY ON A TWO-DIMENSIONAL WAVE GUIDE

Simulating waves in an unbounded domain is a problem with, as yet, no completely satisfactory solution. Even the premier methods for artificially truncating the domain, such as a Perfectly Matched Layer (PML) or a high-order Absorbing Boundary Condition (ABC), produce spurious reflections of outgoing waves. The Double Absorbing Boundary (DAB) is a relatively new alternative that aims to be easier to implement than ABCs, and have better a priori error bounds than PMLs. In this poster, we examine a DAB on a two-dimensional wave guide. We evolve the domain interior with a high-order finite difference method, and the DAB with a recently-invented discontinuous Galerkin discretization. Both discretizations are formulated for wave equations in second-order form.

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STABILITY OF ELECTROLYTE FILMS ON SUBSTRATES WITH SPATIALLY PERIODIC CHARGE DENSITY

The stability of a thin electrolyte film on a substrate characterized by a periodic space-dependent electrical charge density is considered. Using the Debye-Huckel equation to model the electrostatic potential and the Navier-Stokes equations for fluid flow, both steady-state interface shapes and their stability resulting from small perturbations of arbitrary wavelength are considered. Calculations are carried out by two different approaches: an evolution equation is obtained within the framework of a lubrication-type model, and, secondly, Fourier expansion of all terms is used and the corresponding coefficients of the first order correction to the interface shape are found. Stability analysis of the linearized problem is conducted.

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APPLICATIONS OF COMPLETE RADIATION BOUNDARY CONDITIONS

An important issue in the simulation of waves is the ability to truncate unbounded domains into regions of interest that can be simulated efficiently and accurately for long times. In the context of finite difference time domain (FDTD) electromagnetics we demonstrate that complete radiation boundary conditions (CRBC) can be implemented as a Double Absorbing Boundary (DAB). This results in a thin, non-reflecting layer which inherits the desirable properties of CRBCs, namely a clear notion of convergence and an a priori error estimate that allows for the selection of optimized parameters. The performance of the method is demonstrated with numerical experiments. We also briefly discuss ongoing work concerning the application of CRBCs to elastic waves.

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THE IMMERSED INTERFACE METHOD FOR NON-SMOOTH OBJECTS IN 2D INCOMPRESSIBLE VISCOUS FLOW

In the immersed interface method (IIM), singular forces are used to represent the effect of objects immersed in a fluid, and jump conditions induced by the singular forces are incorporated into numerical schemes to simulate the flow. Previously, the IIM was developed to simulate flows with smooth objects. We here present an extension of the method for non-smooth objects. In particular, we describe how to compute necessary jump conditions using line segment representation of 2D objects. Our tests on circular Couette flow, flow past a square cylinder and flow around flapping plates indicate that our method achieves second-order accuracy, uses relatively insignificant time for an extra object and is robust to handle non-smooth complex objects.

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OPTIMIZED EFFICIENT TIME INTEGRATION METHODS FOR MULTIRATE SYSTEMS

This work is in the context of numerical methods for integrating multirate ordinary differential equations. Using our previously proposed framework for multirate methods which leverages Generalized Additive Runge-Kutta theory, we have developed new methods of 4th classical order. These new methods have been optimized for a larger stable stepsize. We will show that these new methods are competitive, and in some areas surpass, current methods.

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WEAK WAVE TURBULENCE IN THE 2D MMT EQUATION

Wave turbulence is exhibited in many physical systems where there are disordered, dispersive, and weakly interacting waves, such as nonlinear optics, fluids, and plasma. It involves the transfer of dynamically conserved quantities like wave action or energy from sources to sinks through a conservative (or inertial) zone. When the wave amplitudes (and thus their interactions) are small, we can compute some of the system's statistical properties analytically. One testable prediction is the relationship between the wavenumber and average wave action density, known as the Kolmogorov-Zakharov (KZ) spectrum. A notable case where this spectrum does not necessarily occur is in the one-dimensional Magda, MacLaughlin, Tabak (MMT) equation. More recent work has suggested that this is due to dominant nonlinear effects in this system rather than an error in the theoretical framework of weak wave turbulence. We have recently simulated the two-dimensional MMT system and shown that the KZ spectrum is robust when another dimension is added under any choice of signs. We also begin to explore the underlying point of contention in the analysis: the four-wave correlator function.

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COMPRESSIVE STRESS AS A STABILIZING MECHANISM IN IRRADIATED THIN FILMS

Irradiation of semiconductor surfaces often leads to the spontaneous formation of rippled structures. However, at high enough energies, these structures are observed to vanish, despite current models predicting their persistence. Here, we examine the effect of a new physical mechanism -- implantation-induced compressive stress -- performing a linear stability analysis to determine if this mechanism is stabilizing over an appropriate range of environmental parameters.

Eric Godat; Fred Olness; Ben Clark; Florian Lyonnet (#111)
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APPLICATIONS FOR MANEPARSE IN NEW PHYSICS SEARCHES AND NUCLEAR PDFS

With Run 2 of the LHC progressing, tools that assist in improving the precision calculations needed for analyzing data and making new predictions are essential. ManeParse is a Mathematica package that serves as an interface for allowing a user to directly access and manipulate Parton Distribution Functions. Parton Distributions Functions are essential in relating theoretical predictions to the new data streaming out of Run 2. Here we illustrate the design of ManeParse as well as several examples of how it is being utilized.

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IMPROVING THE SENSITIVITY OF THE XIA ALPHA COUNTER FOR NEXT-GENERATION DARK MATTER SEARCHES

The XIA UltraLo 1800 Alpha Particle Counter is one of the highest-sensitivity particle detectors commercially available, but it is still not sensitive enough to satisfy the requirements of next-generation dark matter searches. These experiments will need to be constructed from materials with an unprecedentedly high radiopurity in order to achieve their science goals. Such low levels of contamination cannot be presently assessed using the XIA UltraLo 1800. We seek to improve the sensitivity of the instrument by modifying the algorithms for classifying particles.

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VOLTAGE-ASSISTED SEARCH FOR LOW-MASS WIMPS IN THE SUPERCDMS EXPERIMENT

The favored candidate for dark matter is a Weakly Interacting Massive Particle (WIMP). As large amounts of parameter space for high-mass WIMPs have been ruled out, the low mass region has been left largely unexplored. In order to search for a low-mass WIMP, the Super Cryogenic Dark Matter Search (SuperCDMS) uses ultrasensitive germanium crystal detectors cooled to 40 mK with a high voltage (HV) bias of 70V. These detectors take advantage of the Luke-Neganov effect to amplify the ionization signal through phonons, which improves low energy resolution and lowers the ionization energy threshold. I present results from the first data runs of the Low Ionization Threshold Experiment (CDMSlite) in the Soudan Undeground Laboratory in Soudan, MN that produced a world-leading spin-independent limit for WIMP masses between ~1.7 and 6 GeV/c2. I also show plans for analyzing the final CDMSlite run, while showing an outlook for the next generation of SuperCDMS HV detectors in SNOLAB in Sudbury, Ontario.

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ESTIMATION OF THE GAMMA-INDUCED ELECTRON RATE FOR THE SUPERCDMS SOUDAN EXPERIMENT

Dark matter contributes ~26.8% of the universe's mass, and Weakly Interacting Massive Particles (WIMPs) are among the most promising particle dark matter candidates. The Super Cryogenic Dark Matter Search (SuperCDMS) is one of the leading direct dark matter search experiments. Its germanium (Ge) detectors were located deep underground in order to perform a rare-event search in the hope that a WIMP would collide with a Ge nucleus and leave a Ge nuclear recoil signal. It is possible for a gamma-induced

electron to hit the surface of a detector, and this type of event could have incomplete charge collection by the sensors. This reduction of charge signal results from a quenching process that might make the event look like a Ge nuclear recoil event. In this poster, I show a method to estimate the rate of the gamma-induced electrons hitting our detector surfaces.

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MEASURING COSMOLOGICAL DISTANCES TO PROBE THE EXPANSION HISTORY OF THE UNIVERSE

Through observations of baryon acoustic oscillations and various types of supernovae, one can determine distance measurements on cosmological scales in order to chart the expansion history of the universe. The Robotic Optical Transient Search Experiment operates on a telescope owned by SMU, searching for optical light emitted by transient astrophysical events, particularly supernovae. It possess the ability to shed light on systematics affecting distance measurements of these events. Additionally, SMU contributes to the Dark Energy Spectroscopic Experiment, which will begin collecting data in 2019, looking to measure baryon acoustic oscillations throughout the universe. Here, I present an overview of the experiments, as well as analysis contributing to their overall functionality.

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ESTIMATE OF BACKGROUND NEUTRON RATE FROM 210PO DECAYS IN POLYETHYLENE FOR SUPERCDMS SNOLAB

Dark matter is expected to interact weakly with ordinary matter, and with a very low interaction rate. Direct detection will require the lowest possible background, including background neutrons which are difficult to distinguish from dark matter. The CDMS SNOLAB experiment seeks to directly detect dark matter, and uses a polyethylene neutron shield. However, when exposed to naturally occurring 222Rn, we find polyethylene will be contaminated by radon daughter products mainly through plate-out. The 130 Bq/m^3 radon environment at the SNOLAB site will lead to an alpha activity accumulation from 210Po of 379 mBq/day. The alphas from 210Po decay will interact with 13C isotopes present in the polyethylene and release neutrons through the (alpha,n) process, generating 3.009x10^26 neutrons/s/cm^3 for 1ppb 210Pb. To meet the goal of keeping the neutron rate below 3.416x10^-14 neutrons/s/cm^3, the poly must be exposed to the SNOLAB environment for less than 10.72 days before being moved to a radon purged environment. This estimate places potential construction and storage constraints on the experiment. In early 2016, we will be exposing poly samples to the high radon environment at SNOLAB and measuring the surface alpha activity with the XIA UltraLo alpha counter at SMU to verify these estimates in actual conditions.

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NEUTRINO-ELECTRON ELASTIC SCATTERING AND ITS APPLICATION BEYOND STANDARD MODEL

Traditionally, we use the pure weak interaction of numu-electron elastic scattering as a standard method to constrain the neutrino beam flux and check the simulation in standard model of high energy physics, since it is clean unlike the hadronic showers which trends to be effects by known or unknown nuclear effects. Also, the technique of numu-e elastic scattering can be applied into two broad areas of study, neutrino magnetic moments and light dark matter, respectively, to the enhancement of scattered electrons in low energy region(less than 0.3 GeV) and in high energy region (larger than 2 GeV). To measure the upper limits of those values, we may use Feldman & Cousins' method which is highly depending on the average estimation of MC background. In NOvA experiment, we are able to generate lots of MC events to give a better understanding of statistical results and the performance of EL-PIDs were shown good enough, we study and discuss the measurement of numu-electron elastic scattering, numu magnetic moment and light dark matter in this poster.

Keping Xie; Roberto Vega (#118)
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DIPHOTON PRODUCTION IN QCD AND SCTM

Very recently, both ATLAS and CMS reported an excess in the diphoton production events around the invariant mass at 750GeV. We explore the QCD background of this possible new resonance through gluon-gluon fusion, (anti)quark-gluon scattering and quark-antiquark annihilation. We also identify it as a possible new particle in Supersymmetric Custodial Triplet Model, and investigate its behavior in the whole parameter space.

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SPATIAL INTEGRATION OF FUNCTIONAL CONNECTIVITY METHODS IN THE DEFAULT MODE NETWORK OF THE BRAIN

Functional Magnetic Resonance Imaging (fMRI) has become a very powerful research component in the field of neuroscience. Early research works on fMRI data were more focused on detecting brain activation in response to performing a specific task. However, fMRI research goals often are focused on highlighting co-activation patterns across the brain, known as functional connectivity. In the past decade, there has been an increased interest in resting state fMRI. It has the potential to identify brain regions with altered functional connectivity due to certain diseases. In the current literature, there are two commonly used methods of assessing functional connectivity in the resting state fMRI data: seed-based correlation (SCA) analysis and independent component analysis (ICA). However, a common difficultly is the need for voxel-based statistical testing for several thousands of voxels. As a result, one might not see any statistical significance after adjusting for multiple comparisons. We propose to combine neighboring voxels into "blocks" using spatial semivariogram models to produce independent block averages for each time point. It is anticipated that such an approach will reduce the number of multiple comparisons while potentially enabling more powerful statistical tests.

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Mahesh Fernando (#120)
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CONFIDENCE INTERVALS FOR VARIANCE RATIOS FOR THE UNBALANCED LINEAR MIXED MODELS

Our main objective is to calculate confidence intervals for variance ratios (signal to noise) in unbalanced linear mixed models by inverting the hypothesis test for zero variance ratio. We use REstricted Maximum Likelihood (REML) to calculate the variance estimates. Then we use a higer-order asymptotic saddlepoint approximation for the distribution of the REML likelihood ratio test to construct the confidence interval. The general methodology provides confidence intervals for any unbalanced random mixed model with coverage generally accurate to 1% and underage and overage also accurate to 1%. No other methods are capable of giving confidence intervals with such accurate coverage, overage, or underage.

Yu Lan (#121)
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INCORPORATE THE UNCERTAINTY IN COST-EFFECTIVENESS ANALYSIS

Cost-effectiveness analysis is a decision making tool for the allocation of scare health-care resources. We seek to develop methods to correctly and intuitively present and quantify uncertainty in a cost-effectiveness analysis that simultaneously compares multiple treatments. A key element of the analysis is the identification of the cost-effectiveness frontier, or the set of non-dominated, admissible treatments. The method is based on a Bayesian simulation approach that identifies potential frontiers and attaches posterior probabilities to them. We illustrate the method using a micro-simulation model for projecting survival and lifetime healthcare costs for smokers seeking to quit. There are two major stochastic elements: The simulation of lifetime smoking experience, healthcare costs, and survival from otherwise healthy young smokers, and uncertainty about parameters of the simulation model. We adopt quadrature methods to render the simulation methods more efficient. Our analysis demonstrates that there is substantial uncertainty in both the identified frontier elements and in their relative cost-effectiveness.

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RANKED SET SAMPLING ESTIMATORS OF MEAN AND VARIANCE FOR DISCRETE POPULATIONS

Ranked set sampling (RSS), proposed by McIntyre (1952), is a sampling scheme first used to improve the population mean estimation. It is most applicable when units are difficult or costly to measure, but can be easily ranked through a ranker or concomitant variable. As an alternative to simple random sample (SRS), this technique improves the population mean estimation by using extra information through the process of judgment ranking. Ranked set sampling technique has been applied to estimation of the distribution function as well as density function, population variance and population proportion. Although it has been a flourishing research field over the past decades, most of the research only refers to continuous distributions. We propose methods to incorporate tie structures in the sample for discrete data. We showed that the relative efficiency for both mean and variance estimators increases when the ties are used in the estimators.

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AN ADAPTIVE TESTING APPROACH FOR META-ANALYSIS OF GENE SET ENRICHMENT STUDIES

In the field of gene set enrichment analysis (GSEA), meta-analysis has been used to integrate information from multiple studies to improve the power of detecting essential gene sets involved in cancer or other human complex diseases. However, existing methods, Meta-Analysis for Pathway Enrichment (MAPE, Shen and Tseng 2010), may be subject to information loss because of using gross summary statistics for combining end results from component studies. Therefore, we adapt meta-analysis approaches originally developed for genome-wide association studies, which are based on fixed effect (FE) and random effects (RE) models, to integrate multiple GSEA studies. We further propose a mixed strategy via adaptive testing for choosing RE versus FE models to achieve greater statistical efficiency and flexibility. The three methods tend to have much better performance than the MAPE methods, and can be applied to both discrete and continuous phenotypes. Specifically, the performance of the adaptive testing method seems to be most stable in general situations.

Ryan McShane; Ian R. Harris; Ronald W. Butler; Andrew T. A. Wood (#124)
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INFINITY-CALIBRATED LAPLACE APPROXIMATIONS

Laplace approximation is typically used to find integrals of functions which are difficult to evaluate. Using a second-order Taylor expansion, the integral can be re-expressed as the kernel of a normal density. Ultimately, expressing the integral in this way leads to faster calculations as well as fairly accurate values. Laplace approximations are particularly useful in the multivariate setting, for example hypergeometric functions with matrix arguments. The hypergeometric function is an infinite sum with no known closed form. In Butler and Wood (2002), Laplace approximations were calibrated to 0. We give a second calibration option by calibrating the approximations to infinity. We compare the values obtained in Butler and Wood (2002) and the infinity-calibrated values to their true values (obtained by simulation). An example concerning the moments of the non-central Wilk's is given.

Commercial Viability:
Procedure could be used in statistical packages.

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RISK-RETURN RELATIONSHIP: AN EMPIRICAL STUDY OF DIFFERENT STATISTICAL METHODS FOR ESTIMATING THE CAPITAL ASSET PRICING MODEL (CAPM) AND THE FAMA- FRENCH MODEL FOR LARGE CAP STOCKS

The Capital Asset Pricing Model (CAPM) is one of the original models to explain risk-return relationship in the financial market. However, when applying the CAPM into reality, many publications demonstrate a lot of its shortcomings. While improving the performance of the CAPM, some studies, on one hand, attempted to apply different estimation statistical methods; on the other hand, some added more predictors to the model. First, the research focuses on reviewing the CAPM and comparing popular estimation methods, and then compares the predictive power of the CAPM and the Fama-French model, an important extension of the CAPM. Through an empirical study on the data set of large cap stocks, we demonstrated that there was no statistical method that would fully recover the expected relationship between systematic risk (represented by beta) and return from the CAPM, and that the Fama-French model did not have a better predictive performance than the CAPM on individual stocks. Therefore, the thesis provides more evidence to support both the incorrectness of the CAPM and the limitation of the Fama-French model in explaining risk-return relationship.

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RECONSTRUCTING THE USE-LIFE OF AN ANCESTRAL PUEBLOAN WATER RESERVOIR FEATURE, AMOXIUMQUA (LA481), JEMEZ MOUNTAINS, NEW MEXICO

Multiple lines of evidence are used to reconstruct the use-life of a prehistoric water storage feature at the Ancestral Puebloan site of Amoxiumqua (LA481) in the Jemez Mountains of New Mexico. This study demonstrates how integrating a range of geoarchaeological, geophysical, paleoecological, and hydrological datasets can not only test hypotheses about when and how these types of features were used, but when combined with archaeological and ethnographic data can provide insights into how prehistoric communities collectively managed natural resources. Preliminary results indicate that the feature was constructed before the onset of drier than average conditions in the 15th century, and the end of its use-life coincided with village abandonment in the early 17th century. Hydrological modeling and preserved fossil diatoms indicate that the reservoir stored a significant volume of water, but only seasonally. This research approach is being applied to reservoir features at ten sites across the Southern Jemez and Pajarito Plateaus in order to better understand how the collective management of resources factored into the long-term sustainability of Ancestral Puebloan communities.

Jenna Battillo (#127)
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A DISEASE FOR YOUR HEALTH: THE BENEFITS OF EATING CORN SMUT IN THE ANCIENT SOUTHWEST

Corn smut or Ustilago maydis is generally considered a nuisance by the modern agricultural industry. This fungus infects and feeds on corn plants manifesting tumor-like growths with odd discoloration (usually directly on the cob) and reduces overall crop yield. However, in some places this fungus is prized as a delicacy. The cultivation and consumption of corn smut is well-documented among the Maya and Aztec, as well as some Southwestern groups, but it has not been discussed as a constituent of Basketmaker diet. In this study I present evidence from spores found in paleofeces that demonstrates Basketmaker people (the earliest farmers of the Southwest) were purposely consuming and possibly cultivating U. maydis. Furthermore, I argue that this could have served as an advantageous dietary choice that may have augmented the incomplete nutrition in maize prior to bean horticulture and at a site where there is little evidence for meat consumption.

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Katherine Fox (#128)
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EXPERIENCES OF CARE FOR EARLY PSYCHOSIS: SOME PRELIMINARY FINDINGS

This poster draws upon my work on Pathways Through Care, a qualitative study of early psychosis sponsored by the NIMH and under the direction of Dr. Neely Myers (Dept. of Anthropology). We interview young adults between the ages of 18-30 who are experiencing a first-time hospitalization for psychotic symptoms, and we follow up with them over a four-month period to investigate how they are making treatment decisions. After a year of work on the data collection team, I present some preliminary trends that have emerged from this data set.

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BUILDING MULTI-MILLENIAL FIRE CHRONOLOGIES IN DRY SOUTHWESTERN FORESTS

Fire history provides methods to investigate fire regime change in particular ecosystems and has become a vital tool for contemporary land management. I have generated a high-resolution, replicated sedimentary fire history for a wetland site in Lake Fork Canyon in the southern Jemez Mountains of northern New Mexico. Surrounded by mixed conifer and ponderosa pine forests, the sedimentary fire history provides a multi-millennial context for the multi-century tree-ring based fire histories of these ecosystems. I used two methods to quantify sedimentary charcoal in continuous 1cm and 2cm samples from two 1 m cores collected from within the wetland. I measured sediment charcoal content using a nitric acid digestion and loss-on-ignition method that quantified total charcoal by mass, and compared this with wet-sieving and counting macroscopic charcoal (> 125 μm). Results from different methods and comparisons between the two cores suggest that these fire histories are robust and provide information on varying fire activity in the forests surrounding the wetland. Radiocarbon dates on charcoal from the cores were used to build a >4000 year chronology for the charcoal records. Comparisons of these fire histories to local pollen records, regional climate reconstructions, and archaeology elucidate the varying climate and land-use impacts on the fire history.

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MAKING AND UNMAKING CULTURAL DIFFERENCE IN A MENTAL HEALTH CLINIC IN PARIS

France is estimated to be home to more than 6 million Muslim immigrants, but does not collect racial or religious demography data on its populations. Consequently, people are considered to be French or non-French based on a number of factors. The latter category receives specialized healthcare because of perceived cultural differences or barriers to care. This poster explains the ways in which healthcare for immigrants in Paris is both culturally-sensitive and effective, but also how it allows French social service workers to label people as culturally different, and the consequences of each.

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WTO MEMBERSHIP AND CORRUPTION

Despite widespread belief that membership in the World Trade Organization (WTO) is likely to improve the quality of governance, there is no convincing empirical evidence to substantiate this. Here, we investigate whether WTO membership has a causal effect on firm-level reports of political corruption. We overcome self-selection and measurement error issues by applying a nonparametric partial identification approach in order to bound the average treatment effect (ATE). We also analyze conditional ATEs to explore various sources of potential heterogeneity. Contrary to existing thought, we find that WTO membership is likely to increase corruption, particularly by government-owned firms.

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AN EVALUATION OF THE EFFECT OF EDUCATION ON VIOLENCE IN COLOMBIA

In this paper we analyze the impact of education on different outcomes of violence. To do that we exploit the Municipal Panel constructed by Center for Economic Development Studies (CEDE for its acronym in Spanish) that contains information about demography, conflict and violence, agricultural, educational and fiscal variables. Colombia is a country with high levels of violence and a long standing conflict. Moreover those variables have significant temporal and geographical variation. Most of the research has been focused on evaluating the impact of violence on different social and economic variables, dealing with the endogeneity problem but the causality of some social variables on violence has not been addressed. In particular, we are interested in evaluating the role of education in explaining the level of violence at municipality level.

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WHAT'S DRIVING THE LOW-FREQUENCY MOVEMENTS IN STOCK PRICES? A CONSUMPTION BASED ASSET PRICING MODEL WITH RECURSIVE PREFERENCES

The long-run risks (LRR) literature highlights the importance of the predictable long-run component in consumption growth to explaining the fluctuations in asset prices, but overlooks the potential driving forces from the demand side of the economy. So as to understand the asset market phenomena from a wider perspective, this study proposes an asset pricing model with recursive preferenc-

es, accommodating both long-run and valuation risks embedded in the low-frequency movements in consumption growth, dividend growth, and time-preference shocks. In the modeled economy, asset market fluctuates in response to long-run consumption growth, time-preference shocks and their respective volatility; and equity premium reflects the market compensation for households' exposure to consumption growth and valuation risks. Empirical evidence, resting on moment-matching methods and particle smoothing algorithm, indicates that our model can account for the weak correlation puzzle, and justify the joint dynamics of the price-dividend ratio, the stock returns and the equity premium. Moreover, we find that long-run consumption growth and time-preference shocks are the major contributors to asset market fluctuations. In particular, stock market crashes are always associated with quick and substantial declines in long-run consumption growth and the economic measure of investors' patience.

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PEER EFFECTS IN CONSUMPTION

Peer influences have long been considered among the major driving factors of individual consumption behavior by economists and sociologists. However, empirical research on peer influences in consumption is still in its infancy. In this paper, I extend the understanding of this topic with a unique empirical study. Specifically, I examine whether and to what extent individuals' consumption expenditure is affected by consumption expenditure of their peers using micro-data from India. Employing an identification strategy based on instrumental variables/fixed effects, I find robust evidence of significant peer effects in consumption. In particular, I find that a 1 Indian Rupee increase in peer consumption expenditure causes households to increase their own consumption expenditure by 0.7 Indian Rupee. I show that my results are in consonance with the prediction of a model of social conformity rather than that of a model of full risk sharing. My findings suggest the existence of social multiplier effects of policy interventions that affect consumption of only a subset of households of a population.

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THE SPILLOVER EFFECTS OF FOREIGN DEMAND OF SOVEREIGN BONDS ON THE LONG-TERM INTEREST RATES IN THE EURO AREA

This paper expands the literature on the relationship between foreign demand of sovereign bonds and long-term interest rates by analyzing the spillover effect of shocks to the foreign investors' holdings of sovereign bonds in a given euro area country or region on the long-term interest rates of other euro area countries or regions. Using the global vector autoregressive (GVAR) modelling approach, certain spillover effects are observed. And the dynamic simulation results indicate asymmetries in the responses of long-term interest rates in different countries. An unanticipated reduction in the foreign holdings of sovereign bonds in the euro area peripheral countries leads to an increase in the long-term interest rates of the same countries but a decline in the long-term interest rates of the euro area core countries.

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HARSH VERBAL DISCIPLINE IN THE HOME: PREDICTORS OF CHILD COMPLIANCE

To address the absence of a consistent and precise definition of HVD, this study aims to identify specific elements of naturally observed HVD and to assess if these characteristics predict compliance, with consideration of the general parenting climate. Thirty-three mothers of 2- to 5-year-old children wore audio-recorders to record interactions with their children at home. HVD was operationalized as a comment directed at a child that involved increased volume, aggravated tone, and/or negatively valenced content.

Prolonged compliance was defined as the absence of a new conflict for 5 minutes after HVD. The PPQ (Robinson et al., 1995) was used to assess parenting style. There were a total of 893 maternal HVD incidents. A multilevel model with a binomial distribution and logit link function was utilized. There was a significant interaction between mean volume and tone. All three parenting styles significantly predict prolonged compliance. For authoritative and authoritarian parenting, the odds of a child being compliant increase by 1.02. In contrast, for permissive parenting, the odds of a child being compliant decrease by 0.93. Future studies should examine internalization as an outcome. Permissive parents are least likely to elicit prolonged compliance. Research is needed to examine the mechanisms that distinguish permissive parents' inability to elicit compliance.

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IMPACT OF SOCIAL SUPPORT ON RELATIONSHIP SATISFACTION IN BIPOLAR DISORDER

Research has shown that social support impacts physical and psychological well-being. In general, social support from a partner is associated with higher marital satisfaction (e.g., Julien & Markman, 1991). Social support has also been shown to impact the course and functioning of individuals with bipolar disorder (BPD). BPD has been previously associated with impairments in forming and maintaining romantic relationships, and is strongly associated with marital discord (Whisman, 2007). Despite these demonstrated associations, few studies have examined the impact of social support on marital satisfaction within BPD. In addition, many studies collect data only once or twice. We hypothesize that higher social support will be associated with higher average relationship satisfaction and higher stability in relationship satisfaction over time. Observational and self-report data were analyzed from 38 individuals with lifetime diagnoses of bipolar I or II disorder and their heterosexual partners. Participants completed baseline questionnaires and up to 25 weekly diary assessments. Preliminary results showed that higher social support predicted higher relationship satisfaction on average, even controlling for both partners' affective symptoms. Social support was also associated with weekly variability in relationship satisfaction.

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HELICOPTER PARENTING AND COLLEGE STUDENTS' MENTAL HEALTH: EXAMINATION OF SEX DIFFERENCES

A healthy parent-child relationship in which parents instill confidence in their child's capacity to be independent--known as autonomy support--is a key component of successful adulthood (Cullaty, 2011). However, the relationship becomes problematic when a parent resists change and takes on a psychologically and socially overbearing role--a parenting style known as helicopter parenting (LeMoyne & Buchanan, 2011; van Ingen et al., 2015). The current study examined whether the relation between helicopter parenting and autonomy support on college students' mental health differed for boys and girls. Participants were 118 college students (M age=19.82, SD=1.38; 83.1% female). Approximately 57% of the sample was European America, 36.4% were Hispanic, and the remaining students reported another race. Students completed the Helicopter Parenting Behaviors Questionnaire and the Inventory for Depression and Anxiety Symptoms. Regression analyses indicated sex differences in the relation between helicopter parenting and students' well-being, β=.87, p=.018: Helicopter parenting predicted lower levels of well-being, but only for girls. Also, autonomy support predicted lower levels of social anxiety, but only for boys, β=-1.69, p=.016. The findings suggest that helicopter parenting may be a risk factor for girls, whereas autonomy support emerged as a protective factor for boys.

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FAMILY, PEER, AND COGNITIVE PREDICTORS OF EXTERNALIZING BEHAVIOR IN COLLEGE STUDENTS

Externalizing behaviors among emerging adults can have long-lasting repercussions, such as lower academic success and increased risk of injury and suicide (Kerr et al., 2013; Masten et al., 2005). The current study investigated family, peer, and individual cognitive characteristics, to examine which factors uniquely contribute to college students' externalizing behavior. Participants were 118 college students (M age=19.82, SD=1.38; 83.1% female). Students completed surveys measuring externalizing symptoms, family and peer relationship quality, and individual factors of hopelessness, self-esteem, and loneliness. Results from regression analyses found that friendship quality was as the only significant predictor of both relational aggression, B=-.32, p=.011, and rebelliousness, B= -.38, p= .002. Both family and individual characteristics emerged as unique predictors of temper problems: Lower self-esteem, B=-.26, p= .022, hopelessness, B=.32, p= .001, and lower family relationship quality, B=-.25, p= .008, predicted higher levels of temper problems. These findings suggest that family relationship quality, peer relationship quality, and individual cognitive characteristics predict externalizing problems, depending on the domain. Future research should test prospective relations to tease apart the temporal order between risk factors and externalizing behavior.

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EXAMINING THE EFFECTS OF MATCHING AND CHOICE ON EVALUATIONS OF ARGUMENTS FOR SMOKING CESSATION AND CESSATION INTENTIONS

Background: Self-Determination Theory (Ryan & Deci, 2000) and prior evidence (Baldwin et al., 2012) suggest the effect of self-generated arguments in changing attitudes and behavior may be due to either the choice or the matched content. We tested the effects of choice and matching on evaluations of smoking cessation arguments and cessation intentions. Methods: Current smokers (N=201) using MTurk were randomized to a 2 (choice: yes, no) x 2 (matching: yes, no) factorial design to read arguments promoting smoking cessation. Participants selected or were assigned arguments about cessation containing content that was matched or mismatched to their concerns. Participants reported arguments' convincingness, decisional balance (Velicer et al., 1985), and cessation intentions (Biener & Adams, 1991). Results: Results indicated that participants in matched conditions rated arguments as more convincing, $F(1,195)=10.40$, $p=.001$, $d=.459$. There were no significant choice or interaction effects ($ps>.05$). Convincingness was correlated with changes in cessation intentions ($r=.21$, $p=.004$) and smoking pros and cons, respectively ($r=-.27$, $p<.001$; $r=.42$, $p<.001$). Conclusion: The results suggest that choice might influence the persuasiveness of self-generated arguments through the matching of argument content.

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COMPARISON OF TWO MARITAL INTERACTION TASKS: WHAT SPOUSES TALK ABOUT MATTERS

The emotional and physiological effects of marital conflict can have negative implications for spouses' and family members' mental health. However, not all marital conflict is the same. Conflict that is perceived as handled well may not be as harmful to ones' health or the relationship as conflict that is perceived as more difficult for couples to handle. The current study compared emotional and physiological responses during two marital conflict interactions. Participants' pre-ejection period, a measure of physiological arousal, was assessed before and during both interactions. Spouses self-reported on their positive and negative emotions during both interactions. We also examined marital satisfaction as a moderator of the relation between both emotional and physiological responses during conflict and depressive symptoms. Results indicated that husbands and wives reported less positive emotions and more negative emotions during the difficult interaction as compared to the handle-well interaction. Husbands had higher physiological reactivity during the

difficult interaction as compared to the handle-well interaction; however, no significant differences were found for wives. We found partial support for the third hypothesis such that wives marital satisfaction moderated the relation between physiological reactivity during the handle well interaction and depressive symptoms.

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NEUROCOGNITIVE CORRELATES OF WORD RETRIEVAL ABILITY IN YOUNGER AND OLDER ADULTS

Objective: To identify the neurocognitive abilities that relate to word retrieval among adults. Method: Subjects were 30 younger and 30 older adults who were non-depressed, English-speakers, without history of brain injury or cognitive disorder, and who resided in Dallas. Subjects completed a word retrieval task and four neurocognitive tests: Vocabulary, Digit Span, Controlled Oral Word Association Test (COWAT), and Animal Fluency. Results: Vocabulary was significantly correlated ($p<.01$) with retrieval overall and within each age group, so we conducted partial correlations controlling for vocabulary. Overall, retrieval success was significantly correlated with phonemic ($r=.31$, $p=.02$) and semantic ($r=.30$, $p=.02$) fluency, and semantic fluency also correlated with tip-of-the-tongue (TOTs) ($r=-.29$, $p=.03$). Among older adults, semantic fluency correlated with retrieval success ($r=.40$, $p=.03$) and TOTs ($r=-.42$, $p=.02$), phonemic fluency correlated with number of non-retrieved words ($r=-.38$, $p=.04$), and age correlated with retrieval success ($r=-.50$, $p=.01$). Among younger adults, none of these relationships between cognitive performance and retrieval were significant. Conclusion: Cognitive measures may relate differently to retrieval in younger and older adults. Verbal fluency and age predict retrieval ability only among older, but not younger, adults.

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VALIDATION AND APPLICATION OF A NEW MEASURE OF EXPRESSED EMOTION

Many patients diagnosed with mental health disorders often relapse or experience a return of symptoms after initial remission of their diagnosis (Hooley & Teasdale, 1989). Expressed emotion (EE), the amount of "criticism, hostility, or emotional overinvolvement a relative [directs towards] a family member with psychopathology," or a mental or behavioral disorder (Hooley, 2007), is directly correlated with high rates of relapse. The current gold standard assessment for expressed emotion is the Camberwell Family Interview (CFI). However, the CFI is time intensive in several respects and the interview is often impossible to conduct as it requires the patient's family members to have both the willingness and availability to participate. Finally, the CFI was created based on clinical experience without the use of empirical data; as such it is unclear if it assesses all important content relevant to the emotional climate in a family. We used modern scale creation techniques to create a psychometrically sophisticated measure of the EE construct. These analyses led to the creation of a new self-report measure of the EE construct that can be used in research settings, allowing for further examination of this important construct, and to screen in clinical settings. Studies are ongoing to further examine the validity and utility of this measure.

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PREVENTING RACISM ON COLLEGE CAMPUSES: A RANDOMIZED CONTROLLED TRIAL EVALUATING SPEAK UP—A VIDEO PROGRAM

Racial microaggressions are subtle degradations that convey hostile or derogatory messages about minorities. The current study evaluated Speak Up, a 15-minute video intervention designed to increase awareness of racial microaggression. It was hypothesized that

participants who viewed Speak Up, compared to those who viewed a control video, would demonstrate: (1) increased awareness of racial microaggressions at post-intervention and 1-month follow-up assessment, (2) increased cultural sensitivity at post-intervention and 1-month follow-up assessment, and (3) greater knowledge of racial microaggressions at post-intervention and 1-month follow-up assessment. Participants (N = 115) were randomly assigned to view either the Speak Up video or a control video on study skills. A mixed ANOVA revealed that participants who viewed Speak Up, compared to those who viewed the control video, reported increased awareness of racial microaggressions both at post-intervention and at the 1-month follow-up assessment. They also displayed greater knowledge about racial microaggressions at both time points. We view this initial evaluation of Speak Up as a promising step in the development of effective programs to promote awareness and knowledge of racial microaggressions among college students.

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THE PSYCHOBIOLOGICAL RELATIONSHIP OF EXHALED NITRIC OXIDE, SALIVARY HYDROGEN SULFIDE, AND STRESS: PRELIMINARY FINDINGS

Both exhaled nitric oxide (FeNO) and hydrogen sulfide (H2S) are involved in the pathophysiological process in lung disease, and exhaled H2S is correlated with FeNO in lung disease patients (Yun, 2013). To date, the influence of stress on H2S and its relationship with FeNO are unknown. We therefore examined levels of salivary H2S and FeNO in response to a stressful final academic exam period. We hypothesized that both H2S and FeNO would change significantly in response to stress and that FeNO, negative affect, and stress experience would significantly covary with H2S. We collected saliva and FeNO in asthmatic and healthy SMU undergraduate students (n=16) at three time points: low-stress period in the semester, early exam period, and late exam period. Saliva was immediately analyzed for H2S with the fluorescent probe Sulfideflor-4 and FeNO was measured with an electrochemical gas analyzer. The Positive and Negative Affect Schedule was used to measure affect. Mixed effect model analyses with time varying predictors, for within-subject and between-subject effects, showed that as an individual's stress level and negative affect increased, their values of H2S also increased, both in asthma and health. Similarly, changes in FeNO and H2S were positively correlated. Future research needs to elucidate the function of H2S and FeNO during psychological stress in both health and disease.

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INTERPLAY BETWEEN SELF-EFFICACY AND NEGATIVE ATTRIBUTIONS IN PREDICTING CHILD PSYCHOPATHOLOGY

Adolescence is accompanied by an increase in behavioral, emotional, and interpersonal problems; both self-efficacy and negative attributional style are associated with increased psychopathology (Cole et al., 2008; Muris, 2002). Self-efficacy is defined as a person's belief in his or her ability to successfully execute a task (Bandura, 1977), and negative attributional style is defined as the negative causal explanations one makes about a negative event (Beck, 1987). Although they are related constructs, attributional style is often viewed as a trait-like vulnerability, whereas self-efficacy is conceptualized as being more state-dependent (e.g., based on context and type of stressor; Ingram & Luxton, 2005; Rudy et al., 2012). Further, both have been implicated in youth psychopathology: lower self-efficacy is correlated with increased depressive and anxiety symptoms (Muris, 2002), and higher levels of negative attributional style has been shown to predict depression, fear, and hostility (Ciarrochi et al., 2007). Building on previous research, we examined the interaction between children's self-efficacy and negative attributional style as mechanisms predicting children's concurrent depressive symptoms, anxiety symptoms, and internalizing problems. We hypothesized that higher self-efficacy during stress would attenuate the relation between negative attributions and psychopathology.

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EXPERIENTIAL AVOIDANCE MODERATES THE RELATION BETWEEN INTRINSIC ENJOYMENT AND EXERCISE

Experiential avoidance, the tendency to avoid uncomfortable feelings, thoughts, or sensations, may moderate the relation between exercise enjoyment and exercise. Specifically, when enjoyment is low, high experiential avoidance may be associated with a greater likelihood of no exercise than when enjoyment is high. We measured experiential avoidance, exercise enjoyment, and weekly exercise minutes in two samples (Mturk [N = 1,001] and SMU [N = 357]) using online, cross-sectional measures. Data were analyzed using two-part regression models to examine the moderation effect on engagement in zero minutes versus some (binary portion), and on the amount of minutes among exercisers (non-zero gamma portion). Consistent with hypotheses, there was a significant enjoyment x experiential avoidance interaction on the binary portion of the model (Mturk p = .09, SMU p = .03) such that those high in experiential avoidance and low in enjoyment were more likely to report no exercise at all. The interaction was not significant for the non-zero portion of the model (Mturk p = .30, SMU p = .12). Results suggest that experiential avoidance increases the likelihood that people do not exercise at all when exercise enjoyment is low, but has no effect on the amount of minutes for exercisers. Implications include the need to target experiential avoidance in health interventions.

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THE CONVERGENT AND DISCRIMINANT VALIDITY OF AFFECTIVE JUDGMENTS OF PHYSICAL ACTIVITY MEASURES

Affective judgments (i.e., the overall pleasure, enjoyment, and feeling states associated with engaging in physical activity) are emerging as critical to regular physical activity. Various scales have been used as interchangeable assessments of affective judgments of physical activity, although these scales may be measuring distinct constructs. Moreover, it is unclear if affective judgments demonstrate discriminant validity from other conceptually related but theoretically distinct constructs. Therefore, we examined the convergent and discriminant validity of different measures that represent various forms of affective judgments. Participants completed six different affective judgment measures, as well as other measures in order to examine discriminant validity. The measures demonstrated suboptimal convergent validity and poor discriminant validity. Our convergent validity analysis suggests that the various affective judgment measures represent distinct constructs that should be considered independently. The lack of discriminant validity, particularly with regards to exercise self-efficacy, represents an important empirical and theoretical issue in the field of health behavior research. Future research should identify the various experiences and beliefs that underlie affective judgments of physical activity and develop more psychometrically sound measures to assess them.

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EVALUATING TAKECARE, A VIDEO BYSTANDER PROGRAM TO PREVENT HIGH SCHOOL DATING VIOLENCE

Eighteen to 40% of adolescents experience dating violence victimization (DV); 10% of males and 21% of females report physical or sexual DV in the past year. Victimization is associated with negative health consequences. The present study evaluates a video bystander prevention program with high school students using an innovative virtual reality paradigm to collect observational data on bystander behavior. At baseline, students completed measures of bystander behavior, efficacy, and responsibility for intervening. They were randomly assigned to view TakeCARE or control video. One week after video, students participated in virtual reality simulations presenting opportunities to engage in bystander behavior to prevent dating violence. Students who viewed TakeCARE had greater increases in efficacy from baseline to post-treatment and from baseline to 6-month follow-up. They reported greater increases in bystander behavior from baseline to follow-up, and more bystander behavior in virtual reality at post-treatment and follow-up. Efficacy

mediated bystander behavior in the simulations and self-reported bystander behavior at follow-up. These results support the effectiveness of TakeCARE in increasing adolescents' responsive bystander behaviors. A brief video intervention is easy to administer to students, and holds promising implications for reducing rates of dating violence.

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ASSESSING A PROMINENT POSITIVE PARENTING PROGRAM

The goal of this study was to provide preliminary empirical evidence for one prominent parenting program: Attachment Parenting International (API). Three predictions were made: 1) greater exposure to API's principles will be associated with greater adherence to principles; 2) greater adherence to the principles will be associated with a more secure parent-child attachment; and 3) secure parent-child attachments will be associated with fewer internalizing problems and fewer externalizing problems. Mothers answered questions about API involvement and practices, their parent-child relationship, and their children's functioning. As expected, exposure to API principles was significantly associated with adherence to API principles, $\beta = .13$, $p < .001$. Increased exposure (through meeting attendance and materials read, for example) was associated with greater adherence. Also as predicted, adherence to API principles was significantly associated with reported quality of parent-child attachment, $\beta = -.25$, $p < .001$, such that greater API adherence was linked to more secure parent-child attachments. In addition, attachment was significantly related to levels of child internalizing problems, $\beta = .11$, $p < .001$, and child externalizing problems, $\beta = .11$, $p < .001$. The study provides a foundation of research for this popular positive parenting program.

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THE RELATIONSHIP BETWEEN SCHIZOTYPY AND OPENNESS/INTELLECT

There is considerable debate regarding the association between Openness to Experience/Intellect (OE/I) and Schizotypal Personality Disorder (STPD) symptoms. Although two meta-analyses have documented non-significant to small associations between these two constructs (Samuel & Widiger, 2008; Sausman & Page, 2004); others have argued for links between the constructs based on theory or using non-traditional measures of the Big Five (DeYoung, Grazioplene & Peterson, 2012; Kwapil, Barrantes-Vidal & Silvia, 2008; Ross, Lutz & Bailley, 2002; Widiger, 2011). Recently, Chmielewski et al., (2014) found variance relevant to STPD buried within the NEO-PI R, one of the most widely used OE/I measures, using a patient sample. It is therefore important to determine if similar variance is present within other widely used traditional OE/I measures. The current study examines this issue using the Big Five Inventory (BFI) and Goldberg's marker items in 2 student (N = 556, 549) and 1 community (N = 755) samples. Our results failed to replicate the previous findings with the NEO-PI R. Thus, it seems that the variance related to schizotypy may either be unique to the NEO-PI-R OE/I scales or only emerge in patient samples. Future research should examine whether the variance with the NEO-PI R can be replicated in other samples or with other measures.

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CHILDREN'S THREAT APPRAISALS OF INTERPARENTAL CONFLICT: THE ROLE OF INTERPARENTAL CONFLICT, PARENTAL AVAILABILITY, AND CHILDREN'S ANXIETY

Despite the centrality of children's threat appraisals of their parents' conflict in theory linking interparental conflict (IPC) with child internalizing problems, the factors contributing to the development of children's threat appraisals are unclear. We examine four factors that theoretically contribute to children's threat appraisals: destructiveness of the IPC, mother's availability to the child, partner's

availability to the child, and the child's baseline level of anxiety. Children (n = 539; aged 7 to 10) completed measures at 3 assessments, each 6 months apart. Concurrent findings indicate that destructiveness of IPC, partner availability, and children's baseline anxiety related to children's threat appraisals. Prospective findings indicate that destructiveness of IPC and children's baseline anxiety predicted children's threat appraisals. These results replicate prior findings indicating that destructive IPC increases children's threat appraisals. Further, they contribute to the literature by indicating that baseline anxiety increases children's appraisals of IPC as threatening. Perceived closeness to the partner was only associated with threat appraisals in cross-sectional analyses and may function as a short-term protective factor. This research holds important implications for our understanding of the development of children's threat appraisals of IPC.

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ORAL NITRATE SUPPLEMENTATION DURING FINAL EXAM STRESS: ASSOCIATION WITH COLD SYMPTOMS AND EXHALED NITRIC OXIDE

Significant decreases in the fraction of exhaled nitric oxide (FeNO) in both healthy and asthmatic undergraduate students have been found during times of final exam stress. Additionally, research suggests that dietary supplementation of NO may have beneficial effects which offset the physiological consequences of stress. The current study aimed to explore the psychological and physiological effects of dietary NO supplementation via beetroot juice during times of final exam stress. Participants were 76 students (60 healthy, 16 asthmatic) who were randomly assigned to either a control group (no supplementation) or an experimental group which received 7 daily doses of beetroot juice beginning the day before final exams. Participants completed 1 baseline session during a time of low stress and 2 sessions during a time of high stress (final exams). Sessions included self-report questionnaires and physiological measures. Results demonstrate that the experience of cold symptoms after final exams was significantly reduced for those receiving nitrate supplementation, which also corresponded with increases in FeNO. These preliminary results highlight the need for further investigation of the impact of dietary nitrate supplementation on autonomic symptoms of asthmatics during times of stress, as well as potential strategies for also impacting physiological indicators.

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ENGLISH LEARNER VOCABULARY ACQUISITION: PRELIMINARY ANALYSES OF USABILITY AND EFFECTIVENESS

In preparation for a pilot study to be conducted in 2016-2017, this poster will present preliminary results and an outline of the current usability and feasibility study for an English language vocabulary program (ELVA) designed to improve the vocabulary knowledge and language proficiency of second-grade, Spanish-speaking English-language learners (ELLs). ELVA uses an intelligent tutoring system in which an avatar tutor provides prompts and feedback to students on a variety of vocabulary activities connected to abstract words grounded in passages related to science and social studies topics (e.g., Earth Sciences, Organisms and Environment, Famous People, Government). We conducted observations and interviews to evaluate the usability and effectiveness of ELVA. Initial design trials revealed that students were engaged and eager to participate. These findings bolster ELVA's usability, by pointing to the program's learnability, efficiency of use, and user satisfaction. The preliminary analyses of student responses suggest that students improved in three areas of vocabulary development after one week of participation in the program: accuracy of responses to prompts from the intelligent tutor, linguistic quality, and target vocabulary use. ELVA appears to be a valuable tool for providing differentiated instruction to improve student language proficiency.

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INFLUENCES ON AND EFFECTS OF PERSONAL AND PROFESSIONAL STRESS ON FACULTY SATISFACTION

Stress serves as an important predictor of the productivity and satisfaction of faculty members in higher education. If the field of higher education desires to preserve the vitality of the academic professorship, a proper understanding of the influences on and implications of stress remains necessary. The purpose of this study is to understand how institutional and personal characteristics can influence both personal and professional faculty stress and investigate how stress, as well as those factors, impact overall job satisfaction. Using data from the 2010- 2011 Higher Education Research Institute's Faculty Survey, we explore the following research questions: 1) What personal and school characteristics influence the level(s) of stress?, and 2) How do the levels of personal and professional stress influence job satisfaction and other career indicators? Our data includes responses from 28,654 full-time faculty members at 555 four-year colleges and universities in the United States. We aim to understand differences in the influences on and effects of stress across different institutional types based on Carnegie classification. Additionally, we investigate how individual characteristics such as race, gender, age, and tenure status impact faculty stress and how that stress effects their job satisfaction.

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"OUR HANDS ARE NOT IN OUR POCKETS": CHRISTIAN SINGLE MOTHERS AND SOCIAL ACTIVISM IN SOUTH AFRICA'S RURAL WOMEN'S MOVEMENT

In KwaZulu-Natal, South Africa, a 50,000-member grassroots social movement known as the Rural Women's Movement (RWM) is organizing successfully for the reallocation of land, for food security, for the cessation of gendered violence, and for the equipping and empowering of indigenous women in rural areas to create thriving lives for themselves and their families. Interestingly, the members of this movement are predominantly single mothers, perhaps the most vulnerable adult demographic in South Africa, and Christian. Many of these women view their involvement with RWM as a divine calling and as participation in a spiritual community, in contrast to their description of their churches as places they are obligated to attend

In the United States, single mothers also constitute one of the most vulnerable adult demographics, with over fifty percent classified as low-income. While a small number of churches do support single-parent ministries, Christian involvement in activism efforts to better the lives of single mothers is virtually invisible. In this project, I will examine how Christian single mothers in South Africa have been able to organize for political and social action and explore possible reasons why Christian single mothers in the United States have focused on local ministries rather than social and political activism to address their struggles.

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CULTURES IN TRANSITION: A TRANSFORMATIVE EXPERIENCE

Diversity is flourishing in the United States. People from cultures all over the world are residing in America, hoping to achieve citizenship in their attempt to create a better life. In the process of their journey, education plays a huge role in achieving their dreams. It is a difficult, but transformative experience that will enable them to acquire positions of quality and leadership. The goal of cultural research is to identify the strengths these aspiring citizens possess, and the challenges they face in their journey for success in America.

Commercial Viability:
Various cultures are represented in the workplace. Some have achieved corporate level of success, others are either in the process of finishing their education, or beginning their educational journey. Before they begin an educational plan, they must pass comprehensive exams, and prove fluency in the English language. If they do not pass the exams or fluency tests, they must take developmental cours-

es, before they even begin their educational study of choice. These processes delay their progress, and prolong their journey of success in corporate America. The hope of the student is to research methods that will increase the viability of aspiring foreign citizens and English language learners, and enable them to achieve their goals and aspirations. It is important that all Americans, and those aspiring to citizenship in America be equipped to meet the challenges ahead, working in a global community. The student hopes to innovate the educational process, and provide these worthy individuals with the tools necessary to achieve their education, by developing a more streamlined process that meets their needs, and builds an efficient bridge of cultural integration.

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"[O]BLIGED TO YIELD": THE LANGUAGE OF PATRIARCHY AND THE SYSTEM OF SLAVERY IN JANE AUSTEN'S MANSFIELD PARK

This essay and digital presentation will join the chorus of scholarly voices arguing that Mansfield Park is first and foremost a romance about slavery. Using Samuel Johnson's Dictionary, I will contend that a close reading of language in Mansfield Park—especially the words "duty," "gratitude," "obligation," and, to a lesser extent, "ought"—correlates patriarchy with slavery and marks Fanny Price as the text's representative slave. Yet the same linguistic "mind forg'd manacles" that enchain Fanny also constrict the rest of the romance's characters. In Mansfield Park, no person is free. In addition to Johnson's Dictionary, I will use Mary Wollstonecraft's A Vindication of the Rights of Woman to contextualize my readings of patriarchy as a system of slavery. Ultimately, I will show that Austen's purported "country-house romance" offers the "daylight equivalent" of traditional Gothic romance, unmasking patriarchy as a horrific, inescapable system of slavery.

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REMOVING POLITICS FROM ENVIRONMENTAL STEWARDSHIP FOR A COLLABORATIVE APPROACH

In the political arena, the decision-making process is inherently adversarial which creates immediate polarization. The net result for environmentatlism is that it has become a political football. It is my thesis that a grass roots coalition-building approach is needed to generate buy-in and interest in Environmental Stewardship. To this end, I am looking at the doctrinal statements of several churches which support Environmental Stewardship. For example, the Methodist Book of Discipline states in paragraph 160: All creation is the Lord's and we are responsible for the ways in which we use and abuse it... Resources....are to be valued and conserved because they are God's creation...God has granted us stewardship...and we should meet these duties through acts of loving care and respect. To achieve this coalition I am investigating methods for collaboration because research shows that the 4 most basic human desires for Respect, Understanding, Compassion and Fairness can be exercised to find common interests. Interests can then be used to find common ground and get things done. The common ground found in doctrinal statements of leading churches could be a starting point to effectively build momentum for public awareness and buy-in. Figures illustrate the collaborative approach versus adverserial decision-making and solutions.

Commercial Viability:
The collaborative approach can be applied to any controversial decision and most pointedly could be helpful in breaking through gridlock in our political system or between groups of apparent disparate interests such industry and environmentalists.

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PAUL AND MATTHEW: BINDING AND LOOSENING THE LAW

The Apostle Paul wrote his letter scolding the Galatians around 54 C.E. Paul details his message to the churches against those who wanted to force the gentile population to convert to Judaism. Most synagogues did not require gentiles to convert fully to Judaism in order to participate in religious life. (Meeks) Therefore, Paul's message of non-enforcement of circumcision holds within the tradition of Judaism for those wishing to participate in community life. In his commentary on the Gospel of Matthew, Eugene Boring states that as early as 85 when the Gospel may have been written, "This community must both answer the charges of outsiders and clarify its own understanding of the relationship of Christian discipleship and Torah observance." Pharisees at the time, (Paul was a member of this group), practiced exegesis by relaxing and tightening observances of the law. Due to the non-Jewish population in Galatia and the influx of gentiles to the Matthean community, both Paul and the author of the Gospel of Matthew understand the need for a specific interpretation of the Law, not its abolishment.